

A schematic model of scattering in \mathcal{PT} –symmetric Quantum Mechanics

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Abstract

One-dimensional scattering problem admitting a complex, \mathcal{PT} –symmetric short-range potential $V(x)$ is considered. Using a Runge-Kutta-discretized version of Schrödinger equation we derive the formulae for the reflection and transmission coefficients and emphasize that the only innovation emerges in fact via a complexification of one of the potential-characterizing parameters.

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1 Introduction

Standard textbooks describe the stationary one-dimensional motion of a quantum particle in a real potential well $V(x)$ by the ordinary differential Schrödinger equation

$$\left[-\frac{d^2}{dx^2} + V(x) \right] \psi(x) = E \psi(x), \quad x \in (-\infty, \infty) \quad (1)$$

which may be considered and solved in the bound-state regime at $E < V(\infty) \leq +\infty$ or in the scattering regime with, say, $E = \kappa^2 > V(\infty) = 0$. In this way one either employs the boundary conditions $\psi(\pm\infty) = 0$ and determines the spectrum of bound states or, alternatively, switches to the different boundary conditions, say,

$$\psi(x) = \begin{cases} A e^{i\kappa x} + B e^{-i\kappa x}, & x \ll -1, \\ C e^{i\kappa x}, & x \gg 1. \end{cases} \quad (2)$$

Under the conventional choice of $A = 1$ the latter problem specifies the reflection and transmission coefficients B and C , respectively [1].

The conventional approach to the quantum bound state problem has recently been, fairly unexpectedly, generalized to many unconventional and manifestly non-Hermitian Hamiltonians $H \neq H^\dagger$ which are merely quasi-Hermitian, i.e., which are Hermitian only in the sense of an identity $H^\dagger = \Theta H \Theta^{-1}$ which contains a nontrivial “metric” operator $\Theta = \Theta^\dagger > 0$ as introduced, e.g., in ref. [2]. The key ideas and sources of the latter new development in Quantum Mechanics incorporate the so called \mathcal{PT} –symmetry of the Hamiltonians and have been summarized in the very fresh review by Carl Bender [3]. This text may be complemented by a sample [4] of the dedicated conference proceedings.

In this context we intend to pay attention to a very simple \mathcal{PT} –symmetric *scattering* model where

$$V(x) = Z(x) + i Y(x), \quad Z(-x) = Z(x) = \text{real}, \quad Y(-x) = -Y(x) = \text{real}$$

and where the ordinary differential equation (1) is replaced by its Runge-Kutta-discretized, difference-equation representation

$$-\frac{\psi(x_{k-1}) - 2\psi(x_k) + \psi(x_{k+1}))}{h^2} + V(x_k)\psi(x_k) = E\psi(x_k) \quad (3)$$

with

$$x_k = k h, \quad h > 0, \quad k = 0, \pm 1, \dots$$

as employed, in the context of the bound-state problem, in refs. [5].

2 Runge-Kutta scattering

Once we assume, for the sake of simplicity, that the potential in eq. (3) vanishes beyond certain distance from the origin,

$$V(x_{\pm j}) = 0 \quad j = M, M+1, \dots,$$

we may abbreviate $\psi_k = \psi(x_k)$, $V_k = h^2 V(x_k)$ and $2 \cos \varphi = 2 - h^2 E$ in eq. (3),

$$-\psi_{k-1} + (2 \cos \varphi + V_k) \psi_k - \psi_{k+1} = 0. \quad (4)$$

In the region of $|k| \geq M$ with vanishing potential $V_k = 0$ the two independent solutions of our difference Schrödinger eq. (4) are easily found, via a suitable ansatz, as elementary functions of the new “energy” variable φ ,

$$\psi_k = \text{const} \cdot \varrho^k \implies \varrho = \varrho_{\pm} = \exp(\pm i \varphi).$$

This enables us to replace the standard boundary conditions (2) by their discrete scattering version

$$\psi(x_m) = \begin{cases} A e^{i m \varphi} + B e^{-i m \varphi}, & m \leq -(M-1), \\ C e^{i m \varphi}, & m \geq M-1 \end{cases} \quad (5)$$

with a conventional choice of $A = 1$.

Two comments may be added here. Firstly, one notices that the condition of the reality of the new energy variable φ imposes the constraint upon the original energy itself, $-2 \leq 2 - h^2 E \leq 2$, i.e., $E \in (0, 4/h^2)$. At any finite choice of the lattice step $h > 0$ this inequality is intuitively reminiscent of the spectra in relativistic quantum systems. Via an explicit display of the higher $\mathcal{O}(h^4)$ corrections in eq. (3), this connection has been given a more quantitative interpretation in ref. [6].

The second eligible way of dealing with the uncertainty represented by the $\mathcal{O}(h^4)$ discrepancy between the difference- and differential-operator representation of the Schrödinger's kinetic energy is more standard and lies in its disappearance in the limit $h \rightarrow 0$. This is a purely numerical recipe known as the Runge-Kutta method [7]. In the present context of scattering one has to keep in mind that the two “small” parameters h and $1/M$ may and, in order to achieve the quickest convergence, should be chosen and varied independently.

3 The matching method of solution

3.1 The simplest model of the scattering with $M = 1$

Once we are given the boundary conditions (5) the process of the construction of the solutions is straightforward. Let us first illustrate its key technical ingredients on the model with the first nontrivial choice of the cutoff $M = 1$. In this case our difference Schrödinger eq. (4) degenerates to the mere three nontrivial relations,

$$\begin{aligned} -\psi_{-2} + 2 \cos \varphi \psi_{-1} - \psi_0^{(-)} &= 0 \\ -\psi_{-1} + (2 \cos \varphi + Z_0) \psi_0 - \psi_1 &= 0 \\ -\psi_0^{(+)} + 2 \cos \varphi \psi_1 - \psi_2 &= 0 \end{aligned} \tag{6}$$

where we may insert, from eq. (5),

$$\psi_{-1} = e^{-i\varphi} + B e^{i\varphi}, \quad \psi_0^{(-)} = 1 + B, \quad \psi_0^{(+)} = C, \quad \psi_1 = C e^{i\varphi} \tag{7}$$

and where we have to demand, subsequently,

$$\begin{aligned}\psi_0^{(-)} &= 1 + B = \psi_0^{(+)} = C = \psi_0, \\ -e^{-i\varphi} - B e^{i\varphi} + (2 \cos \varphi + Z_0) C - C e^{i\varphi} &= 0.\end{aligned}\tag{8}$$

Thus, at an arbitrary “energy” φ one identifies $B = C - 1$ and gets the solution

$$C = \frac{2i \sin \varphi}{2i \sin \varphi - Z_0}, \quad B = \frac{Z_0}{2i \sin \varphi - Z_0}.$$

Of course, as long as we deal just with the real “interaction term” Z_0 , our $M = 1$ toy problem remains Hermitian since no \mathcal{PT} –symmetry has entered the scene yet.

3.2 \mathcal{PT} –symmetry and the scattering at $M = 2$

In the next, $M = 2$ version of our model we have to insert the four known quantities

$$\psi_{-2} = e^{-2i\varphi} + B e^{2i\varphi}, \quad \psi_{-1} = e^{-i\varphi} + B e^{i\varphi}, \quad \psi_1 = C e^{i\varphi}, \quad \psi_2 = C e^{2i\varphi}$$

in the triplet of relations

$$\begin{aligned}-\psi_{-2} + (2 \cos \varphi + Z_{-1} - i Y_{-1}) \psi_{-1} - \psi_0^{(-)} &= 0 \\ -\psi_{-1} + (2 \cos \varphi + Z_0) \psi_0 - \psi_1 &= 0 \\ -\psi_0^{(+)} + (2 \cos \varphi + Z_{-1} + i Y_{-1}) \psi_1 - \psi_2 &= 0\end{aligned}\tag{9}$$

where the three symbols ψ_0 , $\psi_0^{(-)}$ and $\psi_0^{(+)}$ defined by these respective equations should represent the same quantity and must be equal to each other, therefore.

Having this in mind we introduce $\xi_0^{(-)} = 1 + B$ and $\xi_0^{(+)} = C$ and decompose

$$\psi_0^{(-)} = \xi_0^{(-)} + \chi_0^{(-)}, \quad \psi_0^{(+)} = \xi_0^{(+)} + \chi_0^{(+)}.$$

This enables us eliminate

$$\chi_0^{(-)} = V_{-1} \psi_{-1}, \quad \chi_0^{(+)} = V_1 \psi_1$$

and eq. (9) becomes reduced to the pair of conditions,

$$\begin{aligned} 1 + B + V_{-1} \psi_{-1} &= C + V_1 \psi_1 = \psi_0, \\ -\psi_{-1} + (2 \cos \varphi + Z_0) \psi_0 - \psi_1 &= 0 \end{aligned} \quad (10)$$

They lead to the two-dimensional linear algebraic problem which defines the reflection and transmission coefficients B and C at any input energy φ . The same conclusion applies to all the models with the larger M .

4 The matrix-inversion method of solution

Let us now re-write our difference Schrödinger eq. (4) as a doubly infinite system of linear algebraic equations

$$\begin{pmatrix} \ddots & \ddots & \ddots & \vdots & & \\ \ddots & S_{-1} & -1 & 0 & \dots & \\ \ddots & -1 & S_0 & -1 & \ddots & \\ \dots & 0 & -1 & S_1 & \ddots & \\ & \vdots & \ddots & \ddots & \ddots & \end{pmatrix} \begin{pmatrix} \vdots \\ \psi_{-1} \\ \psi_0 \\ \psi_1 \\ \vdots \end{pmatrix} = 0, \quad (11)$$

where

$$S_k \ (\equiv S_{-k}^*) = \begin{cases} 2 \cos \varphi + Z_k + i Y_k \operatorname{sign} k, & |k| < M, \\ 2 \cos \varphi, & |k| \geq M \end{cases} \quad (12)$$

and where the majority of the elements of the “eigenvector” are prescribed, in advance, by the boundary conditions (5). Once we denote all of them by a different symbol,

$$\psi(x_m) = \begin{cases} A e^{i m \varphi} + B e^{-i m \varphi} \equiv \xi_m^{(-)}, & m \leq -(M-1), \\ C e^{i m \varphi} \equiv \xi_m^{(+)}, & m \geq M-1, \end{cases} \quad (13)$$

we may reduce eq. (11) to a finite-dimensional and tridiagonal non-square-matrix problem

$$\begin{pmatrix} -1 & S_{(M-1)}^* & -1 & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & -1 & S_1^* & -1 & & \\ & & & -1 & S_0 & -1 & \\ & & & & -1 & S_1 & -1 & \ddots \\ & & & & \ddots & \ddots & \ddots & \ddots \\ & & & & & -1 & S_{(M-1)} & -1 \end{pmatrix} \begin{pmatrix} \xi_{-M}^{(-)} \\ \xi_{-(M-1)}^{(-)} \\ \psi_{-(M-2)} \\ \vdots \\ \psi_{M-2} \\ \xi_{M-1}^{(+)} \\ \xi_M^{(+)} \end{pmatrix} = 0 \quad (14)$$

or, better, to a non-homogeneous system of $2M - 1$ equations

$$\mathbf{T} \cdot \begin{pmatrix} \xi_{-(M-1)}^{(-)} \\ \psi_{-(M-2)} \\ \vdots \\ \psi_{M-2} \\ \xi_{M-1}^{(+)} \end{pmatrix} = \begin{pmatrix} \xi_{-M}^{(-)} \\ 0 \\ \vdots \\ 0 \\ \xi_M^{(+)} \end{pmatrix} \quad (15)$$

where the $(2M - 1)$ -dimensional square-matrix of the system can be partitioned as follows,

$$\mathbf{T} = \left(\begin{array}{c|ccc|c} S_{(M-1)}^* & -1 & & & \\ \hline -1 & S_{(M-2)}^* & -1 & & \\ & -1 & \ddots & \ddots & \\ & & \ddots & S_0 & \ddots \\ & & & \ddots & \ddots & -1 \\ & & & & -1 & S_{(M-2)} & -1 \\ \hline & & & & & -1 & S_{(M-1)} \end{array} \right). \quad (16)$$

Whenever this matrix proves non-singular, it may assigned the inverse matrix $\mathbf{R} = \mathbf{T}^{-1}$, the knowledge of which enables us to re-write eq. (15), in the same partitioning, as

follows,

$$\begin{pmatrix} \xi_{-(M-1)}^{(-)} \\ \vec{\Psi} \\ \xi_{M-1}^{(+)} \end{pmatrix} = \mathbf{R} \cdot \begin{pmatrix} \xi_{-M}^{(-)} \\ \vec{0} \\ \xi_M^{(+)} \end{pmatrix}, \quad \vec{\Psi} = \begin{pmatrix} \psi_{-(M-2)} \\ \vdots \\ \psi_{M-2} \end{pmatrix}. \quad (17)$$

In the next step we deduce that the matrix \mathbf{R} has the following partitioned form

$$\mathbf{R} = \left(\begin{array}{c|c|c} \alpha^* & \vec{t}^T & \beta \\ \hline \vec{u} & \mathbf{Q} & \vec{v} \\ \hline \beta & \vec{w}^T & \alpha \end{array} \right).$$

We may summarize that in the light of the overall partitioned structure of eq. (17), the knowledge of the $(2M - 3)$ -dimensional submatrix \mathbf{Q} as well as of the two $(2M - 3)$ -dimensional row vectors \vec{t}^T and \vec{w}^T (where T denotes transposition) is entirely redundant. Moreover, the knowledge of the other two column vectors \vec{u} and \vec{v} only helps us to eliminate the “wavefunction” components $\psi_{-(M-2)}, \psi_{-(M-3)}, \dots, \psi_{M-3}, \psi_{M-2}$. In this sense, equation (15) degenerates to the mere two scalar relations

$$\begin{aligned} \xi_{-(M-1)}^{(-)} - \alpha^* \xi_{-M}^{(-)} - \beta \xi_M^{(+)} &= 0, \\ \xi_{M-1}^{(+)} - \beta \xi_{-M}^{(-)} - \alpha \xi_M^{(+)} &= 0. \end{aligned} \quad (18)$$

Once we insert the explicit definitions from eq. (13) we get the final pair of linear equations

$$\begin{aligned} e^{-i(M-1)\varphi} + B e^{i(M-1)\varphi} - \alpha^* (e^{-iM\varphi} + B e^{iM\varphi}) - C \beta e^{iM\varphi} &= 0, \\ C e^{i(M-1)\varphi} - \beta (e^{-iM\varphi} + B e^{iM\varphi}) - C \alpha e^{iM\varphi} &= 0 \end{aligned} \quad (19)$$

which are solved by the elimination of

$$B = -e^{-2iM\varphi} + \frac{C}{\beta} (e^{-i\varphi} - \alpha) \quad (20)$$

and, subsequently, of

$$C = \frac{2i\beta e^{-2iM\varphi} \sin \varphi}{\beta^2 - (e^{-i\varphi} - \alpha^*)(e^{-i\varphi} - \alpha)}. \quad (21)$$

This is our present main result.

5 Coefficients α and β

Our final scattering-determining formulae (20) and (21) indicate that the complex coefficient α and the real coefficient β carry all the “dynamical input” information. At any given energy parameter φ these matrix elements are, by construction, rational functions of our $2M - 1$ real coupling constants Z_0, Z_1, \dots, Z_{M-1} and Y_1, \dots, Y_{M-1} . In particular, β is equal to $1/\det \mathbf{T}$ and α has the same denominator of course. An explicit algebraic determination of the determinant $\det \mathbf{T}$ and of the numerator (say, γ) of α is less easy. Let us illustrate this assertion on a few examples.

5.1 $M = 2$ once more

$$\det \mathbf{T} = Z_0 Z_1^2 - 2 Z_1 + Y_1^2 Z_0$$

$$\operatorname{Re} \gamma = Z_0 Z_1 - 1$$

$$\operatorname{Im} \gamma = -Z_0 Y_1$$

5.2 $M = 3$

$$\det \mathbf{T} = Z_0 Z_1^2 Z_2^2 - 2 Z_0 Z_1 Z_2 - 2 Z_1 Z_2^2 +$$

$$+ Y_1^2 Z_0 Z_2^2 + 2 Z_2 + Y_2^2 Z_0 Z_1^2 - 2 Y_2^2 Z_1 + Y_2^2 Y_1^2 Z_0 + 2 Z_0 Y_1 Y_2 + Z_0$$

$$\operatorname{Re} \gamma = Z_0 Z_1^2 Z_2 - 2 Z_1 Z_2 + Y_1^2 Z_0 Z_2 - Z_1 Z_0 + 1$$

$$\operatorname{Im} \gamma = -Z_0 Z_1^2 Y_2 + 2 Z_1 Y_2 - Y_1^2 Z_0 Y_2 - Y_1 Z_0$$

5.3 $M = 4$

The growth of complexity of the formulae occurs already at the dimension as low as $M = 4$. The determinant $\det \mathbf{T}$ and the real and imaginary parts of γ are then represented by the sums of 15 and 14 and 32 products of couplings, respectively.

A simplification is only encountered in the weak coupling regime where one finds just two terms in the determinant which are linear in the couplings,

$$\det \mathbf{T} = -2 Z_3 - 2 Z_1 + \dots$$

being followed by the 10 triple-product terms,

$$\begin{aligned} & \dots + Y_1^2 Z_0 + 4 Z_1 Z_2 Z_3 - 4 Z_1 Y_2 Y_3 + Z_1^2 Z_0 + 2 Y_3^2 Z_2 + 2 Y_1 Z_0 Y_3 + \\ & + 2 Z_1 Z_0 Z_3 + Z_3^2 Z_0 + Y_3^2 Z_0 + 2 Z_3^2 Z_2 + \dots \end{aligned}$$

etc. Similarly, we may decompose, in the even-number products,

$$\text{Re } \gamma = -1 + 2 Z_2 Z_3 + Z_0 Z_1 + Z_0 Z_3 + 2 Z_2 Z_1 + \dots$$

and continue

$$\begin{aligned} & \dots + -2 Z_0 Z_1 Z_2 Z_3 + 2 Z_0 Y_1 Y_2 Z_3 - \\ & - Z_2 Y_1^2 Z_0 - 2 Z_2^2 Z_1 Z_3 - Z_2 Z_1^2 Z_0 - 2 Y_2^2 Z_1 Z_3 + \dots \end{aligned}$$

etc, plus

$$\text{Im } \gamma = -2 Z_2 Y_3 + 2 Y_2 Z_1 - Z_0 Y_1 - Z_0 Y_3 - \dots$$

with a continuation

$$\begin{aligned} & \dots - Y_2 Y_1^2 Z_0 - Y_2 Z_1^2 Z_0 + \\ & + 2 Y_2^2 Z_1 Y_3 + 2 Z_0 Z_1 Z_2 Y_3 + 2 Z_2^2 Z_1 Y_3 - 2 Z_0 Y_1 Y_2 Y_3 + \dots \end{aligned}$$

etc. Symbolic manipulations on a computer should be employed at all the higher dimensions $M \geq 4$ in general.

6 Discussion

The main inspiration of the activities and attention paid to the \mathcal{PT} -symmetry originates from the pioneering 1998 letter by Bender and Boettcher [8] where the

operator \mathcal{P} meant parity and where the (antilinear) \mathcal{T} represented time reversal. Its authors argued that the *complex* model $V(x) = x^2 (ix)^\delta$ seems to possess the *purely real* bound-state spectrum at all the exponents $\delta \geq 0$. After a rigorous mathematical proof of this conjecture by Dorey, Duncan, Tateo and Shin [9] and after the (crucial) clarification of the existence of a nontrivial, “physical” Hilbert space \mathcal{H} where the Hamiltonian remains self-adjoint [2, 10, 11, 12], the bound-state version of eq. (1) may be considered more or less well understood, especially after it has been clarified that the physics-inspired concept of \mathcal{PT} –symmetry of a Hamiltonian H should in fact be understood, in the language of mathematics, as a \mathcal{P} –pseudo-Hermiticity of H specified by the property $H^\dagger = \mathcal{P} H \mathcal{P}^{-1}$ [10, 11, 13].

In the spirit of the latter generalization, current literature abounds in the studies of the potentials which are analytically continued [14], singular and multisheeted [15], multidimensional [16], manybody [17], relativistic [18], supersymmetric [19] and channel-coupling [20]. Among all these developments, a comparatively small number of papers has been devoted to the problem of the scattering. For a sample one might recollect the key reviews [21] and various Kleefeld’s conceptual conjectures [22] as well as a very explicit study of the scattering by the separable \mathcal{PT} –symmetric potentials of rank one [23] or by the rectangular or reflectionless barriers [24], or the motion considered along the so called tobogganic (i.e., complex *and* topologically nontrivial) integration contours [25]. In this context our present difference-equation-based study may be understood just as another attempt to fill the gap.

Technically we felt inspired by our old Runge-Kutta-type discretization of the \mathcal{PT} –symmetric Schrödinger equations [5] as well as by our recent chain-model approximations of bound states in a finite-dimensional Hilbert space [26]. In a certain unification of these two approaches we succeeded here in showing that there exists a close formal parallelism between the description of the (one-dimensional, Runge-Kutta-approximated) scattering by a real (i.e., Hermitian) potentials and by their complex, \mathcal{PT} –symmetric generalizations. We showed that in both these contexts,

the definition of the transmission and reflection coefficients has the same form [cf., e.g., eq. (21)], with all the differences represented by the differences in the form of the “dynamical input” information. It has been shown to be encoded, in *both* the Hermitian and non-Hermitian cases, in the two functions α and β of the lattice potentials, with the vanishing or non-vanishing coefficients Y_k , respectively (cf. a few samples of the concrete form of α and β in section 5).

On the level of physics we would like to emphasize that one of the main distinguishing features of the scattering problem in \mathcal{PT} -symmetric quantum mechanics lies in the manifest asymmetry between the “in” and “out” states [22]. In its present solvable exemplification we showed that such an asymmetry is merely formal and that the problem remains tractable by the standard, non-matching and non-recurrent techniques of linear algebra. A key to the success proved to lie in the partitioning of the Schrödinger equation which enabled us to separate its essential and inessential components and to reduce the construction of the amplitudes to the mere two-dimensional matrix inversion [cf. eq. (18)] where all the dynamical input is represented by the four corners of the inverse matrix $\mathbf{R} = \mathbf{T}^{-1}$ [cf. the definition (16)].

We believe that the merits of the present discrete model were not exhausted by its present short analysis and that its further study might throw new light, e.g., on the non-Hermitian versions of the inverse problem of scattering.

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