Honours Literature review

$\mathcal{PT}$-symmetric quantum mechanics

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Contents

Abstract

Introduction

This work reflects on a possible extension to the canonical formalism of quantum mechanics. The main goal of this extension is to allow us to access a much larger class of interesting Hamiltonians which are non-Hermitian but nevertheless physical.This extension has the potential to be of great importance to the advancement of new and physically significant theories.
In "The principles of quantum mechanics", Paul Dirac advises us that"it is important to remember that science is concerned only with *observable* things and that we can observe an object only by letting it interact with some outside influence"[1]. This means that in order to study valid physical systems, these systems must satisfy the fundamental postulates of quantum mechanical theory. Nearly all these postulates are based in physical properties. For example, one postulate establishes that time evolution of a quantum system must be *unitary* (i.e. probability conserving). Another requires that the energy spectrum of the system is bounded below so a lowest energy state can be measured. In quantum mechanics, the Hamiltonian operator ($\hat{H}$) encapsulates the total energy of a system. As explained already, a system's energy spectrum is required to be bounded and real in order to be measurable. According to the fundamental postulates of the standard theory, if the operator $\hat{H}$ satisfies the mathematical property known as Hermiticity –these operators are also known as self-adjoint in mathematics–, then $\hat{H}$ will be an adequate physical observable. Interestingly, the Hermiticity postulate stands out from others in the conventional theory of quantum mechanics because it is mathematical rather than physical in its character[2]. An operator $\hat{O}$ that is Hermitian has the property that its effect on the vectors of the Hilbert space in which $\hat{O}$ is defined is independent of the order in which $\hat{O}$ acts on said vectors[3]

$$\hat{O}\,|\psi\rangle = \langle\psi|\,\hat{O}^{\dagger}. \tag{1.1}$$

Despite of the correctness of Hermiticity, some believe that perhaps we have ended up with an overly restrictive quantum theory. The aim of this review is to summarize the present developments of a more physical alternative to Hermiticity. This alternative postulate is referred to as space–time reflection symmetry ($\mathcal{PT}$ symmetry)[4].

1.1 $\mathcal{PT}$-symmetry

In the late nineties, Carl Bender et al presented a $\mathcal{PT}$-symmetric theory of quantum mechanics. Their aim was to explain a conjecture on the reality and positiveness of the spectrum of a non-Hermitian Hamiltonian proposed by Bessis[5]. $\mathcal{PT}$-symmetric theory can be viewed as an analytical continuation of the conventional theory from real into the complex phase space[6].

An important question that must be answered, is whether a $\mathcal{PT}$-symmetric Hamiltonian defines a valid physical theory of quantum mechanics. By a physical theory we mean that the following conditions must be satisfied; The energy spectra of a system described by $\hat{H}$ must be real and bounded below. Another condition is related to the probabilistic interpretation of the norm of a state, a norm must be always positive to be a valid probability. Finally time evolution under the theory must be unitary. This means that as a state vector evolves in time the state's probability does not leak away[4][2].

1.1.1 The $\mathcal{PT}$ operator

The $\mathcal{PT}$ operator is the anti-linear operator composed of the linear parity operator ($\mathcal{P}$), which performs spatial reflection, and the anti-linear time-reversal operator ($\mathcal{T}$). These operators act on position and momentum operators in the following form

$$\begin{aligned} \mathcal{P}: &\quad \hat{x} \to -\hat{x}, \quad \hat{p} \to -\hat{p}, \\ \mathcal{T}: &\quad \hat{x} \to \hat{x}, \quad\quad \hat{p} \to -\hat{p}, \quad \mathrm{i} \to -\mathrm{i}. \end{aligned} \tag{1.2}$$

Some Hamiltonians may not be symmetric under $\mathcal{P}$ or $\mathcal{T}$ separately, but Hamiltonians that remain invariant under the influence of the $\mathcal{PT}$ operator are labelled as $\mathcal{PT}$-symmetric. A Hamiltonian $\hat{H}$ will possess unbroken $\mathcal{PT}$ symmetry if it's eigenstates are simultaneously eigenstates of the $\mathcal{PT}$ operator, or in other words, if $\hat{H}$ and the $\mathcal{PT}$ operator commute. If the $\mathcal{PT}$ operator and $\hat{H}$ do not commute we say that the Hamiltonian's $\mathcal{PT}$-symmetry is broken[2][7][4]. If the symmetry is unbroken, then the eigenspectrum of $\hat{H}$ is fully real and bounded below –This is also known as exact $\mathcal{PT}$-symmetry–. The effectiveness of $\mathcal{PT}$ symmetry as a tool to investigate the spectra of some non-Hermitian Hamiltonians has been proved rigorously in various works, such as Dorey et al[8], Bender and Boettcher[5], Brody[9], Bender and Mannheim [10], Bender et al[6], Mostafazadeh[11][12] amongst several others.

1.1.2 The $\mathcal{CPT}$ inner product

To be able to describe precisely the nature of $\mathcal{PT}$-symmetric quantum mechanics, we must delve briefly into the inner-product under which our theory satisfies the postulates of conventional quantum mechanics. It is important to note that $\mathcal{PT}$-symmetric quantum mechanics is a kind of 'bootstrap' theory[2], since infinitely many inner-products exist for a given vector space, we can construct an inner product whose associated norm is positive definite by design. This inner-product is in general dependent on the characteristics of the Hamiltonian in question and it guarantees that the underlying dynamics of any $\mathcal{PT}$-symmetric Hamiltonian satisfies unitarity[4]. Firstly, it is necessary to solve for the eigenstates of the Hamiltonian before knowing the Hilbert space and consequentially the associated inner product. To guarantee a positive norm for our theory, we will construct a new linear operator $\mathcal{C}$ that commutes with both $\hat{H}$ and $\mathcal{PT}$. We use the symbol $\mathcal{C}$ to represent this symmetry because it's properties are similar to those of the charge conjugation operator in particle physics[2].

The $\mathcal{C}$ operator

When the $\mathcal{PT}$-symmetry of $\hat{H}$ is exact, then $\hat{H}$ and $\mathcal{PT}$ commute. This statement is equivalent to saying that the eigenfunctions $\phi_n(x)$ of $\hat{H}$ are simultaneously eigenstates of

$\mathcal{PT}$[13].

$$\mathcal{PT}\phi_n(x) = \lambda_n\phi_n(x), \tag{1.3}$$

Where λ_n is a pure phase. Without loss of generality, for each n the phase can be absorbed into $\phi_n(x)$ and this makes the eigenvalue of the $\mathcal{PT}$operator unity[13]:

$$\mathcal{PT}\phi_n(x) = \phi_n^*(-x) = \phi_n(x). \tag{1.4}$$

There is strong numerical evidence of the completeness of the eigenfunctions $\phi_n(x)$[7][13][14]. In the coordinate basis, the completeness statement reads:

$$\sum_n (-1)^n \phi_n(x)\phi_n(y) = \delta(x-y), \quad x, y \in \mathbb{R} \tag{1.5}$$

the unconventional $(-1)^n$ factor in 1.5 can be explained if we define the $\mathcal{PT}$ inner product as

$$\begin{aligned}(f, g) &= \int dx \left[\mathcal{PT} f(x)\right] g(x) \\ &= \int dx f^*(-x) g(x).\end{aligned} \tag{1.6}$$

where the integral above follows a path in the complex plane. Under this definition the eigenstate norms alternate in sign depending on the value n. This means that the metric associated with the $\mathcal{PT}$ inner product is indefinite[13][15]. In quantum theory, the norm of states is interpreted as a probability and this means that the indefinite metric described above presents a serious problem for the validity of $\mathcal{PT}$-symmetric quantum theory. The solution to this problem lies in finding an interpretation for the negative valued norms[6]. The general claim presented in the literature is that for any theory with unbroken $\mathcal{PT}$-symmetry there exists a symmetry of the Hamiltonian that describes the negative and positive norm states. To describe this symmetry of $\hat{H}$ it is necessary to construct a linear operator denoted by $\mathcal{C}$[4][7][13]. When represented in position space $\mathcal{C}$ is a sum over the energy eigenstates of $\hat{H}$:

$$\mathcal{C} = \sum_n \phi_n(x)\phi_n(y) \tag{1.7}$$

From this definition, and the relation $(\phi_m(y), \phi_n(y)) = \int dy\, \phi_m(y)\phi_n(y)$ we can verify that the eigenvalues of $\mathcal{C}$ are ± 1

$$\begin{aligned}\mathcal{C}\phi_n(x) &= \int dy\, \mathcal{C}\, \phi_n(y) \\ &= \sum_m \phi_m(x) \int dy\, \phi_m(y)\phi_n(y) \\ &= (-1)^n \phi_n(x)\end{aligned} \tag{1.8}$$

The $\mathcal{PT}$ norms signatures can therefore be interpreted as the "charge" of the states, while $\mathcal{C}$ is the operator used to measure this charge[13].

The $\mathcal{C}$ operator commutes with the $\mathcal{PT}$ operator, but it does not commute with the parity operator $\mathcal{P}$. Notice that $\mathcal{C}$ and $\mathcal{P}$ operators are square roots of $\delta(x-y)$ the unity operator[7]

$$\mathcal{P}^2 = \mathcal{C}^2 = \mathbb{1}, \tag{1.9}$$

where $\mathcal{P} \neq \mathcal{C}$, since $\mathcal{P}$ is real and $\mathcal{C}$ is complex valued[4][13].

Using the newly constructed $\mathcal{C}$ operator, we can redesign the $\mathcal{PT}$ inner product to suit the conventional probabilistic interpretation of the vector norms in quantum mechanics

$$(f, g) = \int dx \left[\mathcal{CPT} f(x)\right] g(x). \tag{1.10}$$

1.2 Bi-orthogonal systems

WHY IS THIS COOL?

Suppose that a diagonalizable non-Hermitian Hamiltonian $\tilde{H}$ has a discrete spectrum and it commutes with the $\mathcal{PT}$ operator. This means that $\tilde{H}$ has unbroken $\mathcal{PT}$-symmetry. There exists a Hilbert space $\mathcal{H}$ spanned by the eigenvectors of $\tilde{H}$ but because $\tilde{H}$ is non-Hermitian –with respect to a complete positive-definite inner product of $\mathcal{H}$– the time evolution generated by $\tilde{H}$ will not be unitary[11]. As explained in section 1.1.2. For the assumed $\tilde{H}$ above we can construct a different complete positive-definite inner product by constructing and using the antisymmetric $\mathcal{C}$ operator that corresponds to $\tilde{H}$. The assumed diagonalizability condition of $\tilde{H}$ may be viewed as a physical requirement without which an energy eigenbasis would not exist. To our knowledge all known non-Hermitian Hamiltonians that are used in physical applications are diagonalizable and therefore admit a complete bi-orthonormal set of eigenvectors. This set of bi-orthonormal eigenvectors is $\{(|\psi_n, a\rangle, |\phi_n, a\rangle)\}$ and will satisfy the following defining relations[16]

$$\tilde{H} |\psi_n, a\rangle = E_n |\psi_n, a\rangle, \quad \tilde{H}^\dagger |\phi_n, a\rangle = E_n^* |\phi_n, a\rangle, \tag{1.11}$$

$$\langle \phi_m, b | \psi_n, a\rangle = \delta_{mn}\delta_{ab}, \tag{1.12}$$

$$\sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle \langle \phi_n, a| = \hat{\mathbb{I}} \tag{1.13}$$

$$\tilde{H} = \sum_n \sum_{a=1}^{d_n} E_n |\psi_n, a\rangle \langle \phi_n, a|, \quad \tilde{H}^\dagger = \sum_n \sum_{a=1}^{d_n} E_n^* |\phi_n, a\rangle \langle \psi_n, a| \tag{1.14}$$

where n and a are the spectral degeneracy levels, d_n is the degree of degeneracy of E_n and $\hat{\mathbb{I}}$ is the identity operator[16].

PT NORMALISATION

Equivalent Hamiltonians with distinct symmetries

In parallel to the work of Bender is the research of Mostafazadeh who introduced the notion of pseudo-Hermiticity in [11]. A Hamiltonian is said to be pseudo-Hermitian with respect to a positive-definite, Hermitian operator η if it satisfies

$$\tilde{H}^\dagger = \eta^{-1}\tilde{H}\eta. \tag{2.1}$$

In the case of Hamiltonians with $\mathcal{PT}$-symmetry, the role of η is played by the combines action of $\mathcal{P}$ and $\mathcal{C}$. A convenient way to write the $\mathcal{C}$ operator was proposed in [17]

$$\mathcal{C} = e^{Q}\mathcal{P} = \eta^{-1}\mathcal{P}, \tag{2.2}$$

here Q is an antisymmetric Hermitian operator. Mostafazadeh [12] has shown that the square root of the positive-definite Hermitian operator $\eta = e^{-Q}$ can be used to transform any non-Hermitian Hamiltonian with unbroken $\mathcal{PT}$-symmetry into a spectrally equivalent Hermitian Hamiltonian by means of a unitary "similarity transformation"[18][19]. The transformation is as follows, the invertible operator $\rho = \sqrt{\eta}$ acts on the non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian $\tilde{H}$ and returns an equivalent Hermitian Hamiltonian $\hat{H}$

$$\hat{H} = \rho^{-1}\tilde{H}\rho = e^{-Q/2}\tilde{H}e^{Q/2}. \tag{2.3}$$

To verify that the similar Hamiltonian $\hat{H}$ is Hermitian we take the Hermitian conjugate of $\hat{H}$

$$\begin{aligned}\hat{H}^\dagger &= (e^{-Q/2}\tilde{H}e^{Q/2})^\dagger, \\ &= e^{Q/2}\tilde{H}^\dagger e^{-Q/2},\end{aligned} \tag{2.4}$$

If we "swap" Hermiticity: $\tilde{H}^\dagger$ in 2.4 for $\mathcal{PT}$-symmetry, and we use equation 2.2

$$\begin{aligned}\hat{H}^\dagger &= e^{Q/2}\mathcal{P}\tilde{H}\mathcal{P}^{-1}e^{-Q/2}, \\ &= e^{-Q/2}\mathcal{C}\tilde{H}\mathcal{C}^{-1}e^{Q/2},\end{aligned} \tag{2.5}$$

Finally we recall that $\mathcal{C}$ and $\tilde{H}$ commute

$$\hat{H}^\dagger = e^{-Q/2}\tilde{H}e^{Q/2} = \hat{H}. \tag{2.6}$$

Mostafazadeh [11], conjectures that because $\mathcal{CPT}$-symmetry satisfies the postulates of quantum mechanics –whilst only "swapping" the Hermiticity of a Hamiltonian by $\mathcal{CPT}$-symmetry– then this must mean that non Hermitian $\mathcal{CPT}$-symmetric theories are equivalent to certain non local Hermitian field theories. It is natural to notice that this equivalence feature between both theories could provide an advantage to simplify quantum

mechanical calculations, this is explored in references [11],[20],[16],[19],[21].

MORE HERE??????

2.1 Comparing time evolution

In this section I illustrate some features of non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians. Time-evolution in conventional quantum mechanics is implemented using the unitary operator $\hat{U} = e^{-i\hat{H}t/\hbar}$. $\hat{U}$ is unitary because the Hamiltonian $\hat{H}$ is Hermitian. This means that as the state $\vec{\psi}$ evolves in time, the norm of $\vec{\psi}$ remains constant in time. Time evolution of a state $\vec{\psi}$ from time $0 \to t$ is written as

$$\vec{\psi}(t) = \hat{U}\vec{\psi}(0). \tag{2.7}$$

In quantum mechanics, the norm of a state is interpreted as a probability, and this probability must remain constant in time. Probability growth or decay in time, means that the theory violates unitarity. As explained in section 1.1, when the $\mathcal{PT}$-symmetry of $\hat{H}$ is unbroken we still have positive norm states. This means that time evolution under the unbroken $\mathcal{PT}$-symmetric framework is also unitary[3][7][12]. Since both Hermitian and $\mathcal{PT}$-symmetric theory satisfy unitarity, it makes sense to compare their dynamics. In "Faster than Hermitian Quantum mechanics" ([22]) Bender et al compare the time evolution under two distinct Hamiltonians.

2.1.1 Two 2×2 Hamiltonians

In [22] two two-level systems are compared. One is described by Hermitian Hamiltonian $\hat{H}$ and the other by a (unbroken) $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian $\tilde{H}$. The main purpose of this comparison is to identify which kind of Hamiltonian promotes the "speediest" time evolution in a Hilbert space $\mathcal{H}$ spanned by $|\psi_i\rangle$ and $|\psi_f\rangle$, or in other words, we aim to find whether the shortest lapsed time for the time evolution occurs when we use either a $\hat{H}$ or $\tilde{H}$. The premise of Hermitian dynamics is that evolution of states requires a non zero amount of time, provided that the difference between the largest and smallest eigenvalues of the hermitian Hamiltonian $\hat{H}$ remains fixed[22]

$$\omega = E_{\max} - E_{\min} > 0 \tag{2.8}$$

Since the $\mathcal{PT}$-symmetry of the non-Hermitian Hamiltonian $\tilde{H}$ is unbroken, its eigenvalues are also real valued, therefore we can also impose 2.8 when dealing with the dynamics under $\tilde{H}$. We choose the basis so that the initial and final states are

$$|\psi_i\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\psi_f\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \tag{2.9}$$

where a and b are chosen such that $|a|^2 + |b|^2 = 1$[22]. The Hamiltonians we use in this exercise are written most generally in matrix form as

$$\hat{H} = \begin{pmatrix} s & re^{-i\theta} \\ re^{i\theta} & u \end{pmatrix} \quad \text{and} \quad \tilde{H} = \begin{pmatrix} re^{i\theta} & s \\ s & re^{-i\theta} \end{pmatrix} \tag{2.10}$$

where the parameters r, s, u, and θ are real. An interesting geometric picture becomes evident when the eigenvalue problem for both Hamiltonians is solved separately. When we

square equation 2.8, it is clear that ω^2 emphasizes the key difference between Hermitian and $\mathcal{PT}$-symmetric Hamiltonians[22]. The corresponding equation for $\hat{H}$: $\hat{\omega}^2$ is a sum of squares, while in the case of $\tilde{H}$: $\tilde{\omega}^2$ is a difference of squares

$$\hat{\omega}^2 = (s-u)^2 + 4r^2 \quad \text{and} \quad \tilde{\omega}^2 = 4s^2 - 4r^2\sin^2\theta, \tag{2.11}$$

The positivity of $\tilde{\omega}^2$ is ensured by the condition of unbroken $\mathcal{PT}$-symmetry[22] that we imposed on $\tilde{H}$. These equations demonstrate that Hermitian Hamiltonians exhibit elliptic behaviour, which leads to a non zero lower bound for the optimal time[22] as we will see soon. On the other hand, $\mathcal{PT}$-symmetric Hamiltonian states live in a hyperbolic Hilbert space which can be used to make the optimal time arbitrarily small.

Both $\hat{H}$ and $\tilde{H}$ can also be expressed in terms of Pauli matrices

$$\hat{H} = \frac{1}{2}(s+u)\mathbb{1} + \frac{\omega}{2}\vec{\sigma}\cdot\vec{n_1} \quad \text{and} \quad \tilde{H} = (r\cos\theta)\mathbb{1} + \frac{\omega}{2}\vec{\sigma}\cdot\vec{n_2}, \tag{2.12}$$

here each corresponding unit vector is $\vec{n_1} = \frac{2}{\omega}(r\cos\theta, r\sin\theta, \frac{(s-u)}{2})$ and $\vec{n_2} = \frac{2}{\omega}(s, 0, ir\sin\theta)$ and $\vec{\sigma}$ is the vector of Pauli matrices.

Using the matrix identity $e^{-i\phi\vec{\sigma}\cdot\vec{n}} = (\cos\phi)\mathbb{1} + i\sin\phi\vec{\sigma}\cdot\vec{n}$, we can write the Hermitian time evolution expression as

$$\begin{pmatrix} a \\ b \end{pmatrix} = e^{\frac{-i(s+u)t}{2\hbar}} \begin{pmatrix} \cos(\frac{\omega t}{2\hbar}) - i\frac{s-u}{\omega}\sin(\frac{\omega t}{2\hbar}) \\ -i\frac{2r}{\omega}e^{i\theta}\sin(\frac{\omega t}{2\hbar}) \end{pmatrix}. \tag{2.13}$$

To find the time required to transform to the final state $|\psi_f\rangle$, we take the second component in 2.13 and obtain $t = \frac{2\hbar}{\omega}\arcsin(\frac{\omega|b|}{2r})$. The shortest evolution time for all $r > 0$ that satisfies $\hat{\omega}^2$ in 2.11 is

$$\tau = \frac{2\hbar}{\omega}\arcsin|b|, \tag{2.14}$$

τ is known as the *passage time*[23].

To perform the same optimization for the $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian in 2.12 we let $\mathcal{T}$ be the operation of complex conjugation and define the $\mathcal{P}$ operator as the $\mathcal{PT}$-symmetric 2×2 matrix

$$\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{2.15}$$

Since we are only concerned with the region of unbroken $\mathcal{PT}$-symmetry the eigenvalues of $\tilde{H}$: $E_\pm = r\cos\theta \pm \sqrt{s^2 - r^2\sin^2\theta}$ are fully real. The corresponding $\mathcal{PT}$ normalised eigenstates of $\tilde{H}$ are

$$|E_+\rangle = \frac{1}{\sqrt{2\cos\alpha}}\begin{pmatrix} e^{i\alpha/2} \\ e^{-i\alpha/2} \end{pmatrix} \quad \text{and} \quad |E_-\rangle = \frac{1}{\sqrt{2\cos\alpha}}\begin{pmatrix} ie^{-i\alpha/2} \\ -ie^{i\alpha/2} \end{pmatrix} \tag{2.16}$$

here the change of variables is $\sin\alpha = \frac{r}{s}\sin\theta$.

The hyperbolic nature of the $\tilde{\omega}^2$ in 2.12 allows t to approach zero because the matrix elements of the $\mathcal{PT}$-symmetric Hamiltonian can be made large without violating the energy constraint in 2.8[22]. The $\mathcal{PT}$-symmetric analogue of the evolution in 2.13 is

$$\begin{pmatrix} a \\ b \end{pmatrix} = \frac{e^{\frac{-itr\cos\theta}{\hbar}}}{\cos\alpha}\begin{pmatrix} \cos(\frac{\omega t}{2\hbar} - \alpha) \\ -i\sin(\frac{\omega t}{2\hbar}) \end{pmatrix}. \tag{2.17}$$

As an example, let the final state be $|\psi_f\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Once again, finding the smallest t can be done by using one of the equations in the 2.17 matrix system. Here we will use the equation

$$|a| = \frac{\cos(\frac{\omega t}{2\hbar} - \alpha)}{\cos\alpha} \sin\left(\frac{\omega t}{2\hbar}\right),$$
$$\Rightarrow t = \frac{\hbar}{\omega}(2\alpha + \pi). \tag{2.18}$$

the minimal passage time in the $\mathcal{PT}$-symmetric framework must also satisfy the fixed energy constraint in 2.8. From the relationship between θ and α, we can rewrite $\tilde{\omega}^2$ in equation 2.11 as $\tilde{\omega}^2 = 4s^2\cos^2(\alpha)$. This demonstrates that the time evolutions in 2.14 and 2.18 differ mostly in that the shortest passage time in the Hermitian framework is $\tau = \frac{\pi\hbar}{\omega}$, while for the $\mathcal{PT}$-symmetric case in the limit $\alpha \to -\frac{\pi}{2}$ its possible to make the passage time arbitrarily small. This result does not violate the uncertainty principle because of the intrinsic difference in the Hilbert space geometry and its defined metric. In $\mathcal{PT}$-symmetric quantum theory, the inner-product depends directly on the Hamiltonian. As a consequence, it is possible to set the α parameter to a value such that we can have instantaneous evolution from $|\psi_i\rangle$ to $|\psi_f\rangle$.

Conclusion

Appendix

One-to-one equivalence: PT-symmetric and Hermitian quantum theories

parametric family of PTsNHH

Stokes wedges and boundary conditions

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