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1998 J. Phys. A: Math. Gen. 31 10105

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Strong-coupling expansions for the \mathcal{PT} -symmetric oscillators $V(x) = a(ix) + b(ix)^2 + c(ix)^3$

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Received 7 October 1998

Abstract. We study the traditional problem of convergence of perturbation expansions when the hermiticity of the Hamiltonian is relaxed to a weaker \mathcal{PT} symmetry. An elementary and quite exceptional cubic anharmonic oscillator is chosen as an illustrative example of such models. We describe its perturbative features paying particular attention to the strong-coupling regime. Efficient numerical perturbation theory proves suitable for such a purpose.

1. Introduction and summary

The analysis of convergence of perturbation expansions is one of the most exciting mathematical problems in quantum physics. Its relevance ranges from the phenomenology of bound states in atomic and molecular physics up to abstract methodical considerations which concern quantum fields [1]. Often, the convergence of perturbation series is studied by means of an elementary anharmonic oscillator model in one dimension:

$$V(x) = Bx^2 + Cx^3 + Dx^4 \quad x \in (-\infty, \infty) \quad (1)$$

because of its apparent simplicity. The application of textbook Rayleigh–Schrödinger (RS) perturbation theory is remarkably simple in the so called weak coupling regime dominated by harmonic oscillations when $B \gg |C|$ and $B \gg |D|$.

In more sophisticated approaches based on an extensive numerical re-processing of the RS series one considers the strong-coupling regime in which the quartic term is not only important but also dominating [2, 3]. This is of particular importance in field theory where perturbation expansions are one of the few available constructive means. The strong-coupling approach may also be of value in a quantitative description of seemingly non-perturbative quantum mechanical systems of physical interest [4]. Allowing complex values of the couplings of model (1) further enriches its physical meaning and scope [5]. It opens new phenomenological possibilities. Energies may acquire purely imaginary components, bound states may ‘dissolve’ into unstable resonances, etc. Various mathematical techniques have to be combined in order to treat these extended models with non-Hermitian Hamiltonians (see [6] for a review of some relevant literature).

In particular, Bender and Boettcher [7] recently discovered, among all the complex quartic potentials (1), a large two-parametric family of non-Hermitian forces which are partially, *quasi-exactly* [8] solvable. The parity-violating Bender and Boettcher example is already slightly counterintuitive and exceptional. Its appeal comes from field theory as it conserves the product \mathcal{PT} of parity and time reversal. In the context of quantum mechanics this just means the symmetry with respect to the simultaneous reflection of the coordinate $x \rightarrow -x$ and complex conjugation which, formally, replaces i by $-i$ [9].

Strictly speaking, a rigorous treatment of quartic potentials and, in general, of all their higher-power \mathcal{PT} -symmetric generalizations $(ix)^N$ with $N \geq 4$ already requires a nontrivial deformation of the integration path into the complex plane [10]. A slight formal simplification is achieved, therefore, when the dominant quartic anharmonicity in (1) vanishes [11]. In this setting, trying to bridge the gap between the Hermitian and non-Hermitian Hamiltonians in what follows, we will analyse only the non-Hermitian and \mathcal{PT} -symmetric shifted version of (1) with $D = 0$:

$$V(x) = a(ix) + b(ix)^2 + c(ix)^3 \quad x \in (-\infty, \infty). \quad (2)$$

Historically, the empirical and numerically oriented studies of interactions (2) with $a = 0$ go back to Daniel Bessis who conjectured, several years ago, that the purely imaginary cubic coupling keeps the ‘resonant’ anharmonic energies discrete and, what is even more surprising, *purely real* [12]. This property makes these models immediately eligible for perturbative description.

A new, additional motive for perturbative analysis of non-Hermitian oscillators of Bessis type lies in unexpected difficulties related to their weak coupling perturbative interpretation. Indeed, one cannot allow the cubic *and* quadratic coupling to vanish simultaneously since the spectrum of linear $V_0(x) = ix$ is null [13]. In this sense, besides a far reaching analogy between equations (1) and (2) (which was the original inspiration for our present paper) there also exist certain differences.

Several particular cases of potential (2) with real couplings are discussed here. In section 2 we recall the ideas of numerical perturbation theory [14, 15]. Section 3 then shows that their application to the class of non-Hermitian examples (2) is straightforward. Finally, in section 4, we add more observations regarding re-summations of perturbative expansions for our \mathcal{PT} symmetric Hamiltonians, motivated by their possible methodical connection to field theory, etc.

We may summarize by stating that even our utterly schematic examples confirm that many \mathcal{PT} -symmetric non-Hermitian oscillators similar to (2) may be understood and described in a way which strictly parallels the existing extensive studies of the ordinary anharmonic oscillator (1).

The continuation of real Hamiltonians to the complex plane while preserving their \mathcal{PT} symmetry opens a new and almost unexplored field of mathematical analysis of Schrödinger equation. In this context we have resorted to the simple numerical algorithm to compute perturbation series. For Hermitian Hamiltonians, such a numerical form of perturbation theory proved convenient as a stable source of expansions that are suitable for all values of the coupling constant. Our present results extend this numerical experience to a few extremely interesting non-Hermitian examples.

The numerical perturbative approach is again shown to offer a reliable computational tool. In the strong-coupling and, possibly, renormalized regime the possibility of using a virtually arbitrary zero-order system of Bessis type is well matched by the ‘perturbation friendly’ real and discrete character of the spectra of its \mathcal{PT} -symmetric perturbations. Of course, the eigenfunctions are complex valued, with the only requirement being that of

giving square-integrable wavefunctions. One may appreciate the role of the \mathcal{PT} symmetry of Hamiltonians which not only provide *real* eigenvalues, but also their perturbation form with *real* coefficients.

2. Perturbation series by numerical techniques

Traditional textbooks on quantum mechanics pay a thorough attention to the construction of perturbative expansions based on the expansion in a complete set of eigenvectors of the unperturbed Hamiltonian H_0 . For this reason, the perturbation series

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \dots \quad (3)$$

for the eigenvalues of Hamiltonians $H(\lambda) = H_0 + \lambda W$ are commonly restricted to a small range of a few available exactly solvable models.

In contrast, a purely numerical approach is both straightforward and more widely applicable to the determination of perturbation expansions like (3). A simple and efficient procedure for obtaining RS perturbation expansions for the solutions of the Schrödinger equation with Hamiltonians

$$H = -\frac{d^2}{dx^2} + V(x) + \lambda W(x) \quad (4)$$

consists in a replacement of the second derivative operator by the centred second difference operator,

$$\frac{d^2}{dx^2} \approx \frac{\delta^2}{h^2}$$

h being the distance between adjacent points in a suitable uniform mesh. In principle, the problem reduces to the diagonalization of a *symmetric* and *tridiagonal* matrix, well known and understood in the case of real potentials [16].

Many open questions regarding numerical methods for complex potentials still exist [17]. In particular, our Hamiltonian matrices cease to be Hermitian even after discretization. One must test and verify the very reality of their eigenvalues, as well as the rate of their $h \rightarrow 0$ convergence with much greater care. A word of warning may come from both the elementary analytical arguments (illustrating, for example, the subtleties of discretization in the complex plane by the—very discontinuous—square well example) and the numerical tests we offer here.

From this point on, upper-case bold sans-serif and lower-case bold italic letters denote square matrices and column vectors, respectively. In such a notation we solve the matrix eigenvalue problem

$$[\mathbf{H}_0 + \lambda \mathbf{H}_I] \mathbf{v} = E \mathbf{v}$$

where the Hamiltonian matrix $\mathbf{H}_0 + \lambda \mathbf{H}_I$ is symmetric, with

$$\mathbf{H}_0 = \begin{bmatrix} \frac{2}{h^2} + V_0 & -\frac{1}{h^2} & 0 & 0 & \dots \\ -\frac{1}{h^2} & \frac{2}{h^2} + V_1 & -\frac{1}{h^2} & 0 & \dots \\ 0 & -\frac{1}{h^2} & \frac{2}{h^2} + V_2 & -\frac{1}{h^2} & \\ \vdots & & \ddots & \ddots & \ddots \end{bmatrix}$$

and

$$\mathbf{H}_I = \begin{bmatrix} W_0 & 0 & \dots \\ 0 & W_1 & \\ \vdots & & \ddots \end{bmatrix}.$$

When applying perturbation theory one first solves the eigenvalue equation for the unperturbed problem

$$\mathbf{H}_0 \mathbf{v}_0 = E_0 \mathbf{v}_0 \quad (5)$$

and then a hierarchy of inhomogeneous equations for the perturbation corrections of higher order:

$$\mathbf{H}_0 \mathbf{v}_k + \mathbf{H}_I \mathbf{v}_{k-1} = E_0 \mathbf{v}_k + E_k \mathbf{v}_0 + \sum_{p=1}^{k-1} E_p \mathbf{v}_{p-k}. \quad (6)$$

Notice that \mathbf{v}_0 is both a left and right eigenvector because of the symmetry of \mathbf{H}_0 . We find it convenient to use the scalar product $[\mathbf{v}^T \mathbf{w}] \equiv \sum \mathbf{v}_i \mathbf{w}_i$, although it does not produce a real norm, and resort to the *intermediate normalization* condition

$$[\mathbf{v}_0^T \mathbf{v}_k] \equiv \sum_i \mathbf{v}_{0i} \mathbf{v}_{ki} = \delta_{k0}$$

that leads to simpler expressions for the energy coefficients. The intermediate normalization condition is based on the observation that if \mathbf{v}_k is a solution of the perturbation equation, then $\mathbf{v}_k + \alpha \mathbf{v}_0$ is also a solution for arbitrary values of α . The computational scheme is straightforward:

- (i) Solve the eigenvalue equation (5).
- (ii) Project (6) onto \mathbf{v}_0^T and obtain the k th perturbative correction to the energy

$$E_k = [\mathbf{v}_0^T \mathbf{H}_I \mathbf{v}_{k-1}].$$

- (iii) Once E_k is known, solve the inhomogeneous equation for \mathbf{v}_k .
- (iv) Orthogonalize \mathbf{v}_k with respect to \mathbf{v}_0 :

$$\mathbf{v}_k \leftarrow \mathbf{v}_k - [\mathbf{v}_0^T \mathbf{v}_k] \mathbf{v}_0.$$

3. Application to the two \mathcal{PT} symmetric models

Table 1 shows some perturbation corrections to the energies of the \mathcal{PT} symmetric Hamiltonians

$$H^{(1)} = p^2 + ix^3 + i\lambda x \quad (7)$$

and

$$H^{(2)} = p^2 + ix^3 + \lambda x^2. \quad (8)$$

In both cases the coefficients $E_n^{(1,2)}$ of the powers of λ are *real*, as expected from the \mathcal{PT} symmetry. We used complex arithmetics for the numerical calculation observing that the imaginary parts vanished within the rounding errors. The code was successfully tested with the exactly solvable model

$$H = p^2 + x^2 + i\lambda x \quad (9)$$

obtaining the known expansion

$$E(\lambda) = 1 + \frac{1}{4}\lambda^2$$

which one can easily derive by means of the coordinate translation $x \rightarrow x + i\lambda/2$ in the Hamiltonian $H = p^2 + x^2$. The agreement between the numerical and exact result suggests that the method is sufficiently accurate and stable.

Table 1. Energy coefficients for the ground states of the Hamiltonians (7) and (8).

n	$E_n^{(1)}$ for $p^2 + ix^3 + i\lambda x$	$E_n^{(2)}$ for $p^2 + ix^3 + \lambda x^2$
0	1.156 267 071 982	1.156 267 071 982
1	0.590 072 533 078	0
2	0.119 413 858 091	0.196 690 844 356
3	$-1.142\ 128\ 489\ 951 \times 10^{-2}$	$-7.407\ 407\ 406\ 938 \times 10^{-2}$
4	$2.197\ 147\ 795\ 152 \times 10^{-3}$	$1.326\ 820\ 645\ 262 \times 10^{-2}$
5	$-5.299\ 287\ 434\ 734 \times 10^{-4}$	0
6	$1.432\ 651\ 458\ 960 \times 10^{-4}$	$-4.230\ 105\ 523\ 351 \times 10^{-4}$
7	$-4.148\ 903\ 908\ 710 \times 10^{-5}$	0
8	$1.257\ 939\ 817\ 338 \times 10^{-5}$	$2.712\ 528\ 133\ 232 \times 10^{-5}$
9	$-3.941\ 134\ 497\ 194 \times 10^{-6}$	0
10	$1.265\ 478\ 160\ 326 \times 10^{-6}$	$-2.180\ 776\ 735\ 057 \times 10^{-6}$
11	$-4.141\ 789\ 581\ 668 \times 10^{-7}$	0
12	$1.376\ 462\ 051\ 952 \times 10^{-7}$	$1.965\ 228\ 322\ 941 \times 10^{-7}$
13	$-4.632\ 126\ 852\ 199 \times 10^{-8}$	0
14	$1.575\ 200\ 873\ 072 \times 10^{-8}$	$-1.897\ 075\ 421\ 079 \times 10^{-8}$
15	$-5.404\ 290\ 239\ 370 \times 10^{-9}$	0
16	$1.868\ 293\ 677\ 263 \times 10^{-9}$	$1.917\ 298\ 897\ 845 \times 10^{-9}$
17	$-6.501\ 605\ 918\ 143 \times 10^{-10}$	0
18	$2.275\ 683\ 198\ 987 \times 10^{-10}$	$-2.002\ 303\ 776\ 843 \times 10^{-10}$
19	$-8.006\ 218\ 039\ 652 \times 10^{-11}$	0
20	$2.829\ 596\ 711\ 623 \times 10^{-11}$	$2.143\ 098\ 365\ 950 \times 10^{-11}$

The two perturbative expansions of table 1 are connected, because the Hamiltonians (7) and (8) are related by a complex translation of the coordinate. The substitution $x \rightarrow x + i\lambda/3$ in (8) results in a Hamiltonian like equation (7):

$$H \rightarrow p^2 + ix^3 + \left(\frac{i\lambda^2}{3}\right)x - \frac{2}{27}\lambda^3.$$

Consequently, the energy coefficients $E_n^{(1)}$ and $E_n^{(2)}$ of table 1 satisfy

$$E_{2n}^{(2)} = \frac{1}{3^n} E_n^{(1)} \quad E_{2n+1}^{(2)} = -\frac{2}{27} \delta_{n1} \tag{10}$$

indicating that the expansion $E_n^{(2)}$ has only even coefficients except for $E_3^{(2)} = -\frac{2}{27}$. Our numerical coefficients shown in table 1 obey the exact relations (10) with an accuracy close to 1 part in 10^{10} . This test is an additional confirmation of the stability and accuracy of our numerical method.

We may conclude that the application of a numerical version of perturbation theory to non-Hermitian Hamiltonians is straightforward as long as their spectrum is discrete. The demonstrated feasibility of a reliable *quantitative* perturbative description of our unusual models (2) with \mathcal{PT} -symmetric forces is encouraging.

4. Renormalized perturbation expansions

From the magnitude of the energy coefficients in the tests of section 3 we may estimate the radii of convergence to be about 1.7 and 3 for the Hamiltonians (7) and (8), respectively.

Table 2. Renormalized perturbation expansion for the Hamiltonian (12) corresponding to the variable $(1 - \kappa)$, for $\omega = 1$, without the factor $[\lambda/(1 - \kappa)]^{1/2}$.

n	$E_n^{(r)}$	n	$E_n^{(r)}$	n	$E_n^{(r)}$
0	$1.156\ 267\ 07 \times 10^{+0}$	30	$-6.171\ 354\ 80 \times 10^{-4}$	60	$-5.421\ 861\ 48 \times 10^{-5}$
1	$-4.625\ 068\ 29 \times 10^{-1}$	31	$-8.974\ 095\ 09 \times 10^{-4}$	61	$-1.397\ 002\ 06 \times 10^{-5}$
2	$5.793\ 879\ 57 \times 10^{-2}$	32	$-1.054\ 718\ 29 \times 10^{-3}$	62	$2.193\ 137\ 29 \times 10^{-5}$
3	$8.795\ 384\ 66 \times 10^{-2}$	33	$-1.096\ 628\ 61 \times 10^{-3}$	63	$5.129\ 700\ 44 \times 10^{-5}$
4	$7.665\ 126\ 27 \times 10^{-2}$	34	$-1.038\ 846\ 74 \times 10^{-3}$	64	$7.274\ 120\ 89 \times 10^{-5}$
5	$5.723\ 695\ 34 \times 10^{-2}$	35	$-9.025\ 336\ 00 \times 10^{-4}$	65	$8.567\ 778\ 88 \times 10^{-5}$
6	$3.810\ 370\ 38 \times 10^{-2}$	36	$-7.116\ 803\ 94 \times 10^{-4}$	66	$9.025\ 593\ 62 \times 10^{-5}$
7	$2.188\ 533\ 70 \times 10^{-2}$	37	$-4.907\ 264\ 98 \times 10^{-4}$	67	$8.724\ 869\ 94 \times 10^{-5}$
8	$9.294\ 671\ 98 \times 10^{-3}$	38	$-2.625\ 529\ 92 \times 10^{-4}$	68	$7.790\ 895\ 89 \times 10^{-5}$
9	$2.694\ 862\ 28 \times 10^{-4}$	39	$-4.693\ 584\ 53 \times 10^{-5}$	69	$6.380\ 829\ 04 \times 10^{-5}$
10	$-5.590\ 411\ 45 \times 10^{-3}$	40	$1.405\ 040\ 96 \times 10^{-4}$	70	$4.667\ 329\ 11 \times 10^{-5}$
11	$-8.824\ 428\ 31 \times 10^{-3}$	41	$2.888\ 589\ 70 \times 10^{-4}$	71	$2.823\ 216\ 47 \times 10^{-5}$
12	$-1.000\ 845\ 22 \times 10^{-2}$	42	$3.920\ 389\ 67 \times 10^{-4}$	72	$1.008\ 185\ 15 \times 10^{-5}$
13	$-9.697\ 245\ 68 \times 10^{-3}$	43	$4.484\ 903\ 39 \times 10^{-4}$	73	$-6.416\ 947\ 26 \times 10^{-6}$
14	$-8.391\ 244\ 75 \times 10^{-3}$	44	$4.606\ 096\ 91 \times 10^{-4}$	74	$-2.021\ 260\ 36 \times 10^{-5}$
15	$-6.518\ 279\ 89 \times 10^{-3}$	45	$4.339\ 467\ 92 \times 10^{-4}$	75	$-3.060\ 201\ 07 \times 10^{-5}$
16	$-4.425\ 314\ 87 \times 10^{-3}$	46	$3.762\ 890\ 89 \times 10^{-4}$	76	$-3.723\ 809\ 71 \times 10^{-5}$
17	$-2.377\ 298\ 32 \times 10^{-3}$	47	$2.967\ 152\ 78 \times 10^{-4}$	77	$-4.010\ 908\ 85 \times 10^{-5}$
18	$-5.611\ 495\ 17 \times 10^{-4}$	48	$2.046\ 940\ 55 \times 10^{-4}$	78	$-3.949\ 485\ 37 \times 10^{-5}$
19	$9.066\ 333\ 51 \times 10^{-4}$	49	$1.092\ 891\ 25 \times 10^{-4}$	79	$-3.590\ 670\ 12 \times 10^{-5}$
20	$1.969\ 985\ 43 \times 10^{-3}$	50	$1.851\ 445\ 90 \times 10^{-5}$	80	$-3.001\ 741\ 30 \times 10^{-5}$
21	$2.621\ 962\ 98 \times 10^{-3}$	51	$-6.113\ 406\ 29 \times 10^{-5}$	81	$-2.258\ 814\ 43 \times 10^{-5}$
22	$2.893\ 001\ 70 \times 10^{-3}$	52	$-1.249\ 614\ 53 \times 10^{-4}$	82	$-1.439\ 818\ 69 \times 10^{-5}$
23	$2.839\ 486\ 51 \times 10^{-3}$	53	$-1.701\ 769\ 02 \times 10^{-4}$	83	$-6.182\ 586\ 40 \times 10^{-6}$
24	$2.533\ 219\ 73 \times 10^{-3}$	54	$-1.958\ 360\ 70 \times 10^{-4}$	84	$1.418\ 646\ 77 \times 10^{-6}$
25	$2.052\ 219\ 67 \times 10^{-3}$	55	$-2.026\ 502\ 29 \times 10^{-4}$	85	$7.897\ 365\ 74 \times 10^{-6}$
26	$1.473\ 132\ 26 \times 10^{-3}$	56	$-1.926\ 959\ 92 \times 10^{-4}$	86	$1.289\ 916\ 17 \times 10^{-5}$
27	$8.653\ 970\ 89 \times 10^{-4}$	57	$-1.690\ 619\ 44 \times 10^{-4}$	87	$1.623\ 056\ 01 \times 10^{-5}$
28	$2.871\ 842\ 60 \times 10^{-4}$	58	$-1.354\ 679\ 88 \times 10^{-4}$	88	$1.785\ 289\ 84 \times 10^{-5}$
29	$-2.169\ 887\ 80 \times 10^{-4}$	59	$-9.589\ 016\ 14 \times 10^{-5}$	89	$1.786\ 508\ 77 \times 10^{-5}$

It is sometimes possible to extend the perturbative prediction beyond these limits. One of the most common techniques for such an improvement in the convergence of a perturbation series is its renormalization. It consists of a nonlinear mapping of the original perturbation parameter (λ in the equations above) onto a more convenient one. There are many equivalent mappings (see, e.g., [3]). Here we consider one which has lately received detailed attention [18, 19] in connection to strong-coupling expansions. It changes the perturbation parameter $\lambda \in [0, \infty]$ into $\kappa \in [0, 1]$ according to

$$\lambda^{5/4} = \frac{\omega(1 - \kappa)^{5/4}}{\kappa} \quad (11)$$

where the exponent $\frac{5}{4}$ is appropriate for the Hamiltonian in (8), and ω is a free parameter. Application of the scale transformation $x \rightarrow x\sqrt{1 - \kappa}$ to the Hamiltonian (8) leads to a new Hamiltonian

$$H^{(r)} = \sqrt{\frac{\lambda}{1 - \kappa}} \left[p^2 + (1 - \kappa) \left(x^2 - \frac{\text{i}x^3}{\omega} \right) + \frac{\text{i}x^3}{\omega} \right]. \quad (12)$$

The algorithm used to calculate the original perturbation expansion also applies to the renormalized series generated by the Hamiltonian (12). The resulting expansion coefficients

are shown in table 2. After searching for an optimal value of ω we chose $\omega = 1$ in all our calculations.

Table 3. Ground-state energy calculated by the renormalized series and by direct numerical integration of the Schrödinger equation for a wide range of values of the coupling constant λ .

λ	κ	$E(\text{perturbative})$	$E(\text{numerical})$
0.1	0.907 47	1.158 161 23	1.158 161 23
1	0.461 40	1.291 754 16	1.291 754 16
10	0.052 56	3.169 095 62	3.169 096 16
100	0.003 15	9.999 968 45	10.000 068 74

In the language of perturbation theory the \mathcal{PT} symmetry of our models and the related phenomenon of existence of real energies is reflected by the reality of the perturbative coefficients. The renormalized coefficients in table 2 exhibit a surprising oscillatory behaviour with an amplitude that decreases slowly with the perturbation order. We find this resummation-friendly behaviour remarkable, as it does not occur in similar expansions for real Hamiltonians [19].

By absolute value, the coefficients of the renormalized series decrease with the order more slowly than the coefficients of the standard expansion. Nonetheless, the former series exhibits better convergence properties because the new perturbation parameter $(1 - \kappa)$ is limited to the interval $[0, 1]$. For an immediate check one may recall a direct numerical integration of Schrödinger equation for comparison. A small sample of such a test is given in table 3. For the ground-state energy and using the coefficients in table 2 we can see that the relative difference between the exact result and its renormalized perturbative approximant is always smaller than 10^{-5} , even for huge values of the original unrenormalized coupling λ .

Clearly, renormalization is successful in this case. Let us emphasize that such an observation is non-trivial. Indeed, in contrast to the current experience with unitary equivalence of Hermitian operators, the explicit form of relationship between our present models (8) and (12) may only be characterized in terms of their \mathcal{PT} -symmetry in general.

Acknowledgments

RG and JR acknowledge financial support from the Dirección General de Investigación Científica y Tecnológica (DGICYT, Spain) under grant No PB97/1139. MZ acknowledges financial support from the Grantová agentura AV ČR, Praha under grant A 104 8602.

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