THE IMAGINARY CUBIC PERTURBATION: A NUMERICAL AND ANALYTIC STUDY

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ABSTRACT

In

J. Zinn-Justin and U.D. Jentschura, **J. Math. Phys.** 51 (2010) 072106; *ibidem* **J. Phys. A: Math. Theor.** 43 (2010) 425301,

we present a systematic analytic and numerical investigation of the lowest eigenvalue of the quantum harmonic oscillator perturbed by an imaginary cubic term $i\sqrt{g}x^3$, leading to one of the simplest PT symmetric, non-Hermitian, Hamiltonian. The Hamiltonian is known to have a real spectrum.

A key numerical tool is the summation of the perturbative expansion by the Order-Dependent Mapping method (ODM),

R. Seznec and J. Zinn-Justin, **Journal of Math. Phys.** 20 (1979) 1398; J. Zinn-Justin, **Applied Numerical Mathematics** 60 (2010) 1454,

in a form that takes full advantage of the properties of the potential. It happens to be very efficient in the strong coupling regime and, in particular, allows to determine a number of terms of the strong coupling expansion.

The expansion is related to the expansion of another PT symmetric Hamiltonian with the potential $ix^3 + \mathrm{i}vx$, $v = g^{-4/5}$ real, in powers of the parameter v. However, both Hamiltonians are directly related only for v positive. Studying the continuation to $v < 0$, one discovers that for a negative value v_c two eigenvalues merge and then become complex conjugate, a phenomenon that can be interpreted as a spontaneous breaking of the PT symmetry.

The Lee–Yang edge singularity

An initial motivation to study a potential with an imaginary cubic term comes from statistical physics. The partition function of a general Ising model, as a function of the magnetic field H, has singularities on the imaginary axis, *i.e.*, in $z = \mathrm{e}^{H}$ on the circle $|z| = 1$. For $T > T_c$, the circle has a gap while for $T > T_c$, the circle separates two distinct analytic functions. It is expected (Fisher) that near T_{c+} the nature of the singularity closest to the real axis (the edge singularity) can be studied by renormalization group methods. Starting from the ϕ^4 field theory, known to describe universal properties of the Ising model, shifting ϕ by its imaginary expectation value to cancel the linear magnetic term, and keeping only the most relevant terms at large distance, one finds in d dimensions a Hamiltonian of the form

$$\mathcal{H}(\phi) = \int \mathrm{d}^d x \left[\tfrac{1}{2}\left(\partial_\mu \phi(x)\right)^2 + \tfrac{1}{2} r \phi^2(x) + \tfrac{1}{6} i \lambda \phi^3(x)\right].$$

The imaginary cubic potential

The properties of such a model are rather intriguing and suggest to first study a toy model corresponding to $d = 1$, and the quantum Hamiltonian

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{(\mathrm{d}x)^2} + \frac{1}{2}x^2 + i\sqrt{g}\frac{x^3}{6}\,, \quad g > 0\,. \tag{1}$$

The model has been the subject of a number of investigations since it has been conjectured by Bessis and Zinn-Justin (1992) to have a real spectrum, a property that was later proved. It provides one of the simplest examples of a PT symmetric Hamiltonian, that is, invariant under the simultaneous transformations complex conjugation and $x \mapsto -x$.

The perturbative expansion of the energy eigenvalues E_n for $g \to 0$ contains only integer powers of g:

$$E_n(g) = \frac{n}{2} + \sum_{k=1} E_{n,k}\, g^k\,, \quad E_{n,k} \text{ real}\,.$$

The series are divergent with a large order behaviour of the form

$$E_{n,k} \underset{k\to\infty}{\sim} C_n(-1)^{k+1}A^{-k}\Gamma(k+n+1/2)\,, \quad A=24/5\,,$$

but Borel summable. Padé summability has also established: $\operatorname{Im} E_n(g) > 0$ for $g = -|g| + \mathrm{i}0$.

By a simple affine transformation on x, one can relate the Hamiltonian to another PT symmetric Hamiltonian

$$\mathcal{H}(v) = g^{-1/5}\left(H + \frac{1}{3g}\right) = -\frac{1}{2}\frac{\mathrm{d}^2}{(\mathrm{d}x)^2} + i\left(\frac{1}{6}x^3 + \frac{1}{2}vx\right) \text{ with } v = g^{-4/5}.$$

The ODM summation method (defined later) has been applied to the small g expansion to determine a number of coefficients of the large g, small v, expansion.

As a result of our numerical investigations, we conjecture that the lowest eigenvalue $\mathcal{E}_0(v)$ of $\mathcal{H}(v)$, which is a real analytic function, has singularities only on the real negative axis with a discontinuity on the cut that is negative.

The singularity closest to the origin, a square-root singularity, has for the Hamiltonian $\mathcal{H}(v)$ the interpretation of a spontaneous breaking of the PT symmetry: the two lowest eigenvalues merge at the singularity and then become complex conjugate.

A direct confirmation of these conjectures is obtained by studying the continued fraction expansion derived from the small v expansion.

Finally, combining all methods, we have a general numerical control on the function $\mathcal{E}_0(v)$ in a cut-plane or equivalently $E_0(g)$ in the first Riemann sheet of the uniformization variable $g^{-1/5}$.

Related Hamiltonians: Strong coupling expansion

To the cubic Hamiltonian H corresponds the time-independent Schrödinger equation

$$-\frac{1}{2}\psi''(x)+\left(\frac{i}{6}\sqrt{g}x^3+\frac{1}{2}x^2\right)\psi(x)=E(g)\psi(x),$$

which, with proper boundary conditions at infinity, determines the eigenvalues $E(g)$ of the operator.

After a rescaling of the variable x, the equation can be rewritten as

$$-\frac{1}{2}\psi''(x)+\left(\frac{i}{6}x^3+\frac{1}{2}ux^2\right)\psi(x)=\varepsilon(u)\psi(x),$$

in which $u=g^{-2/5}$ and $E(g)=g^{1/5}\varepsilon(g^{-2/5})$.

We then shift the coordinate $x\mapsto x+iu$. The equation becomes

$$-\frac{1}{2}\psi''(x)+i\left(\frac{1}{6}x^3+\frac{1}{2}vx\right)\psi(x)=\mathcal{E}(v)\psi(x) \tag{2}$$

with $v=g^{-4/5}$ and

$$\varepsilon(u)=-\frac{1}{3}u^3+\mathcal{E}(u^2). \tag{3}$$

$\mathcal{E}(v)$ is an eigenvalue of the second PT symmetric Hamiltonian $\mathcal{H}(v)$. The expansion of $\mathcal{E}(v)$ in powers of v, $\mathcal{E}(v) = \sum_{\ell=0} \mathcal{E}_\ell v^\ell$, unlike the perturbative expansion in g, is convergent in a disk. Therefore, $E(g)$ has a convergent large g expansion of the form

$$E(g) = -\frac{1}{3g} + g^{1/5} \sum_{\ell=0} \mathcal{E}_\ell g^{-4\ell/5}. \tag{4}$$

Since $\epsilon(u)$ has only one term odd in u, which, moreover, is explicitly known, for g large, the relevant expansion variable is $g^{-4/5}$ rather than $g^{-2/5}$. In the uniformizing variable $g^{-1/5}$, it is sufficient to determine the eigenvalues for $-\pi/4 \le g^{-1/5} \le \pi/4$ to know them in the whole first Riemann sheet.

Remark. The Hamiltonian $\mathcal{H}(v)$ is PT symmetric for all v real but corresponds to the cubic Hamiltonian only for $v \ge 0$. The numerical determination of the small v expansion allows studying its spectrum also in the region $v < 0$, which corresponds to the analytic continuation $g = |g| \, \mathrm{e}^{i5\pi/4}$.

Order-dependent mapping (ODM) summation method

We briefly explain the ODM summation method, a method based on some prior knowledge of the analytic properties of the expanded function. It applies both to convergent and divergent series, though it is mainly useful in the latter case.

The ODM method. We consider a $E(g)$ function analytic in a sector and mappings $g \mapsto \lambda$ of the form

$$g = \rho\zeta(\lambda)\,,$$

where $\zeta(\lambda)$ is a real analytic function increasing on $0 \le \lambda < 1$, such that $\zeta(\lambda) = \lambda + O(\lambda^2)$ and, for $\lambda \to 1$, $\zeta(\lambda) \propto (1-\lambda)^{-\alpha}$ with $\alpha > 1$. The parameter α has to be chosen in accordance with the analytic properties of the function and ρ is an adjustable parameter.

For the series under study here, one chooses mappings such that, for $g \to \infty$ and, thus $\lambda \to 1$, $g^{-1/\alpha}$ has a regular expansion in powers of $1-\lambda$.

After the mapping, E is given by a Taylor series in λ of the form

$$E\bigl(g(\lambda)\bigr) = \sum_{k=0} P_k(\rho)\lambda^k,$$

where the coefficients $P_k(\rho)$ are polynomials of degree k in ρ. Since the result is formally independent of ρ, ρ can be chosen freely. At ρ fixed, the series in λ is still divergent, but it has been verified on a number of examples (all Borel summable), and proved in certain cases that, by adjusting ρ order by order, one can devise a convergent algorithm.

The k-th approximant $E^{(k)}(g)$ is then constructed in the following way: one truncates the expansion at order k and chooses ρ as to cancel the last term. Since $P_k(\rho)$ has k roots (real or complex), one chooses, in general, for ρ the largest possible root (in modulus) ρ_k for which $P'_k(\rho)$ is small. This leads to a sequence of approximants

$$E^{(k)}(g) = \sum_{\ell=0}^{k} P_\ell(\rho_k)\lambda^\ell(g,\rho_k) \quad \text{with} \quad P_k(\rho_k) = 0.$$

In the case of convergent series, it is expected that ρ_k has a non-vanishing limit for $k \to \infty$. By contrast, for divergent series it is expected that ρ_k goes to zero for large k as

$$\rho_k = O\left(E_k^{-1/k}\right).$$

The intuitive idea is that ρ_k corresponds to a 'local' radius of convergence.

Remarks.

(i) Alternatively, one can choose the largest roots ρ_k of the polynomials $P'_k(\rho)$ for which P_k is small. Indeed, the approximant is not very sensitive to the precise value of ρ_k, within errors. Finally, $P_{k+1}(\rho_k)$ gives an estimate of the error.

(ii) In the ODM method, determining the sequence of the ρ_k's is the most time-consuming task. Indeed, once the ρ_k are known, for each value of g the calculation reduces to inverting the mapping $g \mapsto \lambda$ and simply summing the Taylor series in λ to the relevant order.

Convergence analysis

A semi-rigorous analysis of the convergence of the ODM method provides quantitative asymptotic estimates of the convergence as a function of the choice of the ρ_k's.

We now consider functions $E(g)$ analytic in a cut-plane with an expansion

$$E(g) = \sum_k E_k g^k,$$

where the coefficients E_k have a large order behaviour of the form

$$E_k \underset{k\to\infty}{\propto} (-A)^{-k}\Gamma(k+b+1) \sim (-A)^{-k} k^b k!\,.$$

We have studied several mappings including three relevant for this problem:

$$g = \rho\frac{\lambda}{(1-\lambda)^\alpha} \text{ for } \alpha = 5/4, 5/2 \text{ and } g = \rho\frac{\lambda(1-\lambda/2)}{(1-\lambda)^\alpha} \text{ for } \alpha = 5/2\,.$$

Semi-rigorous arguments confirmed by numerical data suggest the behaviour

$$\rho_k \underset{k\to\infty}{\sim} A\mu/k\,,\;\; \mu > 0\,.$$

(with this definition, the parameter μ is independent of the normalization of g.) Error estimates then determine optimal values $\mu = \mu_c$. For the cubic potential,

$$g = \rho\frac{\lambda}{(1-\lambda)^{5/4}} \;\;\Rightarrow\;\; \mu_c = 3.811522\ldots\,,$$

$$g = \rho\frac{\lambda}{(1-\lambda)^{5/2}} \;\;\Rightarrow\;\; \mu_c = 4.895690\ldots\,,$$

$$g = \rho\frac{\lambda(1-\lambda/2)}{(1-\lambda)^{5/2}} \;\;\Rightarrow\;\; \mu_c = 4.445762\ldots\,,$$

values asymptotically consistent with numerical data.

The error at order k is then governed by a factor of the form

$$\mathrm{e}^{Ck^{1-1/\alpha}} \text{ with } C = \mathrm{Re}(C_1 + C_2 g^{-1/\alpha}),$$

where C_2 can be determined analytically and C_1 numerically.

This form also determines the domain of convergence. Here it is found, for $\alpha = 5/4$,

$$\mathrm{Re}\, g^{-4/5} > -0.48 \ \Leftrightarrow\ \mathrm{Re}\, v > -1.351\ldots\,,$$

and for $\alpha = 5/2$,

$$\mathrm{Re}\, g^{-2/5} > 0 \ \Leftrightarrow\ \mathrm{Re}\sqrt{v} > 0\,.$$

Therefore, from numerical evidence we conjecture that the function $\mathcal{E}_0(v)$ is analytic in a cut-plane, the first singularity being at $v = v_c \approx -1.35$ We also notice $\mathrm{Im}\,\mathcal{E}_0(v) < 0$ near the cut. Finally, at order 150, the best convergence is obtained for $|v| < 1$ for $\alpha = 5/4$ and for $|v| \geq 1$ for $\alpha = 5/2$.

The ix^3 perturbation: ODM summation

We have mainly studied the first eigenvalue E_0 but, because we guessed that the first singularity at $v = v_c$ could be due to an eigenvalue merger, we have also determined $(E_0 + E_1)$ and $(E_0 - E_1)^2$.

For example, the first terms of the expansion of E_0 are:

$$E_0(g) = \tfrac{1}{2} + \tfrac{11}{288} g - \tfrac{930}{(288)^2} g^2 + O(g^3).$$

We have first determined the large g, small v expansion by using the ODM method with $\alpha = 5/4$.

We have applied the ODM method to the function

$$F(g) = \tfrac{1}{3} + gE(g),$$

which has a regular small g expansion and a large g expansion of the form

$$F(g) = g^{6/5} \mathcal{E}(g^{-4/5}) = g^{6/5} \sum_{k=0} \mathcal{E}_k g^{-4k/5}.$$

We have introduced the mapping

$$g = \rho \frac{\lambda}{(1-\lambda)^{5/4}} \text{ and set } F\big(g(\lambda)\big) = (1-\lambda)^{-3/2}\phi(\lambda, \rho).$$

The function $\phi(\lambda, \rho)$ then has a regular expansion both at $\lambda = 0$, determined by the small g expansion, and $\lambda = 1$ $(g \to \infty)$.

To characterize the nature of the first singularity, we have then also expanded the second eigenvalue $E_1(g)$ and summed the series for $(E_1 + E_0)$ and $(E_1 - E_0)^2$. As expected, the singularity disappears in these symmetric functions and $(E_1 - E_0)^2$ vanishes linearly at

$$v_c = -1.3510415966(3).$$

Evidence is found for a new singularity at a more negative value of v. As an additional result, the precision of the small v expansion is improved.

ODM summation: A few numerical results

We first report the values of the coefficients of the large g expansion of $E_0(g)$ as determined by the ODM method with $\alpha = 5/4$ obtained from 150 term series. This is equivalent to determine the small v expansion (v refers to the potential $i(\frac{1}{6}x^3 + \frac{1}{2}vx)$) of

$$\mathcal{E}_0(v) = \sum_p \mathcal{E}_{0,p} v^p \,.$$

The successive coefficients of the small v expansion are related to the function $\phi(\lambda, \rho)$ defined before and its derivatives at $\lambda = 1$. We have stopped the expansion at order $p = 20$ because the precision deteriorates with p until no new information is left.

Since the convergence of the ODM method with $\alpha = 5/4$ is very smooth, we have improved the convergence with an additional extrapolation. Further improvement came from summing $(E_0 + E_1)$ and $(E_0 - E_1)^2$.

One infers

$$
\begin{aligned}
&\mathcal{E}_0(v)\\
&\quad = 0.37254579045220709825060011(5) + 0.36753580554419360353004(6)v\\
&\quad + 0.14378770041506651583339(0)v^2 - 0.026586105627059387135 2(9)v^3\\
&\quad + 0.00988716507920088729 05(5)v^4 - 0.00461001929362315160 2(3)v^5\\
&\quad + 0.00240934263504847521 1(7)v^6 - 0.00134885152931985498(8)v^7\\
&\quad + 0.00079061197681697837(2)v^8 - 0.00047884784141457 25(4)v^9\\
&\quad + 0.00029723755842671 45(5)v^{10} - 0.0001880657953267 13(9)v^{11}\\
&\quad + 0.00012082554956058 7(6)v^{12} - 7.8604558627946(5) \times 10^{-5}v^{13}\\
&\quad + 5.167446464 2199(1) \times 10^{-5}v^{14} - 3.4272947828030(3) \times 10^{-5}v^{15}\\
&\quad + 2.290502086987(5) \times 10^{-5}v^{16} - 1.540915921976(3) \times 10^{-5}v^{17}\\
&\quad + 1.0426603452042(4) \times 10^{-5}v^{18} - 0.709138753556(4) \times 10^{-5}v^{19}\\
&\quad + 0.484508166066(0) \times 10^{-5}v^{20} + O(v^{21}).
\end{aligned}
$$

Continued fraction

Guessing that the function $\mathcal{E}(v)$ is analytic in a cut-plane with a negative discontinuity, we introduce the function

$$\tilde{\mathcal{E}}(v) = \frac{\mathcal{E}_0(v) - \mathcal{E}_0(0)}{\mathcal{E}_0'(0)v}$$

which is expected to be a Stieltjes function. We calculate the coefficients of its continued fraction expansion:

$$f_0(v) = \tilde{\mathcal{E}}(v), \quad f_{p-1}(v) = 1 + \frac{a_p v}{f_p(v)}, \; f_p(0) = 1\,.$$

All coefficients a_p are positive within errors, a result consistent with a Stieltjes function (see table 1). They seem to settle around 0.1850424, the value expected for a square root singularity at v_c. Some of the results obtained by summing the continued fraction are included in tables 3 and 4.

Table 1

Coefficients a_p of the continued fraction for $k = 150$.

p = 1	**2**	**3**
0.39122093207263598993	0.18489832962286956168	0.18699386165533376095
p = 4	**5**	**6**
0.18768406689188109149	0.1851910686950779010(9)	0.1847749761419447774(1)
7	**8**	**9**
0.18470222481783684(5)	0.1850738286033382(9)	0.185134240394894(8)
10	**11**	**12**
0.18510363919575(7)	0.1849998937209(1)	0.185015894534(4)
13	**14**	**15**
0.18504172330(4)	0.18506432329(6)	0.1850419101(5)

A few numerical results

We now display a few typical results obtained for g finite, positive and negative, by the ODM methods at order 150 with $\alpha = 5/4, 5/2$ as well as the variant with $\alpha = 5/2$ and, finally, by using the continued fraction expansion of the small v expansion.

The real g axis

For $g > 0$, two results are given below; a few others are reported in table 2. For $g < 0$, a few results are reported in tables 3 and 4. We verify that the imaginary part itself is a simple positive decreasing function, analytic with singularities on the real negative axis only at $g = 0$ and at infinity.

At order 150, for values of $|g| \leq 1$, the method with $\alpha = 5/2$ gives the most precise results. By contrast, for $g > 1$ the method with $\alpha = 5/4$, especially after extrapolation, eventually takes over.

For $g = 0.5$ and $g = 1$, at order 150, with the ODM method $\alpha = 5/4$ (a) after additional extrapolation (b), with the ODM method with $\alpha = 5/2$ (c), with the modified method with $\alpha = 5/2$ (d), one finds

$$
\begin{aligned}
E_0(0.5) &= 0.516891764253171978211158895662177(5), && \text{(a)} \\
&= 0.516891764253171978211158895662177609999(9)\,, && \text{(b)} \\
&= 0.516891764253171978211158895662177609999961207(4) && \text{(c)} \\
&= 0.5168917642531719782111588956621775(8) && \text{(d)} \\
E_0(1) &= 0.530781759304176671135561 81(7) && \text{(a)} \\
&= 0.53078175930417667113556181803222 5(7) && \text{(b)} \\
&= 0.530781759304176671135561818032222595(1) && \text{(c)}
\end{aligned}
$$

For $g = 1$, a numerical solution of the Schrödinger equation yields

$$
E_0 = 0.53078175930417667113556181803222 5\,.
$$

Table 2

$E_0(g)$, values on the real positive axis, order 150.

g	**0.5**	**1**
$\alpha = 5/4$(a)	0.516891764253171978211588	0.530781759304176671135561
$\alpha = 5/2$(c)	0.516891764253171978211588	0.530781759304176671135561
$\alpha = 5/2$(d)	0.516891764253171978211588	0.530781759304176671135561
continued fraction	0.51689176425317(3)	0.53078175930417667(4)
g	**5**	**21.6**
$\alpha = 5/4$(a) $\alpha = 5/4$(b)	0.601683933205191961 58(6) 0.6016839332051919615 89356	0.7334099204854279 64(2) 0.73340992048542796459 24(0)
$\alpha = 5/2$(c)	0.601683933205191961 58(9)	0.7334099204854(3)
$\alpha = 5/2$(d)	0.601683933205191961 59(0)	0.73340992048542(8)
continued fraction	0.601683933205191961 58(9)	0.7334099204854279645(9)

Table 3

$\mathrm{Re}\, E_0(g)$, *values on the real negative axis, order 150.*

$-\mathbf{g}$	**0.5**	**1**
ODM $\alpha = 5/4$	0.4764273(9)	0.442520045124(6)
ODM $\alpha = 5/2$	0.476427408327179(5)	0.442520045124(7)
continued fraction	0.476427408(0)	0.442520045124(6)
$-\mathbf{g}$	**5**	**21.6**
ODM $\alpha = 5/4$	0.43389066781036312812(2)	0.55405351846101380318(0)
ODM $\alpha = 5/2$	0.433890667(9)	0.5540535(2)
continued fraction	0.433890667810363128(1)	0.554053518461013803(1)

Table 4

$\mathrm{Im}\, E_0(g)$, *values on the real negative axis, order 150. The positivity is verified.*

$-\mathbf{g}$	**0.5**	**1**
ODM $\alpha = 5/4$	0.0002667(0)	0.015517925820(5)
ODM $\alpha = 5/2$	0.000266661882408(1)	0.015517925820(6)
continued fraction	0.000266661(3)	0.0155179258205(0)
$-\mathbf{g}$	**5**	**21.6**
ODM $\alpha = 5/4$	0.1838580861861711729(0)	0.35140177759369193624(4)
ODM $\alpha = 5/2$	0.183858086(0)	0.3514018(0)
continued fraction	0.1838580861861711729(9)	0.351401777593691936(2)

Table 5

$\mathcal{E}_0(v)$, values on the real negative v axis, order 150.

$\mathbf{v}$	$\mathbf{-2^{4/5} = -1.741\ldots}$	$\mathbf{-1}$
ODM $\alpha = 5/4$	does not converge	0.1957508157(1)
ODM $\alpha = 5/2$	$0.38(1) - 0.36(8)i$	0.195(5)
cont. fraction	$0.3898(5) - 0.3644(3)i$	0.195750815716171 9(6)
$\mathbf{v}$	$\mathbf{-5^{-4/5} = -0.275\ldots}$	$\mathbf{-(21.6)^{-4/5} = -0.085\ldots}$
ODM $\alpha = 5/4$	0.28269925819327490989 9(0)	0.34215801861934042140767(3)
ODM $\alpha = 5/2$	0.2827(1)	0.34215(6)
cont. fraction	0.28269925819327490989 90(1)	0.34215801861934042140767(6)