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# An iterative perturbation theory with a Hamiltonian modifier

**J. Chaves · J. M. Barroso · E. Besalú**

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**Abstract** The aim of this paper is to show that the so-called Autoadjusting Perturbation Theory presented years ago [E. Besalú and R. Carbó-Dorca, *J. Math. Chem.*, **22**, 85 (1997)] can be modified and expressed in terms of operators, opening the possibility to define diverse variants with better convergence properties. This methodology is called here modified autoadjusting perturbation theory which is superior, at least numerically, to Rayleigh Schrödinger perturbation theory and the superconvergent perturbation theory [W. Scherer, *Phys. Rev. Lett.*, **74**, 1495 (1995)] applied to the one-dimensional quartic anharmonic oscillator. The new feature of this method is the Hamiltonian modifier which can be chosen in a proper way in order to improve the calculations and to obtain convergent energy series and wavefunction when Rayleigh Schrödinger perturbation theory gives divergent ones. Resummation techniques are used to check whether the correction terms of modified autoadjusting perturbation theory series resums similarly to the Rayleigh Schrödinger perturbation one. The iterative nature of the proposed method allows for a linear time scaling and for memory economization when it is numerically implemented.

**Keywords** Iterative perturbation theory · Autoadjusting perturbation theory · Hamiltonian modifier · Convergent perturbation series · Anharmonic oscillator

J. Chaves (✉) · J. M. Barroso · E. Besalú
Institute of Computational Chemistry, University of Girona Campus Montilivi,
17071 Girona, Catalonia, Spain
e-mail: jchavema@gmail.com

E. Besalú
e-mail: besalu@udg.edu

## 1 Introduction

Let $\hat{H}^{(0)}$ be an unperturbed Hamiltonian, which is also assumed to have no time dependence. The respective discrete energy levels and eigenstates, arising from the time-independent Schrödinger equation, are known

$$\hat{H}^{(0)}|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle, \qquad n = 0, 1, 2, \ldots \tag{1}$$

Let $\hat{V}$ be a Hamiltonian representing a weak physical disturbance, such a potential energy produced by an external field (thus, $\hat{V}$ is formally a Hermitian operator). Let $\lambda$ be a dimensionless parameter, called coupling constant, that can take on values ranging continuously from 0 (no perturbation) to 1 (the full perturbation). The perturbed Hamiltonian is defined as

$$\hat{H}(\lambda) = \hat{H}^{(0)} + \lambda\hat{V}. \tag{2}$$

The energy levels and eigenstates of the perturbed Hamiltonian are again given by the Schrödinger equation

$$\hat{H}(\lambda)|\psi_n\rangle = E_n|\psi_n\rangle, \qquad n = 0, 1, 2, \ldots \tag{3}$$

Thus, an approximated solution of Eq. 3 may be obtained by perturbative methods. One of the most widely used techniques is the Rayleigh Schrödinger perturbation theory (RSPT) which can be found in any textbook related with quantum mechanics such as Levine [1] or Galindo and Pascual [2]. The method starts with the explicit knowledge of Eq. 1, which is the solution of a known Hamiltonian. Another approach is the so-called superconvergent perturbation theory (SCPT) developed by W. Scherer [3] within the context of quantum mechanics and being inspired in Kolmogorov's perturbation theory, called superconvergent as well, and developed by A. N. Kolmogorov [4] for classical systems. In Scherer's paper, it is affirmed that SCPT converges faster than RSPT. But Weniger [5] showed that the perturbed series of the quantum quartic anharmonic oscillator calculated with RSPT has better resummation results than resummed series obtained with SCPT.

In this paper, it has been taken into account the iterative autoadjusting perturbation theory (APT) of Besalú [6,7], which has a successful aplication in a vibrational calculation made by E. Matito et al. [8], the traditional iterative RSPT (see Feenberg [9], Löwdin [10] or Besalú [11,12]) and the Kolmogorov's idea of recalculating the unperturbed Hamiltonian. A mitxure of the three ideas has brought a new method called modified autoadjusting perturbation theory which is introduced in this paper. As in SCPT, the main point in APT is that the unperturbed Hamiltonian is recalculated in order to construct new unperturbed virtual Hamiltonians: $\hat{H}^{(0)} \to \hat{H}^{[1]} \to \cdots \to \hat{H}^{[l]} \to \cdots \to \hat{H}$, with new unperturbed wavefunctions, which progressively becomes nearer to the perturbed Hamiltonian $\hat{H}$ and this new unperturbed wavefunction becomes nearer to the original perturbed one of Eq. 3. Simultaneously, the perturbation is made progressively smaller $\hat{V}^{(0)} \to \hat{V}^{[1]} \to \cdots \to \hat{V}^{[l]} \to \cdots \to 0$.

In our notation, squared brackets denote accumulated corrected unperturbed Hamiltonian and perturbation.

In present work, APT formulation is modified and expressed in operator formalism conserving similarities with RSPT in order to obtain the new modified APT. Additionally, in our formulation, a degree of freedom is left: the definition of a modifier of the unperturbed Hamiltonian and perturbation which will be called mutant operator. This is connected with the partition of the Hamiltonian concept in the field of perturabtion theories (see Møller and Plesset [13], Epstein [14], Nesbet [15] and Szabados [16]) and it is extended to each correction of the iterative procedure following Kolmogorov's genuine idea [4].

One of the touchstones for perturbation theories is the quantum quartic anharmonic oscillator, and here analytical and numerical results are presented, supporting the idea that modified APT converges in energy and, what is more interesting, in wavefunction where RSPT and SCPT are known to be divergent.

The main difference of modified APT from RSPT is found in the computation of the mutant operator, which is, in fact, the approximated correction of energies of the remaining states left apart from the studied one.

## 2 RSPT with accumulated wavefunctions

RSPT technique suposes that the unknown wavefunction can be developed in terms of a continuous paramenter $\lambda$:

$$|\psi_n\rangle = \sum_{m=0}^{l} \lambda^m |\psi_n^{(m)}\rangle + O(\lambda^{l+1}) = |\psi_n^{[l]}\rangle + O(\lambda^{l+1}). \tag{4}$$

Squared brackets $[l]$, as it was mentioned above, denote accumulated elements up to $l-th$ order. Similarly for the energy:

$$E_n = \sum_{m=0}^{l} \lambda^m E_n^{(m)} + O(\lambda^{l+1}) = E_n^{[l]} + O(\lambda^{l+1}). \tag{5}$$

Terms $|\psi_n^{(l)}\rangle$ are corrections of order $l$ of the wavefunction and $E_n^{(l)}$ are corrections of order $l$ of the energy. Insertion of Eqs. 4 and 5 in Eq. 3 provides with the following relationship

$$\left[\hat{H}^{(0)} + \lambda \hat{V} - E_n\right] |\psi_n\rangle = 0, \tag{6}$$

which must be satisfied for each value of the parameter $\lambda$ so that we get the unperturbed equation complemented, term by term, by the system of equations

$$\hat{H}^{(0)} |\psi_n^{(l)}\rangle + \hat{V} |\psi_n^{(l-1)}\rangle = \sum_{m=0}^{l} E_n^{(m)} |\psi_n^{(l-m)}\rangle, \quad l = 1, 2, \ldots \tag{7}$$

Alternative expressions of Eq. 7 may be found using the accumulated wavefunctions notation $|\psi_n^{[l]}\rangle$ from Eq. 4. By analogy to Eq. 7 and setting up $\lambda = 1$ without losing any generality, the corresponding expressions are

$$\hat{H}^{(0)}|\psi_n^{[l]}\rangle + \hat{V}|\psi_n^{[l-1]}\rangle = \sum_{m=0}^{l} E_n^{(m)}|\psi_n^{[l-m]}\rangle \quad l = 1, 2, \ldots \tag{8}$$

which are possible to be decuced by summing all the iterations of the Eq. 7 up to $l$-th order plus Eq. 6 to complete the system. The resulting system of Eq. 8 produces the same solution as the standard RSPT because RSPT with accumulated wavefunctions are only a linear combination of standard RSPT system Eq. 7. The choice of accumulated energies and wavefunctions arises from the fact that iterative corrections in APT and in modified APT are better computed by the accumulated wavefunctions than the simple corrected ones.

Manipulating expression (8) and isolating the $l-th$ correction of the wavefunction results in

$$(\hat{H}^{(0)} - E_n^{(0)})|\psi_n^{(l)}\rangle = (E_n^{(0)} - \hat{H})|\psi_n^{[l-1]}\rangle + \sum_{m=1}^{l} E_n^{(m)}|\psi_n^{[l-m]}\rangle \quad l = 1, 2, \ldots \tag{9}$$

In order to obtain the correction energies, in Eq. 9, it is projected to $\langle\psi_n^{(0)}|$ for any $l$. The first correction $l = 1$ is

$$E_n^{(1)} = \langle\psi_n^{(0)}|\hat{H}|\psi_n^{(0)}\rangle - E_n^{(0)} \tag{10}$$

Finally, for the $l - th$ correction energy:

$$E_n^{(l)} = \langle\psi_n^{(0)}|(\hat{H} - E_n^{(0)})|\psi_n^{[l-1]}\rangle - \sum_{m=1}^{l-1} E_n^{(m)}\langle\psi_n^{(0)}|\psi_n^{[l-m]}\rangle, \quad l = 1, 2, \ldots \tag{11}$$

The deduction of the matrix expression for this new formalism needs the resolution of the identity

$$\hat{I} = \sum_k |\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|, \tag{12}$$

the projection operator of state $n$

$$\hat{P}_n = |\psi_n^{(0)}\rangle\langle\psi_n^{(0)}| \tag{13}$$

and its complementary projection operator of the same state

$$\hat{Q}_n = \hat{I} - \hat{P}_n = \sum_{i \neq n} |\psi_i^{(0)}\rangle\langle\psi_i^{(0)}|. \tag{14}$$

All the terms of Eq. 9 are expressed in matrix formalism, which is more convenient to perform computational calculations. Starting with the left-hand side of Eq. 9

$$\begin{aligned}(\hat{H}^{(0)} - E_n^{(0)})|\psi_n^{(l)}\rangle &= \hat{Q}_n(\hat{H}^{(0)} - E_n^{(0)})|\psi_n^{(l)}\rangle \\ &= \sum_{i\neq n} |\psi_i^{(0)}\rangle\langle\psi_i^{(0)}|(\hat{H}^{(0)} - E_n^{(0)})|\psi_n^{(l)}\rangle \\ &= \sum_{i\neq n} |\psi_i^{(0)}\rangle(E_i^{(0)} - E_n^{(0)})\langle\psi_i^{(0)}|\psi_n^{(l)}\rangle \\ &= \sum_{i\neq n} |\psi_i^{(0)}\rangle(E_i^{(0)} - E_n^{(0)})z_{in}^{(l)}, \quad \text{for} \quad l > 0. \end{aligned} \tag{15}$$

where $z_{in} = \langle\psi_i^{(0)}|\psi_n^{(l)}\rangle$ is the vector $n$ of the projected states into the unperturbed basis set.

The right-hand side of (9) is treated separately into two summands

$$\begin{aligned}\hat{H}|\psi_n^{[l-1]}\rangle &= \hat{Q}_n\hat{H}\hat{I}|\psi_n^{[l-1]}\rangle \\ &= \sum_{i\neq n}\sum_k |\psi_i^{(0)}\rangle\langle\psi_i^{(0)}|\hat{H}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\psi_n^{[l-1]}\rangle \\ &= \sum_{i\neq n} |\psi_i^{(0)}\rangle \sum_k h_{ik} z_{kn}^{[l-1]}, \end{aligned} \tag{16}$$

where

$$h_{ik} = \langle\psi_i^{(0)}|\hat{H}|\psi_k^{(0)}\rangle \tag{17}$$

are matrix elements of the discrete Hamiltonian, and

$$z_{kn}^{[l-1]} = \langle\psi_k^{(0)}|\psi_n^{[l-1]}\rangle = \sum_{m=0}^{l-1}\langle\psi_k^{(0)}|\psi_n^{(m)}\rangle = \sum_{m=0}^{l-1} z_{kn}^{(m)} \tag{18}$$

are the accumulated coefficients of the linear combination of the corrected wavefunction in terms of the unperturbed wavefunctions. Finally the last term of Eq. 9 is transformed into

$$\begin{aligned}\sum_{m=1}^{l} E_n^{(m)}|\psi_n^{[l-m]}\rangle &= \sum_{m=1}^{l} E_n^{(m)}\hat{Q}_n|\psi_n^{[l-m]}\rangle = \sum_{m=1}^{l}\sum_{i\neq n} E_n^{(m)}|\psi_i^{(0)}\rangle\langle\psi_i^{(0)}|\psi_n^{[l-m]}\rangle \\ &= \sum_{i\neq n}|\psi_i^{(0)}\rangle\sum_{m=1}^{l} E_n^{(m)} z_{in}^{[l-m]}. \end{aligned} \tag{19}$$

Inserting expressions (15), (16) and (19) in Eq. 9, after straightforward algebra, the accumulated RSPT in matrix formalism is obtained

$$z_{in}^{(l)} = \frac{-\sum_{k=0}^{\infty}(h_{ik} - E_n^{(0)}\delta_{ik})z_{kn}^{[l-1]} + \sum_{m=1}^{l} E_n^{(m)} z_{in}^{[l-m]}}{E_i^{(0)} - E_n^{(0)}} \tag{20}$$

if $i \neq n$ and $z_{nn}^{(l)} = 0$ if $l \neq 0$.

## 3 Modified autoadjusting Perturbation Theory

The foundations of APT theory have been reported in several works in the references, see for instance Besalú [6,17]. Here, an alternative formulation similar to the usual APT but based on operator formalism, that is modified APT, is developed.

Taking advantage of RSPT expressed with accumulated wavefunctions, our laboratory has developed another iterative equation inspired only in an ansatz. The main idea is that, at each iteration, a new partition of the Hamiltonian is considered generating a new unperturbed Hamiltonian $H^{[l]}$ and a new perturbation $V^{[l]}$:

$$\hat{H}^{[l]} = \hat{H}^{(0)} + \hat{\Delta}^{[l]}(n) \tag{21}$$

$$\hat{V}^{[l]} = \hat{V}^{(0)} - \hat{\Delta}^{[l]}(n), \tag{22}$$

in such a way that the perturbed Hamiltonian remains unchanged:

$$\hat{H} = \hat{H}^{[l]} + \hat{V}^{[l]} = \hat{H}^{(0)} + \hat{V}. \tag{23}$$

The requirement being that this new operator attached to the studied state $n$, $\Delta^{[l]}(n)$, has to commute with the unperturbed Hamiltonian producing the same unperturbed solutions. Then, the known unperturbed eigenvectors can be used in the iterative procedure. This is a typical prescription for renormalization thecniques since it involves an iterative reformation of the original Hamiltonian.

Using this new partition of the Hamiltonian in each iteration, Eq. 8 turns into

$$\hat{H}^{[l]}|\psi_n^{[l]}\rangle + \hat{V}^{[l]}|\psi_n^{[l-1]}\rangle = \sum_{m=0}^{l} E_n^{(m)}|\psi_n^{[l-m]}\rangle \quad l = 1, 2, \ldots. \tag{24}$$

From the last expression, it is found the $l - th$ correction of state $n$

$$(\hat{H}^{[l]} - E_n^{(0)})|\psi_n^{(l)}\rangle = (E_n^{(0)} - \hat{H})|\psi_n^{[l-1]}\rangle + \sum_{m=1}^{l} E_n^{(m)}|\psi_n^{[l-m]}\rangle \quad l = 1, 2, \ldots \tag{25}$$

The proposed mutant operator, $\hat{\Delta}^{[l]}(n)$, is

$$\hat{\Delta}^{[l]}(n) = \sum_{m=1}^{l} \hat{\Delta}^{(m-1)}(n)$$
$$= \sum_{m=1}^{l} \sum_{i} |\psi_i^{(0)}\rangle \left( \langle \psi_i^{(0)} | \hat{V} | \psi_i^{(m-1)} \rangle - \langle \psi_n^{(0)} | \hat{V} | \psi_n^{(m-1)} \rangle \right) \langle \psi_i^{(0)}|. \quad (26)$$

Other choices of $\hat{\Delta}^{[l]}$ have been tested, many of them giving good and valuable results, but here it is only presented the one we have found having good convergence properties and fulfilling with the additional requirement of presenting good behavior in resummation techniques.

Now, Eq. 26 is transformed into a matrix expression

$$\hat{\Delta}^{[l]}(n)|\psi_n^{(l)}\rangle = \sum_i \psi_i^{(0)} \sum_{m=1}^{l} \left( E_i^{(m)} - E_n^{(m)} \right) z_{in}^{(l)} \quad (27)$$

where, for instance for a state $j$

$$E_j^{(l)} = \sum_{k=0}^{\infty} v_{jk} z_{kj}^{(l-1)}. \quad (28)$$

Due to the fact that last expression (27) requires the knowledge of the wavefunction of all corrected eigenstates in each step ($z_{in}^{(l)}, \forall i \neq n$), it demands for a lot of computational effort making it nonefficient. Due to that, only the two first corrections of the $z_{ik}$ for the rest of states distinct of $n$ are considered here, giving simple analytical expressions

$$E_i^{(1)} = v_{ii} \quad (29)$$
$$E_i^{(2)} = \sum_{k \neq i} v_{ik} \frac{v_{ki}}{h_{kk} - h_{ii}} \quad (30)$$
$$E_i^{(m)} = 0 \quad for \quad m \geq 3. \quad (31)$$

Then, expression (25) is written as

$$(\hat{H}^{(0)} + \hat{\Delta}^{[l]}(n) - E_n^{(0)})|\psi_n^{(l)}\rangle = (E_n^{(0)} - \hat{H})|\psi_n^{[l-1]}\rangle + \sum_{m=1}^{l} E_n^{(m)} |\psi_n^{[l-m]}\rangle$$
$$l = 1, 2, \ldots \quad (32)$$

and using Eq. 27, in the unperturbed basis set, takes the form

$$z_{in}^{(l)} = \frac{-\sum_{k=0}^{\infty} h_{ik} z_{kn}^{[l-1]} + E_n^{(0)} z_{in}^{[l-1]} + \sum_{m=1}^{l} E_n^{(m)} z_{in}^{[l-m]}}{E_i^{[l]} - E_n^{[l]}} \tag{33}$$

if $i \neq n$ and $z_{nn}^{(l)} = 0$ if $l \neq 0$. Working with this expression we need to keep the accumulated wavefunctions instead of the correction ones. This modified APT version demands for a little bit more computational cost than RSPT because $E_i^{[l]}$ depends of corrections up to second order.

## 4 Anharmonic oscillator

In 1952, Dyson [18] showed that perturbation expansions in quantum electrodynamics diverge. After a few years, Bender and Wu [19] demonstrated in their seminal work that, in nonrelativistic quantum mechanics, perturbation series for the anharmonic oscillator and, in consequence, for factorially divergent perturbation expansions, with a nonzero coupling constant diverges.

Kato [20] demonstrated that the convergence of $E(\lambda)$ obtained by RSPT method in a neighborhood of $\lambda = 0$ is guaranteed only if perturbation operator $\hat{V}$ is bounded with respect to the unperturbed Hamiltonian $\hat{H}^{(0)}$. But in many quantum mechanical and field theory problems, which use perturbation theory, perturbation $\hat{V}$ does not satisfy this condition, so the energy expansion $E(\lambda)$ diverges. The case of anharmonic oscillator is one of them.

Physicists had invested a lot of work for avoiding this difficulty because this model is important in theoretical physics. For instance, in quantum electrodynamics the field $\phi^4$ is a starting point of the theory, furthermore, quantum electrodynamics is build based on perturbation theory. Renormalization techniques were developed in order to solve the problem, see for instance Killinbeck [21] or Austin [22]. Related to our work, it is interesting the paper of Weniger et al. [23], which focuses in the quantum anharmonic oscillator.

The use of summation techniques is a relevant way of avoiding divergences, see for instance Sergeev [24] and references therein.

Our goal is to skip the divergence by using another approach, without renormalization techniques or summation algorithms. Here, it will be shown how some relevant convergence improvements appear thanks to the modified APT approach.

The model of quantum quartic anharmonic oscillator is our touchstone. Consider the anharmonic oscillator with the Hamiltonian

$$\hat{H}^{(0)} = \hat{p}^2 + \hat{x}^2, \tag{34}$$

$$\hat{V} = \lambda \hat{x}^4. \tag{35}$$

Using creation and annihilation operators taken from the second quantization (see Peskin and Schroeder [25] for a more detailed development) the Hamiltonian and the perturbation are rewritten as

$$\hat{H}^{(0)} = 2a^{\dagger}a + 1 = 2\hat{N} + 1, \tag{36}$$

$$\hat{V} = \frac{\lambda}{4}(a^{\dagger} + a)^4. \tag{37}$$

Within this derivation, one obtains the nonzero matrix elements of the Hamiltonian $\mathbf{H} = \{h_{nm} = \langle n|H|m\rangle\}$,

$$\begin{aligned}
\langle\psi_n|\hat{H}|\psi_n\rangle &= 2n + 1 + \frac{\lambda}{4}(6n^2 + 6n + 3),\\
\langle\psi_n|\hat{H}|\psi_{n-2}\rangle &= \langle\psi_{n-2}|\hat{H}|\psi_n\rangle = \frac{\lambda}{4}\sqrt{n(n-1)}(4n-2),\\
\langle\psi_n|\hat{H}|\psi_{n-4}\rangle &= \langle\psi_{n-4}|\hat{H}|\psi_n\rangle = \frac{\lambda}{4}\sqrt{n(n-1)(n-2)(n-3)}.
\end{aligned} \tag{38}$$

## 5 Resummation methods

At this point, it is necessary to check if the new perturbation theory discussed in this paper, the modified APT, is able to be resummed as the traditional RSPT is. An alternative perturbation theory is taken into account, the so-called SCPT by Scherer [3]. Weniger [5] compared SCPT with traditional one from the point of view of summation methods. Weniger showed that SCPT apparently diververges less strongly than RSPT but the performance decreases when the series is resummed using rigorous mathematical tools. This might be because RSPT is a Taylor series expansion of the unknown solution of the system, while SCPT is not. In this part it is checked if modified APT can be resummed in a similar way as RSPT. Three well known summation techniques have been used: the first one is the Wynn's epsilon algorithm [26], whilst second one is a variant of the Levin-type sequence transformation (see Weniger [27,28]) and finally, the third one is based on Borel summability of divergent series. Some examples are pointed out in the monographs by Balser [29,30]

A widely used summation technique relies on Padé approximants [31,32] which approximate partial sums of a series expansion to a rational function. In this work it has been used Wynn's epsilon algorithm [26], which is an easy algorithm to be implemented. Wynn's epsilon algorithm is codified as

$$\epsilon_{-1}^{(n)} = 0, \quad \epsilon_{0}^{(n)} = s_n, \tag{39}$$

$$\epsilon_{k+1}^{(n)} = \epsilon_{k-1}^{(n+1)} + 1/[\epsilon_{k}^{(n+1} - \epsilon_{k}^{(n)}], \tag{40}$$

where $s_n$ are the partial sums $f_n(z) = \sum_{m=0}^{l} \gamma_m z^m$. Elements $\epsilon_{2k}^{(n)}$ with even subscripts are Padé approximants of the order

$$\epsilon_{2k}^{(n)} = [n + k/k]_f(z). \tag{41}$$

Elements $\epsilon_{2k+1}^{(n)}$ with odd subscripts are auxiliary quantities that diverge if the whole process converges.

One Levin-type sequence transformation that appears in Weniger's report [Eq. (8.4-4) of Ref. [27]] has been considered for this

$$\delta_k^{(n)}(\zeta, s_n) = \frac{\sum_{j=0}^{k}(-1)^j \binom{k}{j} \frac{(\zeta+n+j)_{k-1}}{(\zeta+n+k)_{k-1}} \frac{s_{n+j}}{\Delta s_{n+j+1}}}{\sum_{j=0}^{k}(-1)^j \binom{k}{j} \frac{(\zeta+n+j)_{k-1}}{(\zeta+n+k)_{k-1}} \frac{1}{\Delta s_{n+j+1}}}, \tag{42}$$

for $\zeta = 1$. The symbol $\Delta$ is the forward difference operator: $\Delta s_{n+j} = s_{n+j+1} - s_{n+j}$. This sequence of transformations has been shown to be effective for summing strongly divergent quantum mechanical perturbation expansions and divergent asymptotic series of special functions (for a more detailed discussion see Ref. [5] and references therein). From now on, this method will be called $\delta$ algorithm.

The last studied summation method is Borel transformation, which deals with factorial series. Mathematical conditions can be found in Graffi [33] and Simon [34]. Let supose a function $f(z, l)$ has a Taylor expansion around $z = 0$ truncated at $l - th$ correction:

$$f(z, l) \sim \sum_{n=0}^{l} \gamma_n z^n \tag{43}$$

it can be transformed

$$F(z, l, m) = \sum_{n=0}^{l} \frac{\gamma_n}{(nm)!} z^n \tag{44}$$

and resummed by integration

$$f(z, l, m) = \frac{1}{m} \int_0^\infty e^{-x} F(zx, l, m) dx. \tag{45}$$

Due to the coefficients of the energy series of the quantum quartic anharmonic oscillator the ground state obtained from modified APT series expansion does not present factorial behavior like RSPT one and Borel summation has not to be neccessarily applied. In fact modified APT coefficients, $\gamma_n = C_{MA}^{(n)}(\lambda)$, of its series expansion of the ground state have a dependence on the coupling constant $\lambda$, making it hard to be integrated analytically, so that numerical integration has been considered. Nevertheless, this approach has been used here to accelerate the convergence and for comparing purposes.

## 6 Results and discussion

From the iterative RSPT matrix expression (20) and using Mathematica 5.2 [35] for the algebraic footing, the series up to the $4-th$ correction of the energy for the ground state of the quantum quartic anharmonic oscillator has the form

$$E_{RS}^{[4]} = 1 + \frac{3}{4}\lambda - \frac{21}{16}\lambda^2 + \frac{333}{64}\lambda^3 - \frac{30885}{1024}\lambda^4 \tag{46}$$

In the case of SCPT, the correction energy up to the $4-th$ order for the same system is

$$E_{SC}^{[4]} = 1 + \frac{3}{4}\lambda - \frac{21}{16}\lambda^2 + \frac{333}{64}\lambda^3 + C_{SC}^{(4)}(\lambda)\lambda^4 \tag{47}$$

with

$$C_{SC}^{(4)}(\lambda) = -\frac{3(1317760 + 12935472\lambda + 36433368\lambda^2 + 25183305\lambda^3)}{2048(4+9\lambda)(4+15\lambda)(4+21\lambda)} \tag{48}$$

what is taken from Scherer's paper [3].

In the case of modified APT the expression is more complex than in RSPT and SCPT cases:

$$E_{MA}^{[4]} = 1 + \frac{3}{4}\lambda + C_{MA}^{(2)}(\lambda)\lambda^2 + C_{MA}^{(3)}(\lambda)\lambda^3 + C_{MA}^{(4)}(\lambda)\lambda^4, \tag{49}$$

where some corrections are rational expressions. The coefficient for second order correction is

$$C_{MA}^{(2)}(\lambda) = -\frac{3(28+99\lambda)}{4(4+9\lambda)(4+15\lambda)}. \tag{50}$$

The third order coupling constant dependent coefficient is

$$C_{MA}^{(3)}(\lambda) = \frac{63\sum_{m=0}^{7} p_m^{(3)}\lambda^m}{4\sum_{m=0}^{9} q_m^{(3)}\lambda^m}, \tag{51}$$

$p_m^{(3)}$ and $q_m^{(3)}$ coefficients are listed in Table 1. Similarly, for the fourth order correction

$$C_{MA}^{(4)}(\lambda) = -\frac{3\sum_{m=0}^{30} p_m^{(4)}\lambda^m}{4\sum_{m=0}^{34} q_m^{(4)}\lambda^m}, \tag{52}$$

where the $p_m^{(4)}$ and $q_m^{(4)}$ coefficients can be found in Table 2.

Expression (49) is numerically convergent meanwhile (46) or (47) are not, as can be observed in Table 3. Futhermore, modified APT expression of the ground state energy (49) and RSPT one (46) share similar resummation behavior, meanwhile SCPT ones are clearly the worst as it can be observed in Tables 4, 5 and 6.

An interesting feature of the obtained modified APT series is that the energy up to $n$-th order is also a rational function similar to the ones obtained using resummation methods for RSPT series.

**Table 1** Modified APT exact coefficients appearing in Eq. 51

| $m$ | $p_m^{(3)}$ | $q_m^{(3)}$ | $m$ | $p_m^{(3)}$ | $q_m^{(3)}$ |
|---|---|---|---|---|---|
| 0 | 131072 | 1048576 | 5 | 19093462560 | 565307479296 |
| 1 | 5406720 | 49545216 | 6 | 36662993388 | 2025741037248 |
| 2 | 95296512 | 1049346048 | 7 | 29579452749 | 4649788549872 |
| 3 | 932219136 | 13067587584 | 8 | | 6166775666520 |
| 4 | 5461423488 | 105147371520 | 9 | | 3566441757879 |

**Table 2** Modified APT coefficients appearing in Eq. 52

| $m$ | $p_m^{(4)}$ | $q_m^{(4)}$ | $m$ | $p_m^{(4)}$ | $q_m^{(4)}$ |
|---|---|---|---|---|---|
| 0 | $1.693006798 \times 10^{1}$ | $1.26765060 \times 10^{0}$ | 23 | $3.178795505 \times 10^{30}$ | $2.06454596 \times 10^{30}$ |
| 1 | $4.305234830 \times 10^{3}$ | $3.39413448 \times 10^{2}$ | 24 | $1.394396042 \times 10^{31}$ | $1.063219144 \times 10^{31}$ |
| 2 | $5.331845526 \times 10^{5}$ | $4.43911730 \times 10^{4}$ | 25 | $5.533061829 \times 10^{31}$ | $4.99794291 \times 10^{31}$ |
| 3 | $4.284534978 \times 10^{7}$ | $3.77865785 \times 10^{6}$ | 26 | $1.982892087 \times 10^{32}$ | $2.14285054 \times 10^{32}$ |
| 4 | $2.511181533 \times 10^{9}$ | $2.35336957 \times 10^{8}$ | 27 | $6.404262200 \times 10^{32}$ | $8.37011633 \times 10^{32}$ |
| 5 | $1.144107730 \times 10^{11}$ | $1.143032858 \times 10^{10}$ | 28 | $1.859156432 \times 10^{33}$ | $2.97407063 \times 10^{33}$ |
| 6 | $4.217192247 \times 10^{12}$ | $4.50648444 \times 10^{11}$ | 29 | $4.835066912 \times 10^{33}$ | $9.59425254 \times 10^{33}$ |
| 7 | $1.292388412 \times 10^{14}$ | $1.48223702 \times 10^{13}$ | 30 | $1.121931042 \times 10^{34}$ | $2.80329487 \times 10^{34}$ |
| 8 | $3.358359737 \times 10^{15}$ | $4.14856146 \times 10^{14}$ | 31 | $2.311284317 \times 10^{34}$ | $7.39693218 \times 10^{34}$ |
| 9 | $7.510098827 \times 10^{16}$ | $1.002881365 \times 10^{16}$ | 32 | $4.201743342 \times 10^{34}$ | $1.75638513 \times 10^{35}$ |
| 10 | $1.461859596 \times 10^{18}$ | $2.11830314 \times 10^{17}$ | 33 | $6.690414165 \times 10^{34}$ | $3.73694131 \times 10^{35}$ |
| 11 | $2.499274342 \times 10^{19}$ | $3.94532172 \times 10^{18}$ | 34 | $9.244734851 \times 10^{34}$ | $7.08762844 \times 10^{35}$ |
| 12 | $3.780014403 \times 10^{20}$ | $6.52716222 \times 10^{19}$ | 35 | $1.095643320 \times 10^{35}$ | $1.190855878 \times 10^{36}$ |
| 13 | $5.087022127 \times 10^{21}$ | $9.64960701 \times 10^{20}$ | 36 | $1.097045731 \times 10^{35}$ | $1.75903974 \times 10^{36}$ |
| 14 | $6.120199824 \times 10^{22}$ | $1.28104300 \times 10^{22}$ | 37 | $9.096436426 \times 10^{34}$ | $2.26283488 \times 10^{36}$ |
| 15 | $6.607721513 \times 10^{23}$ | $1.53332036 \times 10^{23}$ | 38 | $6.076016272 \times 10^{34}$ | $2.50520712 \times 10^{36}$ |
| 16 | $6.421707185 \times 10^{24}$ | $1.66016139 \times 10^{24}$ | 39 | $3.140248854 \times 10^{34}$ | $2.35092334 \times 10^{36}$ |
| 17 | $5.631371786 \times 10^{25}$ | $1.63036561 \times 10^{25}$ | 40 | $1.177836288 \times 10^{34}$ | $1.83271995 \times 10^{36}$ |
| 18 | $4.464306904 \times 10^{26}$ | $1.45538806 \times 10^{26}$ | 41 | $2.851141370 \times 10^{33}$ | $1.154465344 \times 10^{36}$ |
| 19 | $3.203802765 \times 10^{27}$ | $1.182970378 \times 10^{27}$ | 42 | $3.341952864 \times 10^{32}$ | $5.64351312 \times 10^{35}$ |
| 20 | $2.083281179 \times 10^{28}$ | $8.76664131 \times 10^{27}$ | 43 | | $2.00792206 \times 10^{35}$ |
| 21 | $1.228043714 \times 10^{29}$ | $5.92865032 \times 10^{28}$ | 44 | | $4.62363274 \times 10^{34}$ |
| 22 | $6.562947124 \times 10^{29}$ | $3.66089192 \times 10^{29}$ | 45 | | $5.16980368 \times 10^{33}$ |

For checking purposes, one can perform the Taylor development series for SCPT and modified APT. Then it is obtained a series which coincides until the 4th order with RSPT one. It can be compared until 7th order of RSPT

$$E_{RS}^{[7]} = E_{RS}^{[4]} + \frac{916731}{4096}\lambda^5 - \frac{65518401}{32768}\lambda^6 + \frac{2723294673}{131072}\lambda^7. \tag{53}$$

**Table 3** Errors respect to exact energy ($\Delta x = \text{Exact} - x$) of RSPT, superconvergent (SC) and modified autoadjusting perturbation theory (MA) energies of the QQAHO ground state corrected up to fourth and seventh order in terms of the coupling constant

| $\lambda$ | Exact | $\Delta E^{[4]}_{RS}$ | $\Delta E^{[4]}_{SC}$ | $\Delta E^{[4]}_{MA}$ | $\Delta E^{[7]}_{RS}$ | $\Delta E^{[7]}_{SC}$ | $\Delta E^{[7]}_{MA}$ |
|---|---|---|---|---|---|---|---|
| 0.010 | 1.0073736721 | 2.06E−08 | 1.57E−08 | 3.40E−09 | 0.00E+00 | −7.00E−10 | 0.00E+00 |
| 0.025 | 1.0180010006 | 1.80E−06 | 1.26E−06 | 1.97E−07 | −2.84E−08 | −1.58E−07 | −6.00E−10 |
| 0.050 | 1.0347296973 | 4.91E−05 | 3.01E−05 | 2.41E−06 | −5.87E−06 | −1.04E−05 | −4.23E−08 |
| 0.075 | 1.0504339643 | 3.26E−04 | 1.76E−04 | 4.65E−06 | −1.27E−04 | −1.30E−04 | −3.71E−07 |
| 0.100 | 1.0652855095 | 1.22E−03 | 5.89E−04 | −5.20E−06 | −1.09E−03 | −8.24E−04 | −1.50E−06 |
| 0.150 | 1.0929050098 | 7.64E−03 | 3.00E−03 | −1.30E−04 | −2.21E−02 | −1.17E−02 | −9.10E−06 |
| 0.200 | 1.1182926544 | 2.74E−02 | 9.10E−03 | −4.70E−04 | −1.82E−01 | −7.88E−02 | −3.02E−05 |
| 0.250 | 1.1419018395 | 7.30E−02 | 2.12E−02 | −1.04E−03 | −9.26E−01 | −3.47E−01 | −7.51E−05 |
| 0.300 | 1.1640471574 | 1.61E−01 | 4.22E−02 | −1.79E−03 | −3.47E+00 | −1.16E+00 | −1.56E−04 |
| 0.350 | 1.1849584844 | 3.13E−01 | 7.60E−02 | −2.66E−03 | −1.06E+01 | −3.21E+00 | −2.88E−04 |
| 0.400 | 1.2048103274 | 5.54E−01 | 1.27E−01 | −3.61E−03 | −2.76E+01 | −7.74E+00 | −4.83E−04 |
| 0.450 | 1.2237391189 | 9.15E−01 | 2.03E−01 | −4.58E−03 | −6.42E+01 | −1.68E+01 | −7.55E−04 |
| 0.500 | 1.2418540597 | 1.43E+00 | 3.09E−01 | −5.56E−03 | −1.37E+02 | −3.35E+01 | −1.11E−03 |
| 0.550 | 1.2592442502 | 2.14E+00 | 4.57E−01 | −6.54E−03 | −2.70E+02 | −6.24E+01 | −1.57E−03 |
| 0.600 | 1.2759835663 | 3.08E+00 | 6.56E−01 | −7.52E−03 | −5.03E+02 | −1.10E+02 | −2.13E−03 |
| 0.650 | 1.2921340995 | 4.31E+00 | 9.19E−01 | −8.49E−03 | −8.89E+02 | −1.86E+02 | −2.80E−03 |
| 0.700 | 1.3077486511 | 5.88E+00 | 1.26E+00 | −9.46E−03 | −1.51E+03 | −3.01E+02 | −3.59E−03 |
| 0.750 | 1.3228725815 | 7.85E+00 | 1.69E+00 | −1.04E−02 | −2.46E+03 | −4.71E+02 | −4.50E−03 |
| 0.800 | 1.3375452081 | 1.03E+01 | 2.24E+00 | −1.14E−02 | −3.90E+03 | −7.17E+02 | −5.52E−03 |
| 0.850 | 1.3518008817 | 1.32E+01 | 2.92E+00 | −1.24E−02 | −5.99E+03 | −1.06E+03 | −6.67E−03 |
| 0.900 | 1.3656698258 | 1.67E+01 | 3.75E+00 | −1.35E−02 | −8.99E+03 | −1.54E+03 | −7.93E−03 |
| 0.950 | 1.3791788017 | 2.10E+01 | 4.76E+00 | −1.46E−02 | −1.32E+04 | −2.19E+03 | −9.32E−03 |
| 1.000 | 1.3923516415 | 2.59E+01 | 5.97E+00 | −1.57E−02 | −1.90E+04 | −3.05E+03 | −1.08E−02 |

For SCPT the obtained Taylor series is

$$E^{[4]}_{SC} = E^{[4]}_{RS} + \frac{354249}{8192}\lambda^5 - \frac{3795201}{32768}\lambda^6 + \frac{43986969}{131072}\lambda^7 + O(\lambda^8), \tag{54}$$

and for modified APT

$$E^{[4]}_{MA} = E^{[4]}_{RS} + \frac{724203}{4096}\lambda^5 - \frac{122266809}{262144}\lambda^6 + \frac{8733880593}{1048576}\lambda^7 + O(\lambda^8). \tag{55}$$

It is also worth of mention the behaviour of the analytic resummation results. Results for SCPT and RSPT are found in Ref. [5] in the cases of epsilon and $\delta$ algorithm. The expressions for modified APT using Wynn's epsilon algorithm are

$$(\epsilon^{(0)}_4)_{MA}(\lambda) = \frac{\sum_{n=0}^{53} p_{\epsilon n}\lambda^n}{\sum_{n=0}^{52} q_{\epsilon n}\lambda^n} \tag{56}$$

**Table 4** Errors respect to exact energy ($\Delta x = \text{Exact} - x$) of RSPT, SCPT and modified APT transformed energies with Wynn's epsilon algorithm of the QQAHO ground state corrected up to the fourth order in terms of the coupling constant

| $\lambda$ | Exact | $\Delta(\epsilon_4^{(0)})_{RS}$ | $\Delta(\epsilon_4^{(0)})_{SC}$ | $\Delta(\epsilon_4^{(0)})_{MA}$ | $\Delta(\epsilon_6^{(1)})_{RS}$ | $\Delta(\epsilon_6^{(1)})_{SC}$ | $\Delta(\epsilon_6^{(1)})_{MA}$ |
|---|---|---|---|---|---|---|---|
| 0.000 | 1.0000000000 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| 0.010 | 1.0073736721 | 2.80E−09 | −8.00E−10 | 1.43E−08 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| 0.025 | 1.0180010006 | 2.05E−07 | −7.90E−08 | 9.15E−07 | −3.00E−10 | −2.00E−10 | −1.00E−10 |
| 0.050 | 1.0347296973 | 4.27E−06 | −2.19E−06 | 9.95E−06 | −2.53E−08 | −5.00E−09 | −8.00E−09 |
| 0.075 | 1.0504339643 | 2.24E−05 | −1.40E−05 | 1.51E−05 | −2.98E−07 | 2.71E−07 | −8.09E−08 |
| 0.100 | 1.0652855095 | 6.77E−05 | −4.92E−05 | −8.49E−06 | −1.51E−06 | 4.64E−06 | −3.55E−07 |
| 0.150 | 1.0929050098 | 2.90E−04 | −2.66E−04 | −1.72E−04 | −1.24E−05 | 2.70E−04 | −2.15E−06 |
| 0.200 | 1.1182926544 | 7.52E−04 | −8.26E−04 | −4.72E−04 | −4.84E−05 | −2.76E−03 | −5.83E−06 |
| 0.250 | 1.1419018395 | 1.50E−03 | −1.92E−03 | −8.68E−04 | −1.29E−04 | −3.50E−03 | −9.24E−06 |
| 0.300 | 1.1640471574 | 2.56E−03 | −3.73E−03 | −1.33E−03 | −2.73E−04 | −6.61E−03 | −6.37E−06 |
| 0.350 | 1.1849584844 | 3.94E−03 | −6.48E−03 | −1.82E−03 | −4.98E−04 | −1.24E−02 | 1.38E−05 |
| 0.400 | 1.2048103274 | 5.62E−03 | −1.04E−02 | −2.34E−03 | −8.19E−04 | −2.26E−02 | 6.90E−05 |
| 0.450 | 1.2237391189 | 7.61E−03 | −1.56E−02 | −2.88E−03 | −1.25E−03 | −3.98E−02 | 1.85E−04 |
| 0.500 | 1.2418540597 | 9.87E−03 | −2.25E−02 | −3.44E−03 | −1.79E−03 | −6.85E−02 | 4.02E−04 |
| 0.550 | 1.2592442502 | 1.24E−02 | −3.13E−02 | −4.03E−03 | −2.46E−03 | −1.18E−01 | 7.75E−04 |
| 0.600 | 1.2759835663 | 1.52E−02 | −4.25E−02 | −4.63E−03 | −3.25E−03 | −2.05E−01 | 1.39E−03 |
| 0.650 | 1.2921340995 | 1.82E−02 | −5.64E−02 | −5.27E−03 | −4.18E−03 | −3.79E−01 | 2.37E−03 |
| 0.700 | 1.3077486511 | 2.14E−02 | −7.35E−02 | −5.95E−03 | −5.24E−03 | −8.07E−01 | 3.91E−03 |
| 0.750 | 1.3228725815 | 2.48E−02 | −9.47E−02 | −6.67E−03 | −6.43E−03 | −2.90E+00 | 6.36E−03 |
| 0.800 | 1.3375452081 | 2.83E−02 | −1.21E−01 | −7.44E−03 | −7.76E−03 | 4.39E+00 | 1.03E−02 |
| 0.850 | 1.3518008817 | 3.21E−02 | −1.53E−01 | −8.26E−03 | −9.22E−03 | 1.68E+00 | 1.70E−02 |
| 0.900 | 1.3656698258 | 3.59E−02 | −1.93E−01 | −9.14E−03 | −1.08E−02 | 1.21E+00 | 2.91E−02 |
| 0.950 | 1.3791788017 | 3.99E−02 | −2.43E−01 | −1.01E−02 | −1.25E−02 | 1.03E+00 | 5.52E−02 |
| 1.000 | 1.3923516415 | 4.41E−02 | −3.07E−01 | −1.11E−02 | −1.44E−02 | 9.45E−01 | 1.37E−01 |

whose coefficients $p_{\epsilon n}$ and $q_{\epsilon n}$ are listed in Table 7.

For the case of $\delta$ algorithm

$$(\epsilon_3^{(1)})_{MA}(\lambda) = \frac{\sum_{n=0}^{53} p_{\delta n}\lambda^n}{\sum_{n=0}^{52} q_{\delta n}\lambda^n} \tag{57}$$

where $p_{\delta n}$ and $q_{\delta n}$ are stored in Table 8.

Numerical results for the quantum quartic anharmonic oscillator ground state are presented in Tables 3, 4 ,5 and 6. The so-called *exact* value is calculated by a diagonalization of $50 \times 50$ matrices $\mathbf{H}(\lambda)$ on the unperturbed quantum harmonic oscillator basis set. This diagonalization is carried out with the function of the symbolic program `Mathematica`.

From the analysis of numerical results of Table 3, the best method is modified APT one, moreover, it shows convergent behaviour while the other two are known to be

**Table 5** Errors respect to exact energy ($\Delta x = \text{Exact} - x$) of RSPT, SCPT and modified APT transformed energies with delta algorithm of the QQAHO ground state corrected up to the fourth order in terms of the coupling constant

| $\lambda$ | Exact | $\Delta(\delta_3^{(1)})_{RS}$ | $\Delta(\delta_3^{(1)})_{SC}$ | $\Delta(\delta_3^{(1)})_{MA}$ | $\Delta(\delta_6^{(1)})_{RS}$ | $\Delta(\delta_6^{(1)})_{SC}$ | $\Delta(\delta_6^{(1)})_{MA}$ |
|---|---|---|---|---|---|---|---|
| 0.000 | 1.0000000000 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| 0.010 | 1.0073736721 | 8.00E−10 | −2.70E−09 | −2.50E−09 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| 0.025 | 1.0180010006 | 5.17E−08 | −2.15E−07 | −1.77E−07 | 0.00E+00 | −3.60E−09 | −5.00E−10 |
| 0.050 | 1.0347296973 | 8.52E−07 | −4.92E−06 | −3.39E−06 | −6.00E−10 | −4.02E−07 | −4.23E−08 |
| 0.075 | 1.0504339643 | 3.55E−06 | −2.76E−05 | −1.66E−05 | −4.60E−09 | −5.09E−06 | −4.57E−07 |
| 0.100 | 1.0652855095 | 8.59E−06 | −8.82E−05 | −4.80E−05 | −1.59E−08 | −2.75E−05 | −2.16E−06 |
| 0.150 | 1.0929050098 | 2.29E−05 | −4.10E−04 | −1.95E−04 | −6.57E−08 | −2.51E−04 | −1.60E−05 |
| 0.200 | 1.1182926544 | 3.38E−05 | −1.13E−03 | −4.92E−04 | −1.30E−07 | −1.06E−03 | −5.72E−05 |
| 0.250 | 1.1419018395 | 2.95E−05 | −2.35E−03 | −9.76E−04 | −1.44E−07 | −3.00E−03 | −1.38E−04 |
| 0.300 | 1.1640471574 | 1.06E−06 | −4.14E−03 | −1.67E−03 | −1.61E−08 | −6.72E−03 | −2.46E−04 |
| 0.350 | 1.1849584844 | −5.72E−05 | −6.53E−03 | −2.59E−03 | 3.39E−07 | −1.29E−02 | −2.67E−04 |
| 0.400 | 1.2048103274 | −1.48E−04 | −9.52E−03 | −3.74E−03 | 9.76E−07 | −2.20E−02 | 1.02E−03 |
| 0.450 | 1.2237391189 | −2.71E−04 | −1.31E−02 | −5.14E−03 | 1.90E−06 | −3.48E−02 | −5.20E−03 |
| 0.500 | 1.2418540597 | −4.24E−04 | −1.72E−02 | −6.77E−03 | 3.06E−06 | −5.16E−02 | −4.17E−03 |
| 0.550 | 1.2592442502 | −6.06E−04 | −2.19E−02 | −8.65E−03 | 4.34E−06 | −7.29E−02 | −4.81E−03 |
| 0.600 | 1.2759835663 | −8.12E−04 | −2.70E−02 | −1.08E−02 | 5.60E−06 | −9.91E−02 | −5.85E−03 |
| 0.650 | 1.2921340995 | −1.04E−03 | −3.26E−02 | −1.31E−02 | 6.62E−06 | −1.30E−01 | −7.13E−03 |
| 0.700 | 1.3077486511 | −1.28E−03 | −3.86E−02 | −1.57E−02 | 7.17E−06 | −1.67E−01 | −8.62E−03 |
| 0.750 | 1.3228725815 | −1.54E−03 | −4.49E−02 | −1.84E−02 | 7.00E−06 | −2.09E−01 | −1.03E−02 |
| 0.800 | 1.3375452081 | −1.80E−03 | −5.16E−02 | −2.14E−02 | 5.83E−06 | −2.57E−01 | −1.22E−02 |
| 0.850 | 1.3518008817 | −2.08E−03 | −5.85E−02 | −2.46E−02 | 3.39E−06 | −3.10E−01 | −1.42E−02 |
| 0.900 | 1.3656698258 | −2.35E−03 | −6.58E−02 | −2.80E−02 | −6.01E−07 | −3.69E−01 | −1.64E−02 |
| 0.950 | 1.3791788017 | −2.62E−03 | −7.32E−02 | −3.16E−02 | −6.41E−06 | −4.34E−01 | −1.88E−02 |
| 1.000 | 1.3923516415 | −2.88E−03 | −8.08E−02 | −3.54E−02 | −1.43E−05 | −5.04E−01 | −2.14E−02 |

divergent. The modified APT convergence has been tested numerically for corrections until 200-th order with an own `Fortran 77` program with $1{,}000 \times 1{,}000$ matrices as Figs. 1 and 2 show for energy and wavefunction, respectively. The convergence of the wavefunction is not a traditional goal for perturbation theories when the series is divergent. In our case the energy series is convergent and, additionally, the wavefunction is convergent too.

If RSPT and modified APT are compared, the last one is clearly better as Table 3 lists. In fact, modified APT is numerically convergent for a tested range of the coupling constant $\lambda \in [0, 20]$, as shown. But when Wynn's epsilon algorithm (Table 4), $\delta$ algorithm (Table 5) or Borel transformation (Table 6)are being considered, RSPT is more effective resummed than modified APT. This is due to the fact that RSPT is a Taylor series and it keeps all analytical properties in this kind of developments.

The comparison of SCPT and modified APT can be done in its development stage. The seminal idea is to transform the unperturbed Hamiltonian at each correction for

**Table 6** Errors respect to exact energy ($\Delta x = \text{Exact} - x$) of Borel summation of RSPT, SCPT and modified APT energies of the QQAHO ground state corrected up to the fourth order in terms of the coupling constant

| $\lambda$ | Exact | $\Delta(f(\lambda,4,1))_{RS}$ | $\Delta(f(\lambda,4,1))_{SC}$ | $\Delta(f(\lambda,4,1/10))_{MA}$ | $\Delta(f(\lambda,7,1))_{RS}$ | $\Delta(f(\lambda,7,1))_{SC}$ | $\Delta(f(\lambda,7,1/10))_{MA}$ |
|---|---|---|---|---|---|---|---|
| 0.000 | 1.0000000000 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| 0.010 | 1.0073736721 | 1.00E−10 | 1.80E−09 | 7.23E−08 | 0.00E+00 | −1.34E−08 | 6.89E−08 |
| 0.025 | 1.0180010006 | 1.23E−08 | 2.61E−07 | 1.20E−06 | −1.00E−10 | −9.68E−07 | 9.90E−07 |
| 0.050 | 1.0347296973 | 2.78E−07 | 9.94E−06 | 1.04E−05 | −1.40E−09 | −2.18E−05 | 6.92E−06 |
| 0.075 | 1.0504339643 | 1.55E−06 | 7.78E−05 | 3.47E−05 | −1.69E−08 | −1.36E−04 | 2.05E−05 |
| 0.100 | 1.0652855095 | 4.94E−06 | 3.23E−04 | 7.66E−05 | −8.64E−08 | −5.33E−04 | 4.28E−05 |
| 0.150 | 1.0929050098 | 2.33E−05 | 2.28E−03 | 2.01E−04 | −7.35E−07 | −4.55E−03 | 1.14E−04 |
| 0.200 | 1.1182926544 | 6.52E−05 | 8.76E−03 | 3.38E−04 | −2.99E−06 | −2.50E−02 | 2.15E−04 |
| 0.250 | 1.1419018395 | 1.39E−04 | 2.44E−02 | 4.34E−04 | −8.33E−06 | −1.02E−01 | 3.37E−04 |
| 0.300 | 1.1640471574 | 2.52E−04 | 5.58E−02 | 4.42E−04 | −1.84E−05 | −3.35E−01 | 4.64E−04 |
| 0.350 | 1.1849584844 | 4.08E−04 | 1.11E−01 | 3.26E−04 | −3.51E−05 | −9.32E−01 | 5.82E−04 |
| 0.400 | 1.2048103274 | 6.11E−04 | 2.01E−01 | 6.01E−05 | −6.00E−05 | −2.28E+00 | 6.74E−04 |
| 0.450 | 1.2237391189 | 8.63E−04 | 3.37E−01 | −3.74E−04 | −9.48E−05 | −5.05E+00 | 7.26E−04 |
| 0.500 | 1.2418540597 | 1.16E−03 | 5.34E−01 | −9.87E−04 | −1.41E−04 | −1.03E+01 | 7.25E−04 |
| 0.550 | 1.2592442502 | 1.52E−03 | 8.07E−01 | −1.79E−03 | −2.00E−04 | −1.97E+01 | 6.58E−04 |
| 0.600 | 1.2759835663 | 1.92E−03 | 1.18E+00 | −2.77E−03 | −2.73E−04 | −3.57E+01 | 5.18E−04 |
| 0.650 | 1.2921340995 | 2.37E−03 | 1.66E+00 | −3.95E−03 | −3.61E−04 | −6.16E+01 | 2.94E−04 |
| 0.700 | 1.3077486511 | 2.88E−03 | 2.28E+00 | −5.32E−03 | −4.65E−04 | −1.02E+02 | −1.75E−05 |
| 0.750 | 1.3228725815 | 3.43E−03 | 3.06E+00 | −6.88E−03 | −5.86E−04 | −1.64E+02 | −4.23E−04 |
| 0.800 | 1.3375452081 | 4.03E−03 | 4.02E+00 | −8.63E−03 | −7.25E−04 | −2.55E+02 | −9.26E−04 |
| 0.850 | 1.3518008817 | 4.68E−03 | 5.20E+00 | −1.05E−02 | −8.82E−04 | −3.87E+02 | −1.53E−03 |
| 0.900 | 1.3656698258 | 5.37E−03 | 6.62E+00 | −1.27E−02 | −1.06E−03 | −5.73E+02 | −2.23E−03 |
| 0.950 | 1.3791788017 | 6.11E−03 | 8.32E+00 | −1.49E−02 | −1.25E−03 | −8.31E+02 | −3.04E−03 |
| 1.000 | 1.3923516415 | 6.89E−03 | 1.03E+01 | −1.74E−02 | −1.47E−03 | −1.18E+03 | −3.95E−03 |

**Table 7** Coefficients appearing in Eq. 56 obtained from the Wynn's epsilon algorithm (39)

| $m$ | $p_m^{(3)}$ | $q_m^{(3)}$ | $m$ | $p_m^{(3)}$ | $q_m^{(3)}$ |
|---|---|---|---|---|---|
| 0 | $1.9513152049 \times 10^{0}$ | $1.9513152049 \times 10^{0}$ | 33 | $2.9239954545 \times 10^{43}$ | $2.6350247614 \times 10^{43}$ |
| 1 | $6.8388371194 \times 10^{2}$ | $6.8242022553 \times 10^{2}$ | 34 | $1.5184132406 \times 10^{44}$ | $1.3608022240 \times 10^{44}$ |
| 2 | $1.1811690091 \times 10^{5}$ | $1.1760764685 \times 10^{5}$ | 35 | $7.3868672593 \times 10^{44}$ | $6.5817613927 \times 10^{44}$ |
| 3 | $1.3406134772 \times 10^{7}$ | $1.3318814560 \times 10^{7}$ | 36 | $3.3649911244 \times 10^{45}$ | $2.9799745775 \times 10^{45}$ |
| 4 | $1.1250291538 \times 10^{9}$ | $1.1151909110 \times 10^{9}$ | 37 | $1.4345201706 \times 10^{46}$ | $1.2622371823 \times 10^{46}$ |
| 5 | $7.4469431064 \times 10^{10}$ | $7.3649927381 \times 10^{10}$ | 38 | $5.7190047178 \times 10^{46}$ | $4.9981198918 \times 10^{46}$ |
| 6 | $4.0506869796 \times 10^{12}$ | $3.9968474335 \times 10^{12}$ | 39 | $2.1303913898 \times 10^{47}$ | $1.8485418313 \times 10^{47}$ |
| 7 | $1.8624898515 \times 10^{14}$ | $1.8334260771 \times 10^{14}$ | 40 | $7.4078964795 \times 10^{47}$ | $6.3791614405 \times 10^{47}$ |
| 8 | $7.3901764990 \times 10^{15}$ | $7.2575650337 \times 10^{15}$ | 41 | $2.4017620479 \times 10^{48}$ | $2.0516032337 \times 10^{48}$ |
| 9 | $2.5706997704 \times 10^{17}$ | $2.5184879467 \times 10^{17}$ | 42 | $7.2509073628 \times 10^{48}$ | $6.1407865016 \times 10^{48}$ |
| 10 | $7.9367999688 \times 10^{18}$ | $7.7566005263 \times 10^{18}$ | 43 | $2.0352900577 \times 10^{49}$ | $1.7079436560 \times 10^{49}$ |
| 11 | $2.1964827104 \times 10^{20}$ | $2.1412885134 \times 10^{20}$ | 44 | $5.3025256667 \times 10^{49}$ | $4.4061779894 \times 10^{49}$ |
| 12 | $5.4926508487 \times 10^{21}$ | $5.3411291600 \times 10^{21}$ | 45 | $1.2796978627 \times 10^{50}$ | $1.0522003202 \times 10^{50}$ |
| 13 | $1.2492922126 \times 10^{23}$ | $1.2117106414 \times 10^{23}$ | 46 | $2.8544748855 \times 10^{50}$ | $2.3204090886 \times 10^{50}$ |
| 14 | $2.5985439350 \times 10^{24}$ | $2.5137739360 \times 10^{24}$ | 47 | $5.8698565463 \times 10^{50}$ | $4.7129777113 \times 10^{50}$ |
| 15 | $4.9651365002 \times 10^{25}$ | $4.7903033085 \times 10^{25}$ | 48 | $1.1095324741 \times 10^{51}$ | $8.7893005445 \times 10^{50}$ |
| 16 | $8.7475517496 \times 10^{26}$ | $8.4163737689 \times 10^{26}$ | 49 | $1.9213456649 \times 10^{51}$ | $1.4996917444 \times 10^{51}$ |
| 17 | $1.4254147424 \times 10^{28}$ | $1.3675833430 \times 10^{28}$ | 50 | $3.0362932412 \times 10^{51}$ | $2.3316128206 \times 10^{51}$ |
| 18 | $2.1538424240 \times 10^{29}$ | $2.0604599677 \times 10^{29}$ | 51 | $4.3592104574 \times 10^{51}$ | $3.2873130092 \times 10^{51}$ |
| 19 | $3.0243734111 \times 10^{30}$ | $2.8845839956 \times 10^{30}$ | 52 | $5.6562211027 \times 10^{51}$ | $4.1794208910 \times 10^{51}$ |
| 20 | $3.9534933659 \times 10^{31}$ | $3.7590866416 \times 10^{31}$ | 53 | $6.5921354924 \times 10^{51}$ | $4.7597691741 \times 10^{51}$ |
| 21 | $4.8183350264 \times 10^{32}$ | $4.5667170231 \times 10^{32}$ | 54 | $6.8505903339 \times 10^{51}$ | $4.8169315588 \times 10^{51}$ |
| 22 | $5.4817865283 \times 10^{33}$ | $5.1782560002 \times 10^{33}$ | 55 | $6.2922038355 \times 10^{51}$ | $4.2896613648 \times 10^{51}$ |
| 23 | $5.8278048419 \times 10^{34}$ | $5.4861221469 \times 10^{34}$ | 56 | $5.0531900914 \times 10^{51}$ | $3.3209359559 \times 10^{51}$ |
| 24 | $5.7945241164 \times 10^{35}$ | $5.4352355666 \times 10^{35}$ | 57 | $3.5008482055 \times 10^{51}$ | $2.2006448829 \times 10^{51}$ |
| 25 | $5.3922090196 \times 10^{36}$ | $5.0390038067 \times 10^{36}$ | 58 | $2.0566439916 \times 10^{51}$ | $1.2230317322 \times 10^{51}$ |
| 26 | $4.6989441140 \times 10^{37}$ | $4.3741023436 \times 10^{37}$ | 59 | $1.0015711703 \times 10^{51}$ | $5.5435186292 \times 10^{50}$ |
| 27 | $3.8363215976 \times 10^{38}$ | $3.5566699438 \times 10^{38}$ | 60 | $3.9194717378 \times 10^{50}$ | $1.9676873238 \times 10^{50}$ |
| 28 | $2.9353491062 \times 10^{39}$ | $2.7098986206 \times 10^{39}$ | 61 | $1.1780403450 \times 10^{50}$ | $5.1287072150 \times 10^{49}$ |
| 29 | $2.1054190397 \times 10^{40}$ | $1.9351590756 \times 10^{40}$ | 62 | $2.5320342590 \times 10^{49}$ | $8.7271325447 \times 10^{48}$ |
| 30 | $1.4158336810 \times 10^{41}$ | $1.2953591385 \times 10^{41}$ | 63 | $3.4199005056 \times 10^{48}$ | $7.2725668564 \times 10^{47}$ |
| 31 | $8.9268740088 \times 10^{41}$ | $8.1280533797 \times 10^{41}$ | 64 | $2.1311135862 \times 10^{47}$ | |
| 32 | $5.2768697683 \times 10^{42}$ | $4.7805277388 \times 10^{42}$ | | | |

wavefunction and energy. SCPT accounts for this transformation using unitary transformations of the operators as Kolmogorov [4] pointed in his celebrated work in classical mechanics. In the case of modified APT, the foundations were born from the properties of easy matrix inversions, see Besalú [6,17]. The coefficients of both series are coupling constant dependent. For SCPT, Eq. 47 shows this dependence from the

**Table 8** Coefficients appearing in Eq. 57 obtained from the $\delta$ algorithm (42)

| $m$ | $p_m^{(3)}$ | $q_m^{(3)}$ | $m$ | $p_m^{(3)}$ | $q_m^{(3)}$ |
|---|---|---|---|---|---|
| 0 | $5.463682574 \times 10^{0}$ | $5.463682574 \times 10^{0}$ | 33 | $4.6043744100 \times 10^{43}$ | $4.1242195984 \times 10^{43}$ |
| 1 | $2.023987061 \times 10^{3}$ | $2.0198893 \times 10^{3}$ | 34 | $2.2403444115 \times 10^{44}$ | $1.9950121541 \times 10^{44}$ |
| 2 | $3.684788328 \times 10^{5}$ | $3.669710869 \times 10^{5}$ | 35 | $1.0211077947 \times 10^{45}$ | $9.0373070249 \times 10^{44}$ |
| 3 | $4.3943881489 \times 10^{7}$ | $4.3671275850 \times 10^{7}$ | 36 | $4.3578235176 \times 10^{45}$ | $3.8321310408 \times 10^{45}$ |
| 4 | $3.8607750401 \times 10^{9}$ | $3.8284928878 \times 10^{9}$ | 37 | $1.7405293353 \times 10^{46}$ | $1.5202326128 \times 10^{46}$ |
| 5 | $2.6645447511 \times 10^{11}$ | $2.6363857412 \times 10^{11}$ | 38 | $6.5016034488 \times 10^{46}$ | $5.6383029567 \times 10^{46}$ |
| 6 | $1.5042605354 \times 10^{13}$ | $1.4849684658 \times 10^{13}$ | 39 | $2.2695453757 \times 10^{47}$ | $1.9534032797 \times 10^{47}$ |
| 7 | $7.1425959144 \times 10^{14}$ | $7.0344966196 \times 10^{14}$ | 40 | $7.3964329210 \times 10^{47}$ | $6.3155142471 \times 10^{47}$ |
| 8 | $2.9108539336 \times 10^{16}$ | $2.8599175794 \times 10^{16}$ | 41 | $2.2479437857 \times 10^{48}$ | $1.9032379037 \times 10^{48}$ |
| 9 | $1.0339397539 \times 10^{18}$ | $1.0133434663 \times 10^{18}$ | 42 | $6.3630501202 \times 10^{48}$ | $5.3389817485 \times 10^{48}$ |
| 10 | $3.2397484986 \times 10^{19}$ | $3.1671743417 \times 10^{19}$ | 43 | $1.6749963876 \times 10^{49}$ | $1.3919671132 \times 10^{49}$ |
| 11 | $9.0420056810 \times 10^{20}$ | $8.8164600937 \times 10^{20}$ | 44 | $4.0934379344 \times 10^{49}$ | $3.3668923985 \times 10^{49}$ |
| 12 | $2.2656167128 \times 10^{22}$ | $2.2031945868 \times 10^{22}$ | 45 | $9.2691367169 \times 10^{49}$ | $7.5400006291 \times 10^{49}$ |
| 13 | $5.1300815886 \times 10^{23}$ | $4.9750137606 \times 10^{23}$ | 46 | $1.9404285441 \times 10^{50}$ | $1.5596941761 \times 10^{50}$ |
| 14 | $1.0555326538 \times 10^{25}$ | $1.0207287584 \times 10^{25}$ | 47 | $3.7458984702 \times 10^{50}$ | $2.9721437952 \times 10^{50}$ |
| 15 | $1.9827139636 \times 10^{26}$ | $1.9117486207 \times 10^{26}$ | 48 | $6.6488644521 \times 10^{50}$ | $5.2014771324 \times 10^{50}$ |
| 16 | $3.4137160965 \times 10^{27}$ | $3.2816461036 \times 10^{27}$ | 49 | $1.0814800370 \times 10^{51}$ | $8.3305006644 \times 10^{50}$ |
| 17 | $5.4059232231 \times 10^{28}$ | $5.1806887887 \times 10^{28}$ | 50 | $1.6058106499 \times 10^{51}$ | $1.2159650661 \times 10^{51}$ |
| 18 | $7.8973547275 \times 10^{29}$ | $7.5441475138 \times 10^{29}$ | 51 | $2.1668798634 \times 10^{51}$ | $1.6099039911 \times 10^{51}$ |
| 19 | $1.0670525316 \times 10^{31}$ | $1.0159693996 \times 10^{31}$ | 52 | $2.6434855418 \times 10^{51}$ | $1.9225060736 \times 10^{51}$ |
| 20 | $1.3364686591 \times 10^{32}$ | $1.2681567734 \times 10^{32}$ | 53 | $2.8977329430 \times 10^{51}$ | $2.0569717660 \times 10^{51}$ |
| 21 | $1.5547117026 \times 10^{33}$ | $1.4700559516 \times 10^{33}$ | 54 | $2.8334426846 \times 10^{51}$ | $1.9561474156 \times 10^{51}$ |
| 22 | $1.6826619609 \times 10^{34}$ | $1.5852524906 \times 10^{34}$ | 55 | $2.4498266580 \times 10^{51}$ | $1.6373456410 \times 10^{51}$ |
| 23 | $1.6968319589 \times 10^{35}$ | $1.5925854300 \times 10^{35}$ | 56 | $1.8529465945 \times 10^{51}$ | $1.1916851366 \times 10^{51}$ |
| 24 | $1.5963433857 \times 10^{36}$ | $1.4924304386 \times 10^{36}$ | 57 | $1.2097374593 \times 10^{51}$ | $7.4256071855 \times 10^{50}$ |
| 25 | $1.4025871791 \times 10^{37}$ | $1.3059891370 \times 10^{37}$ | 58 | $6.7020434029 \times 10^{50}$ | $3.8814861029 \times 10^{50}$ |
| 26 | $1.1519850704 \times 10^{38}$ | $1.0681511150 \times 10^{38}$ | 59 | $3.0807044796 \times 10^{50}$ | $1.6550897370 \times 10^{50}$ |
| 27 | $8.8512997465 \times 10^{38}$ | $8.1714496880 \times 10^{38}$ | 60 | $1.1392795184 \times 10^{50}$ | $5.5279670335 \times 10^{49}$ |
| 28 | $6.3661535690 \times 10^{39}$ | $5.8506066887 \times 10^{39}$ | 61 | $3.2412770938 \times 10^{49}$ | $1.3560897468 \times 10^{49}$ |
| 29 | $4.2880922175 \times 10^{40}$ | $3.9222941158 \times 10^{40}$ | 62 | $6.6108457047 \times 10^{48}$ | $2.1723080390 \times 10^{48}$ |
| 30 | $2.7059408195 \times 10^{41}$ | $2.4629840535 \times 10^{41}$ | 63 | $8.5075916229 \times 10^{47}$ | $1.7045326960 \times 10^{47}$ |
| 31 | $1.6000553891 \times 10^{42}$ | $1.4489537959 \times 10^{42}$ | 64 | $5.0900987553 \times 10^{46}$ | |
| 32 | $8.8665798019 \times 10^{42}$ | $7.9864556848 \times 10^{42}$ | | | |

fourth corrected order. In modified APT, this dependence already appears from the second corrected order of the energies, see Eq. 49. Numerical results show a convergent behaviour for modified APT for the quantum quartic anharmonic oscillator in both energy and wavefunction. The excited states will be studied in a forthcoming work.

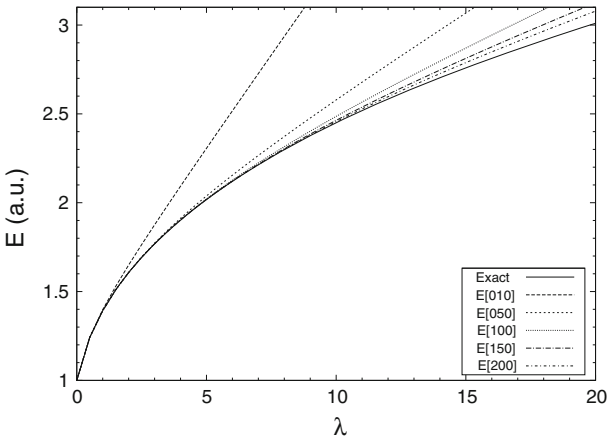


**Fig. 1** Modified APT ground state corrected energies in terms of the coupling constant for the quantum quartic anharmonic oscillator for a range of values between 0 and 20. Corrections are performed up to 200th order

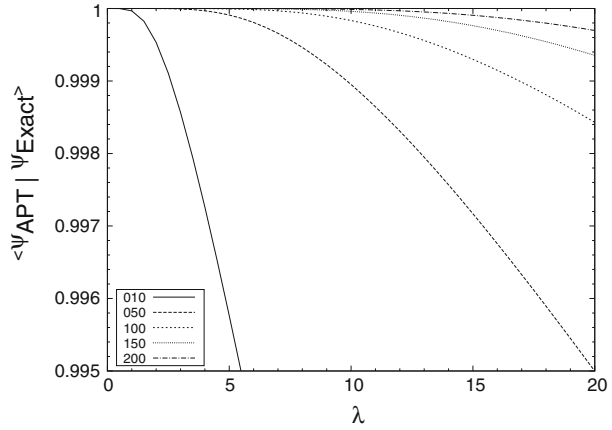


**Fig. 2** Overlaps between modified APT ground state corrected wavefunction and the exact wavefunction in terms of the coupling constant of the quantum quartic anharmonic oscillator (range between 0 and 20). Corrections are performed up to 200th order

Resummation algorithms, i.e., Wynn's epsilon, $\delta$ algorithms and Borel transformation have been codified using `Mathematica`. It is desirable that perturbation theories generate resummable series, that is, these theories should have a good foundation in their developments allowing to be manipulated in order to get a better prediction for corrected energies. This requirement is not totally fullfilled by SCPT which is clearly worse than modified APT and RSPT resummations for $\lambda > 0.1$ (see Tables 4, 5 and 6). The best series to be manipulated is the RSPT one. It resumms in a proper way with all three methods employed in this paper, see Tables 4, 5 and 6. In the case of modified APT, some poles appear in terms of the coupling constant as Table 4 puts it in evidence, consequently it resumms fine sometimes except when a pole is found.

On the other hand, $\delta$ algorithm and Borel transformation works properly for modified APT. In any case APT series does not need to be resummed because it shows to be convergent.

## 7 Conclusions

As a whole, the powerful power of modified APT is that the energy and wavefunction are convergent without needing to rely on resumation procedures whereas RSPT diverges, as Figs. 1 and 2 show. A new and flexible perturbation theory has been deduced from the foundations of RSPT, APT and SCPT: the definition of the so-called mutant Hamiltonian operator Eq. 26 is not unique, that is, several choices can be considered. Thus, a promising door for perturbation theories is being opened.

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