Convergence enhancement in perturbation theory *

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Abstract

The Frobenius norm of operator QW is minimized with respect to level shift parameters applied to the zero order spectrum, where W is the perturbation while Q is the reduced resolvent of the zero order Hamiltonian. The stationary condition leads to a simple formula for the level shifts which eliminates degeneracy-induced singularities. Such level shifts may increase the radius of convergence of the perturbation series, and may improve low-order perturbative estimations – as it is found on the cases of a simple matrix eigenvalue problem and the one-dimensional quartic (anharmonic) oscillator.

Keywords: Perturbation theory, convergence, partitioning, level shifts, anharmonic oscillator.

* Dedicated to Professor Rudolf Zahradník on the occasion of his 70^{th} birthday

I. INTRODUCTION

Perturbation theory (PT) continues to attract investigations due to its unsolved problems concerning convergence properties, the flexibility of partitioning, and related questions [1–4]. The theory of resolvents, or Green functions, may serve as a powerful tool to develop new solutions to open problems in PT. Green function theory being somewhat misterious to many chemists, a well written didactic survey on the quantum chemical application of Green functions has been topical for some time and would be highly appreciated. In this connection, one of the present authors (PRS) feels it necessary to mention that 17 years ago, looking for a publisher for his book on second quantization[5], Professor Rudolf Zahradník, to whom this article is dedicated, kindly offered many invaluable advises in this matter. Among other propositions, he suggested to cover also Green function theory in the same volume. It may be a shame, but PRS was not able to follow this advise, not being well prepared for this task at that time. Since then, we have performed some research in this area[6, 7], but the aforementioned didactic introduction is still in delay. In the present paper, however, we briefly review an important aspect of Green function (GF) theory, discussed by Kato[4] a long time ago, namely its application to the convergence problem in PT. It will be seen that, although GF theory alone does not solve the problem of convergence, its suggestive formal results may induce useful thoughts towards enhancing convergence properties of the PT series. The encouragement of Professor Rudolf Zahradník is herewith gratefully acknowledged.

A. Level shifts in perturbation theory

In PT, one starts with an (arbitrary) split applied to the total Hamiltonian

$$H = H^0 + W \tag{1}$$

and normally assumes that the spectrum of H^0 is known:

$$H^0\Psi_i^0 = E_i^0\Psi_i^0. \tag{2}$$

The well-known PT formulae emerge in terms of these zero order quantities and the matrix elements of W in the basis of Ψ_i^0.

It has been realized a long time ago, that for any given splitting expressed by Eq.(1), the partitioning of H can be freely changed by adding and substracting an operator that is diagonal in basis Ψ_i^0:

$$H = \underbrace{H^0 + \sum_i \eta_i |\Psi_i^0\rangle\langle\Psi_i^0|}_{H^{0\prime}} + \underbrace{W - \sum_i \eta_i |\Psi_i^0\rangle\langle\Psi_i^0|}_{W^\prime} \tag{3}$$

where η_i-s are arbitrary parameters called level shifts. The level shifts obviously do not affect the zero order wave functions, they merely shift the zero order energy levels.

Level shift parameters have been applied previously in a number of works with various purposes. With the aim of improving the convergence properties in particular Feenberg, Goldhammer[8, 9], Amos[10], Dietz et al.[11, 12], Finley et al.[13**?** , 14] have introduced appropriately chosen shift parameters. Recently, optimal level shifts have been determined from the condition that the energy perturbed up to the third order should be stationary with respect to η_i-s [1, 2, 15–18]. Here we shall investigate the applicability of level shift parameters deduced in a different manner.

B. On the convergence of the PT series

It has been known for a long time[4] that the theory of Green functions provides a suffcient condition for the convergence of the PT series. To see this, we consider the operator

$$G(z) = (z - H)^{-1} \tag{4}$$

where H is the Hamiltonian operator, and z is a complex scalar variable. Accordingly, $G(z)$ is an operator-valued function of z which is called the resolvent of H or the Green function. The resolvent is an analytic function of z except for the points where z coincides an eigenvalue of H. In these points $G(z)$ has simple poles.

An important property of the resolvent operator is that eigenvalues of H can be extracted from $G(z)$ by a contour integration:

$$E_k = \frac{1}{2\pi i} \oint z \ \mathrm{Tr}\ G(z)\ dz \tag{5}$$

where the integration has to be extended to a path which contains exclusively the k-th (isolated) eigenvalue (cf. Fig. 1.). Validity of this statement can be immediately seen by inserting the spectral resolution of H and performing the integration via Cauchy's theorem for contour integrals.

If one splits the Hamiltonian to a zero order part (H^0) and a perturbation (W) as in Eq.(1), and defines

$$G^0(z) = (z - H^0)^{-1} \tag{6}$$

as the GF of H^0, than $G(z)$ fulfills the relation

$$G(z) \;=\; G^0(z) \;+\; G^0(z)W\; G(z) \tag{7}$$

which is called the (simple form of) Dyson equation[1]This result is easily proved by multiplyting Eq.(7) by the inverse of $G^0(z)$ (from the left) and the inverse of $G(z)$ (from the right), when simply the definition of the partitioning $H = H^0 + W$ is recovered.

Eq.(7) has A formal solution of Eq.(7) looks:

$$G \;= \left(1 - G^0 W\right)^{-1} G^0 \tag{8}$$

which can be expanded into a Taylor series

$$G \;= G^0 + G^0 W G^0 + G^0 W G^0 W G^0 + \ldots \tag{9}$$

Upon integrating this equation on the appropriate contour and making use of Eq.(5), one gets:

$$E_k = E_k^0 + E_k^1 + E_k^2 + \ldots \tag{10}$$

with E^i denoting the i-th PT correction to the energy. Accordingly, the convergence of this series depends upon the validity of expansion (9) for all z values touched during the integration[2]. At a given z value, the convergence of Eq.(9) is known to depend on the norm of operator G^0W : if and only if $||G^0(z)W|| < 1$, the series is convergent.

The above observation is quite interesting since it appears as if we formulated the condition for convergence of the PT series. However, there are an infinite number of ways how

[1] The true Dyson equation emerges after projecting Eq.(7) into a subspace; after this projection the simple peturbation operator W has to be replaced by a much more complicated self-energy operator.

[2] This contour should embed the k-th pole of both G and G^0

an 'appropriate' contour can be set up, and finding the necessary and sufficient condition for convergence assumes that one has specified the most suitable path for the integration, which is usually unknown. Therefore, in practice, this observation yields only sufficient but not necessary criteria for the convergence of the PT series. The punctual convergence conditions, necessary and sufficient, therefore, still remain unknown in the Rayleigh-Schrödinger perturbation theory.

II. THE NORM OF QW

Apart from the problem of finding the most appropriate integration path, i.e. the appropriate z values, it is evident that quantity $||G^0W||$ plays a determining role in the problem of convergence. One may hope for example that its minimization for a certain selected z value may improve the convergence properties.

An important quantity, related to G^0 is the reduced resolvent Q defined for the ground state as

$$Q(E_0^0 - H^0) \;=\; 1 - |\Psi_0^0\rangle\langle\Psi_0^0|. \tag{11}$$

In spectral resolution Q can be expressed as

$$Q = -\sum_{i\neq 0} \frac{|\Psi_i^0\rangle\langle\Psi_i^0|}{E_i^0 - E_0^0}. \tag{12}$$

In words, Q is the inverse of $(E_0^0 - H^0)$ in the subspace orthogonal to the ground state. Unlike $G^0(z)$, Q is a regular quantity if the ground state is nondegenerate in the zero order spectrum. As its name refers to, Q can be deduced from $G^0(z)$ by applying the aforementioned reduction and taking it at $z = E_0^0$. The role of the reduced resolvent in PT can be summarized by recalling the compact PT energy formulae at the lowest orders:

$$E^2 = \langle WQW\rangle \tag{13}$$

$$E^3 = \langle WQ(W - \langle W\rangle)QW\rangle \tag{14}$$

etc. In these formulae, as well as in higher orders, the PT corrections are constructed from the powers of operator QW. It appears, therefore, a natural idea to minimze the square norm of this operator, $||QW||^2$ with respect to any free parameters that are at our disposal.

As discussed above, free level shift parameters can always be introduced in PT, these therefore can be utilized to minimize $||QW||^2$. The first thing one has to do is to choose a

norm in the operator space. In this work, we define the norm of operator A as

$$||A||^2 = \text{Tr } (AA^\dagger) \tag{15}$$

In a basis set representation this norm is expanded as

$$||A||^2 = \sum_{ik} A_{ik} A^*_{ik} = \sum_{ik} |A_{ik}|^2, \tag{16}$$

that is the 2-norm or Frobenius norm in matrix theory.

Evaluating $||QW||^2$ with this definition we get:

$$\begin{aligned} ||QW||^2 &= \sum_{ik} |\langle i|QW|k\rangle|^2 \\ &= \sum_{ik} \langle i|QW|k\rangle\langle k|WQ|i\rangle \\ &= \sum_{i} \langle i|QW^2Q|i\rangle \\ &= \sum_{i\neq 0} \frac{\langle i|W^2|i\rangle}{(E_i^0 - E_0^0)^2}, \end{aligned}$$

where the resolution of identity was used to get rid of the summation over k. Applying now the level shifts (3) we get

$$||QW||^2 = \sum_{i\neq 0} \frac{\langle i|W^2|i\rangle - 2\eta_i\langle i|W|i\rangle + \eta_i^2}{(E_i^0 - E_0^0 + \eta_i)^2} \tag{17}$$

where the level shift of the ground state, η_0, was set zero to fix the energy origin.

To determine η_i values that are optimal in this sense, we require

$$\frac{\partial}{\partial \eta_k} ||QW||^2 = 0, \tag{18}$$

which yields

$$\eta_k = \frac{\langle k|W^2|k\rangle + \langle k|W|k\rangle(E_k^0 - E_0^0)}{\langle k|W|k\rangle + (E_k^0 - E_0^0)}. \tag{19}$$

In what follows, level shifts obtained from this relation will be identified as QW-optimized ones. Similarly, the partitioning defined by them will be referred to as QW-optimized (shortly: QW-opt) partitioning.

III. PROPERTIES OF THE QW-OPTIMIZED PARTITIONING

First we intend to show that the QW-opt partitioning is unique, that is the resulting shifted denominators do not depend on the initial partitioning. To see this, we evaluate

the shifted denominators using abbreviations $\Delta_k = E_k^0 - E_0^0$, $W_{kk} = \langle k|W|k\rangle$ and $W_{kk}^2 = \langle k|W^2|k\rangle$

(20)

$$\begin{aligned}
\Delta_k + \eta_k &= \Delta_k + \frac{W_{kk}^2 + W_{kk}\Delta_k}{W_{kk} + \Delta_k} \\
&= \frac{\Delta_k^2 + W_{kk}^2 + 2W_{kk}\Delta_k}{W_{kk} + \Delta_k} \\
&= \frac{(W_{kk} + \Delta_k)^2 - (W_{kk})^2 + W_{kk}^2}{W_{kk} + \Delta_k} \\
&= W_{kk} + \Delta_k + \frac{\langle W_{kk}^2\rangle_c}{W_{kk} + \Delta_k} \qquad (21)
\end{aligned}$$

where the second connected moments of the perturbation operator,

$$\langle W_{kk}^2\rangle_c = W_{kk}^2 - (W_{kk})^2 \qquad (22)$$

are introduced. To arrive at our final formula for the shifted denominators we observe that

$$W_{kk} + \Delta_k = H_{kk} - E_0^0, \qquad (23)$$

by which

$$\Delta_k + \eta_k = H_{kk} - E_0^0 + \frac{\langle W_{kk}^2\rangle_c}{H_{kk} - E_0^0} \qquad (24)$$

In this expression, both the quantities $H_{kk} - E_0^0$ and the connected moments $\langle W_{kk}^2\rangle_c$ are independent on the initial partitioning[3]. Therefore we see that the QW-optimization results uniquely defined energy denominators.

A second property of the QW-opt partitioning can be inferred from (19) or (24) observing that these formulae do not present explicit coupling between the states k. (There is, however, and implicit coupling expressed by the presence of the square of W in the connected moments.) This uncoupled nature of QW-optimization makes it markedly different from the energy-optimized partitionings[1, 2, 15–19] where the coupling between different states represents a serious computational difficulty. The simplicity exhibited by Eqs. (19) or (24) is a great advantage from the computational point of view, but gives us a warning that the power of this simple optimization might not be strong enough.

[3] With no loss of generality, one can choose $W_{00} = 0$. This can always be achieved – without affecting the partitioning – by a simple shift of the origin of the energy scale. Then, $E_0^0 = H_{00}$ which clearly expresses a partitioning-independence of Eq.(24).

The same conclusion is supported by the observation that the QW-opt denominators are numerically often quite close to the so called Epstein-Nesbet (EN) [20, 21] denominators $H_{kk} - H_{00}$. Namely, if $W_{00} = 0$, the EN partitioning results from Eq.(24) simply by neglecting the second connected moment of W, which is supposedly a small quantity. The results obtained in the QW-opt partitioning for modest perturbations will thus be close to those of the EN partitioning. Moreover since the correction term $\langle W_{kk}^2 \rangle_c / (H_{kk} - E_0^0)$ is always positive, the QW-opt denominators are slightly larger than the EN ones. Low order corrections, therefore, are expected to be in absolute value smaller in QW-opt partitioning as compared to EN corrections.

An interesting property of the QW-opt partitioning is connected to the fact that all shifted denominators are definitely positive. This is because $(H_{kk} - E_0^0) \geq 0$ by definition and the second connected moments $\langle W_{kk}^2 \rangle_c$ are always positive quantities (these moments are zero if and only if evaluated with an exact eigenfunction of H, when all PT corrections are zero anyway). Accordingly, any eventual degeneracy of the zero order spectrum will be lifted upon QW-optimization.

To have a closer look into the degeneracy problem, let us evaluate the limit of the second order QW-opt correction when a particular state k becomes degenerate with the ground state. As Eq.(24) indicates, $\eta_k \to \infty$ in this limit, thus the contribution of this state to the second order correction becomes zero. This is not the accurate value that would be obtained from degenerate PT, but it is certainly a better etimate than the divergent result of non-degenerate PT. The result of QW-opt partitioning in such a degenerate limit will be the elimination of the effect of degenerate levels, a damping of quasidegeneracies, while summing up slightly modified EN-type contributions from non-degenerate states.

Difference between the EN and QW-opt partitionings is expected to be major if the perturbation is strong, i.e., $\langle W_k^2 k \rangle_c$-s are large. In these cases QW-optimization appears to be a promising tool. The accuracy of the results, however, can only be checked by numerical calculations.

IV. NUMERICAL ILLUSTRATION

Due to the close relation between QW-opt and EN partitionings, we cannot expect the former to be very useful to treat electron correlation effects where the Møller-Plesset[22]

partitioning is usually superior to the EN partitioning. There are however, special situations when QW-optimization is advantageous. In this paper we shall illustrate this on a matrix diagonalization problem and on the example of the anharmonic oscillator.

A. Perturbing a 2x2 matrix

First we study a simple 2-by-2 matrix eigenvalue problem. This is a rather special example but allows us a detailed investigation on the performance of QW-optimization.

Consider the Hermitian matrix and its splitting to a zero order part and a perturbation

$$H = \begin{pmatrix} a & w \\ w & b \end{pmatrix} = \underbrace{\begin{pmatrix} a & 0 \\ 0 & b+\eta \end{pmatrix}}_{H^0} + \underbrace{\begin{pmatrix} 0 & w \\ w & -\eta \end{pmatrix}}_{W}. \tag{25}$$

The reduced resolvent is

$$Q = \frac{1}{b-a+\eta} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{26}$$

The second, third and fourth order corrections, respectively, turn out to be:

$$E^2 = -\frac{w^2}{b-a+\eta} \tag{27}$$

$$E^3 = -\frac{\eta w^2}{(b-a+\eta)^2} \tag{28}$$

and

$$E^4 = w^2 \frac{w^2-\eta^2}{(b-a+\eta)^3} \tag{29}$$

From the condition that $||QW||^2$ is minimal, one obtains the optimal value of η:

$$\eta = \frac{w^2}{b-a}. \tag{30}$$

Substituting this value into the above results, one obtains the QW-opt corrections, while the standard Rayleigh-Schrödinger PT formulae in the EN partitioning emerge by setting $\eta = 0$. These should be compared to the exact eigenvalue

$$E = \frac{b+a}{2} - \sqrt{\left(\frac{b-a}{2}\right)^2 + w^2} \tag{31}$$

In Fig.2. we plot the energy corrections up to the 4th order as a function of w, choosing a=1 and b=2. Fig. 2.a. shows that for small w values all low-order energies are accurate, but

they behave differently as w increases. The standard second and fourth order corrections (i.e., those with $\eta = 0$ deviate from the exact curve to the greatest extent. When using optimal η-s, the second and fourth order curves remain close to the exact one, while the third order result is less accurate (note that odd order corrections are zero in the standard partitioning).

In a wider interval, Fig.2.b. depicts the energy errors of the same energies. Again, the standard second and third order results diverge very soon, while the optimized curves exhibit a systematically improving behaviour with increasing order.

B. Anharmonic oscillator

A physically more interesting example is provided by the quartic anharmonic oscillator having the Hamiltonian

$$H(\gamma) = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + \gamma x^4, \tag{32}$$

where the coupling parameter γ is a measure of anharmonicity. This system has been extensively studied[23–27], and it is known[23, 28] that if choosing $H^0 = H(\gamma = 0)$ as the zero order Hamiltonian, the Rayleigh-Schrödinger PT series is divergent for any $\gamma \neq 0$. It appears to be interesting, therefore, to study the convergence properties of the QW-opt partitioning for this case. In the present work, we performed a numerical study by evaluating large order energy corrections, for various γ values.

The choice $H^0 = H(\gamma = 0)$ will be referred to as the 'standard' partitioning. If we put all diagonal perturbations to the zero order, i.e., requiring $W_{kk} = 0$ for all states k, we can speak about an EN partitioning. Finally, the QW-opt partitioning results if using the shifted denominators of Eq.(24).

Fig. 3. shows the convergence of the PT expansion for small and medium γ values. It is well illustrated that the PT series in the standard partitioning is never convergent, while the EN partitioning may converge for small γ. (It may of course also be possible that the EN result also start to diverge at larger orders.) However, the results obtained in the QW partitioning turn out to be the best for all cases as to their convergence properties, althought its small-order estimations are not necessarily more accurate.

To see the convergence numerically for a large value of the coupling constant, we evaluated the PT corrections in QW-opt partitioning for $\gamma = 50$ up to order 2500. The results are

plotted in Fig. 4 for the large-order part and some of them are collected in Table I. (The results of the EN partitioning are not computed here since the corresponding PT series is divergent even for smaller γ values). At order 2500, the energy does not seem to be converged to 4 digits, since the energy contributions are in the 10^{-5} order of magnitude. This shows that the convergence is very slow, but there is no apparent sign of divergence.

The above results indicate that, while the convergence radius for the quartic oscillator in the standard partitioning is zero, the EN and QW-optimized partitionings may result finite convergence radii. In the case of the QW-opt partitioning the convergence radius can be quite large, and it might also be possible that it is infinite. To decide this, further numerical and – preferably – analytic calculations are required.

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Figure legends

Fig.1 Integration contour to get the energy of state k

Fig.2 Eigenvalue corrections for matrix (25) as a function of parameter w measuring the strength of perturbation. (a): eigenvalue estimates, (b) differences of estimated eigenvalues from the exact one

Fig.3

Fig.4 Large order behaviour of perturbed energies of quartic oscillator in the strong-copuling limit ($\gamma = 50$)

n	E^n	$\sum_{i=1}^{n} E^i$
1	38.0000000	38.0000000
2	-6.79284227	31.2071577
3	-4.11989193	27.0872658
4	-2.77990065	24.3073652
5	-2.01212717	22.2952380
6	-1.52904999	20.7661880
7	-1.20396842	19.5622196
8	-0.97398290	18.5882367
9	-0.80487850	17.7833582
10	-0.67667558	17.1066826
20	-0.20208716	13.6355834
40	-0.05365966	11.6116823
60	-0.02326577	10.9166085
80	-0.01246184	10.5801887
100	-0.00752193	10.3884604
200	-0.00136293	10.0577779
300	-0.00044720	9.97848353
400	-0.00019358	9.94884744
500	-0.00010029	9.93488668
600	-0.00005955	9.92716938
700	-0.00003946	9.92233745
800	-0.00002853	9.91899457
900	-0.00002208	9.91649326
1000	-0.00001797	9.91450714
1500	-0.00000934	9.90814155
2000	-0.00000600	9.90439782
2500	-0.00000407	9.90192042

TABLE I: Convergence of the PT series for the quantic anharmonic oscillator in the QW-optimized partitioning for $\gamma = 50$

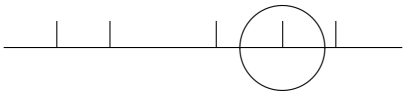

Fig.1.

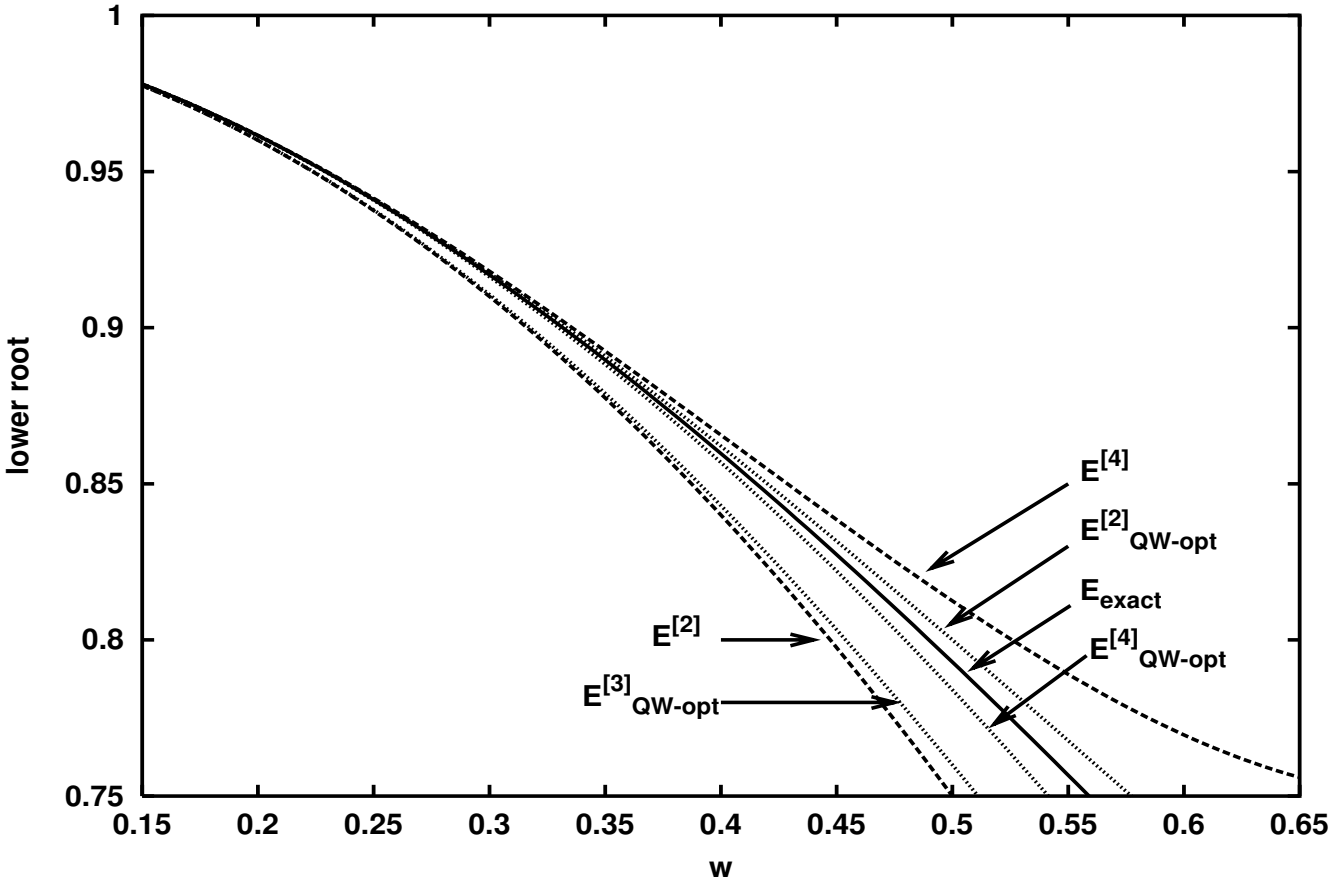
1
0.95
0.9
0.85
0.8
0.75
lower root
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0.55
0.6
0.65
w
E[4]
E[2]QW-opt
Eexact
E[4]QW-opt
E[2]
E[3]QW-opt

Fig.2a.

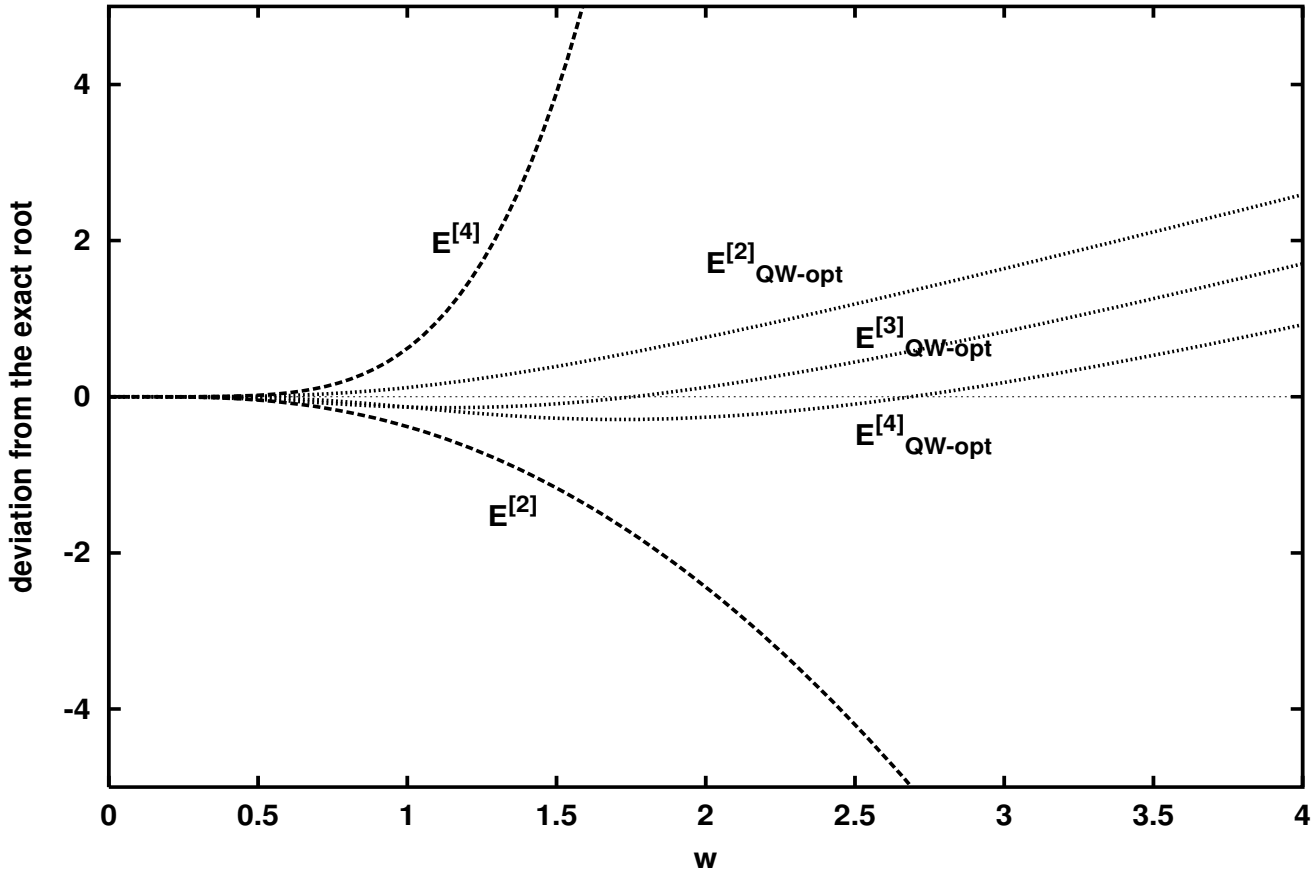
deviation from the exact root
w
E[4]
E[2]QW-opt
E[3]QW-opt
E[4]QW-opt
E[2]
4
2
0
-2
-4
0
0.5
1
1.5
2
2.5
3
3.5
4

Fig.2b.

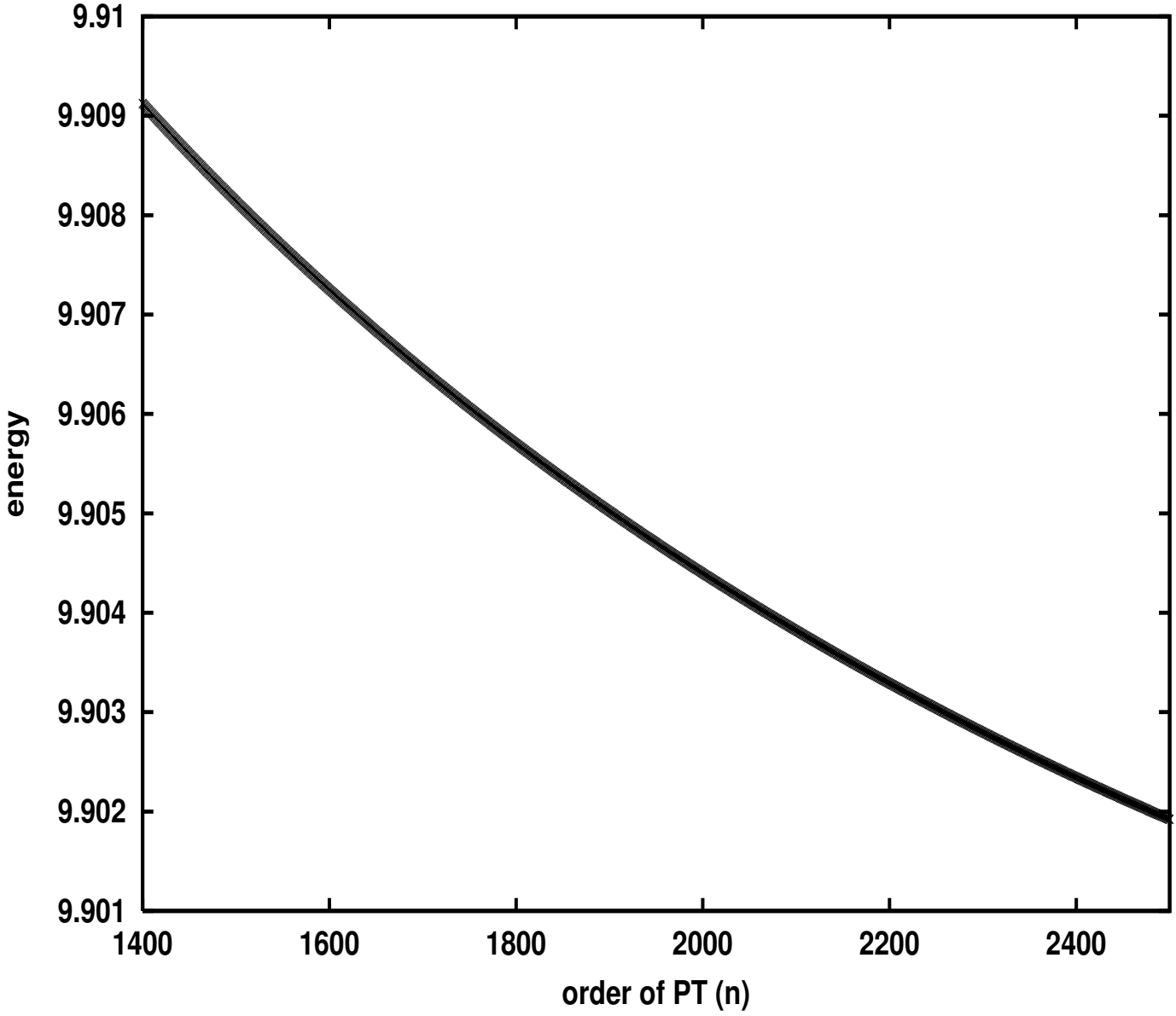
9.91
9.909
9.908
9.907
9.906
9.905
9.904
9.903
9.902
9.901
energy
1400
1600
1800
2000
2200
2400
order of PT (n)

Fig.4.