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Review

Generalized Rayleigh–Schrödinger perturbation theory in matrix form*

Emili Besalú and Ramon Carbó

Institute of Computational Chemistry, University of Girona, 17071 Girona, Spain

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The *nested summation symbols* (NSS) formalism is used as a starting point to formulate a completely general Rayleigh–Schrödinger perturbation theory (RSPT) scheme. In order to make the theoretical framework practical from a computational point of view, the matrix form for the theory is given in every case. As a result, an algorithmic iterative recipe to compute eigenvalue and eigenvector corrections up to any order is described. Degenerate systems are also treated. At the same time the described procedure allows the computation of eigenvalue and eigenvector derivatives with respect to a set of parameters.

1. Introduction

We have recently proposed a quite general Rayleigh–Schrödinger (RS) perturbation theory (PT) formalism [1] based on the definition of a simple device which we named *nested summation symbols* (NSS) [2]; also the algorithmic counterpart, *generalized nested do loops* (GNDL), was discussed [2]. This connected our recent research development [2,3] with earlier ideas published in the early seventies by one of us [4].

The present paper is another consequence of such a connection. The practical algorithm to solve the general RSPT problem from a matrix point of view is the leading feature of the present study. The problem is presented here from a completely general point of view and, as examples of application, simpler cases and related mathematical properties are discussed. Degenerate spectral secular systems are also discussed and a solution allowing the use of the non-degenerate PT framework with slight modifications is proposed.

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2. Preliminary definitions

2.1. NESTED SUMMATION SYMBOL

The NSS concept corresponds to a linear operator attached to an arbitrary number of nested sums. In other words, an NSS represents a set of summation symbols where their number can be variable. Ample information about this topic can be found in refs. [2,3]. Here, a simple notation for NSSs will be used. They will be written as

$$\sum_k(\boldsymbol{i} = \boldsymbol{u}, \boldsymbol{v}), \tag{1}$$

where the meaning of this convention corresponds to performing all the sums involved in the generation of all the possible values of the index vector $\boldsymbol{i}$. The elements of vector $\boldsymbol{i}$ have the following limits:

$$\{u_p \leqslant i_p \leqslant v_p\}, \quad \forall p = 1, k, \tag{2}$$

where the i_p indices are incremented one step at a time. The index k is the *dimension of the NSS*, that is, the number of summation symbols embedded in the operator, and thus the dimension of the vectors $\boldsymbol{i}$, $\boldsymbol{u}$ and $\boldsymbol{v}$ involved. The operator $\sum_0(\boldsymbol{i} = \boldsymbol{u}, \boldsymbol{v})$ is assumed to be the same as the unit operator.

```
      Parameter (k=?)   !  Dimension of the NSS
      Integer p,i(k),u(k),v(k)

* < Initial parameter values >

      do p=1,k
         u(p)=?
         v(p)=?
         i(p)=u(p)
      end do

* < GNDL procedure >

      p=k
      do while (p.gt.0)
         if (i(p).gt.v(p)) then
            i(p)=u(p)
            p=p-1
         else
            call Application(k,i,u,v)
            p=k
         end if
         if (p.gt.0) i(p)=i(p)+1   ! Step
      end do
      END
```

Program 1. FORTRAN codification of the GNDL implementing an NSS like $\sum_k(\boldsymbol{i} = \boldsymbol{u}, \boldsymbol{v})$.

An NSS has a computational implementation which we called a GNDL [2,3]. The GNDL algorithm constitutes the link between the mathematical notation of the NSS and the computer codification of this operator. As a short example, the

FORTRAN codification of the operator outlined in eq. (1) corresponds to the listing given in Program 1. There, the question marks stand for integer values which depend on a concrete application of the algorithm. The code generates all the $\boldsymbol{i}$ vector forms and, for each case, calls for an *Application* routine which depends on the NSS operator parameters.

2.2. TAYLOR SERIES EXPANSION OF AN n-VARIABLE FUNCTION

The complete formula for the Taylor series expansion [5] of an n-variable function $f(\boldsymbol{x})$ in the neighbourhood of the point $\boldsymbol{x}_0$ possesses the following peculiar simple structure when using the NSS formalism:

$$f(\boldsymbol{x}) = \sum_{k=0}^{\infty} f^{(k)}(\boldsymbol{x}) , \tag{3}$$

where the following relationship between the sum of the kth order derivatives of the function $f(\boldsymbol{x})$ evaluated at the point $\boldsymbol{x}_0$ and the kth perturbation correction has been taken into account:

$$f^{(k)}(\boldsymbol{x}) = (k!)^{-1} \sum_k (\boldsymbol{i} = \mathbf{1}, n\mathbf{1}) \Pi^{(k)}(\boldsymbol{i}, \boldsymbol{x} - \boldsymbol{x}_0) f^{k)}(\boldsymbol{i}) , \tag{4}$$

where

$$f^{k)}(\boldsymbol{i}) = \partial^{(k)}(\boldsymbol{i})[f(\boldsymbol{x}_0)] , \tag{5}$$

where the $\Pi^{(k)}(\boldsymbol{i}, \boldsymbol{z})$ terms appearing in eq. (4) are defined by means of the following product:

$$\Pi^{(k)}(\boldsymbol{i}, \boldsymbol{z}) = \prod_{j=1}^{k} z_{ij} , \quad k \neq 0 \quad \wedge \quad \Pi^{(0)}(\boldsymbol{i}, \boldsymbol{z}) = 1 . \tag{6}$$

Also, the $\partial^{(k)}(\boldsymbol{i})[f(\boldsymbol{x}_0)]$ expression in eq. (5) depends on the high order partial derivative operators, acting first over the function $f(\boldsymbol{x})$ and then evaluated at the point $\boldsymbol{x}_0$. The differential operators can be defined in the same manner as the terms appearing eq. (6), but using as a second argument the nabla vector, that is,

$$\partial^{(k)}(\boldsymbol{i}) = \Pi^{(k)}(\boldsymbol{i}, \nabla), \quad k \neq 0 \quad \wedge \quad \partial^{(0)}(\boldsymbol{i}) = \boldsymbol{I} . \tag{7}$$

Expression (3) is very useful in the sense that one can control the series truncation. This is so because the parameter k gives the order of the derivatives appearing in the expansion.

Here, this formulation will be used to deal with a generalized RSPT formalism. The study presented here includes the framework of multiple perturbations as in the earlier double perturbations treatment of Dalgarno [6a] and Fu-Tai Tuan [6b,c] or those discussed recently by Kutzelnigg [6d].

3. Generalized matrix perturbation theory (MPT)

3.1. PERTURBATION HAMILTONIAN AND TAYLOR SERIES

The goal is to solve the secular equation in the matrix form,

$$\boldsymbol{H}(\boldsymbol{x})\boldsymbol{V}(\boldsymbol{x}) = \boldsymbol{V}(\boldsymbol{x})\boldsymbol{E}(\boldsymbol{x}), \tag{8}$$

where all the involved matrices depend on n variables, collected in the vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$, and where $\boldsymbol{H}(\boldsymbol{x})$ is Hermitian; so the eigenvector matrix $\boldsymbol{V}(\boldsymbol{x})$, being unitary, satisfies

$$\boldsymbol{V}^{+}(\boldsymbol{x})\boldsymbol{V}(\boldsymbol{x}) = \boldsymbol{V}(\boldsymbol{x})\boldsymbol{V}^{+}(\boldsymbol{x}) = \boldsymbol{I} \tag{9}$$

and $\boldsymbol{E}(\boldsymbol{x})$ is a diagonal real matrix.

Using the Taylor series expansion (3) for the Hamiltonian and expanding it around the point $\boldsymbol{x}_0 = \boldsymbol{0}$, it can be written as

$$\boldsymbol{H}(\boldsymbol{x}) = \sum_{k=0}^{\infty} \boldsymbol{H}^{(k)}(\boldsymbol{x}), \tag{10}$$

where the following term has also been defined:

$$\boldsymbol{H}^{(k)}(\boldsymbol{x}) = (k!)^{-1} \textstyle\sum_k (\boldsymbol{i} = \boldsymbol{1}, n\boldsymbol{1}) \Pi^{(k)}(\boldsymbol{i}, \boldsymbol{x}) \boldsymbol{H}^{k)}(\boldsymbol{i}), \tag{11}$$

with

$$\boldsymbol{H}^{k)}(\boldsymbol{i}) = \partial^{(k)}(\boldsymbol{i})[\boldsymbol{H}(\boldsymbol{0})], \tag{12}$$

and $\Pi^{(k)}(\boldsymbol{i}, \boldsymbol{x})$, $\partial^{(k)}(\boldsymbol{i})$ have the same meanings as in eqs. (6) and (7), respectively.

Expressions similar to eq. (10) can be given for the matrices $\boldsymbol{V}(\boldsymbol{x})$ and $\boldsymbol{E}(\boldsymbol{x})$.

In this manner, once the perturbation corrections are known, it is easily possible to compute the derivatives of the matrices $\boldsymbol{V}(\boldsymbol{x})$ and $\boldsymbol{E}(\boldsymbol{x})$. Therefore, the RSPT can be directly related to the computation of derivatives [7]. This feature can be applied to several quantum chemical topics related to Taylor expansions as the ones outlined in ref. [8].

3.2. PT IN A MATRIX FORM

Supposing the matrix derivatives $\{\boldsymbol{H}^{(k)}(\boldsymbol{x})\}$ and the $\boldsymbol{V}^{(0)} = \boldsymbol{V}(\boldsymbol{0})$ and $\boldsymbol{E}^{(0)} = \boldsymbol{E}(\boldsymbol{0})$ matrices are known, as well as the following equation satisfied:

$$\boldsymbol{H}^{(0)}\boldsymbol{V}^{(0)} = \boldsymbol{V}^{(0)}\boldsymbol{E}^{(0)}, \tag{13}$$

where

$$\boldsymbol{V}^{(0)+}\boldsymbol{V}^{(0)} = \boldsymbol{V}^{(0)}\boldsymbol{V}^{(0)+} = \boldsymbol{I}, \tag{14}$$

then, combining eqs. (8) and (10), with the Taylor expansions of $\boldsymbol{V}(\boldsymbol{x})$ and $\boldsymbol{E}(\boldsymbol{x})$ the set of nth order equations is obtained:

$$\sum_{p=0}^{n} \boldsymbol{H}^{(p)}(x)\boldsymbol{V}^{(n-p)}(x) = \sum_{p=0}^{n} \boldsymbol{V}^{(n-p)}(x)\boldsymbol{E}^{(p)}(x), \quad n \geqslant 1 . \tag{15}$$

A linear transformation, $\boldsymbol{Z}^{(n)}(x)$, from the unperturbed vector matrix to the perturbed ones can be envisaged:

$$\boldsymbol{V}^{(n)}(x) = \boldsymbol{V}^{(0)}\boldsymbol{Z}^{(n)}(x) , \tag{16}$$

or using eq. (14),

$$\boldsymbol{V}^{(0)+}\boldsymbol{V}^{(n)}(x) = \boldsymbol{Z}^{(n)}(x) , \tag{17}$$

where the Taylor expansion of $\boldsymbol{Z}(x)$ has been defined as

$$\boldsymbol{Z}(x) = \sum_{k=0}^{\infty} \boldsymbol{Z}^{(k)}(x) , \tag{18}$$

and the following expression holds:

$$\boldsymbol{V}(x) = \boldsymbol{V}^{(0)}\boldsymbol{Z}(x) . \tag{19}$$

From (17) and (14) it follows that $\boldsymbol{Z}^{(0)}(x) = \boldsymbol{Z}(\boldsymbol{0}) = \boldsymbol{I}$. Without loss of generality, a correction vector of any order can be expanded as a linear combination of the unperturbed ones except those related to the same eigenvector column. Then, the matrices $\boldsymbol{Z}^{(n)}(x)$ should bear a null diagonal for $n \geqslant 1$.

In this manner, the role of $\boldsymbol{Z}^{(n)}(x)$ matrices is similar to the Hirschfelder and Silverstone definition of resolvent operators [9].

Equation (15) can be multiplied on the left by $\boldsymbol{V}^{(0)+}$ and the following expression is obtained:

$$\begin{aligned} \boldsymbol{Q}^{(n)}(x) &= [\boldsymbol{E}^{(0)}, \boldsymbol{Z}^{(n)}(x)] \\ &= \sum_{p=1}^{n} (\boldsymbol{Z}^{(n-p)}(x)\boldsymbol{E}^{(p)}(x) - \boldsymbol{J}^{(p)}(x)\boldsymbol{Z}^{(n-p)}(x)), \quad n \geqslant 1 , \end{aligned} \tag{20}$$

where $\boldsymbol{Q}^{(n)}(x)$ is a zero-diagonal matrix and the $\{\boldsymbol{J}^{(p)}(x)\}$ matrix collection is defined as

$$\boldsymbol{J}^{(p)}(x) = \boldsymbol{V}^{(0)+}\boldsymbol{H}^{(p)}(x)\boldsymbol{V}^{(0)} , \tag{21}$$

the equivalent matrix set to the pth order perturbation Hamiltonians throughout the matrix $\boldsymbol{V}^{(0)}$.

Because of the nature of $\boldsymbol{Z}^{(n)}(x)$ matrices, it follows from eq. (20) that

$$\begin{aligned} \boldsymbol{E}^{(n)}(x) &= \operatorname{diag}\left\{ \sum_{p=1}^{n} \boldsymbol{J}^{(p)}(x)\boldsymbol{Z}^{(n-p)}(x) \right\} \\ &= \operatorname{diag}\left\{ \boldsymbol{V}^{(0)+} \sum_{p=1}^{n} \boldsymbol{H}^{(p)}(x)\boldsymbol{V}^{(n-p)}(x) \right\} . \end{aligned} \tag{22}$$

Equation (20) allows the computation of the $\boldsymbol{Q}^{(n)}(x)$ matrix involving $\boldsymbol{Z}^{(p)}(x)$ matrices of orders from 0 up to $n-1$. In this manner, once $\boldsymbol{Q}^{(n)}(x)$ is known, it is possible to compute the elements of the $\boldsymbol{Z}^{(n)}(x)$ matrix using

$$z_{ij}^{(n)}(x) = q_{ij}^{(n)}(x)/(e_{ii}^{(0)} - e_{jj}^{(0)}), \quad \forall i \neq j \quad \wedge \quad z_{ii}^{(n)}(x) = 0\,, \tag{23}$$

where $e_{ii}^{(0)}$ are the diagonal elements of the $\boldsymbol{E}^{(0)}$ matrix assuming a non-degenerate spectral form for $\boldsymbol{H}^{(0)}$.

Therefore, it is possible to compute all the energy corrections, iterating over eqs. (22), (20) and (23) in this order. If needed, eq. (16) can provide the vector corrections.

From eq. (20), it can be deduced that $\boldsymbol{Q}^{(1)}(x)$ is a symmetric matrix, then, from eq. (23), $\boldsymbol{Z}^{(1)}(x)$ appears as a skew-symmetric matrix.

3.3. APPLICATION TO DEGENERATE SYSTEMS

Degenerate systems can be treated using a non-degenerate framework such as the one previously described. The present recipe can be found in ref. [10], transforming the perturbed system by simultaneously adding and subtracting a matrix $\boldsymbol{M}(x)$. The perturbed problem becomes

$$\boldsymbol{H}(x) = (\boldsymbol{H}^{(0)}(x) + \boldsymbol{M}(x)) + \left(\sum_{k=1}^{\infty} \boldsymbol{H}^{(k)}(x) - \boldsymbol{M}(x)\right), \tag{24}$$

and this is equivalent to redefining the unperturbed system as

$$\boldsymbol{H}^{(0)}(x)' = \boldsymbol{H}^{(0)}(x) + \boldsymbol{M}(x)\,, \tag{25}$$

compensating this sum in the perturbation. It is possible to chose $\boldsymbol{M}(x)$ in a convenient form which allows the erasure of degeneracies. This can be achieved by defining the matrix $\boldsymbol{M}(x)$ as the spectral decomposition:

$$\boldsymbol{M}(x) = \sum_{p} \epsilon_p \boldsymbol{P}_p^{(0)}(x)\,, \tag{26}$$

where every ϵ_p is a small arbitrary number and $\boldsymbol{P}_p^{(0)}(x)$ is a projector associated to the pth eigenvector of the unperturbed system $\boldsymbol{H}^{(0)}(x)$. It is easy to show that this choice for the $\boldsymbol{M}(x)$ matrix converts the new unperturbed system (25) in such a way that the eigenvectors are kept invariant with respect to the original system, $\boldsymbol{H}^{(0)}(x)$, and the set of eigenvalues $\{e_{pp}^{(0)}\}$ transforms to the set $\{e_{pp}^{(0)} + \epsilon_p\}$. The eigenvalue shifting allows the overriding of degeneracies, making possible the use of the non-degenerate PT formalism to the new defined system.

Some numerical tests have been done in our laboratory showing this procedure is valid. Nevertheless, the set of $\{\epsilon_p\}$ shift values must be chosen carefully and some

particular cases may present numerical instabilities making the procedure difficult, but this is perhaps preferable to the usual complex formalism involving degenerate PT. This can be made even clearer by consulting Hirschfelder and Certain [11].

4. Generalized finite order matrix perturbation theory (FOMPT)

It is possible to truncate the series (10) up to the mth term. So, it is assumed that

$$\boldsymbol{H}^{(k)}(\boldsymbol{x}) = \boldsymbol{0}, \quad \forall k > m, \tag{27}$$

and, the expression for the Taylor expansion of the Hamiltonian matrix reads

$$\boldsymbol{H}(\boldsymbol{x}) = \sum_{k=0}^{m} \boldsymbol{H}^{(k)}(\boldsymbol{x}); \tag{28}$$

in this manner, the $\boldsymbol{J}^{(p)}(\boldsymbol{x})$ matrices, as defined in eq. (21), vanish for $p > m$.

In this case, the counterpart of eqs. (20) and (22) is

$$\boldsymbol{Q}^{(n)}(\boldsymbol{x}) = \sum_{p=1}^{n} \boldsymbol{Z}^{(n-p)}(\boldsymbol{x}) \boldsymbol{E}^{(p)}(\boldsymbol{x}) - \sum_{p=1}^{\min(m,n)} \boldsymbol{J}^{(p)}(\boldsymbol{x}) \boldsymbol{Z}^{(n-p)}(\boldsymbol{x}), \quad n \geqslant 1, \tag{29}$$

and

$$\begin{aligned} \boldsymbol{E}^{(n)}(\boldsymbol{x}) &= \operatorname{diag}\left\{ \sum_{p=1}^{\min(m,n)} \boldsymbol{J}^{(p)}(\boldsymbol{x}) \boldsymbol{Z}^{(n-p)}(\boldsymbol{x}) \right\} \\ &= \operatorname{diag}\left\{ \boldsymbol{V}^{(0)+} \sum_{p=1}^{\min(m,n)} \boldsymbol{H}^{(p)}(\boldsymbol{x}) \boldsymbol{V}^{(n-p)}(\boldsymbol{x}) \right\}, \end{aligned} \tag{30}$$

respectively.

5. Wigner theorem for the generalized first order MPT

A particular case of the FOMPT is reached when one truncates the sum (28) for $m = 1$. Then, one is dealing with the first order MPT. In this case, starting from eq. (30), using eq. (27), eq. (15) for $n = 1$ and transposing the involved matrices, the following result is obtained:

$$\begin{aligned} \boldsymbol{E}^{(n)}(\boldsymbol{x}) = &- \operatorname{diag}\{ \boldsymbol{V}^{(1)}(\boldsymbol{x})^{+} \boldsymbol{H}^{(0)} \boldsymbol{V}^{(n-1)}(\boldsymbol{x}) \} \\ &+ \operatorname{diag}\left\{ \sum_{p=0}^{1} \boldsymbol{V}^{(n-1)}(\boldsymbol{x})^{+} \boldsymbol{V}^{(1-p)}(\boldsymbol{x}) \boldsymbol{E}^{(p)}(\boldsymbol{x}) \right\}. \end{aligned} \tag{31}$$

This process can be repeated over the first term of eq. (31) using eq. (15) for n substituted by the values: $\{n-k, k+1\}$ $(k=1,m)$. The following expression is obtained:

$$\begin{aligned} \boldsymbol{E}^{(n)}(\boldsymbol{x}) = & -\operatorname{diag}\{\boldsymbol{V}^{(m)}(\boldsymbol{x})^{+}\boldsymbol{H}^{(0)}\boldsymbol{V}^{(m)}(\boldsymbol{x})\} \\ & +\operatorname{diag}\left\{\sum_{k=1}^{m}\sum_{p=0}^{k}\boldsymbol{V}^{(n-k)}(\boldsymbol{x})^{+}\boldsymbol{V}^{(k-p)}(\boldsymbol{x})\boldsymbol{E}^{(p)}(\boldsymbol{x})\right\} \\ & -\operatorname{diag}\left\{\sum_{k=1}^{m-1}\sum_{p=0}^{n-k}\boldsymbol{V}^{(n-k-p)}(\boldsymbol{x})^{+}\boldsymbol{V}^{(k)}(\boldsymbol{x})\boldsymbol{E}^{(p)}(\boldsymbol{x})\right\}, \end{aligned} \tag{32}$$

where n is considered even and $m = n/2$. The invariance upon commutation of the diagonal elements of a product between a diagonal matrix and an arbitrary one has been also used.

Induction can prove that terms involving vector corrections of order greater than m vanish in eq. (32). In this manner, the expression for the nth order energy correction involves corrections to the vectors up to the order $n/2$ only:

$$\begin{aligned} \boldsymbol{E}^{(n)}(\boldsymbol{x}) = & -\operatorname{diag}\{\boldsymbol{V}^{(m)+}(\boldsymbol{x})\boldsymbol{H}^{(0)}\boldsymbol{V}^{(m)}(\boldsymbol{x})\} \\ & +\operatorname{diag}\left\{\sum_{p=0}^{m}\boldsymbol{V}^{(m)+}(\boldsymbol{x})\boldsymbol{V}^{(m-p)}(\boldsymbol{x})\boldsymbol{E}^{(p)}(\boldsymbol{x})\right\} \\ & -\operatorname{diag}\left\{\sum_{k=1}^{m-1}\sum_{p=m-k}^{n-k}\boldsymbol{V}^{(n-k-p)+}(\boldsymbol{x})\boldsymbol{V}^{(k)}(\boldsymbol{x})\boldsymbol{E}^{(p)}(\boldsymbol{x})\right\}. \end{aligned} \tag{33}$$

A similar and straightforward result can be obtained when n is odd. In this case, eigenvector corrections up to order $(n-1)/2$ are needed to evaluate nth eigenvalue corrections.

6. Monodimensional case

A particular case of the general formalism outlined in section 3 is obtained when the monodimensional framework is envisaged. Then, the $\boldsymbol{x}$ vector becomes a scalar: x. One can proceed in the same manner as in the general theory in order to derive the PT equations. The main differences are such that eq. (11) becomes

$$\boldsymbol{H}^{(k)}(x) = (k!)^{-1}x^{k}\frac{d^{k}}{dx^{k}}\boldsymbol{H}(x)\Big|_{x=0}, \tag{34}$$

and the term x^k is a common factor on both sides of eq. (15); so it is no longer necessary. The nth order equation now reads

$$\sum_{p=0}^{n}\boldsymbol{H}^{(p)}\boldsymbol{V}^{(n-p)} = \sum_{p=0}^{n}\boldsymbol{V}^{(n-p)}\boldsymbol{E}^{(p)}, \quad n\geqslant 1, \tag{35}$$

where in this case, the constant matrix has been defined:

$$\boldsymbol{H}^{(k)} = x^{-k}\boldsymbol{H}^{(k)}(x) = (k!)^{-1}\frac{d^k}{dx^k}\boldsymbol{H}(x)\Big|_{x=0}, \tag{36}$$

and similar expressions hold for $\boldsymbol{V}^{(k)}$, $\boldsymbol{E}^{(k)}$ and $\boldsymbol{Z}^{(k)}$ matrices.

The expression for the nth order energy correction is

$$\boldsymbol{E}^{(n)} = \mathrm{diag}\left\{\sum_{p=1}^{n}\boldsymbol{J}^{(p)}\boldsymbol{Z}^{(n-p)}\right\} = \mathrm{diag}\left\{\mathrm{V}^{(0)}+\sum_{p=1}^{n}\boldsymbol{H}^{(p)}\boldsymbol{V}^{(n-p)}\right\}, \tag{37}$$

which is the counterpart of eq. (22). The companions of eqs. (20) and (23) are trivially defined.

The usual RSPT [12] scheme in the matrix form is nothing else but a particular case of the formalism outlined above. Series (28) is truncated using $m = 1$ and, thus, eq. (28) is transformed into the monodimensional case. The expression for the Taylor expansion of the $\boldsymbol{H}(x)$ matrix takes the following well-known form:

$$\boldsymbol{H}(x) = \boldsymbol{H}^{(0)} + x\boldsymbol{H}^{(1)}, \tag{38}$$

and the counterpart of eqs. (29) and (30) becomes

$$\boldsymbol{Q}^{(n)} = \sum_{p=1}^{n}\boldsymbol{Z}^{(n-p)}\boldsymbol{E}^{(p)} - \boldsymbol{J}^{(1)}\boldsymbol{Z}^{(n-1)}, \quad n \geqslant 1, \tag{39}$$

and

$$\boldsymbol{E}^{(n)} = \mathrm{diag}\{\boldsymbol{J}^{(1)}\boldsymbol{Z}^{(n-1)}\} = \mathrm{diag}\{\boldsymbol{V}^{(0)}+\boldsymbol{H}^{(1)}\boldsymbol{V}^{(n-1)}\}, \tag{40}$$

respectively.

7. Conclusions

A general RSPT framework in the matrix form allowing a perturbation matrix series, useful in any eigenvalue occurrence, has been described. The connection with Taylor series expansions has been made at all levels. The result is a simple reliable set of algorithms involving matrix operations and allowing automatized calculation of eigenvalues and eigenvector corrections.

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