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Asymptotics of eigenvalues and eigenvectors of some infinite three-diagonal matrices

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Abstract. We consider the eigenvalue problem for an infinite three-diagonal matrix whose main diagonal is a sequence tending to infinity. We derive asymptotic expansions for the eigenvalues and eigenvectors. The small parameter of the asymptotics is determined by quotient of second-diagonal elements to the differences between the main-diagonal elements. Some applications to molecular spectroscopy are considered.

1. Introduction

1.1. Motivation: molecular physics

The Schrödinger equation is one of the most important concepts in modern physics and chemistry, as well to quantum computing. At the same time there exists only a small set of potentials (as a rule, one-dimensional) which allow exact solutions of the corresponding Schrödinger equations [1]. The set of exactly solvable two- and three-dimensional non-central potentials is much smaller [2]. Therefore searching for exactly solvable Schrödinger equations with non-central potentials is an important problem.

One of exactly solvable three-dimensional Schrödinger equations with non-central potential describes one-electron model of a highly excited (Rydelberg) molecule [3–5] or dipole-bound anion [6, 7]. In this model implies that the molecular is a source of central potential, $U(r)$ and non-central potential, $V(r, \vartheta)$, where $r, \vartheta, \varphi$ are the polar coordinates characterizing the position of electron with respect to the center of charge of the molecular core, local $z$ axis being directed along the core dipole moment vector, $\vec{\mu}$. Hence the Schrödinger equation for the Rydberg electron has the following form (atomic units are used henceforward):

$$H\Psi = E\Psi, \quad H = T_{el} + U(r) + V(r, \vartheta),$$

where the kinetic energy operator

$$T_{el} = -\frac{\Delta}{2} = -\frac{1}{2r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{\vec{l}^2}{2r^2}$$

is expressed in terms of the electron’s squared orbital momentum operator, $\vec{l}^2$, which, in turn, is proportional to the Legendrian (angular part of the Laplacian) operator:

$$\vec{l}^2 = -\Delta_{\vartheta,\varphi} = -\frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left( \sin \vartheta \frac{\partial}{\partial \vartheta} \right) - \frac{1}{\sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2}.$$


For the point dipole potential

\[ V(r, \vartheta) = -\frac{(\vec{\mu} \cdot \vec{r})}{r^3} = -\frac{\mu \cos \vartheta}{r^2}, \]

one can separate the variables in (1). Indeed, assuming \( \Psi(r, \vartheta, \varphi, \eta) \)
we obtain the following eigenvalue problem for the angular function \( Z \):

\[ \left( \hat{L}^2 - 2\mu \cos \vartheta \right) Z = \eta Z, \quad Z(\vartheta, \varphi + 2\pi) = Z(\vartheta, \varphi), \quad |Z(\vartheta, \varphi)| < \infty \quad \text{when} \quad |\cos \vartheta| = 1. \quad (5) \]

The eigenfunction of the problem (5), so called dipole-spherical functions, play an important role in molecular physics. It seems that the dipole-spherical angular functions mentioned above were used for the first time by Debye [8] in the analysis of the problem of the Stark effect for a symmetric rotator. Zon [3] and Watson [9] used these functions for the description of the Rydberg states of polar molecules. Dipole-spherical functions appear in the theory of electron photodetachment from atomic anions in a strong field [10] as well as in theoretical models of dipole-bound anion photodetachment [6] and collisions [7]. Dipole-spherical functions are convenient basis for calculation of dynamic polarizability of polar molecules [4].

At \( \mu = 0 \) the dipole-spherical functions are reduced to the well-known spherical functions \( Y_{\ell\lambda}(\vartheta, \varphi) \) and the eigenvalues \( \eta_{\ell} = \ell(\ell + 1) \). The orbital quantum number \( \ell = 0, 1, 2 \ldots \) and the magnetic quantum number \( \lambda = -\ell, -\ell + 1, \ldots, \ell \) are integers.

At \( \mu \neq 0 \) it is natural to expand the dipole-spherical functions (5) over the spherical harmonics:

\[ Z(\vartheta, \varphi) = \sum_{l=0}^{\infty} x_{\ell\lambda} Y_{\ell\lambda}(\vartheta, \varphi). \quad (6) \]

After substituting Eq. (6) into the angular Schrödinger equation (5) we obtain a recurrence relation (or, mathematically, a difference equation) of the type (7a) below for the coefficients \( x_{\ell\lambda, l}[\mu] \) which are responsible for all the properties of the dipole-spherical functions.

Recurrence relations of the type (6) occur, e.g. in analyzing the spectrum of asymmetric top [11, § 18] or a symmetric top in an external field [12]. In the latter case the problem, the three-diagonal matrix of the recurrence relation (7a) has constant (i.e. independent of the representation index \( l = l \)) elements, while in the former case the matrix elements are weakly dependent on \( l \), that corresponds to the semiclassical approximation in \( l \)-representation.

1.2. Mathematical formulation of the problem

Consider a second-order difference equation

\[ -2\mu\beta_l x_{l-1} + 2\mu\gamma_l x_l - 2\mu\alpha_{l+1} x_{l+1} = \eta x_l, \quad l = l_0, l_0 + 1, \ldots, \quad (7a) \]

with the boundary conditions

\[ x_{l_0 - 1} = 0, \quad \sum_{l=l_0}^{+\infty} |x_l|^2 < \infty. \quad (7b) \]

Let \( \gamma_l \) be mutually distinct and grow rapidly enough:

\[ l \neq l' \Rightarrow \gamma_l \neq \gamma_{l'}; \quad \gamma_l \rightarrow \infty, \quad \beta_{l+1} \gamma_l = O(\gamma_l), \quad \frac{\alpha_{l+1}}{\gamma_l} = O(\gamma_l) \quad \text{at} \ l \rightarrow \infty. \quad (8) \]

We will treat Eqs. (7) as an eigenvalue, \( \eta \), and eigenvector, \( \vec{x} = \{ x_l \} \), problem for the operator

\[ (Q\vec{x})_l = (Q[\mu]\vec{x})_l = \sum_{l'=l_0}^{\infty} q_{l,l'} x_{l'}, \quad l = l_0, l_0 + 1, \ldots, \quad (9) \]
The operator defined by the infinite three-diagonal matrix \( Q \) with the elements

\[
q_{l',l} = -2\mu \beta_l \delta_{l-1,l'} + \gamma_l \delta_{l,l'} - 2\mu \alpha_l \delta_{l+1,l'}, \quad l = l_0, l_0 + 1, \ldots
\]  

(10)

The Kronecker delta \( \delta_{i,j} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \) is used henceforward.

To the authors’ knowledge [13, Eq. (1.4.14), p. 14], all orthogonal polynomials \( x_l(\eta) \) of a continuous variable \( \eta \) satisfy some difference equation of the type (7a) treated as a recurrence relation without initial/boundary conditions in the discrete variable \( l \). The classical orthogonal polynomials of discrete variable \( l \) [13, tables 2.1–2.3] satisfy a recurrence relation (7a), provided \( \alpha_l, \beta_l, \gamma_l = O(l^2) \) at \( l \to \infty \), that does not match the last requirement (8). The case \( \gamma_l = \text{const} \cdot l^2 \) is close to the recurrence relation for the Fourier coefficients of the Mathieu functions [14, sec. 16.2].

This work studies the dependence of eigenvalues and eigenvectors of infinite three-diagonal matrices (10) on the parameter \( \mu \). For the eigenvalues and eigenvectors we obtain simple approximate analytic expressions which are their asymptotic estimates at \( \mu \to 0 \). We also prove some symmetry properties of eigenvalues and eigenvectors related to their behaviour with respect to the substitution \( \mu \to -\mu \). A continuous fraction representation is given for the eigenvectors. The efficiency of the proposed approximation is demonstrated on the example of Fourier coefficients of the dipole-spherical functions which has wide application in molecular spectroscopy.

2. Methods

2.1. Properties of the operator \( Q \)

According to the boundary conditions, we shall treat the operator \( Q \) to act in the \( l_2 = l_2([l_0, \infty)) \) space and to have the domain of definition \( D(\mathcal{Q}) = \{ x : \mathcal{Q}x \in l_2 \} \).

**Proposition 1.** The domain of the operator \( \mathcal{Q}[\mu] \), which is defined by the formula (9), consists of the sequences \( x \in l_2 \), such that \( \sum_{l=l_0}^{\infty} |\gamma_l|^2 |x_l|^2 < \infty \).

**Proposition 2.** The operator \( \mathcal{Q}[\mu] \), defined by the formula (9), is closed.

**Proof.** Let \( \bar{x}_k = (x_{k,l_0}, x_{k,l_0+1}, \ldots) \in D(\mathcal{Q}), \mathcal{Q}\bar{x}_k = \bar{y}_k = (y_{k,l_0}, y_{k,l_0+1}, \ldots) \) and \( \bar{x}_k \) converges in norm to \( \bar{x}_s = (x_{s,l_0}, x_{s,l_0+1}, \ldots) \in l_2 \) and \( \bar{y}_k \) converges in norm to \( \bar{y}_s = (y_{s,l_0}, y_{s,l_0+1}, \ldots) \in l_2 \). Let us show that \( \bar{x}_s \in D(\mathcal{Q}) \) and \( \mathcal{Q}\bar{x}_s = \bar{y}_s \).

The convergence of \( \bar{x}_k \) to \( \bar{x}_s \) and \( \bar{y}_k \) to \( \bar{y}_s \) in norm implies the pointwise convergence i.e. \( x_{k,l} \to x_{s,l} \) when \( k \to \infty \) for all \( l = l_0, l_0 + 1, \ldots \) and, similarly, for \( y_k \). Then one can pass to the limit in the following equations:

\[
q_{l-1,l} x_{k,l-1} + q_{l,l} x_{k,l} + q_{l+1,l} x_{k,l+1} = y_{k,l}, \quad l = l_0, l_0 + 1, \ldots
\]

that results in

\[
q_{l-1,l} x_{s,l-1} + q_{l,l} x_{s,l} + q_{l+1,l} x_{s,l+1} = y_{s,l}, \quad l = l_0, l_0 + 1, \ldots
\]

This means that \( \bar{x}_s \in D(\mathcal{Q}) \) and \( \mathcal{Q}\bar{x}_s = \bar{y}_s \).

It is easy to see that the family \( \mathcal{Q}[\mu], \mu \in \mathbb{C} \) is holomorphic in a sense of [15, ch. VII, § 1.2]. The operator \( \mathcal{Q}[0] \) has compact resolvent because of \( \gamma_l \to \infty \) at \( l \to \infty \). Therefore [15, ch. VII, theor. 2.4], the resolvent of the operator \( \mathcal{Q}[\mu] \) is compact for all \( \mu \in \mathbb{C} \).

**Theorem 3.** The spectrum of the operator \( \mathcal{Q}[\mu] \) consists entirely of countable number of isolated eigenvalues with finite multiplicities for all \( \mu \in \mathbb{C} \).
Theorem 4. For all \( n \in \mathbb{N} \) there exists \( \varepsilon_n > 0 \) such that the eigenvalue \( \eta_n[\mu] \) remains isolated at \( |\mu| < \varepsilon \) and the eigenvalues \( \eta_n[\mu] \) and the corresponding eigenprojections depend on \( \mu \) holomorphically.

Proof. Follows from [15, ch. VII, theors. 1.7 and 1.8].

2.2. The behavior of the eigenvalues and eigenvectors under the replacement \( \mu \to -\mu \)

Theorem 5. The replacement \( \mu \to -\mu \) does not change the spectrum of the operator \( Q[\mu] \), while the components of its eigen-sequences are changed according to \( x_l[-\mu] = (-1)^l x_l[\mu] \).

Proof. Consider the operator \( T : l_2([0, \infty]) \to l_2([0, \infty]) \), which acts according to \( (Tx)_l = (-1)^l x_l \); its matrix is clearly consist of the elements \( t_{l,l'} = (-1)^l \gamma_{l,l'} \). Consider now the operator \( Q' = T^{-1}Q'T \), which is similar to the operator \( Q \). The operator \( Q' \) is obviously orthogonal and is defined by the matrix \( Q' \) whose elements are

\[
q'_{l,l'} = (T^{-1}Q'T)_{l,l'} = (-1)^l \delta_{l,i} q_i,j (-1)^j \delta_{j,l'} = (-1)^{l-l'} q_{l,l'}.
\]

The standard summation over repeated indices is assumed in (12). It is easy to see that the transition from \( Q \) to \( Q' \) is brought to the change of signs in the off-diagonal elements, that is equivalent to \( \mu \to -\mu \) replacement. Therefore, \( Q[-\mu] = Q'[\mu] \). This fact, together with the invariance of the spectrum under the similarity transformations, result in the identity of the spectra of the operators \( Q[-\mu] \) and \( Q[\mu] \). To finish the proof, we note that it follows from \( Q'T^{-1} = T^{-1}Q \) that the eigen-sequences, \( x_n \) and \( x'_n \), of the operators \( Q \) and \( Q' \) are related by

\[
x'_n,l[-\mu] = (-1)^n x_n,l[\mu].
\]

Remark 1. We are focused here on the dependence of the eigen-sequences, \( x_n[\mu] \), on the parameter \( \mu \), but the eigen-sequences are defined up to an arbitrary scale factor. It is convenient to choose this factor in such a way that the dependence on \( \mu \) would be continuous in norm and that we would have the eigen-sequence (11) at \( \mu = 0 \) holding the identity \( x_l[-\mu] = (-1)^l x_l[\mu] \) from Theorem 5. These conditions imply the following relationship:

\[
x_n,l[-\mu] = (-1)^{n-l} x_n,l[\mu].
\]

2.3. Continuous fraction representation of the eigenvalues

Theorem 6. If all the off-diagonal elements \( \alpha_l, \beta_l \) are nonzero, then the eigenvalues \( \eta = \eta_n \) of the operator \( Q \) satisfy the following equation:

\[
\gamma_0 - \eta = \frac{(2\mu)^2 \alpha_{l_0+1} \beta_{l_0+1}}{\gamma_{l_0+1} - \eta - \frac{(2\mu)^2 \alpha_{l_0+2} \beta_{l_0+2}}{\gamma_{l_0+2} - \eta - \frac{\cdots}{\gamma_{l-1} - \eta - \frac{(2\mu)^2 \alpha_l \beta_l}{\gamma_l - \eta - \cdots}}}}
\]

or, in a short form

\[
\sum_{l=0}^{\infty} \frac{-(2\mu)^2 \alpha_{l+1} \beta_{l+1}}{\gamma_l - \eta} = 0.
\]

Proof. Follows from [15, ch. III, theor. 6.29].

Clearly, the spectrum of the operator \( Q[\mu] \) consists of the in-diagonal elements, \( \gamma_n \), of \( Q \) matrix. Due to the condition \( \gamma_l \neq \gamma_l' \) at \( l \neq l' \), all the eigenspaces of the operator \( Q[0] \) have dimension 1. Let the points of the spectrum of the operator \( Q[0] \) and the corresponding eigen-sequences are enumerated in the natural way:

\[
\eta_n[0] = \gamma_n, \quad x_{n,l}[0] = \delta_{n,l}.
\]

We emphasize that these eigen-sequences \( \ddot{x}_n[0] \) have norm 1.

Proof. Follows from [15, ch. VII, theors. 1.7 and 1.8].

The proof of this theorem is straightforward.
Proof. Denoting the $n$-th eigen-sequence as $\bar{x}_n$, we rewrite Eq. (7a) in the following form:

$$\frac{x_{n,l}}{x_{n,l+1}} = \frac{2\mu\alpha_{l+1}}{\gamma_l - \eta_n - 2\mu\beta_l \frac{x_{n,l-1}}{x_{n,l}}},$$

$$\frac{x_{n,l}}{x_{n,l-1}} = \frac{2\mu\beta_l}{\gamma_l - \eta_n - 2\mu\alpha_{l+1} \frac{x_{n,l+1}}{x_{n,l}}}.$$  \hspace{1cm} (15)

For the initial $l = l_0$ in (15) one should assume $x_{n,l_0-1} = 0$ and/or $\beta_l = 0$:

$$\frac{x_{n,l_0}}{x_{n,l_0+1}} = \frac{2\mu\alpha_{l_0+1}}{\gamma_{l_0} - \eta_n} \Rightarrow \gamma_{l_0} - \eta_n = 2\mu\alpha_{l_0+1} \frac{x_{n,l_0+1}}{x_{n,l_0}}.$$  \hspace{1cm} (16)

Applying (15) recursively, we obtain (16) in the continuous fraction form (14).

The continuous-fraction expansion (14) can be treated as an implicit equation to determine the eigenvalues $\eta[\mu]$. The parameter $\mu$ appears in (14) squared only, that ensures that the eigenvalues $\eta[\mu]$ are even functions of $\mu$.

2.4. Perturbation theory

If we write formal perturbation series for the eigenvectors $\bar{x}_n$ at $\mu \to 0$, then it is easy to see that, for $k > 0$, the first non-vanishing contribution to $x_{n,l}$ has the order of $\mu^k$ and arise at $l = n \pm k$. It can also be seen that

$$\frac{x_{n,l+1}}{x_{n,l}} = o(\mu), \quad l \geq \text{max}(n, l_0 + 1), \quad \text{and} \quad \frac{x_{n,l-1}}{x_{n,l}} = o(\mu), \quad l_0 \leq l \leq n.$$  \hspace{1cm} (17)

By (17) one can neglect the last terms in the denominators of the expressions (15) and write them approximately (we denote this approximation by the PT mark):

$$x_{n,l}^{(PT)} = \begin{cases} \frac{2\mu\alpha_{l+1}}{\gamma_l - \eta_n} x_{n,l+1}^{(PT)}, & l_0 \leq l \leq n, \\ \frac{2\mu\beta_l}{\gamma_l - \eta_n} x_{n,l-1}^{(PT)}, & l \geq \text{max}(n, l_0 + 1). \end{cases}$$ \hspace{1cm} (18)

Some standard calculations result in the following statement.

**Theorem 7.** The eigenvectors in PT-approximation have the following form ($k \geq 0$):

$$x_{n,l \leq n}^{(PT)} = x_{n,n-k}^{(PT)} = \frac{\begin{pmatrix} (2\mu)^k \prod_{s=n-k+1}^{n} \alpha_s \end{pmatrix}}{\prod_{s=n-k}^{n-1} (\gamma_s - \eta_n)}, \quad x_{n,n}^{(PT)} = \frac{(2\mu)^{n-l} \prod_{s=l+1}^{n} \beta_s}{\prod_{s=l}^{n-1} (\gamma_s - \eta_n)},$$

$$x_{n,l \geq n}^{(PT)} = x_{n,n+k}^{(PT)} = \frac{\begin{pmatrix} (2\mu)^k \prod_{s=n+1}^{n+k} \beta_s \end{pmatrix}}{\prod_{s=n+1}^{n+k} (\gamma_s - \eta_n)}, \quad x_{n,n}^{(PT)} = \frac{(2\mu)^{l-n} \prod_{s=n+1}^{l} \beta_s}{\prod_{s=n+1}^{l} (\gamma_s - \eta_n)}.$$  \hspace{1cm} (19a-b)

As usual, all the products in (19) are assumed to equal to unity when the lower bound of the product is greater than its upper bound.
Theorem 8. PT-approximation is the first non-vanishing term of the order of \( \mu^{\left|l-n\right|} \) in the asymptotics of the eigen-sequences:

\[
x_{n,l} = x_{n,l}^{(PT)} + o \left( \mu^{\left|l-n\right|} \right),
\]

(20)

Note that the expressions (19) satisfy the transformation law (13). It is convenient to chose the component \( x_{n,n}^{(PT)} \) as normalizing factor of the vectors (19).

Proposition 9. If

\[
x_{n,n}^{(PT)} = 1,
\]

(21)

then the vectors with the components calculated according to (19), satisfy approximately the orthogonality conditions

\[
\sum_l x_{n',l}^{(PT)*} x_{n''l}^{(PT)} = \delta_{n',n''} \cdot O(1) + \left( 1 - \delta_{n',n''} \right) \cdot O(\mu^{|n'-n''+2|}).
\]

(22)

Now we proceed to the analogous perturbation series for the eigenvalues \( \eta_n \). Multiplying the difference equation (7a) by \( x_{n,l}^{*} \) and summing it over \( l \), using the conditions (22) and (21), we have in PT-approximation (20):

\[
\eta_n = \gamma_n + S_-^{(PT,k)}(\eta_n) + S_+^{(PT,k)}(\eta_n) + o(\mu^k),
\]

(23)

\[
S_-^{(PT,k)}(\eta_n) = (2\mu)^2 \sum_{l=\max(l_0+1,n-k)}^n \frac{\alpha_l \beta_l |x_{n,l}^{(PT)}|^2}{\eta_n - \gamma_{l-1}},
\]

(24)

\[
S_+^{(PT,k)}(\eta_n) = (2\mu)^2 \sum_{l=n}^{n+k} \frac{\alpha_{l+1} \beta_{l+1} |x_{n,l}^{(PT)}|^2}{\eta_n - \gamma_{l+1}}.
\]

(25)

As usual, the sum (24) turns to zero when the lower bound of summation is greater than the lower bound of summation. In particular, \( \forall k > 0 \) \( S_-^{(PT,k)}(\eta_0) = 0 \).

The relationship (23) has a form of an implicit equation for \( \eta_n \). Given that \( S_\pm^{(PT,k)}(\eta) = O(\mu^{2k+2}) \), it would be reasonable to get the asymptotics (of the same order) of this equation. This can be done by different ways which are characterized by different estimates of the residual term, \( o(\mu^{2k+2}) \), of the asymptotics. One of such ways (we denote it as PT0-approximation) consists in using the non-perturbed values \( \eta_n = \gamma_n \) in formulas (19) and (23), i. e. \( S_\pm^{(PT0,k)} = S_\pm^{(PT,k)}(\eta_n = \gamma_n) \). The second way (we denote it as PT-approximation, in analogy with that for the eigen-sequences (19)) consists in using the PT0-estimate for \( \eta_n = \eta_n^{(PT0,k)} \) in formulas (19) and (23).

Theorem 10. (PT0)- and (PT)-approximations for the eigenvalues

\[
\eta_n^{(PT,k)} = \gamma_n + S_-^{(PT,k)}(\eta_n^{(PT0)}) + S_+^{(PT,k)}(\eta_n^{(PT0)}),
\]

(26a)

\[
\eta_n^{(PT0,k)} = \gamma_n + S_-^{(PT0,k)} + S_+^{(PT0,k)}(\eta_n),
\]

(26b)

are their asymptotic estimates of the order of \( 2k + 2 \):

\[
\eta_n = \eta_n^{(PT,k)} + o(\mu^{2k+2}).
\]

(26c)
3. Numerical results and discussion
A disadvantage of the theory presented above is a lack of explicit estimates for accuracy of the asymptotics (20), (22), (26). To illustrate their accuracy, we consider a particular example appearing in molecular spectroscopy.

The Fourier coefficients of dipole-spherical functions (used in theory of Rydberg states in polar molecules [3] and dipole-bound anions [6]), satisfy the recurrence relation (7a) with the following matrix elements (10):

\[
\alpha_l = \beta_l = \left[ \frac{l^2 - \lambda^2}{4l^2 - 1} \right]^{1/2}, \quad \gamma_l = l(l+1); \quad n = \ell. \tag{27}
\]

The parameter \( \mu \) is the dipole moment of the molecular core (in atomic units); \( n = \ell \) is an integer quantum number which enumerates the eigenvalues in order of growth (at constant \( \lambda \)). In the unperturbed case (11), which physically corresponds to the central potential, \( \ell \) is conserved even if \( \lambda \) projection, \( \ell \) quantum number, so \( \ell \) is merely an integer numerator of the eigenvalue series with the same projection, \( \lambda \), of the orbital angular momentum on the dipole moment direction. This projection is conserved even if \( \mu \neq 0 \). From (27) it is natural to assume \( l_0 = |\lambda| \). We emphasize that the notation \( \ell \) for the eigenvalue enumerator should not be mixed with the discrete variable \( l \) (in quantum mechanics, \( l \) is referred to as the index of the representation, while \( n = \ell \) as the index of the state).

Introducing

\[
P_{\ell \lambda, l} = \frac{(\ell + \lambda)!((l - \lambda)!((2\ell - 1))!/(2\ell + 1))!}{(\ell + \lambda)!((l - \lambda)!((2\ell - 1))!/(2\ell + 1))!}, \tag{28}
\]

and inserting the matrix elements (27) into eqns. (19) we obtain for the eigenvectors in PT0-approximation:

\[
x^{(PT0)}_{\ell \lambda, l}[\mu] = \begin{cases} 
(2\mu)^{\ell - l}[P_{\ell \lambda, l}]^{1/2} \frac{(2\ell + 1)!}{(l - \lambda)!((l + l + 1))!}, & l \geq \ell, \\
(2\mu)^{\ell - l}[P_{\ell \lambda, l}]^{-3/2} \frac{(2\ell + 1)!}{(l - \lambda)!((2\ell))!}, & |\lambda| \leq l \leq \ell;
\end{cases} \tag{29}
\]

Using the PT0-approximation (29) in (23) we can make summation in (24,25) up to \( k = \infty \) and express the result in terms of generalized hypergeometric functions:

\[
\eta^{(PT0)}_{\ell \lambda} = \ell(\ell + 1) \tag{30}
\]

\[
+ \frac{\lambda^2 - (\ell + 1)^2}{(2\ell + 1)(2\ell + 2)(2\ell + 3)} 2F_5 \left( \begin{array}{c} 2 + \ell - \lambda, 2 + \ell + \lambda \\ \frac{3}{2} + \ell, \frac{3}{2} + \ell, 2, 2, 2 \ell + 3, 2 \ell + 2 \end{array} \right| \mu^2 \right)
\]

\[
+ \frac{(1 - \delta_{\ell,0})(\ell^2 - \lambda^2)(2\mu)^2}{(2\ell - 1)(2\ell)(2\ell + 1)} 2F_5 \left( \begin{array}{c} 1 - \ell - \lambda, 1 - \ell + \lambda \\ \frac{3}{2} - \ell, \frac{1}{2} - \ell, 2, 1 - 2\ell, -2\ell \end{array} \right| \mu^2 \right).
\]

Here the factor \((1 - \delta_{\ell,0})\) is zero for \( \ell = 0 \) in accord with (24).

In the first non-vanishing approximation in powers of \( \mu \), the hypergeometric functions in (30) turn to unities, that yields the simple expression for the eigenvalues [9]:

\[
\eta_{\ell \lambda} = \begin{cases} 
\ell(\ell + 1) + \frac{2\mu^2[\ell(\ell + 1) - 3\lambda^2]}{\ell(\ell + 1)(2\ell - 1)(2\ell + 3)} + O(\mu^4), & \ell > 0, \\
-\frac{2}{3}\mu^2 + O(\mu^4), & \ell = 0
\end{cases} \tag{31}
\]
The analogous results in (PT)-approximation can also be obtained. To this end, we define so-called quasiorbital momentum \( \tilde{\ell} \) (in (PT0)-approximation) according to \( \tilde{\ell}(\ell + 1) = \eta^{(\text{PT0},k)}_\mu \), and express the the eigenvectors in PT0-approximation:

\[
x^{(\text{PT})}_{\ell\lambda,j}[\mu] = \begin{cases} (2\mu)^{l-\ell} [P_{\ell\lambda,j}]^{1/2} \frac{\Gamma(1 + \ell - \tilde{\ell})\Gamma(2 + \ell + \tilde{\ell})}{\Gamma(1 + l - \tilde{\ell})\Gamma(2 + l + \tilde{\ell})}, & l \geq \ell, \\ (-2\mu)^{l-\ell} [P_{\ell\lambda,j}]^{-1/2} \frac{\Gamma(1 - \ell + \tilde{\ell})\Gamma(1 + l + \tilde{\ell})}{\Gamma(1 - l + \tilde{\ell})\Gamma(1 + l + \tilde{\ell})}, & |\lambda| \leq l \leq \ell. 
\end{cases}
\]  

(32)

Using the PT-approximation (32) in (23) we again make summation in (24,25) up to \( k = \infty \) and express the result in terms of generalized hypergeometric functions:

\[
\eta^{(\text{PT})}_{\ell\lambda} = \ell(\ell + 1) + \frac{[\lambda^2 - (\ell + 1)^2]}{(2\ell + 1)(2\ell + 3)(\ell - \ell + 1)(\ell + \ell + 2)} (2\mu)^2 \\
\times 3F_6 \left( \begin{array}{c} \frac{1}{2} + \ell, \frac{5}{2} + \ell, 2 - \tilde{\ell} + \ell, 1 + \tilde{\ell} + \ell, 2 + \tilde{\ell} + \ell, 3 + \tilde{\ell} + \ell \\ \mu^2 \end{array} \right) \\
+ \frac{(\ell^2 - \lambda^2)(2\mu)^2}{(2\ell - 1)(2\ell + 1)(\ell - \ell + 1)(\ell + \ell)} \\
\times 3F_6 \left( \begin{array}{c} \frac{1}{2} - \ell, \frac{1}{2} - \ell, 2 - \tilde{\ell} - \ell, 1 - \tilde{\ell} - \ell, 1 + \tilde{\ell} - \ell, -\tilde{\ell} - \ell \\ \mu^2 \end{array} \right)
\]  

(33)

Figure 1. Eigenvalues \( \eta_\mu[\mu] \) for \( \ell = 0..3 \). Dotted lines (· · · · · ·) correspond to PT0-approximation (29); dashed lines (− − − −) correspond to PT-approximation (32); solid lines (——) correspond to the numerical solution of the eigenvector problem (7).
Some plots of eigenvalues, $\eta_{n=\ell,\lambda}$, and eigenvectors, $x_{\ell,l}$, (so called $l$-mixing coefficients) as functions of the dipole moment, $\mu$, and index of the representation, $l$ are given in figures 1 and 2 for different $\ell$ and $\lambda$.

It can bee seen from the figures that, at fixed $l$ and $\ell, \lambda$, the accuracy of our analytical approximations is the better the closer to zero are the values of $\mu$. At fixed $\mu$ the accuracy is improved with increase of $l$ and $\ell$, however this improvement depends non-monotonically on the ratio between $\ell$ and $\lambda$). The plots demonstrate good agreement of the above analytical approximations with the numerical results up to $\mu = 7..10$ Debye units that surpass the dipole moments of most of known molecules.

4. Conclusion
This work studies the dependence of eigenvalues and eigenvectors of infinite three-diagonal matrices depending on the parameter $\mu$. For the eigenvalues and eigenvectors we obtain simple approximate analytic expressions which are their asymptotic estimates at $\mu \to 0$. We also prove some symmetry properties of eigenvalues and eigenvectors related to their behaviour with respect to the substitution $\mu \to -\mu$. A continuous fraction representation is given for the eigenvectors. The efficiency of the proposed approximation is demonstrated on the example of Fourier coefficients of the dipole-spherical functions which has wide application in molecular spectroscopy.

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