On the effective secular equation

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Abstract

We show that the effective secular equation proposed several years ago is suitable for estimating the location of the exceptional points of eigenvalue equations. As an illustrative example we choose the well known Mathieu equation.

1 Introduction

Several years ago, Fried and Ezra [1] developed a method for improving the calculation of eigenvalues by means of their perturbation series. The resummation method consists of the reconstruction of an effective secular equation (ESE) that yields better results than the original perturbation series. They applied the approach to the Barbanis Hamiltonian.

Somewhat later, Zheng [2] presented essentially the same approach and applied it to a trivial tridiagonal $3 \times 3$ matrix representation of a toy Hamiltonian operator. It has been shown that both approaches yield the same result on the just mentioned oversimplified model [3]. However, Zheng [4] put forward some unconvincing arguments with the purpose of showing that there are some relevant differences between both methods. In particular, Zheng focused on the fact that the ESE yielded complex eigenvalues for the Barbanis Hamiltonian [1]. Clearly, Zheng overlooked the fact that the anharmonic oscillator chosen by
Fried and Ezra [1] does not exhibit bound states and, consequently, the appearance of complex eigenvalues is not surprising. What is more, Zheng [4] did not attempt to apply his approach to the Barbanis Hamiltonian or to compare his results with those derived by Fernández [3] using the ESE method.

In a later paper, Zheng [5] proposed a most unclear strategy to improve the ESE approach of Fried and Ezra to which he refers, quite pejoratively, as *cockamamie*. Zheng never attempted to test his new approach on a demanding problem and after three papers [2,4,5] he did not go beyond an extremely simple toy model given by a $3 \times 3$ tridiagonal matrix representation of an Hermitian operator. Zheng’s supposed improvement of ESE [5] is based on the determinant of $\frac{E - H_{\text{eff}}(\lambda)}{E - H_0^P}$. Since the operators $H_{\text{eff}}(\lambda)$ and $H_0^P$ are not expected to commute it is not clear whether he means either $(E - H_0^P)^{-1} [E - H_{\text{eff}}(\lambda)]$ or $[E - H_{\text{eff}}(\lambda)] (E - H_0^P)^{-1}$.

As mentioned above, Fried and Ezra [1] applied ESE to the Barbanis Hamiltonian. Unfortunately, this nontrivial problem is not the most suitable one for testing the approach because the perturbation series exhibit zero radius of convergence. On the other hand, the perturbation series for the eigenvalues of the toy problem chosen by Zheng [2] exhibit finite radii of convergence and one can locate the exceptional point closest to origin by means of ESE [3]. In this paper we apply ESE to a nontrivial problem in which the perturbation expansions exhibit finite radii of convergence, the Mathieu equation.

2 The effective secular equation

In this section we develop ESE following the lines of our earlier paper [3] based on Fried and Ezra’s one [1]. Suppose that we want to obtain the solutions to the Schrödinger equation $H \psi_n = E_n \psi_n$, $n = 1, 2, \ldots$, where $H = H_0 + \lambda H_f$. To this end, we apply perturbation theory and obtain partial sums of the form

$$E_n^{[K]} = \sum_{j=0}^{K} E_{n,j} \lambda^j. \quad (1)$$
The ESE is given by

\[
\prod_{n=1}^{N} \left[ W - E_n^{[K]}(\lambda) \right]^{[K]} = W^N + \sum_{j=1}^{N} p_j(\lambda) W^{N-j},
\]

(2)

where \( \{ \ldots \}^{[K]} \) means that we remove any term with \( \lambda^j \) if \( j > K \). The reason is that the accuracy of the results cannot be greater than \( O(\lambda^K) \) determined by the partial sums (1). The eigenvalues \( E_n \) used in this reconstruction are related to the so-called model space, which is finite, and we leave aside the complement space that is not necessarily so. The states in the model space are strongly coupled among themselves and weakly coupled to the states in the complement space. The roots \( W_n(\lambda) \), \( n = 1, 2, \ldots, N \), of the polynomial (2) are expected to be better approximations to the eigenvalues \( E_n(\lambda) \), \( n = 1, 2, \ldots, N \), that the partial sums \( E_n^{[K]}(\lambda) \) used in the construction of the ESE.

3 The Mathieu equation

As an example we choose the Hermitian operator

\[
H = -\frac{d^2}{dx^2} + 2\lambda \cos(2x),
\]

(3)

so that \( H\psi = E\psi \) yields the well known Mathieu equation. We may consider solutions of period \( \pi \) (\( \psi(x + \pi) = \psi(x) \)) and \( 2\pi \) (\( \psi(x + 2\pi) = \psi(x) \)) and each class can be separated into sub classes with even (\( \psi(-x) = \psi(x) \)) and odd (\( \psi(-x) = -\psi(x) \)) eigenfunctions \( \psi(x) \). In a recent paper Amore and Fernández [6] obtained some of the exceptional points for the Mathieu eigenvalue equation quite accurately. Here, we simply try to estimate the exceptional point \( \lambda_p \) closest to origin by means of ESE.

One can easily obtain the perturbation expansions for the eigenvalues of \( H \) by means of well known suitable approaches [7]. For example, the perturbation series for the two lowest eigenvalues of the \( 2\pi \) even subspace are

\[
E_1 = 1 + \lambda - \frac{\lambda^2}{8} - \frac{\lambda^3}{64} - \frac{\lambda^4}{1536} + O(\lambda^5), \\
E_2 = 9 + \frac{\lambda^2}{16} + \frac{\lambda^3}{64} + \frac{13\lambda^4}{20480} + O(\lambda^5),
\]

(4)
and we can obtain as many perturbation corrections as desired. Straightforward
application of ESE as outlined in section 2 with $N = 2$ and increasing values of $K$
enables us to obtain

$$K \quad |\lambda_p| \quad \lambda_p$$

| 10 | 3.769959083 | 1.931394919 ± 3.237638825i |
| 11 | 3.769957228 | 1.931392571 ± 3.237638065i |
| 12 | 3.769957375 | 1.931392656 ± 3.237638186i |
| 13 | 3.769957431 | 1.931392443 ± 3.237638378i |

(5)

It is understood that $E_1(\lambda)$ and $E_2(\lambda)$ coalesce at the exceptional point $\lambda_p$
and the radius of convergence of the series (4) is $|\lambda_p|$. On the other hand,
the application of the discriminant to the secular equation for $H$ in the $2\pi$
even subspace yielded $|\lambda_p| = 3.769957494$ that is accurate to the last digit [6].
We appreciate that ESE enables us to accurately estimate the exceptional point
closest to origin from the perturbation series as suggested by earlier calculations
on the toy model [2, 3].

Zheng [5] stated that “This reconstruction is also inefficient. Even to order
of $\lambda^2$, one has to perform a second-order perturbation calculation for all the
$E_P^P(\lambda)$, and some of these calculations actually are redundant since we have
proved that terms such as those containing $\frac{1}{\epsilon_i - \epsilon_n}$ must offset each other in the
final effective secular equation.” We must confess that we do not understand
this statement. In our example above, we used perturbations expansions of
order $\lambda^{13}$ without difficulty and the results shown in (5) exhibit a remarkable
rate of convergence.

4 Conclusions

It is clear that Zheng [4] failed to show that his approach is different from the
ESE of Fried and Ezra [1]. One reason for such statement is that he did not
apply his approach to the Barbanis Hamiltonian. In addition to it, the accurate
Fernández’s results for the exceptional point of the toy problem [3] agree with
two of the three results shown by Zheng [2]. The discrepancy for the order $\lambda^2$
appears to be a misprint in Zheng’s paper.

Zheng’s improvement [5] of the ESE approach of Fried and Ezra [1] is based on a wrong expression that does not take into account that the operators involved do not commute. Besides, Zheng did not show any calculation to convince the readers about the advantages of his proposal.

In section 3 we calculated one of the exceptional points of the Mathieu equation by means of the ESE approach of Fried and Ezra [1]. Although this problem is relatively simple, it is not trivial. On the other hand, Zheng [2, 4, 5] did not go beyond the tridiagonal $3 \times 3$ matrix representation of a toy Hermitian Hamiltonian.

References

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