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Chirality of wavefunctions for three coalescing levels

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Abstract

The analytic structure in the vicinity of three coalescing eigenvalues (EP3) of a matrix problem is investigated. It is argued that the three eigenfunctions—also coalescing at the EP3—invoke a true chiral behaviour in the vicinity of the EP3 and that they can be related to a three-dimensional helix. The orientation of the helix depends on the distribution of the widths of the three levels in the vicinity of the EP3.

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Introduction

There is substantial literature from the past decade relating to exceptional points [1], i.e. points where two eigenvalues of an operator coalesce giving rise to a square-root singularity in the spectrum [2]. These singularities are encountered in virtually all physical problems associated with parameter-dependent eigenvalues. They have been discussed in mechanical problems [3], optics [4], for bound states [5] and resonances [6, 7] in quantum mechanics and atomic physics [8, 9]. The mutual influence of neighbouring exceptional points upon the phase behaviour of the associated wavefunctions is dealt with in [10]. Exceptional points also play a crucial role in quantum phase transitions [11]. The chiral behaviour of the eigenfunction [12] as well as effects of time-reversal symmetry breaking are discussed in [13, 14]. Experimental manifestations including chiral behaviour have been achieved with microwave cavities [15] and coupled oscillators in electronic circuits [16]. A more recent mathematical exposé investigates exceptional points in the context of projective Hilbert spaces [17] and extensive numerical work applied to quantum dots is presented in [18], while a connection to \mathcal{PT} -symmetric Hamilton operators [19] is found in [20]. In fact, it is established in [21] that, for a pseudo-Hermitian \mathcal{PT} -symmetric Hamiltonian, the onset of spontaneous symmetry breaking by the wavefunction happens just at an exceptional point.

In many of the papers quoted above, the notation EP was used denoting the simplest exceptional point where two levels coalesce at a square-root branch point. To distinguish it

from the more involved coalescence of three levels being the subject of the present paper, we here denote the simple EP by EP2 and by EP3 the specific situation where the three levels coalesce. While a three-fold diabolic point is mentioned in an earlier experimental paper [22], a genuine investigation of three truly coalescing levels has not—to the best of our knowledge—been dealt with in the literature. We note, however, that EPs of higher order have been implicitly encountered as the coalescence of two or more EP2 in a recent investigation of a complex WKB analysis [23].

Three levels coalescing

The situation of three or more levels coalescing does not seem to have been investigated in great detail, the reason being that there are too many parameters needed to enforce such a higher order coalescence. In fact, while two real parameters (one complex parameter) suffice to invoke the coalescence of two levels, for N levels coalescing $(N^2 + N - 2)/2$ real parameters are needed considering complex symmetric matrices. For $N = 3$ it means that three additional real parameters have to be chosen judiciously to invoke the coalescence of three levels in the complex plane of some complex parameter. Since, as seen below, the coalescence of just three levels has particular attractive features—for the coordinate systems used conventionally a distinction between left and right seems possible—the challenge to implement an experimental arrangement may just fall within reach of realization. To simplify the discussion, we in this paper consider complex symmetric matrices. This is of course not the general situation; in fact, one experimental realization using electronic circuits [16] would yield non-symmetric matrices. A forthcoming paper along those lines is in preparation.

We recall that the wavefunction at a usual EP2 has—for complex symmetric matrices—a fixed phase relationship of its components [15] that can be interpreted as a form of chirality [12]. Considering two coupled dissipative oscillators, a particular EP2 specifies uniquely which of the two oscillators is leading by the phase $\pi/2$. In this particular mode, that is at the EP2, the two oscillators thus specify an orientation in one-dimensional space by simply placing them on a line and using the convention that an arrow points from the oscillator with the leading phase to the one with the lagging phase [16].

When three levels are coalescing the structure becomes richer in comparison with that of an EP2, even though much of it turns out to be an expected generalization. Choosing some convenient complex parameter (denoted by λ below), the EP3 is the point where three levels are analytically connected by an algebraic branch point of third order; to distinguish it from a traditional three-fold degeneracy (as it can occur for Hermitian matrices) we prefer to say, three eigenvalues coalesce. If any of the three additional parameters, that were chosen to invoke the third-root branch point, is now perturbed while keeping all other parameters including λ_{EP3} fixed, three eigenvalues will pop out in the energy plane from the EP3 (just as they do when only λ is moved away from λ_{EP3}). In turn, the EP3 can be seen as a coalescence of two EP2 as the three eigenvalues—obtained from the perturbation—are still analytically connected. In fact, searching for singularities in the chosen parameter λ —using the perturbation mentioned above—one finds two EP2 that sprout from the original EP3 in the λ -plane. Some other parameters could then be used to force a coalescence of the two EP2 into a new (shifted) EP3. We stress that the analytical connectedness is crucial for all properties of an EP3; while three levels were considered in [18, 22], the three levels are not connected analytically as they do not interact.

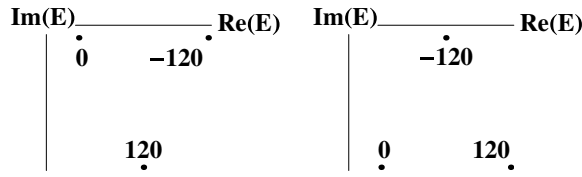


Figure 1. The two basic positions of the three levels for small $|\lambda - \lambda_c|$ in the lower energy plane. The drawing is schematic in that the imaginary parts of two energies are equal: tilting either triangle by less than 30° in either direction still represents the two specific cases as discussed in the text. The lagging (120°) and leading (-120°) phases of the respective wavefunctions are indicated relative to the most left point (the smallest $\text{Re}(E)$). The EP3 lies in the centre of the equilateral triangles.

Of course, the simplest form of an operator giving rise to three levels coalescing is a three-dimensional matrix. Let us assume that any suitable triple of the parameters in

$$H_0 = \begin{pmatrix} e_1 & 0 & 0 \\ 0 & e_2 & 0 \\ 0 & 0 & e_3 \end{pmatrix} \quad \text{and} \quad H_1 = U \begin{pmatrix} o_1 & 0 & 0 \\ 0 & o_2 & 0 \\ 0 & 0 & o_3 \end{pmatrix} U^T, \quad (1)$$

with U a general three-dimensional orthogonal matrix parametrized by three angles, is so chosen that the full problem

$$H_0 + \lambda H_1 \quad (2)$$

has an EP3. If the parameters are all real (except for λ), the EP3 will occur at complex conjugate values of λ . Denoting such point by λ_c , the three levels are connected by a third-root branch point (see the appendix) and there exists the expansion

$$E_j(\lambda) = E_c + \sum_{k=1}^{\infty} a_k (\sqrt[3]{\lambda - \lambda_c})^k, \quad (3)$$

where the label $j = 1, 2, 3$ is specified by the value of $\sqrt[3]{\lambda - \lambda_c}$ on the first, second or third Riemann sheet in the λ -plane. More explicitly, (3) can be written

$$E_j(\lambda) = E_c + \sum_{k=1}^{\infty} a_k (\sqrt[3]{|\lambda - \lambda_c|} \exp(i \arg(\lambda - \lambda_c)/3 + 2i\pi(j - 1)/3))^k, \quad j = 1, 2, 3.$$

As a consequence, for small values of $|\lambda - \lambda_c|$ the three complex energies $E_j(\lambda)$ form an equilateral triangle in the energy plane. The orientation of the triangle depends on $\arg(\lambda - \lambda_c)$ and the parameters of the specific problem (1), which determine the complex coefficient a_1 in (3). Generically, we can order the energies according to their real parts, that is $\text{Re}(E_1) < \text{Re}(E_2) < \text{Re}(E_3)$ (we dismiss the possibility that two real parts are equal as non-generic). In the energy plane we distinguish two different cases of orientation, depicted schematically in figure 1: in (a) $\text{Im}(E_2)$ is smaller than the imaginary parts of the other two energies—in other words it has the largest width (recall that all the energies have negative imaginary parts), whereas in (b) $\text{Im}(E_2)$ has the largest imaginary part (the smallest width).

Now we turn to the eigenfunctions. Three eigenfunctions coalesce, in other words they become aligned when approaching the EP3. There are the expansions

$$|\psi_j(\lambda)\rangle = |\psi_{\text{EP3}}\rangle + \sum_{k=1}^{\infty} (\sqrt[3]{\lambda - \lambda_c})^k |\phi_k\rangle. \quad (4)$$

As in (3), the labels $j = 1, 2, 3$ are specified by the Riemann sheet of the third root, that is (4) can be written more explicitly

$$|\psi_j(\lambda)\rangle = |\psi_{\text{EP3}}\rangle + \sum_{k=1}^2 (\sqrt[3]{|\lambda - \lambda_c|})^k |\phi_k^j\rangle,$$

with $|\phi_k^j\rangle = \exp(i(\arg(\lambda - \lambda_c) + 2(j - 1)\pi)k/3)|\phi_k\rangle$. For any $\lambda \neq \lambda_c$ the eigenfunctions form the usual bi-orthogonal complete system, namely,

$$\langle \tilde{\psi}_i(\lambda) | \psi_j(\lambda) \rangle = N_j(\lambda) \delta_{i,j}, \tag{5}$$

$$\sum_j \frac{|\psi_j(\lambda)\rangle \langle \tilde{\psi}_j(\lambda)|}{\langle \tilde{\psi}_j(\lambda) | \psi_j(\lambda) \rangle} = I. \tag{6}$$

It can be shown (see the appendix) that the scalar product (5) vanishes as

$$N_j(\lambda) \sim \zeta \cdot (\lambda - \lambda_c)^{\frac{2}{3}} \quad \text{for } \lambda \rightarrow \lambda_c \tag{7}$$

and similarly

$$\langle \tilde{\psi}_j(\lambda) | \psi_{\text{EP3}} \rangle \sim \eta \cdot (\lambda - \lambda_c)^{\frac{2}{3}} \quad \text{for } \lambda \rightarrow \lambda_c \tag{8}$$

with some constants ζ, η .

It should be noted that the structure of the eigenvectors at an EP3 is slightly more involved as there are three vectors that coalesce into $|\psi_{\text{EP3}}\rangle$ when $\lambda \rightarrow \lambda_c$. In view of result (8), expansion (4) implies that not only

$$\langle \tilde{\psi}_{\text{EP3}} | \psi_{\text{EP3}} \rangle = 0, \tag{9}$$

but also

$$\langle \tilde{\psi}_{\text{EP3}} | \phi_1 \rangle = 0,$$

where $|\phi_1\rangle$ is the first-order term in (4) associated with the first power of $\sqrt[3]{\lambda - \lambda_c}$.

In contrast to an EP2, the eigenfunction $|\psi_{\text{EP3}}\rangle$ does not bear a chiral behaviour at an EP3. It is rather in its immediate neighbourhood where the chiral phase structure is revealed. Similar to the reasoning in [12], an expansion of $|\psi_{\text{EP}}\rangle$ in terms of the normalized basis

$$|\chi_j(\lambda)\rangle = \frac{|\psi_j(\lambda)\rangle}{\sqrt{\langle \tilde{\psi}_j(\lambda) | \psi_j(\lambda) \rangle}} \tag{10}$$

provides the phase relation of interest. Indeed, while it is always possible for $\lambda \neq \lambda_c$ to write (identically in λ)

$$|\psi_{\text{EP3}}\rangle = \sum_{j=1}^3 c_j(\lambda) \chi_j(\lambda), \tag{11}$$

we find for the leading term for $\lambda \rightarrow \lambda_c$ either

$$\begin{pmatrix} c_1(\lambda) \\ c_2(\lambda) \\ c_3(\lambda) \end{pmatrix} \sim \xi_1 \sqrt[3]{|\lambda - \lambda_c|} \begin{pmatrix} 1 \\ e^{2i\pi/3} \\ e^{-2i\pi/3} \end{pmatrix} \tag{12}$$

or

$$\begin{pmatrix} c_1(\lambda) \\ c_2(\lambda) \\ c_3(\lambda) \end{pmatrix} \sim \xi_2 \sqrt[3]{|\lambda - \lambda_c|} \begin{pmatrix} 1 \\ e^{-2i\pi/3} \\ e^{2i\pi/3} \end{pmatrix} \tag{13}$$

with ξ_1 and ξ_2 some complex constants; what matters are the quotients of the components $c_j(\lambda)$, they are given just by the phases $\exp(\pm 2i\pi/3)$. Recall that the normalized state vectors $\chi_j(\lambda)$ tend to infinity as $1/\sqrt[3]{\lambda - \lambda_c}$ when $\lambda \rightarrow \lambda_c$ thus yielding a finite expression for $|\psi_{\text{EP3}}\rangle$ in (11). The relative phases given in (12) and (13) are due to the analytic structure of the third-root branch point and are thus independent of a particular basis. Note that

$$\sum_j c_j(\lambda)^2 \equiv 0$$

in accordance with (9). We mention that for non-symmetric matrices (12) and (13) have to be modified. In the case of electronic circuits (see also [16]) the phase relations remain.

The essential point is now the unambiguous association of the phases as given in (12) and (13) with the complex values of the energies in the vicinity of the EP3, that is with the frequencies and their widths. This association is illustrated in figure 1. Choosing as reference point the eigenvector of the energy with the smallest real part (frequency), then the eigenstate of the next higher frequency has a lagging phase of 120° if (and only if) its width is larger than the other two; the phase of the eigenstate with the largest frequency would then be leading by 120° . In turn, if the width of the middle frequency is smallest, the role of the leading and lagging phase is interchanged among the two states with the larger frequencies. This result is demonstrated analytically in the following section in a specific setting and confirmed numerically in numerous general examples.

The strict phase relations of the eigenvectors associated with the positions of the frequencies and widths of the three levels allow the interpretation of distinct helices in that we relate a left-hand helix and a right-hand helix with the smaller and larger widths of the middle frequency, respectively. The top row of figure 2 illustrates how a particular right-handed helix is generated. In a three-dimensional coordinate system the points $(\cos(\Phi_k), \sin(\Phi_k), \text{Re}(E_k))$ with $\Phi_{1,2,3} = (0^\circ, 120^\circ, -120^\circ)$ invoke an oriented helix, where $\Phi_{1,2,3}$ are the phase angles of the three eigenvectors associated with the energies $E_{1,2,3}$. The example on the top row of figure 2 refers to the case where the width of the middle frequency is the largest, it generates a right-handed helix. In turn, if the width of the middle frequency is smallest, the helix will be left handed as illustrated in the bottom row of figure 2.

The similarity between the EP2 and EP3 is the fixed phase relations of the eigenvectors in the immediate vicinity of the respective singularity. The particular result for the EP3 is of course related to (4) implying the appealing feature of (12) and (13). We stress that, while the phase relation of the eigenvectors at an EP2 can only give an orientation in one dimension and hence cannot provide a genuine chirality, the eigenvectors of an EP3 do provide just that as their three-dimensionality can be mapped into a three-dimensional coordinate system.

As an aside we note that at an EP2 the phase difference between the two components of the coalescing eigenfunction is $\pi/2$ (recall: for complex symmetric matrices), while at the EP3 the phases of the three components differ by $2\pi/3$. This means that, in contrast to the EP2, where only a four-fold loop around the singularity restores the eigenfunctions, at the EP3 the eigenvectors are retrieved after three loops in the λ -plane just like for the corresponding energies.

Special setting

The all important question is: can a three-fold coalescence be arranged in the laboratory and are the energies and phases amenable to measurement? One suggestion could be a setting similar in spirit to the microwave experiment for an EP2 [15] but now with three chambers

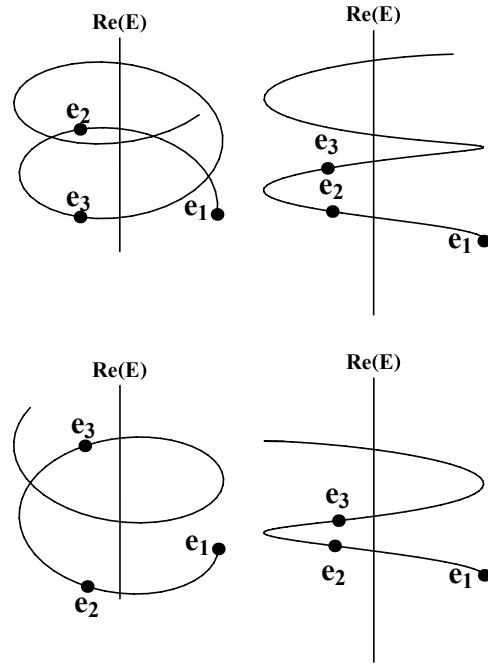


Figure 2. Perspective views of the three-dimensional helix. The right-hand helix at the top row refers to the width of E_2 being larger than the other two, while the left-hand helix at the bottom row refers to the width of E_2 being smaller. The coordinates of the points denoted by e_k are $(\cos(\Phi_k), \sin(\Phi_k), \text{Re}(E_k))$ with $(\Phi_1, \Phi_2, \Phi_3) = (0^\circ, 120^\circ, -120^\circ)$ for the top and $(\Phi_1, \Phi_2, \Phi_3) = (0^\circ, -120^\circ, 120^\circ)$ for the bottom row.

in the cavity. Another, perhaps simpler possibility could use electronic circuits as in [16]. Basically, such settings can be simulated by the simple matrix

$$H = \begin{pmatrix} e_1 & s_1 & s_3 \\ s_1 & e_2 & s_2 \\ s_3 & s_2 & e_3 \end{pmatrix}, \tag{14}$$

where s_j give the couplings and the e_j are the (complex) energies. To facilitate matters, we consider in particular the problem

$$H_0 + \lambda H_1 = \begin{pmatrix} e_1 & 0 & s_3 \\ 0 & e_2 & s_2 \\ s_3 & s_2 & e_3 \end{pmatrix} + \lambda \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{15}$$

and choose the couplings s_2 and s_3 such that H_0 has a three-fold coalescence. The choice

$$s_2 = \pm \sqrt{-\frac{(e_1 - 2e_2 + e_3)^3}{27(e_1 - e_2)}}, \quad s_3 = \pm \sqrt{+\frac{(-2e_1 + e_2 + e_3)^3}{27(e_1 - e_2)}} \tag{16}$$

achieves this goal with

$$E_c^{(1,2,3)} = \frac{1}{3}(e_1 + e_2 + e_3).$$

The perturbation by λ splits the coalescence into three levels and we obtain to the lowest order (note that here $\lambda_c = 0$)

$$E_j = E_c + \frac{2^{1/3} \sqrt{-(-2e_1 + e_2 + e_3)(e_1 - 2e_2 + e_3)}}{3(e_1 - e_2)^{1/3}} \sqrt[3]{|\lambda|} \exp(i \arg(\lambda)/3 + 2i(j - 1)\pi/3) + O((\lambda)^{2/3}), \quad j = 1, 2, 3 \quad (17)$$

and, using the notation as in (4), the corresponding (unnormalized) eigenvectors are

$$|\psi_{\text{EP3}}\rangle = \begin{pmatrix} \frac{\sqrt{-2e_1 + e_2 + e_3}}{\sqrt{3}(e_1 - e_2)} \\ i \frac{\sqrt{e_1 - 2e_2 + e_3}}{\sqrt{3}(e_1 - e_2)} \\ 1 \end{pmatrix}, \quad (18)$$

$$|\phi_1^j\rangle = \begin{pmatrix} i 2^{1/3} \frac{\sqrt{e_1 - 2e_2 + e_3}}{\sqrt{3}(e_1 - e_2)^{5/6}} \\ -2^{1/3} \frac{\sqrt{-2e_1 + e_2 + e_3}}{\sqrt{3}(e_1 - e_2)^{5/6}} \\ 0 \end{pmatrix} \exp(i \arg(\lambda)/3 + 2i(j - 1)\pi/3), \quad (19)$$

and similar algebraic expressions for the higher orders being of no interest here. We note, however, that the leading terms of the $c_j(\lambda)$, defined by (11) and given in (12) and (13), are related to the next order $|\phi_2\rangle$, used in (4), by $c_j(\lambda) \sim \sqrt[3]{\lambda - \lambda_c} \langle \tilde{\psi}_{\text{EP3}} | \phi_2 \rangle$; the $c_j(\lambda)$ therefore have the same phase dependence as the $|\phi_1^j\rangle$ as they are also associated with the first power of the third root.

The essential point revealed in these explicit expressions is the unambiguous association of the relative phases $\exp(2i(j - 1)\pi/3)$ in the energies E_j and the corresponding eigenvectors $|\phi_1^j\rangle$. While the common factor of the energies is some complex number given by the parameters of the Hamiltonian (15) and $\arg(\lambda)$, we may always choose $j = 1$ for the energy with the smallest real part. Once this choice is made, the situation as illustrated in figure 1 naturally emerges. The width (imaginary part) of the second energy of the ordered frequencies (real parts) determines the sequence of the relative phases $\exp(\pm 2i\pi/3)$ of the associated wavefunctions and thus specifies their relative orientation. Depending on whether $\text{Im } E_2$ is smallest or largest a left- or right-hand helix is obtained, respectively, as illustrated in figure 2.

Conclusion

Suppose three coupled damped oscillators are placed in a plane in the form of a triangle and we look upon that plane. It depends now on the measurements of the frequencies and widths of the eigenmodes in the vicinity of an EP3 whether we should arrange the oscillators and their numbering at the corners of the triangle in a clockwise or counterclockwise sense. Once that arrangement is made according to the relative magnitudes of the widths, the measurement of the phase sequence of the associated wavefunctions will then confirm the consistency of the oriented arrangement. A unique and unambiguous orientation is obtained in this way. Apart from the illustration in figure 2, the time behaviour of the eigenstates can also be viewed like that of the leads of a technical three-phase current; in fact, the sequence of the three amplitudes being governed by the time behaviour $\exp(i\omega_{\text{EP3}}t)$ follows just the traditional pattern of the voltage of a three-phase current in one case, and with two phases (leads) interchanged in the other.

Recall that the single eigenstate $|\psi_{EP3}\rangle$ does not carry such information. The relevant phases are found in the part of the eigenstate that is switched on when moving away from the EP3 in the λ -plane. An experimental verification of this subtle behaviour would thus lead to a clear chiral characterization in three-dimensional space. We stress that there is no *a priori* handedness in an experimental setting as suggested above. There is, however, the direction of time that provides the various widths of the dissipative system and the time sequence of the amplitudes mentioned above. In other words, we here suggest that the arrow of time invokes chirality.

Strictly speaking, the two cases merely distinguish one orientation in three dimensions from the other, that is the two situations have a genuine and different chirality. Using our traditional convention for the clockwise motion and left handedness, we associate the larger or smaller width of the middle frequency with right or left handedness, respectively.

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Appendix

For an N -fold coalescence of eigenvalues, the N levels are connected by a branch point of N th order. This follows from the fact that—for an N -dimensional matrix of the form $H_\lambda = H_0 + \lambda H_1$ —the determinant of $H_\lambda - IE$ vanishes linearly in the variable λ , while the requirement of N coalescing levels entails an N -fold vanishing in the variable E , that is the following set of equations is to be satisfied simultaneously:

$$\frac{d^k}{dE^k} \det|H_\lambda - IE| = 0, \quad k = 0, \dots, N - 1.$$

This is possible only if

$$E(\lambda) = E_c + \sum_{m=1}^{\infty} c_m (\sqrt[N]{\lambda - \lambda_c})^m.$$

Here the N eigenvalues are given by the values upon the N sheets of the N th root. We recall that it is one general characteristic of EPs that the matrix cannot be diagonalized. Rather the Jordan normal form reads

$$\begin{pmatrix} E_c & 1 & 0 & & 0 \\ 0 & E_c & 1 & & \\ & & \ddots & \ddots & 0 \\ & & & \ddots & 1 \\ 0 & & & 0 & E_c \end{pmatrix}.$$

The N eigenstates coalesce likewise into one eigenvector. There is the expansion

$$|\psi(\lambda)\rangle = |\psi_{EPN}\rangle + \sum_{m=1}^{\infty} |\phi_m\rangle (\sqrt[N]{\lambda - \lambda_c})^m.$$

Note, however, that for the scalar product the following behaviour prevails

$$\langle \psi(\lambda) | \psi_{EPN} \rangle \sim (\lambda - \lambda_c)^{\frac{N-1}{N}}$$

as follows from considering

$$\begin{aligned}(E(\lambda) - E_c)\langle\psi(\lambda)|\psi_{\text{EPN}}\rangle &= \langle\psi(\lambda)|H_\lambda - H_{\lambda_c}|\psi_{\text{EPN}}\rangle \\ &= (\lambda - \lambda_c)\langle\psi(\lambda)|H_1|\psi_{\text{EPN}}\rangle.\end{aligned}$$

The right-hand side vanishes linearly when $\lambda \rightarrow \lambda_c$, while $(E(\lambda) - E_c) \sim \sqrt[N]{\lambda - \lambda_c}$. Note that these analytic properties imply the relations

$$\langle\psi_{\text{EPN}}|\phi_m\rangle = 0 \quad \text{for } m = 1, \dots, N - 2$$

and

$$\langle\phi_m|\phi_{m'}\rangle = 0 \quad \text{for } m + m' \leq N - 2.$$

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