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Localization of exceptional points with Padé approximants

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Abstract

The strict coalescence of two resonance states may never occur (due to the sensitivity to small external perturbations). However, its existence can have noticeable effects on measurable quantities. The coalescence of resonances is associated with exceptional points (EPs) in the spectrum of the system under study. The determination of exceptional points is often a hard numerical task, due to the need to calculate many eigenvalues of a non-Hermitian Hamiltonian as a function of the potential's parameters which are to be varied adiabatically. The method presented here is based on the Padé algorithm. This enables one to calculate the EPs with a small number of solutions. As an illustrative numerical example an EP of H_2^+ in strong laser fields is calculated.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The fact that non-Hermitian Hamiltonians may have an incomplete spectrum was proved a long time ago [1]. The incomplete spectrum is obtained upon coalescence of two or more eigenvalues and of their corresponding eigenfunctions at a branch point. Such a point is commonly referred to as an exceptional point (EP) [2, 3]. However, for many years it was considered as a mathematical object rather than a physical one. Only recently was it associated with physical phenomena in optics [4], atomic physics [5, 6], electron–molecule collisions [7], superconductors [8], quantum phase transitions in a system of interacting bosons [9], electric field oscillations in microwave cavities [10], PT optical coupled systems [11, 12] and photodissociation of diatomic species [13].

Since these points are in fact branch points in the energy plane, this circumstance imposes limits to the analytic representation of a resonance energy. The Padé formalism [14] is a powerful tool to produce analytic representations. We examine how this formalism behaves in the presence of

EPs. We wish to demonstrate that the breakdown of the Padé analytic continuation can be a tool for localizing an EP. Although we discuss here the calculations of an EP of H_2^+ , the method proposed in this paper for the determination of EPs can be applied to other physical systems. The interest for such a method results from the fact that only for very specific potential parameters (laser parameters in our case) two eigenstates coalesce. Therefore, the search for an EP may require many solutions of the wave equation. We leave aside the cases where the eigenvalues are obtained from the diagonalization of matrices of very small sizes [15, 16]. In such cases the EPs can be obtained from the parameter-dependent analytic expressions of the eigenvalues. In more general cases one may quote several systematic procedures to calculate the values of the potential parameters for which two or more eigenstates coalesce.

- (1) The first one is based on some unpublished work of Byers–Brown which has been first described in [17]. This method uses the fact that a perturbational expansion of the spectrum in the potential parameters is converging provided the parameters get sufficiently small values. Small means here that these potential parameter values are embedded inside a circle/sphere with its radius

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determined by the location of the branch point in the potential's parameter space which is closest to the origin of the circle/sphere. The branch point is an EP in the spectrum, where two eigenvalues and their corresponding eigenfunctions coalesce. The calculation of the branch point requires the calculation of very high-order perturbational corrections to the energy.

- (2) Another method is based on the resonance exchange taking place if the parameters are varied adiabatically along a loop encircling the branch point (see for example [13, 18, 19]). Since the parameters should be adiabatically varied, the calculation requires a large number of eigenfunctions of the non-Hermitian Hamiltonian.
- (3) The third method for calculating the EPs is based on the self-orthogonality property of the eigenfunction which is associated with the EP [20, 21]. This approach requires again many eigenfunctions of the non-Hermitian Hamiltonian for calculating the norm of the almost self-orthogonal state since one has to be close to the EP in order to get extremely large values of the norm.

The method based on the Padé algorithm presented here has some advantages over such procedures since it does not require the calculations of the energy spectra for so many values of the potential parameters. Another point should be mentioned: when the Hamiltonian is time periodic, as in our case, time serves as an additional coordinate rather than as a parameter, as usual [22, 23].

As an illustrative numerical example, we consider a molecule which is exposed to a continuous wave (cw) laser field. Our system is the molecular ion H_2^+ . We have recently shown [13] that, with appropriate laser parameters, pairs of quasi-energies may be driven to coincidence. We will show here how the use of the Padé analytic continuation reduces substantially the task of the determination of the laser parameters for which the EPs are obtained. Using this information one may design an experiment to show the effect of the EP on the vibrational transitions of H_2^+ as the laser is turned off. As explained in [13], if the molecule is driven adiabatically along a loop encircling in the parameter space an EP corresponding to the coalescence of two resonance energies issued from two vibrational states, the undissociated molecules are transferred from one state to another. This behaviour of the Padé continuation procedure is not specific for the photodissociation of H_2^+ studied in this paper. Therefore, we propose the use of the Padé continuation procedure for a systematic search of exceptional points in other physical systems.

In section 2, we recall briefly how the Floquet method provides the photodissociation rate of a diatomic species in a continuous wave (cw) laser field. Section 3 gives the Padé procedure to be used in the search of EPs. In section 4, we are considering the problem in two steps. Since the Padé method is a *one-parameter* algorithm, while the determination of an EP is the search for *two parameters*, we make some preliminary checks about the capacity of this method to determine one of the parameters when the other is already known. The method works as expected: there is a breakdown of the continuation scheme when the unknown parameter reaches the branch point,

thus providing a method to estimate this parameter. We then turn to the determination of the two parameters when they are unknown. In order to turn this two-parameter search into a one-parameter one, we take advantage of a correlation which can be established between the two parameters along an axis passing through the EP in parameter plane. The procedure is shown to yield rather accurate estimates about the location of the EP, with the determination of a small number of solutions of the wave equation. Section 5 illustrates the power of Padé approximants to represent a resonance width when there is no anomaly along the trajectory in the parameter plan. The application is made here to the prediction of the intensity at which there is vanishing of a resonance width. Some conclusions are given in section 6.

2. Floquet formalism for calculating photo-induced resonances

The photodissociation rate of a molecule submitted to a cw field can be calculated with the Floquet formalism. Our model implies the two electronic states $|g\rangle$ and $|u\rangle$ of a diatomic molecule, these being the ground and excited electronic states respectively. The model Hamiltonian is one dimensional. The wavefunction is written as

$$|\Psi(R, t)\rangle = \chi_g(R, t)|g\rangle + \chi_u(R, t)|u\rangle. \quad (1)$$

If the intensity of the field is such as to allow only for absorption of one photon of energy $\hbar\omega$, the Floquet ansatz consists in writing the vector nuclear wavefunction as

$$\begin{bmatrix} \chi_g(R, t) \\ \chi_u(R, t) \end{bmatrix} = e^{-iE_F t/\hbar} \begin{bmatrix} \Psi_g(R) e^{i\omega t} \\ \Psi_u(R) \end{bmatrix}, \quad (2)$$

where E_F is called a quasienergy. Choosing the length gauge for the matter-field interaction one gets the two coupled equations:

$$[T_N + V_g(R) + \hbar\omega - E]\Psi_g(R) - 1/2\mathcal{E}_0\mu(R)\Psi_u(R) = 0, \quad (3)$$

$$[T_N + V_u(R) - E]\Psi_u(R) - 1/2\mathcal{E}_0\mu(R)\Psi_g(R) = 0, \quad (4)$$

where T_N is the nuclear kinetic energy operator, $V_g(R)$ and $V_u(R)$ are the Born-Oppenheimer potentials of the ground and excited states, which for H_2^+ are asymptotically degenerate, and $\mu(R)$ is the electronic transition moment between states $|g\rangle$ and $|u\rangle$. The laser electric field amplitude is of the form $\mathcal{E}_0 \cos(\omega t)$, with a wavelength $\lambda = 2\pi c/\omega$. The solution with Siegert outgoing wave boundary conditions in the open channel produces a complex quasi-energy $E_F = E_R - i\Gamma_R/2$. Γ_R/\hbar is the photodissociation rate, while $\Gamma_R/2$ is the resonance width. The equations are solved with a matching technique based on the Fox-Goodwin propagator [24], with exterior complex scaling ([25] and references therein), applied in [26] to the calculation of the H_2^+ resonances. The potentials of H_2^+ are those of Bunkin and Tugov [27]. It can be shown [28] that in the present context gauge changes have no effect on resonance energies. Finally, it should be stressed that if the laser intensity is such as to impose the consideration of multiphoton processes, EPs are still present, as shown in [29],

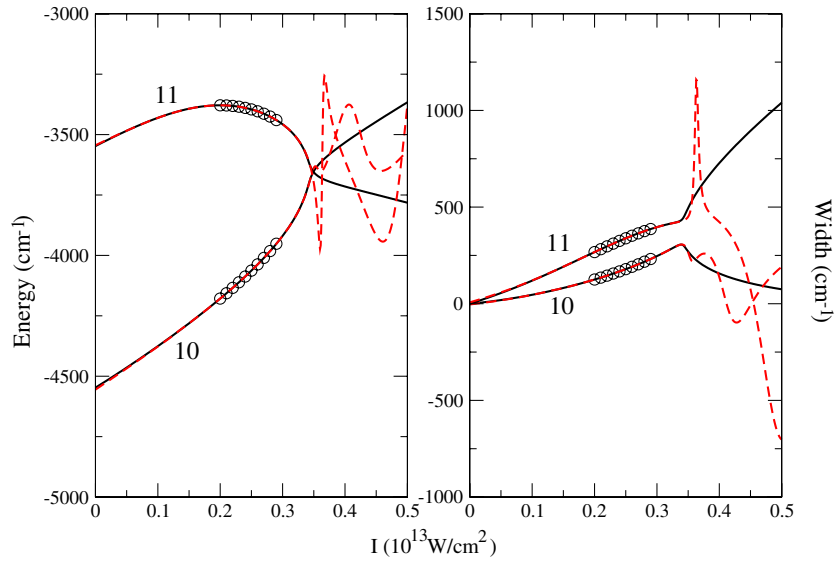


Figure 1. Left panel. The solid curves give the real parts of the Floquet quasi-energies issued from the field-free states $v = 10$ and $v = 11$ as a function of laser intensity, at a fixed wavelength. The wavelength is close to that of the EP (493 instead of 494 nm). There is a crossing of the Floquet energies. The circles mark the input data for the Padé procedure. The dashed curves correspond to the use of the Padé approximants. They agree well with the Floquet results, except beyond the intensity of the EP ($0.334 \times 10^{13} \text{ W cm}^{-2}$). Right panel. The same informations for the widths of these two resonances.

where emission of two virtual photons and absorption of up to three photons have been introduced in the formalism. The loop chosen to produce a state-to-state transfer in the two-channel approximation produces this same transfer in a six-channel calculation. This proves that the EP still exists and is still within this loop.

3. The Padé algorithm

The Padé formalism aims at giving an analytic representation of a function of either a real or a complex coordinate. This representation is in the form of the ratio of two polynomials. It can be used to perform an analytic continuation of a function. Schlessinger [14] has given several procedures to reach such a representation. The first step is to ensure that, given a set of input variables z_i and values of a function $F(z)$ for these values of the variables, the ratio of polynomials reproduces accurately these values at these points. This is not a trivial problem. A straightforward fulfilment of the relation

$$F(z_i) = \frac{P_N(z_i)}{Q_M(z_i)} \quad (5)$$

with

$$P_N(z) = \sum_{k=0}^N p_k z^k; \quad Q_M(z) = 1 + \sum_{k=1}^M q_k z^k \quad (6)$$

and

$$Q_M(z_i)F(z_i) = P_N(z_i) \quad (7)$$

requires the inversion of a matrix which is often ill conditioned. We use instead the procedure given by Schlessinger [14] based on truncated continued fractions. We have tested earlier the reliability of this method [30].

4. Padé continuation of Floquet quasi-energies

Exceptional points in molecular photodissociation have been recently studied [13] in the 1D H_2^+ model described in the section devoted to the Floquet formalism. In particular it has been shown that the two resonance energies issued from the field-free vibrational levels $v = 8$ and $v = 9$ are merging for a wavelength $\lambda_{\text{EP}}^{8,9} \sim 442 \text{ nm}$ and an intensity $I_{\text{EP}}^{8,9} \sim 0.395 \times 10^{13} \text{ W cm}^{-2}$, while for the pair $v = 9$ and $v = 10$ there is merging for $\lambda_{\text{EP}}^{9,10} \sim 442 \text{ nm}$ and $I_{\text{EP}}^{9,10} \sim 0.513 \times 10^{13} \text{ W cm}^{-2}$. We extend this study by a consideration of the pair $v = 10$ and $v = 11$. We examine here the capacity of the Padé procedure to represent the Floquet quasi-energies and to give some useful information about the position of an EP in the parameter plane. Since the Padé procedure is a *one-parameter* method, while estimating the position of an EP in the parameter plane is a *two-parameter* search, some special strategy has to be formulated. The study proceeds in two steps. The first step is to establish that if only one parameter had to be determined, Padé approximants would provide a way to determine the other parameter. For the pair $v = 10$ and $v = 11$ we have established in various ways that $\lambda_{\text{EP}}^{10,11}$ is $\sim 494 \text{ nm}$ and that $I_{\text{EP}}^{10,11}$ is $\sim 0.334 \times 10^{13} \text{ W cm}^{-2}$.

In figure 1 the wavelength is 493 nm, while the intensity runs from zero (in which case the quasi-energies are simply the field-free energies, respectively -4550 cm^{-1} for $v = 10$ and -3551 cm^{-1} for $v = 11$), to $0.5 \times 10^{13} \text{ W cm}^{-2}$. λ being somewhat smaller than λ_{EP} , the left panel shows (for reasons to be given below) that the real parts of the Floquet quasi-energies are crossing each other, while (right panel) the widths show a wide avoided crossing. This shows how the effects can be large even when departing slightly from the EP parameters. The circles on each curve give the position

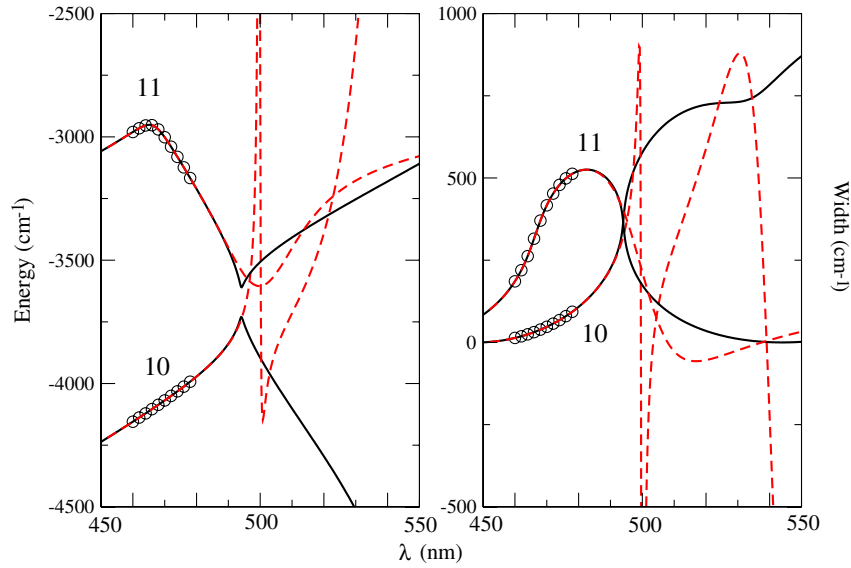


Figure 2. Left panel. The solid curves give the real parts of the Floquet quasi-energies issued from the field-free states $\nu = 10$ and $\nu = 11$ as a function of wavelength at a fixed intensity ($I = 0.334 \times 10^{13} \text{ W cm}^{-2}$). There is an avoided crossing of the energies. The circles mark the input data for the Padé procedure. The dashed curves correspond to the use of the Padé approximants. They agree well with the Floquet results, except beyond the wavelength of the EP (394 nm). Right panel. The same informations for the widths of these two resonances.

of the input values given to the Padé procedure. The input variables consist of ten values of the intensity from $0.2 \times 10^{13} \text{ W cm}^{-2}$ to $0.3 \times 10^{13} \text{ W cm}^{-2}$. The input functions are the ten corresponding complex quasi-energies. Both panels show a clear breakdown of the Padé method as soon as I is approaching I_{EP} . The breaking point allows I_{EP} to be estimated as $\sim 0.347 \times 10^{13} \text{ W cm}^{-2}$ from the left panel, while from the right panel as $\sim 0.338 \times 10^{13} \text{ W cm}^{-2}$. In figure 2 the role of the two parameters is exchanged. The intensity is given the value $0.334 \times 10^{13} \text{ W cm}^{-2}$, while the wavelength is now the parameter given as an input to the Padé procedure. The same conclusion emerges. There is again a breakdown of the Padé method when the wavelength goes beyond λ_{EP} . From both panels λ_{EP} is estimated to be $\sim 494 \text{ nm}$. These preliminary calculations show the failure of the extrapolation procedure when reaching a branch point. If no information about the EP is available, another approach is needed.

To formulate a general one-parameter approach in the parameter plane, we will make use of some properties of the resonance energies close to an EP established by Hernández *et al* [31]. According to their analysis, it is possible to define an axis in the parameter plane passing through the EP, which is such that the EP is the dividing point between two half-axes. On one of them there is equality of the real parts of the resonance energies, while on the other half-axis it is the imaginary parts (or the widths) which are equal. Two points are enough to determine this axis. It has been shown elsewhere [32] that in the present problem $\lambda < \lambda_{EP}$ is a condition for having an equality of the real parts of the quasi-energies, while $\lambda > \lambda_{EP}$ produces an equality of the imaginary parts. A preliminary calculation of the resonance energies at a fixed wavelength (respectively 480 and 490 nm) as a function of intensity has produced crossings of the real

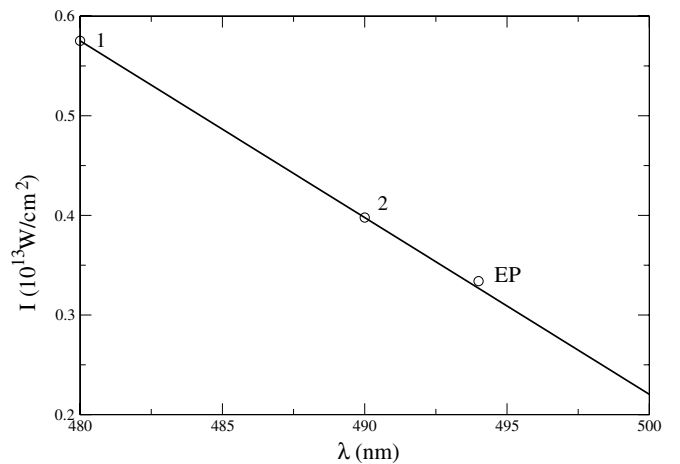


Figure 3. Two trajectories calculated for the wavelengths 480 and 490 nm have produced a crossing of the real parts of the quasi-energies issued from $\nu = 10$ and $\nu = 11$ at the intensities 0.575×10^{13} and $0.397 \times 10^{13} \text{ W cm}^{-2}$. These two points marked 1 and 2 allow for the determination of the axis passing (in principle) through the exceptional point. Shown also is the EP in the parameter plane, which is slightly outside the axis.

parts of the energies at respectively 0.575×10^{13} and $0.397 \times 10^{13} \text{ W cm}^{-2}$. These two points are shown in figure 3. The position of the EP is also indicated. The EP is very close to being on the straight line defined by the two points. The next step is to use these two points corresponding to a crossing of the real parts to relate the intensity to the wavelength along this line, in the form $I = a\lambda + b$, and to take λ as the independent parameter. In figures 4 and 5, there is given, successively for the resonances 10 and 11, the Floquet results along this line,

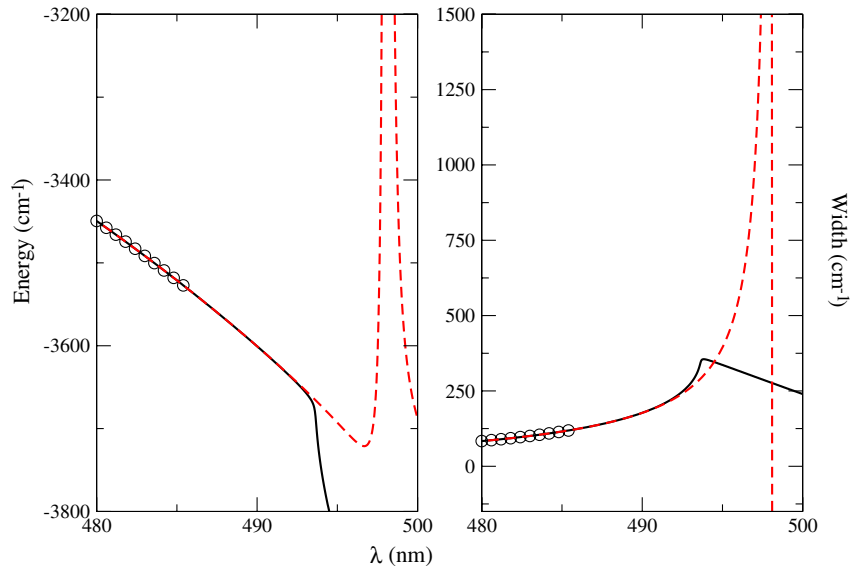


Figure 4. Comparison between Padé approximants (solid curves) and Floquet results (dashed curves) for the energy (left panel) and the width of the resonance $\nu = 10$ (right panel). The intensity is correlated with the wavelength according to equation (8). The circles give the positions chosen for the input data of the Padé method. Padé approximants fail when λ reaches the wavelength of the EP.

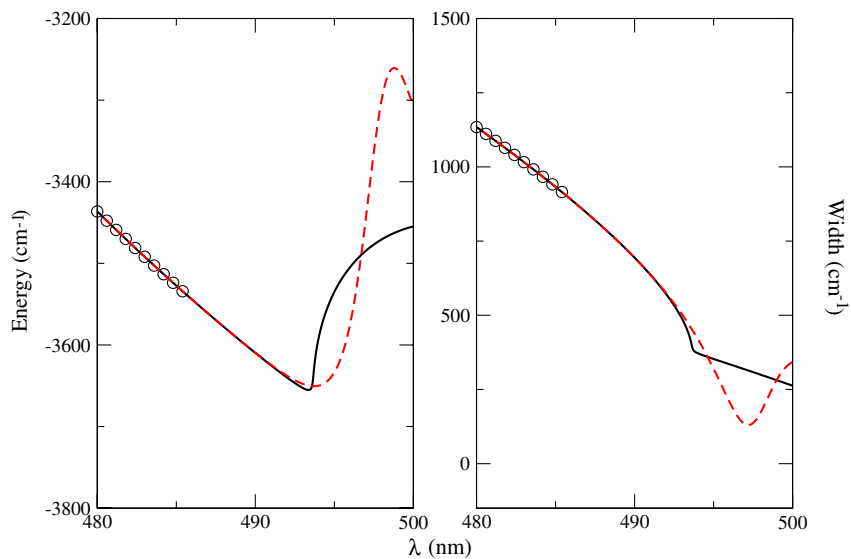


Figure 5. Same comparison between Padé approximants and Floquet results as, in figure 4, now for the resonance $\nu = 11$.

as well as the Padé approximants based on the points indicated by circles. The situation met in the previous one-parameter case is again present. The Padé approximants agree very well with the Floquet results, except beyond the EP. An estimate from the four graphs gives $\lambda_{EP} \sim 493$ nm, yielding, from the relation correlating wavelength and intensity, $I = 0.345 \times 10^{13} \text{ W cm}^{-2}$.

A variant of this procedure would be to start with two values of λ larger than λ_{EP} . This would allow us to obtain two points in the parameter plane with equality of the imaginary parts of the quasi-energies, leading again to the axis passing through the EP. Extrapolation would be backwards towards

λ_{EP} . The failure of the Padé approximants should lead to another determination of λ_{EP} .

5. Padé approximants and zero-width resonances

As an illustration of the power of the Padé method to represent the resonance energies when no branch point is to be met along a trajectory in the parameter plane, we present in figure 6 the width (solid curve) as a function of intensity for the resonance issued from $\nu = 10$ at a wavelength $\lambda = 450$ nm. The width vanishes for an intensity $I = 0.302 \times 10^{13} \text{ W cm}^{-2}$. It has been shown before [33] that this behaviour of the width is typical of those resonances of H_2^+ which are of Feshbach type,

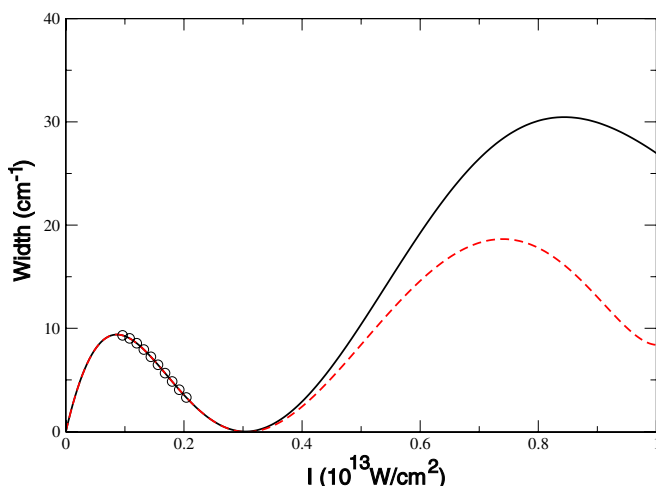


Figure 6. The solid curve represents the width issued from the field-free level $v = 10$ as a function of intensity. The width is vanishing at a critical intensity $I = 0.302 \times 10^{13} \text{ W cm}^{-2}$. The circles give the input points for the building of the Padé approximant. The dashed curve is the Padé approximant. On the left of the critical intensity it agrees fully with the Floquet result. The critical intensity is well accounted for.

that is, which go asymptotically to the levels of the upper of the two potentials obtained by the diagonalization of the radiative coupling. The circles on figure 6 represent the input given to the Padé procedure, while the dashed curve corresponds to the Padé approximant. The critical intensity at which there is vanishing of the width is very-well accounted for by the Padé extrapolation. There is of course a failure of the latter procedure for higher intensities, but far from the input region.

6. Concluding remarks

It is shown that the Padé continuation procedure breaks down, as expected, when approaching a branch point (the so-called exceptional point in the present context), where two resonance states coalesce. By calculating the photo-induced resonance eigenvalues of H_2^+ in strong laser fields for a set of values of correlated laser parameters (intensity and frequency) an EP could be estimated by using the Padé continuation procedure. This behaviour is not specific for the photodissociation of H_2^+ we study in this paper. Therefore, we propose the use of the Padé continuation procedure for a search of exceptional points in other physical systems.

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