Coalescence of two branch points in complex time marks the end of rapid adiabatic passage and the start of Rabi oscillations

Petra Ruth Kaprálová-Ždánská¹,∗, Milan Sindelka² and Nimrod Moiseyev³,⁴

¹ Department of Radiation and Chemical Physics, Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 182 21 Prague 8, Czech Republic
² Institute of Plasma Physics, Academy of Sciences of the Czech Republic, Za Slovankou 1782/3, 182 00 Prague 8, Czech Republic
³ Schulich Faculty of Chemistry, Technion—Israel Institute of Technology, Haifa 32000, Israel
⁴ Faculty of Physics, Technion—Israel Institute of Technology, Haifa 32000, Israel

E-mail: kapralova@fzu.cz, sindelka@ipp.cas.cz and nimrod@tx.technion.ac.il

Received 30 December 2021, revised 11 May 2022
Accepted for publication 8 June 2022
Published 1 July 2022

Abstract
We study theoretically the population transfer in two-level atoms driven by chirped lasers. It is known that in the Hermitian case, the rapid adiabatic passage (RAP) is stable for an above-critical chirp below which the final populations of states Rabi oscillate with varying laser power. We show that if the excited state is represented by a resonance, the separatrix marking this critical phenomenon in the space of the laser pulse parameters emanates from an exceptional point (EP)—a non-Hermitian singularity formed in the atomic system by the fast laser field oscillations and encircled due to slow variations of the laser pulse envelope and instantaneous frequency. This critical phenomenon is neatly understood via extending the ‘slow’ time variable into the complex plane, uncovering a set of branch points which encode non-adiabatic dynamics, where the switch between RAP and Rabi oscillations is triggered by a coalescence of two such branch points. We assert that the intriguing interrelation between the two different singularities—the EP and the branch point coalescence in complex time plane—can motivate feasible experiments involving laser driven atoms.

∗Author to whom any correspondence should be addressed.
Keywords: physics of exceptional points, Dykhne–Davis–Pechukas formula, Rabi oscillations, rapid adiabatic passage, chirped laser pulses, coalescence of transition points, experimental proposal

(Some figures may appear in colour only in the online journal)

1. Introduction

Exceptional points (EPs) represent non-Hermitian degeneracies of a Hamiltonian which form branch points in the plane of external Hamiltonian parameters [1–3]. The non-Hermitian degeneracy is very different from the degeneracy in Hermitian Hamiltonians since the two corresponding eigenvectors coalesce and a self-orthogonal state is obtained. When an EP is stroboscopically encircled in the parameter plane, states are exchanged as the complex energies form Riemann surfaces. This of course sparked interest in quantum dynamics of a system which is forced to encircle EP by changing Hamiltonian parameters in time, a process called dynamical encircling and primarily addressed in the present paper.

EPs have been initially used as a mathematical concept in quantum theory [4, 5]. Their physical significance was first recognized by Berry in 1994 based on an early observation by Pancheratnam in 1955 [6, 7]. A topological structure as a basic phenomenon related to EPs was first predicted in 1998 [8] and verified experimentally in 2001 and 2003 [9, 10]. Since then EPs have been studied in many papers, see reviews [11–14]. A particular interest in the EP physics arose after 2008, when an occurrence of EP has been associated with an explanation for the breakdown of the real spectrum of parity-time (PT) symmetric non-Hermitian Hamiltonian (see references [15, 16]), which takes place in two coupled gain and loss waveguides [17]. Many experimental demonstrations of EPs in optical devices [18, 19] and laser cavities [20–23] followed. Though less often, EP phenomena in atomic and molecular physics have also been measured or proposed theoretically, notably for PT-symmetric systems designed using atomic vapor cells and optical traps [24, 25], and for isolated atoms and molecules perturbed by fields [26–30].

The present study follows up on previous theoretical studies of non-adiabatic dynamics which occurs when dynamically encircling the EP by a contour in the plane of the relevant Hamiltonian parameters. Current literature on this problem has been mainly focused on the state switching phenomenon, where the non-Hermitian components of the energies, preventing the usual application of the adiabatic theorem, induce a chiral behavior [31–36]. Recently, experimental realizations of the time-asymmetric switch phenomena were reported in waveguides [37, 38]. As a matter of fact, it would be difficult to tailor a similar experiment in the scope of atomic and molecular physics.

Here we present a different phenomenon represented by a behavior switch between Rabi oscillations and rapid adiabatic passage (RAP), which is attributed to be inherently associated with the EP encircling, see section 2. This phenomenon is even particularly suitable for an experimental realization in laser driven atoms which is the objective of sections 3 and 4. In section 3 we present a unique experimental strategy to determine the behavior switch, which as we will see is not a straightforward thing due to small variations of the measured quantity. In section 4 we enlist and discuss important requirements on suitable laser–atom systems, demonstrating the behavior switch in a full-dimensional simulation of the driven helium atom. After presenting conclusions we append a theoretical derivation of transformation between frequency and time domains for chirped laser pulses which based on Wigner phase space theory and used within this work.
2. Behavior switch between Rabi oscillations and rapid adiabatic passage

2.1. Dynamical EP encircling resulting in the behavior switch

Let us motivate our considerations by recalling the well known problem, where two bound states of an atom are coupled by a continuous wave laser. Such atoms exhibit Rabi oscillations, which appear also in the more general case of a finite pulse, where the populations of the states oscillate with integer multiples of $\pi$ of the pulse area [39]. On the other hand, a completely different kind of dynamics takes place whenever a (large enough) frequency chirp is added, which leads to the RAP [39, 40]. These facts indicate that some kind of a switch between the monotonic (RAP) and oscillatory (Rabi) behavior must occur at some critical chirp. This assumption is strongly supported by the known instability of RAP for insufficient chirping [41].

The aim of our present work is to explore the switch between the regimes of Rabi oscillations and RAP in the more general case, when the upper atomic level corresponds to a metastable resonance state. A clear cut (yet so far unreported) link between the Rabi-to-RAP switch and the EP-encircling dynamics will be subsequently highlighted.

Our Gaussian chirped pulse is defined in the time-domain by the laser strength $\varepsilon(t)$ and instantaneous frequency $\omega(t)$, such that

$$\varepsilon(t) = \varepsilon^\text{max} e^{-\left(\frac{t}{\gamma}\right)^2/2}.$$  \hspace{1cm} (1)

The two-level atom consists of one bound and one metastable state, where the transition frequency is $\omega_r$, ionization width of the metastable state is $\Gamma$, and the transition dipole moment is $\mu$. We restrict our discussion to the systems where $\mu$ is real valued.

The driven atomic system is described in the rotating wave approximation [42] by the interaction Hamiltonian

$$H(t) = \hbar \begin{bmatrix} 0 & \frac{1}{2}\Omega(t) \\ \frac{1}{2}\Omega(t) & \Delta(t) \end{bmatrix},$$  \hspace{1cm} (2)

where the time-dependence is related to the slow variation of the field frequency and amplitude within the laser pulse. $\Delta(t) = \omega(t) - \omega_r + i\Gamma/2\hbar$ stands for the dynamical frequency detuning; and $\Omega(t) = \mu\varepsilon(t)/\hbar$ is the time-dependent Rabi frequency.

Dynamical quantum state of our laser driven atom can be then described by the formula

$$\psi(t) = e^{-\frac{i}{\hbar} \int_0^t \Omega'(\tau) \Phi_-(\tau) d\tau} a_-(t) \Phi_-(t) + e^{-\frac{i}{\hbar} \int_0^t \Omega'(\tau) \Phi_+(\tau) d\tau} a_+(t) \Phi_+(t),$$  \hspace{1cm} (3)

where $\Phi_{\pm}(t)$ are the two parametrically $t$-dependent eigenvectors of the Hamiltonian (2), associated with complex eigenvalues $\epsilon_{\pm}(t)$,

$$\epsilon_{\pm}(t) = \frac{\hbar}{2} \left[ \Delta(t) \pm \sqrt{\Delta^2(t) + \Omega^2(t)} \right].$$  \hspace{1cm} (4)

If the time-dependence is omitted in equation (2), then such a Hamiltonian would describe an atom driven by a continuous wave laser, with parameters $[\omega, \varepsilon_0]$. This Hamiltonian has an EP where $\epsilon_+ = \epsilon_-$ for $\omega^{\text{EP}} = \omega_r$ and $\varepsilon^{\text{EP}} = \Gamma/2\mu$. If $t$ is taken as an adiabatic parameter in equation (2), the EP is encircled by trajectories $[\omega(t), \varepsilon(t)]$ defined by the pulse of equation (1) for $\varepsilon^{\text{max}} > \varepsilon^{\text{EP}}$, see figure 1. We assign $\Phi_-(t \to -\infty)$ to represent the field free bound state, which is initially populated, $a_-(t \to -\infty) = 1$ and $a_+(t \to -\infty) = 0$. Counterintuitively, the bound state at the end of the pulse is represented by $\Phi_+(t \to \infty)$ due to the adiabatic flip [43].
An EP is formed in a two-level atom including bound and resonance states \( \{ \varepsilon_0 = 2 \mu/\Gamma, \omega = \omega_r \} \) driven by a continuous wave laser for the well defined laser parameters \( \varepsilon_0 \). Gaussian chirped laser pulses define adiabatic encircling contours, which vary for different values of the chirp \( \alpha \) and peak strength \( \varepsilon_{\text{max}} \). The plot is based on system independent parameters, \( \bar{\alpha} \) and \( \bar{\varepsilon}_0 \) are defined below in equation (8).

Accordingly, the final population (survival probability) of the bound state \( p_b \) is given by the ratio of the coefficients in the front of \( \Phi_+ (t \to \infty) \) and \( \Phi_- (t \to -\infty) \) in equation (3), such that

\[
p_b = \left| \frac{a_+(t \to \infty)}{a_-(t \to -\infty)} \cdot e^{-\frac{i}{\hbar} \int_0^\infty dt' \left[ \varepsilon_+ (t') - \varepsilon_- (t') \right]} \right|^2.
\]  

(5)

The non-adiabatic amplitudes \( a_{\pm} (t) \) of equation (3) satisfy the close-coupled equations

\[
\dot{a}_+ (t) = -a_- (t) N(t) e^{-\frac{i}{\hbar} \int_0^t dt' \left[ \varepsilon_+ (t') - \varepsilon_- (t') \right]},
\]

\[
\dot{a}_- (t) = a_+ (t) N(t) e^{\frac{i}{\hbar} \int_0^t dt' \left[ \varepsilon_+ (t') - \varepsilon_- (t') \right]},
\]

(6)

where \( N(t) \) is the non-adiabatic coupling defined as \( \langle \Phi_+ | \partial_\tau | \Phi_- \rangle \), where the non-Hermitian \( c \)-product is used [3].

The adiabatic energies \( \varepsilon_{\pm} \) in equation (6) are complex-valued, which causes a breakdown of the adiabatic theorem [31, 34–36]. Yet, if the initial state is the less dissipative one and the excited state is the more dissipative one, an adiabatic perturbation theory is justified to solve equation (6) and express the non-adiabatic amplitudes for the encircling of EP [44]. Thus the underlying assumption for our present discussion is given by,

\[
a_{\pm} (t \to \infty) = - \int_{-\infty}^\infty dt N(t) e^{\frac{i}{\hbar} \int_0^t dt' \left[ \varepsilon_+ (t') - \varepsilon_- (t') \right]}.
\]

(7)

See our paper [45] for a detailed derivation of equation (7) and a thorough numerical verification of the convergence of the perturbation series for the system under the study here. The survival probability \( p_b \) (equation (5)) is calculated by numerically evaluating the integral equation (7) for different values of the pulse parameters. We conveniently use effective laser
parameters proposed in reference [45], which allow to describe laser induced dynamics for different atomic transitions as a single atom-independent problem. Namely, we set
\[ \theta = \frac{\tau \epsilon_{0}^{\text{max}} \mu}{\hbar} \sqrt{2\pi}, \quad \epsilon_{0} = \frac{\epsilon_{0}^{\text{max}}}{\epsilon_{0}^{\text{EP}}} = \frac{2\mu}{\Gamma}, \]
\[ \bar{\alpha} = \frac{2\hbar}{\epsilon_{0}^{\text{max}} \mu}, \] (8)
where \( \theta \) defines the temporal pulse area [39], \( \epsilon_{0} \) is the peak strength relative to the position of EP, \( \epsilon_{0}^{\text{EP}} = \Gamma/2\mu \), and \( \bar{\alpha} \) represents an effective chirp. The above definition of effective laser parameters is led by the efforts to exclude atomic characteristics such as \( \mu \) and \( \Gamma \) from the evolution equations equation (6). In fact, the pulse area \( \theta \) is known in a similar problem of bound-to-bound transitions without a chirp, where the survival and excitation probabilities depend on \( \theta \) only (in that case, the excitation probability is given by unity in the famous \( \theta = \pi/2 \) pulses [39]). \( \theta \) can be introduced also here to equation (6) via a separation of the pulse length \( \tau \) in all time-dependent variables and integrals. In reference [45] we show that this step leads to specific normalizations of the quasi-energy split \( \epsilon_{-}(t) - \epsilon_{+}(t) \) and non-adiabatic coupling \( N(t) \). The obtained normalized quantities in the case of a linearly chirped Gaussian depend only on the two remaining variables, \( \bar{\alpha} \) and \( \bar{\epsilon}_{0} \), which come out of the equations.

Importantly, figure 2 shows that \( p_{b} \) creates a unique pattern in the \( [\bar{\epsilon}_{0}, \bar{\alpha}] \) plane, where separate areas of oscillatory and monotonous behavior appear. The separatrix \( s \) demarcates between the parametric regions associated with the dynamical regimes of Rabi oscillations and RAP. This observation highlights an emergence of the critical phenomenon associated with dynamical encircling of the EP, and the main topic of this paper. At large values of \( \bar{\epsilon}_{0} \), the separatrix is nearly parallel to the \( \bar{\epsilon}_{0} \)-axis. However, as \( \bar{\epsilon}_{0} \) decreases, the separatrix becomes sharply bent towards the \( \bar{\epsilon}_{0} \)-axis, and intersects this axis at the peak strength \( \bar{\epsilon}_{0} = 1 \), which represents the position of the encircled EP, \( \epsilon_{0}^{\text{max}} = \Gamma/2\mu \). Note that the position of the separatrix is not changed for different values of the pulse area \( \theta \), but with larger \( \theta \), the density of oscillations is increased whereas the average value of \( p_{b} \) is rapidly decreased.

2.2. Coalescence of branch points in complex time

Let us move on to a theoretical explanation of the above described critical phenomenon. This will require moving to a complex plane of adiabatic time, where the change of behavior of \( p_{b} \) is related to a particular non-Hermitian singularity which is formed. Let us start with a definition of the non-adiabatic coupling \( N(t) \) [46]
\[ N(t) = \frac{1}{4i} \frac{d(\Omega/\Delta)}{dt} \left( \frac{1}{i + \Omega/\Delta} + \frac{1}{i - \Omega/\Delta} \right), \] (9)
showing that \( N(t) \) includes poles \( t_{k} \) in the complex plane of time \( t \), where \( \Omega(t_{k}) = \pm i\Delta(t_{k}) \), \( t_{k} \in C \). The poles \( t_{k} \) also represent complex degeneracies of the analytically continued Hamiltonian \( H(t_{k}) \); this becomes clear by putting the relation \( \Omega(t_{k}) = \pm i\Delta(t_{k}) \) to equation (4). Honoring the nomenclature established by Dykhne, Davis and Pechukas, Child [47–49], and others we shall refer to these points as transition points (TPs), though the nature of these points is exactly same as of the EPs. We propose to reserve the latter term to the branch points if the Hamiltonian parameters are other than time.

Let us explore now in more detail the properties of the TPs, their intimate association with the critical phenomenon shown in figure 2, and their relation to the EP. Figure 3 shows the distribution of TPs in the complex time plane for the studied two-level system driven by the
Figure 2. Survival probability $p_b$ of an initial bound state coupled to an unstable resonance by a chirped laser. The laser pulse is defined by effective parameters $\bar{\varepsilon}_0, \bar{\alpha}, \theta$ of equation (8), where the pulse area $\theta$ is held fixed, $\theta \in \{6\pi, 14\pi, 30\pi\}$. The plots are based on numerical results of the first-order perturbation approximation, equation (5). A unique switch between Rabi oscillations and RAP in the survival probability is clearly manifested. The separatrix ($s$) designates an abrupt change of behavior, which is even more profound for larger pulse areas $\theta$. The curve of $s$, however, is independent of $\theta$. It starts at $\bar{\varepsilon}_0 = 1$, which corresponds to the laser amplitude of the encircled EP ($\varepsilon_{0,\text{EP}}^{\text{max}} = \Delta \bar{\varepsilon}_0^0$), and converges asymptotically ($\varepsilon_{0,\text{EP}}^{\text{max}} \gg \varepsilon_{0}^0$) to a constant critical chirp (given by $\bar{\alpha} \to 2\sqrt{e}$ as derived in the main body of the text).

Gaussian linearly chirped pulse of equation (1). The TPs in the upper half of the complex time plane are typically represented by a pair of points near the real axis and two asymptotic sequences of other TPs which unfold within the complex plane at the angles of $\pm \pi/4$ as a gradually condensing series of points, see figure 3. We shall restrain here to a shorthand argument to explain such a distribution of the TPs. The TPs represent zeros of the quasienergy split, namely the sum of $[\Omega_2(t) + \Delta_2(t)]$, see equation (4). We seek points $t_k$ at which contributions of these two terms cancel out. Based on this requirement $\Omega_2(t_k)$ and $\Delta_2(t_k)$ must have an opposite complex phase. Equations (1) and (2) imply

$$\Omega_2(t_k) \propto \exp(-t_k^2/\tau^2),$$

$$\Delta_2(t_k) \propto (\alpha t_k + i\Gamma/2\hbar)^2.$$  

Hence, for large $k$, assuming $|\alpha| |t_k| \gg \Gamma/2\hbar$, the term $[\Omega_2(t) + \Delta_2(t)]$ vanishes iff

$$\left(\frac{t_k}{\tau}\right)^2 = k \cdot 2i\pi \pm i\pi/2 + \beta, \quad \beta \in \mathbb{R}, \quad k \in \mathbb{Z},$$  

where both $\Omega_2(t_k)$ and $\Delta_2(t_k)$ possess purely imaginary values along the progression of the $t_k$’s. Note that the TPs are fixed in the plane of dimensionless time $t/\tau$ according to equation (11) (dimensionless-time axes are also used in figure 3). The large $k$ limit formulated using effective laser parameters (equation (8)) and put together with equation (11) yields a rough estimate of the very applicability of equation (11) in the case of different laser parameters $[\bar{\varepsilon}_0, \bar{\alpha}]$, namely

$$\left|\frac{t_k}{\tau}\right| \gg \frac{2}{\alpha \bar{\varepsilon}_0} \rightarrow k \gg \frac{2}{\pi (\alpha \bar{\varepsilon}_0)^2}.$$  

Using the same argument we will show how the central pair of TPs produces a specific singularity triggering the critical phenomenon of figure 2. Namely, let us assume small values
Figure 3. TPs (▲, ●) arising in the adiabatic Hamiltonian (equation (2)) analytically continued to the complex time plane. The positions of the TPs vary with the pulse parameters $\bar{\alpha}, \bar{\varepsilon}_0$ shown by corresponding markers in the inset. Critical change of behavior of $p_N$ displayed in the inset for $\theta = 30\pi$ is associated with the coalescence of the central TPs.

of $|t_\ell|$, and set for convenience $z_k = -it_k$. Equation (10) imply then

$$\Omega^2(i z_k) \propto 1 + z_k^2/\tau^2 + \cdots,$$

$$\Delta^2(i z_k) \propto -(\alpha z_k + \Gamma/2\hbar)^2,$$

showing that $[\Omega^2(i z_k) + \Delta^2(i z_k)]$ represents approximately a quadratic polynomial. The sought central pair of TPs is determined by roots $z_{1,2}$ of this quadratic polynomial. Depending upon the laser pulse parameters, these roots $z_{1,2}$ are located either at the real axis (blue triangles of figure 2), or they penetrate into the complex $z$-plane (red bullets of figure 2). Critical transition from the real $z$-axis into the complex plane occurs then at those specific laser parameters for which $z_1 = z_2 = \bar{z}$. The degenerate case of $z_1 = z_2 = \bar{z}$ corresponds actually to coalescence of two TPs, i.e., to merging of $z_1$ and $z_2$ into a single TP $\bar{z}$ of a higher Puiseux order, such that $\epsilon_+ (iz) - \epsilon_- (iz) = O(z - \bar{z})$, where the leading square root term in the Puiseux series vanishes. (Note that this is still a second-order non-Hermitian degeneracy, as opposed to other situations where a higher Riemann-order EP is formed [50].) By implication, the coalescence point satisfies not only $[\Omega^2(t) + \Delta^2(t)] = 0$ but also $d/dt [\Omega^2(t) + \Delta^2(t)] = 0$. This problem is readily solved when exact analytical expressions for $\Omega$ and $\Delta$ (below equation (2)) are substituted to both conditions yielding

$$t^\text{coal} = it \left[ \frac{\sqrt{(\bar{\alpha}\bar{\varepsilon}_0)^{-2} + 1} - (\bar{\alpha}\bar{\varepsilon}_0)^{-1}}{2} \right]$$

(see reference [45] for a pictorial derivation of the conditions defining coalescence leading to this equation). As $t^\text{coal}$ is plugged into the equation $[\Omega^2(t^\text{coal}) + \Delta^2(t^\text{coal})] = 0$, we arrive at

$$e^{-a(\bar{\alpha}\bar{\varepsilon}_0)^2/2} \left( \frac{\bar{\alpha}}{2} a(\bar{\alpha}\bar{\varepsilon}_0) + \frac{1}{\bar{\varepsilon}_0} \right) = 1,$$

where $a = -i t^\text{coal}/\tau$, such that

$$a(\xi) = \sqrt{\frac{\xi^{-2} + 1 - \xi^{-4}}{2}}.$$
which is an implicit definition of a curve in the $[\bar{\varepsilon}, \bar{\alpha}]$ parameter plane for which the central TPs coalesce. Shortly we will prove that this equation represents the separator $s$ between Rabi oscillations and RAP in figure 2. Let us meanwhile discuss asymptotic limits of the curve $s$, as parametrized by $\xi$, which include the cases $\xi \to 0$ and $\xi \to \infty$, respectively. The former limit corresponds to the point $[\bar{\varepsilon}_0 = 1, \bar{\alpha} = 0]$, namely the point associated with the peak laser amplitude being equal to the EP (see the corresponding arrow for $\bar{\varepsilon}_0 = 1$ in figure 2). The latter limit represents the asymptotic limit $[\bar{\varepsilon}_0 \to \infty, \bar{\alpha} = 2\sqrt{\gamma}]$ which is also denoted by an arrow in figure 2. Note by passing that bound-to-bound transitions are inherently associated with the latter asymptotic limit where the separator between Rabi oscillations and RAP boils down to this single asymptotic point due to the fact that $\Gamma = 0$ and thus always $\bar{\varepsilon}_0 \to \infty$ (compare equation (8)). Yet bound-to-resonance transitions start to behave as bound-to-bound for large $\bar{\varepsilon}_0$ ($\varepsilon_{\text{max}} \gg \varepsilon_{\text{EP}}$).

Importantly, the just discussed TPs enable us to neatly explain the behavior of the time integral of equation (7) and its changes with varying laser parameters. The corresponding argument is based upon contour integration in the plane of complex time [45]. Mathematical elaborations of reference [45] provide ultimately a simple outcome. Namely, for a sufficiently large pulse area $\theta$, the pair of TPs near the real axis outweighs residual contributions of the other TPs and actually controls the value of the integral of equation (7). The fact that the central pair of TPs may acquire two different configurations in the complex time plane is of a fundamental importance for an explanation of the studied critical phenomenon reported in figure 1. If the two TPs possess nonzero real parts (bullets in figure 3), their residual contributions (given by complex exponentials) sum up into a cosine term, while if they lay on the imaginary axis (triangles in figure 3) they sum up to a single exponential term. The survival probability of equations (5) and (7) takes then the form [45]

$$p_b = \left(\frac{\pi}{3}\right)^2 \exp\left[-\frac{\theta}{\hbar \sqrt{2\pi \bar{\gamma}}}\right] \times Z(\theta, \bar{\varepsilon}_0, \bar{\alpha}), \quad (17)$$

where the term $Z$ acquires two distinct values for the two just mentioned configurations of the two central TPs. Namely, if the TPs possess nonzero real parts, then

$$Z = 4 \cos^2\left[\frac{\theta}{\hbar \sqrt{2\pi \bar{\gamma}}}\phi\right], \quad (18)$$

but if they are located on the imaginary axis then $Z = 1$. $\phi$ and $\bar{\gamma}$ are associated with the residua at the central TPs and must be obtained numerically; note that the residua and thus also $\phi$ and $\bar{\gamma}$ do not depend on the prefactor $\theta$. The regularity of oscillations and decay displayed in figure 2 indicates that $\phi$ as a function of $\bar{\varepsilon}_0$ and $\bar{\alpha}$ has a simple characteristic to which we will refer in section 3.1.

Equations (17) and (18) represent the final output of our theoretical analysis of $p_b$, and enable us to rationalize the corresponding abrupt change of the behavior of $p_b$ from the regime of Rabi oscillations to RAP, as plotted in figure 2. This Rabi-to-RAP transition occurs when crossing the separatrix $s$, which is defined by the coalescence of the two central TPs, figure 3.

Note that equations (17) and (18) are known in the literature as Dykhne–Davis–Pechukas formula [44, 47, 48, 51, 52]. We would like to mention two analytical approaches both ultimately yielding this formula as a result. First, it is possible to use the complex contour integration as proposed for avoided crossings of two real-defined coupled potential energy curves by Dykhne, Davis, and Pechukas long time ago [47, 48], while proving an approximate applicability of such an integration to dissipative states [44, 51, 52]. Nevertheless, below we briefly
Figure 4. First order perturbation approximation to survival amplitude (equation (7)) is analyzed based on complex contour integration. The complex contour (thick solid line) has to encircle poles and branchcuts which are associated with the TPs (▲, •) as the TPs represent both poles and branchpoints. In order to eliminate a diverging behavior of the integrand along the complex contour, the branchcuts must coincide with ‘equivalue lines’ where the integral over imaginary part of the quasienergy split is given by zero, 
\[ \int_{t_{k}}^{t} \left[ \epsilon_{+}(t') - \epsilon_{-}(t') \right] dt' = 0 \]
(equivalence lines not being used to define any branchcut are displayed as dotted curves). Two qualitatively different complex contours are required by the distinct distributions of the central TPs, leading to two different analytical results for the survival amplitudes, predicting Rabi oscillations in one case, while RAP in the other. Note that the complex contours displayed here have been proposed recently in reference [45].

introduce other possible approach, elaborated recently in reference [45], where integration contours are proposed with regard to the dissipative nature of the excited state.

Different distributions of the central TPs require two distinct integration contours which are shown in figure 4 to solve equation (7). The contours encircle the TPs \textit{and} branchcuts—the former as poles of the non-adiabatic coupling \( N(t) \) and the latter because of a discontinuity of quasienergies \( \epsilon_{\pm}(t) \) implied by the presence of the branchpoints. Note that the complex contours follow special curves (‘equivalue lines’ [48]) defined such that imaginary part of the integral over quasienergy split starting at a TP \( (t_{k}) \) is given by zero,

\[ \text{Im} \int_{t_{k}}^{t} \left[ \epsilon_{+}(t') - \epsilon_{-}(t') \right] dt' = 0. \quad (19) \]

Namely, only if condition equation (19) is met, the exponential term in equation (7) represents a non-diverging oscillatory phase factor, allowing for an integration. It is implied that branchcuts must be also chosen to coincide with one of the equivalence lines. Typically, a triplet of different equivalence lines is associated with each TP as marked in figure 4.

As a result of this procedure, the sought integral equation (7) is rewritten as a sum of residual and branchcut contributions by separate TPs. A branchcut contribution \( b_{k} \) represents a result of the contour integration along the two opposite sides of the branchcut associated with the given TP. In the ‘classical limit’ \( \theta \rightarrow \infty \), which is characterized by fast oscillations of the exponential part of the integrand (equation (7)), getting yet faster along the branchcut as the distance from the TP is increased, the only significant contribution to \( b_{k} \) comes from the infinitesimal neighborhood of the TP. One can thus observe a striking similarity between the
branchcut and residual \( (r_k) \) contributions:

\[
\begin{align*}
\frac{N(t \to tk)}{\pi 6} \exp \left\{ -\frac{i}{\hbar} \int_{0}^{\infty} \text{d}t' \left[ \epsilon_-(t') - \epsilon_+(t') \right] \right\}, \\
\lim_{\theta \to \infty} b_k = \left( -\right)^n \frac{\pi 6}{\pi} \exp \left\{ -\frac{i}{\hbar} \int_{0}^{\infty} \text{d}t' \left[ \epsilon_-(t') - \epsilon_+(t') \right] \right\}. \tag{20}
\end{align*}
\]

We observe a non-trivial sign alteration of the prefactors; \( z_k \) represents a sign of non-adiabatic coupling at the given pole, namely \( N(t \to tk) = z_k/4i(t - tk) \) which can be derived \([45]\); \( n \) represents an integer number which defines which one from the triplet of the equivalence lines is associated with the branchcut. Finally, \( \Delta_n \) is a difference between the numbers denoting equivalence lines of the outgoing and incoming integration contour, respectively, between which the complex integration contour encircles a particular pole (TP). For example, in the case of full circles around the pole, \( \Delta_n = 3 \), while if \( 1/3 \) of the circle is accomplished by the integration contour (such as the in the case of central TPs for the RAP integration contour, figure 4), \( \Delta_n = 1 \).

Above we indicated that infinitely many TPs contributing within the complex contour integrations boil down to only two central points in the classical limit which ultimately leads to the Dykhne–Davis–Pechukas formula. Let us be more specific. The magnitude of the TP contributions given by \( r_k \) and \( b_k \) is controlled by the exponential term, i.e. by the imaginary part of the integral within, equation (20). In the case of the Gaussian pulse (equation (1)), where we know analytical expressions for the quasienergies \( \epsilon_\pm \) (equation (4)), we are able to derive an analytical estimate for the integral defining \( r_k \) and \( b_k \) (equation (20)) in the limit of large \( k \), namely:

\[
\text{Im} \int_{0}^{\infty} \text{d}t' \left[ \epsilon_-(t') - \epsilon_+(t') \right] \propto 2k + \frac{1}{2}. \tag{21}
\]

Though we will not give here a comprehensive derivation of this expression which is found in reference \([45]\), we shall briefly outline the logic behind it; the major contribution to the integral comes from integration over the asymptotic regions of \( t' \to tk \), where the quasienergy split \( \epsilon_-(t') - \epsilon_+(t') \propto \sqrt{\Omega^2(t') + \Delta^2(t')} \) is prevailed by the term \( \Delta(t') \) and therefore it may be roughly approximated as

\[
\epsilon_-(t') - \epsilon_+(t') \propto t'. \tag{22}
\]

(We use the fact that \( \text{Im} t' < |\text{Re} t'| \) due to the applicability of equation (11) to the complex phase of \( t_k \), and likewise \( |\text{Re} t'| \gg 0 \), which is applicable in the asymptote of large \( k \). Then the exponential term \( \Omega^2(t') \propto \exp(-t'^2/2) \to 0 \) and thus \( \Delta^2(t') \propto (\alpha t' + i\Gamma/2\hbar)^2 \) prevails in the definition of the quasienergy split, compare equation (10).) Now we substitute the asymptotic expression equation (22) for the quasienergy split on the left-hand side of equation (21) and get

\[
\text{Im} \int_{0}^{\infty} \text{d}t' \left[ \epsilon_-(t') - \epsilon_+(t') \right] \propto \text{Im} \int_{0}^{\infty} \text{d}t' t' \propto \text{Im}(t_k^2). \tag{23}
\]

An asymptotic expression for \( t_k \) (\( k \to \infty \)) has been given in equation (11), from where \( \text{Im} t_k^2 \propto 2k + 1/2 \), by which equation (21) is proved.

Equation (21) demonstrates that the contributions of the TPs, \( r_k, b_k \) given in equation (20), exponentially decrease with increasing \( k \). Yet we did not explain the role of the classical limit
\( \theta \to \infty \) in the applicability of the Dykhne–Davis–Pechukas formula. The key here is to define a dimensionless integral over the quasienergy split \((\phi_k + i \gamma_k)\) such that

\[
\int_0^{\gamma_k} dt \left[ \epsilon_-(t') - \epsilon_+(t') \right] = \tau \int_0^{\gamma_k/\tau} \frac{d}{d} \left[ \epsilon_-(t) - \epsilon_+(t) \right]
\]

\[
\equiv \frac{\mu t_{e\max}}{\hbar} (\phi_k + i \gamma_k) = \frac{\theta}{\hbar \sqrt{2\pi}} (\phi_k + i \gamma_k),
\] (24)

where it can be verified that \(\phi_k\) and \(\gamma_k\) depend no more on the pulse area \(\theta\) but only on the laser parameters \(\xi_0\) and \(\alpha\) (equation (8)), \(\phi_k = \phi_k(\xi_0, \alpha), \gamma_k = \gamma_k(\xi_0, \alpha)\). Now we can see that the magnitudes of the TPs contributions given by \(r_k\) and \(b_k\) (equation (20)) decrease exponentially with \(k\) and the pulse area \(\theta\) as well. Thus in the semiclassical limit, defined by \(\theta \to \infty\), the central TPs \((k = 0)\) contributions are infinitely larger than contributions of the remaining TPs \((k > 0)\).

Finally, the contributions of the central TPs sum up yielding the Dykhne–Davis–Pechukas formula, equations (17) and (18). The central TPs contributions are defined by equation (20) which we rewrite using the functions \(\phi_k, \gamma_k\) defined in equation (24) such that

\[
r_k = -\Delta_k \frac{\pi \sqrt{2}}{6} \exp \left[ \frac{\theta}{\hbar \sqrt{2\pi}} (i\phi_k - \gamma_k) \right],
\]

\[
\lim_{\theta \to \infty} b_k = (-)^n \frac{\pi \sqrt{2}}{6} \exp \left[ \frac{\theta}{\hbar \sqrt{2\pi}} (i\phi_k - \gamma_k) \right].
\] (25)

In the case of the central TPs \(k = \pm 0\), where \(\pm\) just indicates the fact that we deal with two distinct points (the pair of central TPs). Let us start with the distribution of the TPs as displayed in figure 4(a) (Rabi oscillations). Importantly, the sign of \(b_k\) in equation (20) is equal for both contributing TPs (a proof is beyond the scope of this paper and can be found in reference [45]). We substitute \(\Delta_k = 3\) in the definition of \(r_k\) as long as a full circle around the each pole (TP) is accomplished by the integration contour (figure 4(a)). Putting this together, we obtain the pre-exponential factor \((-z_k \pi / 3)\) for the overall contribution \((r_k + b_k)\) of each one of the TPs. The complex exponentials in equation (25) are mutually complex conjugated for the two TPs which is a result of the apparent time-symmetry, see figure 3 while a thorough discussion is given in reference [45]. Thus the two TPs sum up to the cosine term as found in equation (18) with the pre-exponential factor given by \((2\pi / 3)\); the survival probability \(p_k\) is obtained from here using equation (5) which implies an additional normalization, thus \(\gamma_k\) has been replaced by \(\tilde{\gamma}_k\) in equation (17) such that

\[
\tilde{\gamma}_k = \frac{\sqrt{2\pi}}{\theta} \text{Im} \int_{-\infty}^{\gamma_k} dt \left[ \epsilon_-(t') - \epsilon_+(t') \right],
\] (26)

where the lower bound of the integral has been changed from 0 for \(\gamma_k\) to \(-\infty\) for \(\tilde{\gamma}_k\).

Let us now compare this result with the case of the other distribution of TPs as displayed in figure 4(b) (RAP). Interestingly, the contribution of the upper central TP is an identical zero. Namely, the contributions of the branchcut and the parts of the integration contour directing upwards (figure 4(b)) together with the two thirds of the residuum mutually cancel out due an interplay of signs \((-)^n\) in equation (20)). Thus the survival amplitude is determined by the single remaining TP, the point near the real axis in figure 4(b). The pre-exponential factor of its overall contribution \((r_k + b_k)\) is obtained by substituting \(\Delta_k = 3\) and \((-)^n = 1\) into equation (20), and is given by \((-z_k \pi / 3)\). A single contributing TP cannot lead to the interference phenomenon which occurred in the case of Rabi oscillations; as a result, the oscillatory
behavior is ceased while the pre-exponential factor is lowered by a factor of 1/2 due to only one contributing TP. This in accord with the setting $Z = 1$ for the case of RAP as defined above around equations (17) and (18).

3. Proposal of experimental realization of Rabi-to-RAP switch

3.1. Analytical fit for the oscillatory term in the survival probability

Let us provide a more detailed discussion of Rabi oscillations, for which the key is represented by the function $\phi$, see equation (18), where $\phi$ is obtained via numerical integration,

$$
\phi(\varepsilon_0, \alpha) = \frac{\sqrt{2\pi}}{\theta} \Re \int_0^{t_0} dt \left[ \epsilon_-(t) - \epsilon_+(t) \right],
$$

(27)

where $t_0$ represents one of the central TPs for the distribution associated with Rabi oscillations, $t_0 \in \mathcal{C}$, figure 4(a), and is found also numerically. Such numerical calculations have been performed and adapted to the form of an analytical function in reference [45]. For this sake, the parameter space coordinates $[\varepsilon_0, \alpha]$ were replaced by $[R, \Phi]$, more natural to the found numerical behavior. Namely, $R$ has been defined as

$$
R = e^{-A^2/2} \cdot (Y \sqrt{e} A + X),
$$

(28)

where

$$
X = \frac{1}{\varepsilon_0}, \quad Y = \frac{\alpha}{2\sqrt{e}},
$$

(29)

and

$$
A = \frac{1}{2\sqrt{e}} \left( \sqrt{(\tan \Phi)^2 + 4e} - \tan \Phi \right), \quad \Phi = \arctan \frac{X}{Y},
$$

(30)

Equations (28)–(30) are no unknown to us here. We have derived the separator curve in equations (15) and (16), which represents a clear basis for the present definition assuming $R = 1$. Thus $R$ represents an effective distance, a generalized radius, on the $[X, Y]$-plane from the origin $[X = 0, Y = 0]$, where the condition

$$
R = 1,
$$

(31)

defines the separator $s$, wherefore analytical expression for $R$ in equations (28)–(30) is found as a coalescence of zeros (TPs) of the quasi energy split for a Gaussian linear chirp.

The precise numerical fit as taken from reference [45] reads as follows:

$$
\frac{\phi}{\hbar} = -\sqrt{\frac{\pi}{2}} + \sqrt{\frac{\pi}{2}} \sum_{k=1}^{4} a_k R^k
$$

$$
+ b_0 \left[ \left( 1 - \frac{2\Phi}{\pi} \right)^3 + \frac{b_1}{b_0} \right]^{1/3} \sin \left[ \pi R \left( 1 + \frac{8c_0\Phi}{\pi}(R - 1) \right) \right],
$$

(32)

where the dependence on the quasi-radius $R$ given by $a_1 = 0.5129$, $a_2 = 1.2477$, $a_3 = -1.1912$, and $a_4 = 0.4307$ dominates over a mild angular dependence on $\Phi$ given by $b_0 = 0.1093$, $b_1 = 0.03569$, and $c_0 = 0.0912$. This result is illustrated in figure 5 which
Figure 5. The survival probability $p_b$ is displayed as a function of the reciprocal relative intensity ($X$-axis, $X = 1/\varepsilon_0$) and effective chirp ($Y$-axis, $Y = \alpha/2\sqrt{\varepsilon}$), while the temporal pulse area $\theta$ is fixed on a given value (see above the frames). The values of the survival probability $p_b$ are indicated by the shadow-scale (color-scale online) displayed in the bottom. We define generalized radius $R$ as a relative distance from the coordinate center to the separator which occurs for $R = 1$, see the labeled equivalue lines. This figure represents a numerical demonstration of the fact that the wavefronts of Rabi oscillations are approximately given by the equivalue lines of $R$.

displays survival probability $p_b$ as function of $X$ and $Y$. In particular, wavefronts of Rabi oscillations approximately coincide with equivalue lines of $R$, demonstrating that the angular dependence is not prominent.

We aim even yet at a simpler expression for $\phi$ in order to explain our new ideas to detect the Rabi-to-RAP switch in an experiment. Apparently, we are interested in the physical interval of the quasi-radius $R$, $0 \leq R \leq 1$. The value of $\phi$ for $R = 1$ is given by zero, in particular the sum
of coefficients \( a_k \) is given by unity. One can find that a frequency of Rabi oscillations at \( R \),

\[
\frac{1}{\hbar} \frac{d \phi}{dR} = \sqrt{\frac{\pi}{2}} \sum_{k=1}^{4} k a_k R^{k-1},
\]

(33)
is quite close to unity for most of the interval \( 0 \leq R \leq 1 \). This fact allows us to get the sought simple approximation such that,

\[
\frac{1}{\hbar \sqrt{2\pi}} \phi \approx -\frac{1}{2} (1 - R).
\]

(34)

Equation (34) leads to an approximate analytical expression for the term \( Z \) defining Rabi oscillations in equations (17) and (18) such that

\[
Z \propto \cos^2 \left( \theta \cdot \frac{R - 1/2}{2} \right).
\]

(35)
The applicability of equation (35) is confirmed in figure 5 which clearly indicates that survival probability oscillates with a constant Rabi frequency along the quasi-radius \( R \), whereas the Rabi frequency is increased with the pulse area \( \theta \).

3.2. Using infinite pulse area limit to find the separator

In this section we study behavior of Rabi oscillations as function of temporal pulse area \( \theta \). First we compare different panels of figure 5 which illustrate the effect of a gradual increase of the temporal pulse area. The nodes (white spaces in the graphs) get more condensed with \( \theta \) being increased. The node closest to the separator \( s \) seems to approach and merge with the separator line the limit \( \theta \to \infty \). Below we give a prove that this is indeed the case, and even that the same applies to the other subsequent nodes, which all drift towards the separator \( s \) along with increasing \( \theta \).

In order to study oscillations of survival probability \( p_b \) as function of the temporal pulse area \( \theta \) we choose a two-dimensional frame of laser pulse parameters defined by \([x, y]\) such that

\[
x = \sqrt{\frac{2\pi}{\theta}}, \quad y = \frac{\delta \omega}{2}, \quad \delta \omega = \text{const.}
\]

(36)

where \( \delta \omega \) represents a frequency width of the laser pulse. \( \delta \omega \) is used here to fully define the chirped laser pulse instead of the laser strength \( \bar{\varepsilon}_0 \), see equation (1). \( \delta \omega \) has the meaning of frequency interval obtained when the chirped laser pulse defined in equation (1) is Fourier transformed from the time to energy domain, see appendix. \( \delta \omega \) is related to \( \bar{\varepsilon}_0 \) through the equation

\[
\left( \frac{\delta \omega}{\Gamma \bar{\varepsilon}_0} \right)^2 = 2\pi \left( \frac{1}{\bar{\varepsilon}_0} \right)^2 + \left( \frac{\delta \omega}{2} \right)^2,
\]

(37)

which shows that the laser pulse intensity \( \bar{\varepsilon}_0 \) is represented by the reciprocal radius \( 1/r \) in the coordinate system \([x, y]\) such that

\[
\bar{\varepsilon}_0 = \frac{2\delta \omega}{\Gamma} \cdot \frac{1}{r}, \quad r = \sqrt{x^2 + y^2}.
\]

(38)

Survival probability within coordinates \([x, y]\) is displayed in figure 6, where different panels correspond to different frequency widths \( \delta \omega \). The figures show that nodes of Rabi oscillations...
Figure 6. This figure demonstrates the intriguing phenomenon that zeros of Rabi oscillations (marked by magenta curves online) converge and cross in a single point if the frequency width $\delta_{\omega}$ of the chirped pulses is fixed. The crossing point also marks a critical change of behavior, as it lies on the separator $s$ between the regions of Rabi oscillations (below $s$) and RAP (above $s$). Note that as the ratio between the pulse frequency width and the resonance width is varied, the crossing point is represented by different points $[\bar{\alpha}_s, \bar{\epsilon}_s]$ on the separator $s$ (compare figure 2). This characteristic behavior of the zeros is proposed as a suitable experimental means to determine the values $[\bar{\alpha}_s, \bar{\epsilon}_s]$ by an extrapolation of the curves of the zeros starting at accessible regions $p_b > 0.001$ to $x = 0$. Here, the survival probability $p_b$ is displayed as a function of the reciprocal pulse area ($x$-axis, $x = \sqrt{2\pi/\theta}$) and effective chirp ($y$-axis, $y = \bar{\alpha}/2$), where the values of the survival probability are indicated by the shadow-scale (color-scale online) displayed in the bottom right. The value of the frequency width $\delta_{\omega}$ of the pulse is provided above the figures where we give its relative value with respect to the resonance width $\Gamma$ of the excited state.

converge into a single point $[x = 0, y = y_0]$, where this phenomenon takes place for every possible value of $\delta_{\omega}$. The crossing of nodal lines occurs for $x = 0$ which represents the asymptotic limit of the temporal pulse area $\theta$, see equation (36). This fact partially supports our previous considerations based on figure 5 where we assumed that the lines of nodes merge with the separator at the limit $\theta \to \infty$. Let us prove that the crossing point $[0, y_0]$ is indeed found on the separator.

The nodal lines of Rabi oscillations are defined based on equation (35) such that

$$1 - R = x \cdot (1 - 2n) \sqrt{\frac{\pi}{2}} \quad n \in \mathbb{Z},$$

(39)
where \( n \) indicates a particular node and \( R \), defined via equations (28)–(30), is a function of coordinates \( x \) and \( y \) defined in equation (36) such that,

\[
R = 2y \cdot \sqrt{\frac{\xi^2 + 1}{2\xi}} e^{-\frac{\sqrt{\xi^2 + 1}}{2\xi}}. \tag{40}
\]

where

\[
\xi = \frac{4\delta\omega y}{\Gamma}. \tag{41}
\]

\( R \) can be also expressed using a power series of \( \xi \) such that

\[
R \approx y \sqrt{e} \left( 1 + \frac{3}{2} \xi^{-1} + \frac{7}{8} \xi^{-2} + O(\xi^{-3}) \right), \tag{42}
\]

which we will use below to explore the effect of magnitude of the pulse frequency width \( \delta\omega \) on the studied phenomenon.

The first panel in figure 6 illustrates the situation where the pulse frequency width \( \delta\omega \) is far larger than the resonance width \( \Gamma \), namely the ratio of \( \delta\omega/\Gamma \) is as high as 100. This special case represents the limit \( \xi \to \infty \), see equations (41) and (42), where

\[
R \approx y \sqrt{e}. \tag{43}
\]

By substitution of this limiting expression for \( R \) into equation (39) we obtain equations for different nodes \( n \) in the \([x, y]\) plane such that

\[
y = \sqrt{e} - x \cdot (2n - 1) \sqrt{\frac{\pi e}{2}}, \quad n \geq 1. \tag{44}
\]

The fact that \( y \) is linearly dependent on \( x \) is in agreement with the shape of nodes shown in the first panel in figure 6. The curves for different nodes, \( y^{(n)} \), intersect at the point \([x = 0, y^{(0)} = y_0 = \sqrt{e}]\).

Next panel in figure 6 displays the situation where the ratio \( \delta\omega/\Gamma \) is still relatively high being equal to 10. The nodes are still linear but the point of intersection is clearly shifted to a smaller value, \( y_0 < \sqrt{e} \). The shift of \( y_0 \) from the asymptotic value \( \sqrt{e} \) can be derived using the first order expansion of \( R \) based on equations (42) and (41) which is given by,

\[
R \approx y \sqrt{e} \left( 1 + \frac{3}{2} \Gamma^{-1} \delta\omega \right) = \frac{y \sqrt{e}}{\sqrt{e} \delta\omega} \approx \frac{y \sqrt{e}}{\sqrt{e} \delta\omega} \left( 1 + \frac{3}{8} \delta\omega \right). \tag{45}
\]

This expression for \( R \) is substituted to equation (39) which defines the nodes and we obtain

\[
y \approx \sqrt{e} - x \cdot \frac{(1 - 2n) \sqrt{\frac{\pi e}{2}}}{1 + \frac{3}{8} \delta\omega \sqrt{e}} \tag{46}
\]

which shows that the nodal lines in the \([x, y]\) plane remain linear within the first order approximation of \( R \). From here we obtain also the negative shift of the crossing point \( y_0 \) by setting \( x = 0 \) such that

\[
y_0 \approx \sqrt{e} \left( 1 + \frac{3}{8} \delta\omega \right)^{-1} < \sqrt{e}. \tag{47}
\]
As the ratio $\Gamma/\delta\omega$ is even larger, see the third to sixth panels in figure 6, the nodal lines deviate from linearity but we can derive the meaning of the intersecting point $y_0$ in this general case simply by substitution of $x = 0$ to equation (39). Equation (39) shows immediately the fact that nodal curves intersect at criticality, i.e. for $R = 1$, compare equation (31) and the text along with. The value of $y_0$ in the intersection $[x = 0, y = y_0]$ is obtained from the condition $R = 1$ applied to equation (40), where we substitute $y = r$ in the definition of $\xi$ in equation (41).

We find,

$$y_0 = \frac{\xi}{\sqrt{\xi^2 + 1}} e^{\sqrt{\xi^2 + 1} - 1}, \quad \xi = \frac{4\delta\omega}{\Gamma}.$$

Let us summarize; we have just proved that nodal planes of the oscillatory structure in the three-dimensional space of pulse parameters given by temporary pulse area, effective chirp, and frequency width of the pulse, or any other equivalent set of three parameters, collapse into the separator $s$ in the infinite temporal pulse area limit $\theta \to \infty$. This remarkable phenomenon is apparent for survival probability $p_b$ being shown as a function of reciprocal temporal pulse area ($x = \sqrt{2\pi/\theta}$) and effective chirp ($y = \bar{\alpha}/2$) when frequency width of the pulse $\delta\omega$ is held fixed as shown in figure 6. Note that nodal lines of the oscillating survival probability can be found experimentally in this frame, as long as amplitudes of $p_b$ are relatively large in the major part of the $[x, y]$ space, see the scale given below the last frame in figure 6. We refer to this fact when giving our suggestions for experiment below.

3.3. Experimental proposal to localize the critical change of behavior — separator (step 1)

Let us explain how this phenomenon can be applied experimentally. The goal would be to measure the point $[x = 0, y = y_0]$ experimentally and by knowing that this point is a part of the separator $s$, find the corresponding pulse parameters in the $[\bar{\alpha}, \bar{\varepsilon}_0]$ plane which are related to $y_0$ through equations (36) and (38) such that

$$\bar{\alpha}^s = 2y_0, \quad \bar{\varepsilon}_0^s = \frac{2\delta\omega}{\Gamma} \frac{1}{y_0}.$$

Up to now we viewed the problem within the reduced frame, see equation (8), which is also used to define the $[x, y]$ plane. In a practical experimental setup, however, the reduced pulse parameters cannot be applied as long as the transition moment $\mu$ is considered unknown. Therefore system dependent parameters $[x_\mu, y_\mu]$ will be used instead of $[x, y]$ such that

$$x_\mu = \frac{h}{\tau \varepsilon_0^\max}, \quad y_\mu = y \mu = \frac{2h\alpha \tau}{\varepsilon_0^\max}.$$

Note that $x_\mu$ and $y_\mu$ depend on the usual pulse parameters such as peak amplitude $\varepsilon_0^\max$, pulse length $\tau$, and pulse chirp $\alpha$, equation (1).

It is assumed that survival probability $p_b$ will be measured throughout the parametric plane $[x_\mu, y_\mu]$ while frequency width of the pulse $\delta\omega$ will be held fixed. In a realistic experimental setup, chirped laser pulses are often designed by using grating mirrors applied to an original non-chirped pulse, where as a result the frequency spread of the pulse remains the same but the pulse length and peak amplitude are modified. Thus $\delta\omega$ will be naturally defined by the pulse length prior to its chirping, while $x_\mu$ and $y_\mu$ will be varied via the chirp magnitude and field amplitude.

Nodal lines measured in $[x_\mu, y_\mu]$ for a given fixed value $\delta\omega$ will allow to determine the crossing point at $[x_\mu = 0, y_\mu]$. Using different values of the pulse frequency width $\delta\omega$, the function
$\gamma_0(\delta_s)$ shall be obtained from the spectroscopic measurements. From here the separator $s$ can be obtained up to the system dependent scaling via the transition moment $\mu$. The separator is measured in the following form,

$$\bar{\alpha}_\mu(\delta_s) = 2\gamma_0(\delta_s), \quad \varepsilon_{\text{max}}^{(s)} = \frac{\delta_\mu}{\gamma_0(\delta_s)},$$  \hspace{1cm} (51)$$

where $\bar{\alpha}_\mu$ is a system dependent pulse parameter related to the effective chirp $\bar{\alpha}$ such that

$$\bar{\alpha}_\mu = \bar{\alpha} = 2\hbar \alpha \tau \varepsilon_{\text{max}}^{(s)}.$$  \hspace{1cm} (52)$$

Now let us discuss what we expect from this type of measurement. First, it is expected that the separator would display a curvature as the laser amplitude gets near EP, $\varepsilon_{\text{max}}^{(s)} \approx \varepsilon_{\text{EP}}^{(s)}$, where the separator should be found bent towards $\bar{\alpha}_s \to 0$ exactly as predicted in figure 2. Bending of the separator is associated with a small ratio between the pulse frequency width $\delta_\omega$ and resonance width $\Gamma$, $\delta_\omega/\Gamma \lesssim 1$, which is shown in the lower panels in figure 6. On the opposite side, as $\delta_\omega/\Gamma > 1$, $\gamma_0(\delta_s)$ approaches the asymptotic value of $\varepsilon_{\text{EP}}^{(s)}$ from below, see equation (47) and upper panels of figure 6. This regime corresponds with the asymptotic part of the separator $s$, where variations of $\varepsilon_{\text{max}}^{(s)}$ (as long as $\varepsilon_{\text{max}}^{(s)} \gg \varepsilon_{\text{EP}}^{(s)}$) do not affect the critical chirp, $\bar{\alpha}_\mu \approx \text{const.}$, see figure 2.

An experimental verification of this indicated general shape of the separator would provide clear fingerprints of time-symmetric dynamical encircling of EP in frequency-amplitude domain as shown in figure 1.

3.4. Method for experimental verification of the asymptotes of the separator (step 2)

Up to now we have shown how the separator can be measured, while the weight of our argument lies on agreement between a measured and the predicted shape of the separator. An additional experimental approval of the theoretical predictions regarding the separator $s$ would represent a verification of its asymptotes for $\bar{\alpha}_\mu \to 0$ and $\varepsilon_{\text{max}}^{(s)} \to \infty$. In the theoretical prediction they correspond with the quantities $\varepsilon_{\text{EP}}^{(s)}$ and $\mu \sqrt{\tau}$, respectively, which calls for a verification using another experimental method.

Let us propose a measurement of Rabi oscillations where the chirp is not present as such an independent method. The oscillations of survival probability $p_b$ in equation (17) are given by the term $Z$ for which we derived the approximate form equation (35). Now, as the chirp is not present, $R$ is replaced by $X = 1/\varepsilon_0$, see equations (28)–(30). The oscillatory term $Z$ then reads such that

$$Z \propto \cos^2 \left[ \frac{\theta}{2} \left( \frac{1}{\varepsilon_0} - 1 \right) \right].$$  \hspace{1cm} (54)$$

From here, the zeros of $Z$ (corresponding to zeros of survival probability $p_b$ measured for zero chirp) are defined as

$$\theta = (2n + 1) \frac{\pi}{1 - 1/\varepsilon_0}. \hspace{1cm} (55)$$

\hspace{1cm}
Let us substitute for the relative variables $\theta$ and $\varepsilon_0$ using realistic pulse parameters, equation (8). We obtain a theoretical prediction for the zeros on the survival probability $p_b$ given by,

$$
\varepsilon_0^{\max}(n) = \varepsilon_0^{EP} + (2n + 1) \frac{\sqrt{2\pi} \hbar}{2\tau \mu}, \quad \varepsilon_0^{\max}(n) \geq \varepsilon_0^{EP},
$$

(56)

assuming that the pulse length $\tau$ is fixed while field amplitude $\varepsilon_0$ is varied. Note again that equation (56) represents a theoretical prediction for Rabi oscillations when $E_P$ is encircled, i.e. the field amplitude $\varepsilon_0^{\max}$ must be beyond $\varepsilon_0^{EP}$, see figure 1.

We propose to use equation (56) first to determine transition dipole moment $\mu$ from experimental measurement of the periods of Rabi oscillations such that

$$
\mu = \frac{\sqrt{2\pi} \hbar}{\tau \Delta \varepsilon_0^{\max}}, \quad \Delta \varepsilon_0^{\max} = \varepsilon_0^{\max}(n + 1) - \varepsilon_0^{\max}(n).
$$

(57)

Using equation (8) one can prove that the period $\Delta \varepsilon_0^{\max}$ corresponds to the change of temporal pulse area by $\Delta \theta = 2\pi \hbar / \tau \mu$. This phenomenon has been found for bound-to-bound transitions (which correspond with our theory as $\varepsilon_0^{EP} \to 0$) where it has been studied in coherent control [39]. This phenomenon is now found general to bound-to-resonance transitions as well.

Though we do not know the exact equation for the survival probability $p_b$ below $\varepsilon_0^{EP}$, we do know that $p_b$ is not oscillatory there. Therefore the position of the first zero on $p_b$ is given by

$$
\varepsilon_0^{\max}(n = 0) = \varepsilon_0^{EP} + \frac{\sqrt{2\pi} \hbar}{2\tau \mu}
$$

(58)

according to equation (56). Let us see what this equation says about the first zero in bound-to-bound transitions where $\varepsilon_0^{EP} = 0$. It shows the remaining term $\sqrt{\pi/2} \hbar / \tau \mu$ which corresponds to the temporal pulse area $\theta = \pi$, see equation (8). Such pulse is used to be called the $\pi$-pulse in coherent control, where it is used as a method to obtain a maximum transition to the excited state, see reference [39]. As we can see immediately, the first zero of $p_b$ in bound-to-resonance transitions is shifted exactly by $\varepsilon_0^{EP}$, i.e. beyond the encircled $E_P$. After determining the period of Rabi oscillations in the step above one can determine also $\varepsilon_0^{EP}$ using this new theoretical prediction.

Here we outlined an independent experimental method exploring Rabi oscillations of bound-to-resonance transitions without a chirp to determine the transition dipole moment $\mu$ and the position of the EP $\varepsilon_0^{EP}$. This method is independent on the measurement of the separator $s$ described above as there is no search for the critical change of behavior (Rabi-to-RAP) in this method.

The two experimental methods are meant to be used in conjunction: first the critical change of behavior (Rabi-to-RAP) should be measured using the direct method described in section 3.3 where the general shape and limits of the separator $s$ for $\alpha_0 \to 0$ and $\varepsilon_0^{\max(s)} \to \infty$ should be determined. Then these limits, theoretically predicted as given by the quantities $\varepsilon_0^{EP}$ and $\mu \sqrt{\tau}$, respectively, should be compared with measurements of $\varepsilon_0^{EP}$ and $\mu$ based on the Rabi oscillations where chirp is not applied as described in this section.

4. Requirements on suitable atomic systems and laser pulses

4.1. Real valued transition moment—using absorption line profiles

Our above pursued elaborations assumed that the atomic transition moment $\mu$ is real valued, which is assured for any bound-to-bound transition. In bound-to-resonance transitions, the
transition dipole moment is generally complex. It is uniquely defined as [30]

\[ \mu = \sqrt{(1_L | x | 2_R)(2_L | x | 1_R)}, \] (59)

where \((L)\) and \((R)\) denotes left and right eigen-vectors [3] of the field-free states denoted by numbers \((1, 2)\) which are involved in the transition. This definition of transition dipole moment assures symmetry of the two-by-two Floquet Hamiltonian (equation (2)).

Pick et al [30] demonstrated that the complex phase of \(\mu\) is directly related to a spectral shift of the resonance absorption line, the so called Fano profile, also understood as a result of an interference between quasi-bound state and free-particle scattering amplitudes [53]. We reassume here the corresponding asymmetric shifted absorption line profile

\[ S(\omega) \propto \frac{(\omega - \omega_r + q \Gamma/2)^2}{(\omega - \omega_r)^2 + (\Gamma/2)^2}, \] (60)

where \(q\) is an asymmetry parameter. For \(q = 0\) a symmetric Lorentzian profile is obtained with maximum for \(\omega = \omega_r\). Otherwise the absorption peak is shifted from \(\omega_r\), while the line profile is asymmetric. Based on results of reference [30], \(q\) is directly related to the complex phase of the transition dipole moment \(\mu\) such that

\[ q = \frac{\cos \phi - 1}{\sin \phi} \approx \phi, \quad \phi = \arctan \frac{\text{Im} \mu^2}{\text{Re} \mu^2}. \] (61)

This excursion indicates an interrelation between the symmetry of absorption line profiles and obtaining time-symmetric EP encircling using Gaussian chirped pulses. It leaves us with a simple experimental method to determine whether a given bound-to-resonance transition would demonstrate the Rabi-to-RAP switch or not. Such an experimental tool would be particularly useful in situations where precise non-Hermitian theoretical calculations of transition dipole moments do not exist (which is still the case even for larger atoms).

4.2. Isolated two level system—a full dimensional numerical simulation for the helium atom

Physical relevance of the studied phenomenon of the switch between Rabi oscillations and RAP, relies on the assumption that the two coupled levels are sufficiently decoupled from the rest of atomic levels. Allow us therefore approve the proposed phenomenon in a realistic system for which direct (numerically exact) non-perturbative computations of \(p_\theta\) may be simply performed.

We choose a specific class of bound-to-resonance transitions in the helium atom, which is derived from the ionic bound-to-bound transitions,

\[ \text{He}^+(1s)(S) \rightarrow (\text{He}^+)^+(2p)(P), \] (62)

where instead of the ion we assume a neutral Rydberg atom, where the electron is added to a Rydberg orbital \((np)\):

\[ \text{He}^+(1snp)(P) \rightarrow (\text{He})^{++}(2pnp)(S, D). \] (63)

The doubly excited atom is an autoionization resonance which would spontaneously decay to the ionized atom:

\[ (\text{He})^{++}(2pnp)(S, D) \rightarrow \text{He}^+(1s)(S) + e^-. \] (64)
Figure 7. These figures demonstrate the qualitative and even semi-quantitative applicability of the presented analytical solution obtained using a number of approximations, starting from the two level approximation through the first order perturbation method down to the long pulse limit, to a real atomic system, which is represented here by a full dimensional simulation of the helium atom interacting with the laser field. The symbols (▲, •, ■) represent results from numerical simulations using a basis set of 184 field-free helium states, which are coupled by the interaction with the classically approximated field.

These transitions are characterized by almost real valued transition dipole moment. We pick up the transition He\(^{+}\)(1s2p) → He\(^{++}\)(2p\(^2\)) where the transition dipole moment \(\mu\) is given by 
\[
\mu = 0.763643 + 0.0001i.
\]

Numerical method for quantum dynamics of the helium atom in the presence of chirped laser pulse has been described in references [36, 54], here we present particular parameters for the simulations, namely 184 field-free states of helium forming the basis set included the bound states, quasi-discrete continuum (He\(^{+}\)(1s) + e\(^-\)), and the resonances above the first ionization threshold (see reference [55]). The diameter of the space sampled using the ExTG5G primitive Gaussian basis set reached up to 40 Å. The complex scaling parameter was set to \(\vartheta = 0.4\).

The initial state for the simulation is represented by the He\(^{+}\)P (1s2p) state. This state is coupled by the XUV pulse with the central wavelength \(\lambda = 30.322\) nm with the doubly excited resonance He\(^{++}\)S (2p\(^2\)) with the lifetime of \(\tau = 0.11\) ps. The results of the multidimensional simulations displayed in figure 7 represent an evidence that equations (17) and (18) are valid to a good approximation. The sought effect, where the oscillatory behavior changes due to the coalescence of the TPs in the complex plane of adiabatic time, is clearly present in the full-dimensional case.

Let us briefly comment also on the experimental feasibility of the predicted phenomenon in the helium atom. The pulse peak intensity reaches up to 4 TW/cm\(^2\) and the pulse length
reaches up to 5 ps in this case, where these quantities are correlated to obtain the particular laser parameters $\bar{\alpha}, \bar{\varepsilon}_0, \theta$. Such pulses are generally available today. Below we add a discussion of precision demands for frequency, which are high in this case of XUV range.

4.3. Precision demands on the carrier frequency of the Gaussian chirps

The presented phenomenon requires the mean laser frequency being equal to the real energy difference between the two involved field free states. Here we provide a numerical simulation of the system including a static detuning of the laser frequency. The pulse would be modified such that

$$\varepsilon_0(s\tau) = \frac{2\mu}{\Gamma} \bar{\varepsilon}_0 e^{-s^2/2}, \quad \omega(s\tau) = \omega_r + \Delta_\omega + \bar{\alpha} \bar{\varepsilon}_0 s^2 \frac{\mu^2}{\hbar^2}, \quad (65)$$

where $\Delta_\omega$ is a static detuning. If $\Delta_\omega$ is non-zero then the time-symmetry of the energy split is broken. This fact implies that the opposite TPs in the complex adiabatic-time plane (figure 3) are shifted from their original symmetrical layout and therefore the interference phenomenon which is responsible for Rabi oscillations is less efficient, i.e. the oscillatory minima are not exact zeros. An impact of asymmetry due to static detuning is illustrated in figure 8 which has been obtained by solving equation (7) numerically for detuned laser pulses.

Figure 8 shows that nodes of the Rabi oscillations are not so well pronounced but at the same time they stay in place (are not shifted) in the $1/\bar{\varepsilon}_0 - \bar{\alpha}$ plane as a detuning is introduced. From the experimental point of view this means that there is a certain tolerance for the precision of
the carrier frequency $\omega_r$. Based on simulations which are presented in figure 8 we define the tolerance factor $f_p$ which defines the detuning with respect to the resonance lifetime such that

$$\Delta_\omega = f_p \Gamma / \hbar,$$

(66)

where $f_p$ represents the factors 0.01, 0.1, and 0.2 in the panels of figure 8. Let us consider the value of $f_p = 0.1$ as the precision requirement. When this requirement is put in terms of wavelength, the demand on wavelength precision is given by

$$\Delta_\lambda = f_p \cdot \frac{\lambda^2 \Gamma}{4\pi \hbar c}.$$

(67)

According to this formula, for the helium transition which was suggested above, the detuning in an experiment should not exceed $\Delta_\lambda = 0.4$ pm. In other systems where the wavelength of transitions would be in the IR range such as 800 nm, achieving the Rabi-to-RAP phenomenon would be possible with much lesser precision of the carrier frequency of 0.1 nm when about the same resonance width $\Gamma$ is assumed.

5. Conclusions

We have shown that, in particular atomic bound-to-resonance transitions, the dynamical encircling of an EP is manifested by a critical switch between oscillatory and monotonic behavior of the occupancy $p_b$ of the initial atomic bound state. We rationalize this phenomenon theoretically as a consequence of coalescence of TPs (branchpoints of the adiabatic Hamiltonian in complex time plane). Such an intriguing interconnection between EPs and TPs has not yet been discussed in this context of laser driven atoms.

The studied critical phenomenon lends itself well to an experimental realization in driven atoms using linearly chirped Gaussian pulses. We propose a suitable experimental method how the critical change of behavior can be directly localized in the parameter space of the linearly chirped Gaussian pulses. The critical change of behavior defines a typical separating line between the oscillatory and monotonic areas in the pulse parameter space. The starting point of the separator in the pulse parameter space is identical with the laser amplitude associated with the EP in the encircling (frequency–laser amplitude) plane.

Experimental demonstration of the presented phenomenon would represent a novel way how to detect fingerprints of the encircled EP in laser driven atoms and even allow for a direct measurement of the EP position in the encircling space.

Acknowledgments

The work was financially supported in parts by the Czech Ministry of Education, Youth and Sports (Grant LTT17015), the Grant Agency of the Czech Republic (Grant 20-21179S) (PRK and MS), and by the Israel Science Foundation Grant No. 1661/19 (NM).

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).
Appendix A. Linearly chirped Gaussian pulses

A.1. Gaussian pulse chirping based on group velocity dispersion

The practical way of constructing chirped pulse is by using a frequency decomposition of a non-chirped laser pulse, where individual frequencies go through a different path length, after which they are assembled back. The difference between the length of paths for frequencies is given by the group velocity dispersion. The relation between the group velocity dispersion and the chirp is derived here.

Let us define the laser pulse before chirping such that

\[ f(t) = \varepsilon_{0}^{\text{max}} \exp \left( -\frac{t^2}{2\tau_0^2} + i\omega_0 t \right), \tag{A.1} \]

where \( \omega_0 \) represents the carrier frequency, and \( \tau_0 \) represents the pulse length before chirping. By applying the Fourier transform of \( f(t) \) we obtain the frequency distribution of such a pulse given by

\[ \tilde{f}(\omega) = \varepsilon_{0}^{\text{max}} \delta(\omega) \exp \left[ -\frac{(\omega - \omega_0)^2}{2\delta_\omega^2} \right], \tag{A.2} \]

where \( \delta_\omega \) represents the frequency width related to the pulse length \( \tau_0 \) such that

\[ \delta_\omega = \frac{\hbar}{\tau_0}. \tag{A.3} \]

The same pulse can be also defined in the mixed time-energy domain via the Wigner distribution [56–58] (as a Fourier transform over the density matrix \( f^*(t - t'/2)f(t + t'/2) \) over the correlation coordinate \( t' \)) such that

\[ f_w(\omega, t) = \frac{(\varepsilon_{0}^{\text{max}})^2 \tau_0}{\sqrt{\pi}} \exp \left[ -\frac{t^2}{\tau_0^2} - \frac{(\omega - \omega_0)^2}{\delta_\omega^2} \right]. \tag{A.4} \]

General properties of the Wigner distribution [58] assure that

\[ |f(t)|^2 = \int d\omega f_w(\omega, t), \tag{A.5} \]
\[ |\tilde{f}(\omega)|^2 = \int dt f_w(\omega, t). \tag{A.6} \]

The practical way how the chirping is usually done is by imposing the time shift between different frequency components. Mathematically this means that the time \( t \) is replaced by a function related to the frequency component \( \omega \) via the group dispersion velocity \( \nu_{\text{GDV}} \),

\[ t \rightarrow t + \nu_{\text{GDV}}(\omega - \omega_0), \tag{A.7} \]
in equation (A.4). The Wigner distribution for the chirped pulse $g_w$ is then obtained,

$$g_w(\omega, t) = \left( \frac{\varepsilon_{\text{max}}^2 \tau_0}{\sqrt{\pi}} \right) \exp \left[ -\frac{[t + \nu_{\text{GVD}}(\omega - \omega_0)]^2}{\tau_0^2} - \frac{(\omega - \omega_0)^2}{\delta_\omega^2} \right].$$  \hspace{1cm} (A.8)

The chirping does not change the frequency profile of the pulse as one could prove by applying equation (A.6) to the definition of $g_w$ in equation (A.8). The time-profile, on the other hand, is modified which one can see by applying a few algebraical steps on equation (A.8) such that:

$$g_w(\omega, t) = \left( \frac{\varepsilon_{\text{max}}^2 \tau_0}{\sqrt{\pi}} \right) \exp \left[ -\frac{t^2}{\tau_0^2} \gamma^2 + \gamma^2 \left[ \frac{\omega}{\gamma_0^2} \frac{\omega - (\omega_0 + \nu_{\text{GVD}} t)}{\delta_\omega^2} \right]^2 \right],$$  \hspace{1cm} (A.9)

where

$$\gamma^2 = 1 + \frac{\nu_{\text{GVD}}^2}{\tau_0^4}. \hspace{1cm} (A.10)$$

The time-profile of the chirp remains Gaussian with the new pulse length $\tau$, 

$$\tau = \tau_0 \gamma, \hspace{1cm} (A.11)$$

which one can prove by integrating equation (A.9) with respect to $\omega$ based on equation (A.5).

Next we transform the Wigner distribution $g_w$ back to the complex definition of the pulse in the time-domain, which will be denoted as $g(t)$ in order to obtain the chirp $\alpha$, which is defined as the gradient of the complex phase:

$$\omega_0 + \alpha \cdot t = \frac{d \arg g(t)}{dt},$$  \hspace{1cm} (A.12)

The complex phase of the original pulse $f(t)$ (given by $\omega_0$, equation (A.1)) shall differ from that of the new pulse $g(t)$ due to the modification of the pulse ($f \rightarrow g$) via the group velocity dispersion $\nu_{\text{GVD}}$. The right-hand side of equation (A.12) is readily obtained from the Wigner distribution as

$$\frac{d \arg g(t)}{dt} = \int d\omega \omega g(\omega, t).$$  \hspace{1cm} (A.13)

From here we obtain the linear time dependence defining the chirp,

$$\alpha = \frac{\nu_{\text{GVD}}}{\nu_{\text{GVD}}^2 + \tau_0^4}. \hspace{1cm} (A.14)$$

### A.2. Relations between parameters of Gaussian linearly chirped pulses

The definitions that we derived above, in particular equations (A.10) and (A.11) and equation (A.14) help us to derive further relations between different parameters of the Gaussian linearly chirped pulses. Equations (A.10) and (A.11) are combined such that

$$\tau^2 \tau_0^2 = \tau_0^4 + \nu_{\text{GVD}}^2. \hspace{1cm} (A.15)$$

By putting together equations (A.15) and (A.14) we obtain a simple relation for the group velocity dispersion such that

$$\nu_{\text{GVD}} = \frac{\tau^2 \tau_0^2 - \tau_0^4}{\alpha}. \hspace{1cm} (A.16)$$
This definition is substituted back to equation (A.15) where we obtain a relation between chirp, pulse length, and the pulse length of the original pulse such that,

\[ \tau^2 = \tau_0^2 (1 + \tau^4 \alpha^2). \]  

(A.17)

The pulse length of the original pulse \( \tau_0 \) is related to the frequency width \( \delta_\omega \) (equation (A.3)) which is identical for the original and chirped pulses, see equation (A.8) and the text below. Thus using equations (A.17) and (A.3) we obtain a relation between the frequency width of a chirped pulse and the pulse length \( \tau \) and the chirp \( \alpha \) as follows,

\[ \delta_\omega^2 = \hbar^2 \tau^{-2} (1 + \alpha^2 \tau^4). \]  

(A.18)

A.3. Relation between effective parameters of Gaussian linearly chirped pulse

Effective parameters of Gaussian linearly chirped pulse defined in equation (8) allowed us to derive general equations for phenomena related to the symmetric EP encircling quantum dynamics of any two level system. Equation (A.18) can be rewritten in terms of the effective pulse variables \( \bar{\alpha} \) and \( \theta \) (equation (8)) such that

\[ \left( \frac{\delta_\omega}{\Gamma \bar{\varepsilon}_0} \right)^2 = 2\pi \left( \frac{1}{\theta} \right)^2 + \left( \frac{\bar{\alpha}}{2} \right)^2, \]  

(A.19)

where we first substituted for \( \alpha \) in equation (A.18),

\[ \alpha = \frac{\bar{\alpha}}{2} \frac{\varepsilon_{0}^\text{max}}{\tau} \frac{\mu}{\hbar}, \]  

(A.20)

and then for \( \tau \) using \( \theta \),

\[ \tau = \theta \frac{\hbar}{\varepsilon_{0}^\text{max} \mu \sqrt{2\pi}}. \]  

(A.21)

and finally for \( \varepsilon_{0}^\text{max} \) using

\[ \varepsilon_{0}^\text{max} = \bar{\varepsilon}_0 \frac{\Gamma}{2\mu}. \]  

(A.22)

ORCID iDs

Petra Ruth Kaprálová-Zdánšká https://orcid.org/0000-0002-3448-1469
Milan Sindelka https://orcid.org/0000-0003-3370-7507
Nimrod Moiseyev https://orcid.org/0000-0001-6001-4322

References

[1] Kato T 1966 Perturbation Theory for Linear Operators (Berlin: Springer)
[2] Berry M V 2004 Physics of nonhermitian degeneracies Czech. J. Phys. 54 1039
[3] Moiseyev N 2011 Non-Hermitian Quantum Mechanics (Cambridge: Cambridge University Press)
[4] Heiss W D 1970 Analytic continuation of a Lippmann–Schwinger kernel Nucl. Phys. A 144 417
[5] Moiseyev N and Friedland S 1980 Association of resonance states with the incomplete spectrum of finite complex-scaled Hamiltonian matrices Phys. Rev. A 22 618
[6] Berry M 1994 Pancharatnam, virtuoso of the Poincare sphere: an appreciation Curr. Sci. 67 220
https://scholar.google.com/scholar?q=Berry+M+V+1994+Pancharatnam%2C+virtuoso+of+the+Poincare+sphere%3A+an+appreciation+Curr.+Sci.+67+220-3
[7] Zienau S 1976 Collected works of S Pancharatnam Phys. Bull. 27 265
[8] Heiss W D, Müller M and Rotter I 1998 Collectivity, phase transitions, and exceptional points in open quantum systems Phys. Rev. E 58 2894
[9] Dembowski C, Gräf H-D, Harney H L, Heine A, Heiss W D, Rehfeld H and Richter A 2001 Experimental observation of the topological structure of exceptional points Phys. Rev. Lett. 86 787
[10] Dembowski C, Dietz B, Graf H D, Harney H L, Heine A, Heiss W D and Richter A 2003 Observation of a chiral state in a microwave cavity Phys. Rev. Lett. 90 034101
[11] Rotter I 2009 A non-Hermitian Hamilton operator and the physics of open quantum systems J. Phys. A: Math. Theor. 42 153001
[12] Rotter I and Bird J P 2015 A review of progress in the physics of open quantum systems: theory and experiment Rep. Prog. Phys. 78 114001
[13] Heiss W D 2012 The physics of exceptional points J. Phys. A: Math. Theor. 45 444016
[14] Miri M-A and Alu A 2019 Exceptional points in optics and photonics Science 363 7709
[15] Bender C M and Boettcher S 1998 Real spectra in non-Hermitian Hamiltonians having PT symmetry Phys. Rev. Lett. 80 5243
[16] Berry M V and Uzdin R 2011 Slow non-Hermitian cycling: exact solutions and the Stokes phenomenon J. Phys. A: Math. Theor. 44 435302
[33] Berry M V 2011 Optical polarization evolution near a non-Hermitian degeneracy J. Opt. 13 115701
[34] Gilary I, Mailybaev A A and Moiseyev N 2013 Time-asymmetric quantum-state-exchange mechanism Phys. Rev. A 88 010102
[35] Graefe E M, Mailybaev A A and Moiseyev N 2013 Breakdown of adiabatic transfer of light in waveguides in the presence of absorption Phys. Rev. A 88 033842
[36] Kapralova-Zdanska P R and Moiseyev N 2014 Helium in chirped laser fields as a time-asymmetric atomic switch J. Chem. Phys. 141 014307
[37] Doppler J et al 2016 Dynamically encircling an exceptional point for asymmetric mode switching Nature 537 76
[38] Xu H, Mason D, Jiang L and Harris J G E 2016 Topological energy transfer in an optomechanical system with exceptional points Nature 537 80
[39] Vitanov N V, Halfmann T, Shore B W and Bergmann K 2001 Laser-induced population transfer by adiabatic passage techniques Ann. Rev. Phys. Chem. 52 763
[40] Tannor D J 2007 Introduction to Quantum Mechanics—A Time-Dependent Perspective (Mill Valley, CA: University Science Books)
[41] Malinovsky V S and Krause J L 2001 General theory of population transfer by adiabatic rapid passage with intense, chirped laser pulses Eur. Phys. J. D 14 147
[42] Allen L and Eberly J H 1987 Optical Resonance and Two-Level Atoms (New York: Dover)
[43] Lefebvre R, Atabek O, Sindelka M and Moiseyev N 2009 Resonance coalescence in molecular photodissociation Phys. Rev. Lett. 103 123003
[44] Dridi G, Guerin S, Jausslin H R, Viennot D and Jolicard G 2010 Adiabatic approximation for quantum dissipative systems: formulation, topology, and superadiabatic tracking Phys. Rev. A 82 022109
[45] Kapralova-Zdanska P R 2022 Complex time method for quantum dynamics when an exceptional point is encircled in the parameter space Ann. Phys. 443 168939
[46] Shore B W 2008 Coherent manipulations of atoms using laser light Acta Phys. Slovaca 58 243
[47] Dykhne A M 1962 Adiabatic perturbation of discrete spectrum states Sov. Phys. - JETP 14 941 https://scholar.google.com/scholar?q=Dykhne+A+M+1962+Adiabatic+perturbation+of+discrete+spectrum+states+Sov.+Phys.-JETP+14+941-3
[48] Davis J P and Pechukas P 1976 Nonadiabatic transitions induced by a time-dependent Hamiltonian in the semiclassical/adiabatic limit: the two-state case J. Chem. Phys. 64 3129
[49] Child M S 1979 Semiclassical effects in heavy-particle collisions Adv. At. Mol. Phys. 14 225–80
[50] Am-Shallem M, Kosloff R and Moiseyev N 2015 Exceptional points for parameter estimation in open quantum systems: analysis of the Bloch equations New J. Phys. 17 113036
[51] Schilling R, Vogelsberger M and Garanin D A 2006 J. Phys. A: Math. Gen. 39 13727
[52] Dridi G and Guérin S 2012 J. Phys. A: Math. Theor. 45 185303
[53] Fano U 1961 Effects of configuration interaction on intensities and phase shifts Phys. Rev. 124 1866
[54] Kapralova-Zdanska P R, Smydke J and Civis S 2013 Excitation of helium Rydberg states and doubly excited resonances in strong extreme ultraviolet fields: full-dimensional quantum dynamics using exponentially tempered Gaussian basis sets J. Chem. Phys. 139 104314
[55] Kapralova-Zdanska P R and Smydke J 2013 Gaussian basis sets for highly excited and resonance states of helium J. Chem. Phys. 138 024105
[56] Wigner E 1932 On the quantum correction for thermodynamic equilibrium Phys. Rev. 40 749–59
[57] Hillery M, O’Connell R F, Scully M O and Wigner E P 1984 Distribution functions in physics: fundamentals Phys. Rep. 106 121
[58] Lee H-W 1995 Theory and application of the quantum phase-space distribution functions Phys. Rep. 259 147