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Nonadiabatic transitions for a decaying two-level system: geometrical and dynamical contributions

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Abstract

We study the Landau–Zener problem for a decaying two-level system described by a non-Hermitian Hamiltonian, depending analytically on time. Use of a super-adiabatic basis allows us to calculate the survival probability P in the slow-sweep limit, without specifying the Hamiltonian explicitly. It is found that P consists of a 'dynamical' and a 'geometrical' factor. The former is determined by the complex adiabatic eigenvalues $E_{\pm}(t)$, only, whereas the latter solely requires the knowledge of $\alpha_{\pm}(t)$, the ratio of the components of each of the adiabatic eigenstates. Both factors can be split into a universal one, depending only on the complex level crossing points, and a nonuniversal one, involving the full time dependence of $E_{\pm}(t)$ and $\alpha_{\pm}(t)$. This general result is applied to the Akulin–Schleich model where the initial upper level is damped with damping constant γ. For analytic power-law sweeps we find that Stückelberg oscillations of P exist for γ smaller than a critical value γ_c and disappear for $\gamma > \gamma_c$. A physical interpretation of this behaviour will be presented by use of a damped harmonic oscillator.

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

1. Introduction

In many cases one can reduce the quantum behaviour of a system to that of a two-level system (TLS), which corresponds to a (pseudo-)spin one half. The spin-down and spin-up states will be denoted by $|1\rangle$ and $|2\rangle$, respectively. If the TLS is in state $|\Psi_0\rangle$ at time t_0 one obtains $|\Psi(t)\rangle$ by solving the Schrödinger equation

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle \tag{1}$$

with initial condition $|\Psi(t_0)\rangle = |\Psi_0\rangle$. Note that we allow for an explicit time dependence of H. One of the quantities of particular interest is the survival probability

$$P = \lim_{t\to\infty} \lim_{t_0\to-\infty} |\langle\Psi(t_0)|\Psi(t)\rangle|^2 \tag{2}$$

that the system remains in its initial state. For a TLS with a level spacing depending linearly on time the result for P as a function of the sweep rate v has been derived approximately by Landau [1] and Stückelberg [2] and rigorously by Zener [3] and Majorana [4]. P will depend sensitively on the t-dependence of H and cannot be calculated analytically, except in limiting cases only. One of them is the adiabatic limit. In this limit it is known that $|\Psi(t)\rangle$ converges to a superposition of the adiabatic states $|u_{0,\pm}(t)\rangle$ which are solutions of the eigenvalue equation:

$$H(t)|u_{0,\pm}(t)\rangle = E_\pm(t)|u_{0,\pm}(t)\rangle \tag{3}$$

with $E_\pm(t)$ the adiabatic eigenvalues. Although $E_+(t)$ and $E_-(t)$ may not cross in real time (avoided level-crossing) this will happen for complex times t_c^k, $k = 1, 2, \ldots, N$.

In the case of a *real-symmetric* Hamiltonian matrix $\langle\nu|H(t)|\nu'\rangle$, $\nu, \nu' = 1, 2$ which is analytic in t and for a single crossing point t_c in the upper complex t-plane ($\mathrm{Im}\, t_c > 0$) it was shown by Dykhne [5] (see also earlier work by Pokrovskii *et al* [6]) that

$$P \cong \exp[-2\,\mathrm{Im}\, z(t_c)] \tag{4}$$

in the adiabatic limit. The new variable $z(t)$ is given by

$$z(t) = \int_0^t \mathrm{d}t'[E_+(t') - E_-(t')]. \tag{5}$$

Davis and Pechukas [7] have performed an exact proof of result (4), (5). Particularly, these authors have proven that the pre-exponential factor equals 1. Therefore, it is sometimes called the Dykhne–Davis–Pechukas (DDP) formula. For more than one crossing point with $\mathrm{Im}\, z_c^k = \mathrm{Im}\, z\big(t_c^k\big) > 0$ a generalization of (4) has been suggested [7, 8] and tested by Suominen and co-workers ([9] and references where-in). A rigorous proof of the generalization of DDP formula including even *Hermitian* Hamiltonians has been provided by Joye *et al* [10]. More than one crossing point leads to interferences which generate oscillations in P as a function of control parameters, like the sweeping rate (see below).

For Hamiltonian matrices which are not real-symmetric, but Hermitian, Berry [11] and Joye *et al* [12] made an interesting observation which is that P obtains also a 'geometrical' factor besides the 'dynamical' one, equation (4), where the former also depends on the crossing points t_c^k, only. For those who are less familiar with this kind of physics let us explain the choice of this nomenclature. Below we will see that one of the factors of P is entirely determined by the adiabatic eigenvalues and the other by the adiabatic eigenstates. Since the former is important for the time evolution it is called 'dynamical' whereas the latter is related to the geometry in the Hilbert space, particularly through a condition for parallel transport (equation (21)), and accordingly it is called 'geometrical'.

TLS will be influenced by their environment, e.g. by phonons. The spin–phonon coupling leads to dissipation of the (pseudo-)spin dynamics which will influence the probability P. Although there exist microscopic models for the spin–boson system [13, 14], and simplified models where the bath is described by fluctuating fields [15–19], we will use a dissipative Schrödinger equation. This will be achieved by using a *non-Hermitian* Hamiltonian for the TLS. A particular version of such a model has been suggested by Akulin and Schleich [20]. In their model, called AS model in the following, the upper level (at the initial time t_0) experiences a damping (see section 3).

The survival and transition probability for non-Hermitian TLS Hamiltonians has already been investigated by Moyer [21]. This has been done by mapping the original differential equation to the Weber equation, which can be solved exactly. By use of the Weber equation as the appropriate 'comparison equation' it was shown how the DDP formula, equations (4) and (5), can be extended [21]. However, this extension does not contain a 'geometric' contribution, although one expects that it exists similarly to what has been proven for Hermitian matrices [11, 12]. On the other hand, Garrison and Wright [22] have investigated the geometrical phase for dissipative systems but not the non-adiabatic transition probability.

It is one of our main goals to derive a generalized DDP formula in the adiabatic limit containing a 'geometrical' and a 'dynamical' contribution for a *general* non-Hermitian TLS Hamiltonian. We will demonstrate that both contributions consist of a universal and a non-universal part. The former depends only on the complex crossing points whereas the latter requires the knowledge of the complete time dependence of H. Instead of using a 'comparison equation' we apply the concept of a *superadiabatic* basis, put forward by Berry [23], to non-Hermitian TLS Hamiltonians. As a result, we will find that the 'dynamical' contribution to the survival probability is determined by the complex, adiabatic eigenvalues $E_{\pm}(t)$ only. The corresponding 'geometrical' part solely requires the knowledge of $\alpha_{\pm}(t)$), the ratio of the components of each of the *adiabatic* eigenstates.

A second motivation is the application of our results to the AS model. It has been shown that the survival probability P does not depend on the damping coefficient γ of the upper level, provided the bias of the TLS varies *linearly* in time, and the coupling Δ between both levels is time-independent [20]. Therefore, it is interesting to investigate *nonlinear* time dependence and to check whether or not P remains insensitive on γ. For nonlinear time dependence more than one complex crossing points may occur, such that interference effects can govern the dependence of P on the sweeping rate [10]. Specific examples with $\gamma = 0$ for which this happens were discussed in recent years [9, 14, 24]. There it was found that critical values for the sweeping rate exist at which the survival probability vanishes, i.e. complete transitions occur between both quantum levels. Consequently, one may ask: are these oscillations reduced or even suppressed in the presence of damping? The authors of [14] have studied interference effects (Stückelberg oscillations) due to phase changes between two resonances of the diabatic levels. In the adiabatic limit they have also shown, e.g. for a non-dynamical environment of TLS, by numerical computation that the oscillations are reduced and that their amplitude exhibits a non-monotonic dependence on the system–environment coupling strength. The same has been found for a dynamical environment (spin–phonon model) but restricted to the fast sweep limit.

Our paper is organized as follows. The next section will contain the general treatment of the non-Hermitian Hamiltonian and the presentation of the generalized DDP formula. In section 3, we will apply the results from the second section to the AS model with power law time dependence. The results for the AS model for power law sweeps can be interpreted by the dynamics of a damped harmonic oscillator. This will be shown in section 4. A short summary and some conclusions are given in the final section.

2. General formula for survival probability

In this section, we will derive a generalized DDP formula for the non-adiabatic transition problem of a decaying TLS. The Hamiltonian can be represented as follows,

$$H(\delta t/\hbar) = \frac{1}{2}\sum_{j=1}^{3} B_j(\delta t/\hbar)\sigma_j \tag{6}$$

with σ_j, the Pauli matrices and B_j a time-dependent field. $\delta > 0$ is the adiabaticity parameter. Because this model should be dissipative, at least one of the B_j must contain a nonzero imaginary part. Accordingly H is non-Hermitian. In the following we will assume that B_j is analytic in t. Introducing a new time variable

$$\tau = \delta t/\hbar \tag{7}$$

equation (1) becomes

$$\mathrm{i}\delta d_\tau|\Psi(\tau)\rangle = H(\tau)|\Psi(\tau)\rangle, \tag{8}$$

where $d_\tau = \partial/\partial\tau$. $|\Psi(\tau)\rangle$ can be expanded with respect to $|\nu\rangle$

$$|\Psi(\tau)\rangle = \sum_{\nu=1}^{2} c_\nu(\tau)|\nu\rangle. \tag{9}$$

With $|\Psi(\tau_0)\rangle$, the initial state, its survival probability is

$$P \equiv P(\delta) = \lim_{\tau\to\infty}\lim_{\tau_0\to-\infty}|\langle\Psi(\tau_0)|\Psi(\tau)\rangle|^2. \tag{10}$$

Note that P is the survival probability with respect to the *diabatic* basis. With respect to the *adiabatic* basis P is the nonadiabatic transition probability.

To calculate P for $\delta \ll 1$ we introduce the *adiabatic basis* of $H(\tau)$. This can be done as in [22] where a biorthonormal set of right-eigenstates was used or alternatively by use of left- and right-eigenstates. We will use the latter, as it turns out to be more elegant. Let

$$|u_{0,\pm}(\tau)\rangle = \sum_{\nu=1}^{2} e_\pm^\nu(\tau)|\nu\rangle \tag{11}$$

be the adiabatic *right*-eigenstates. They are solutions of

$$H(\tau)|u_{0,\pm}(\tau)\rangle = E_\pm(\tau)|u_{0,\pm}(\tau)\rangle \tag{12}$$

with $E_\pm(\tau)$, the adiabatic eigenvalues. Note that $E_\pm(\tau)$ are complex in general and that the norm of $|u_{0,\pm}(\tau)\rangle$ and of $|\Psi(\tau)\rangle$ is *not* conserved, since $H(\tau)$ is non-Hermitian. Following Berry [23], we introduce a hierarchy of *superadiabatic* right-eigenstates $|u_{n,\pm}(\tau)\rangle, n = 0, 1, 2, \ldots$, and expand the solutions $|\Psi_\pm(\tau)\rangle$ of equation (8) with respect to the superadiabatic basis:

$$|\Psi_\pm(\tau)\rangle = \exp\left[-\frac{\mathrm{i}}{\delta}\int_{\tau_0}^{\tau}\mathrm{d}\tau' E_\pm(\tau')\right]\sum_{m=0}^{\infty}\delta^m|u_{m,\pm}(\tau)\rangle. \tag{13}$$

Substituting $|\Psi_\pm(\tau)\rangle$ into equation (8) yields the recursion relations

$$[H(\tau) - E_\sigma(\tau)]|u_{0,\sigma}(\tau)\rangle = 0, \quad \sigma = \pm \tag{14}$$

$$\mathrm{i}d_\tau|u_{m-1,\sigma}(\tau)\rangle = [H(\tau) - E_\sigma(\tau)]|u_{m,\sigma}(\tau)\rangle, \qquad m \geqslant 1. \tag{15}$$

Equation (14) is already fulfilled, due to equation (12). To make progress we introduce the adiabatic *left*-eigenstates

$$\langle\tilde{u}_{0,\sigma}(\tau)| = \sum_{\nu=1}^{2}\tilde{e}_\sigma^\nu(\tau)\langle\nu| \tag{16}$$

which are solutions of

$$\langle\tilde{u}_{0,\sigma}(\tau)|H(\tau) = E_\sigma(\tau)\langle\tilde{u}_{0,\sigma}(\tau)| \tag{17}$$

and are normalized such that

$$\langle\tilde{u}_{0,\sigma}(\tau)|u_{0,\sigma'}(\tau)\rangle = \delta_{\sigma\sigma'}. \tag{18}$$

Let

$$\alpha_\sigma(\tau) = \frac{e_\sigma^2(\tau)}{e_\sigma^1(\tau)} \tag{19}$$

be the ratio of the components of the adiabatic right-eigenstate $|u_{0,\sigma}(\tau)\rangle$. Then it is straightforward to prove that

$$\tilde{e}_\sigma^\nu(\tau) = \frac{\sigma}{[\alpha_+(\tau) - \alpha_-(\tau)]e_\sigma^1(\tau)} \begin{cases} -\alpha_\mp(\tau), & \nu = 1 \\ 1, & \nu = 2 \end{cases} \tag{20}$$

which defines the left-eigenstate from the right-eigenstate. Multiplication of equation (15) for $m = 1$ with $\langle\tilde{u}_{0,\sigma}(\tau)|$ leads to

$$\langle\tilde{u}_{0,\sigma}(\tau)|d_\tau|u_{0,\sigma}(\tau)\rangle \equiv 0, \qquad \sigma = \pm. \tag{21}$$

This is the condition for 'parallel transport' [11, 25] now generalized to non-Hermitian Hamiltonians.

In order to solve recursion (15) we expand $|u_{m,\sigma}(\tau)\rangle, m \geqslant 1$ with respect to $|u_{0,\sigma}(\tau)\rangle$:

$$|u_{m,\sigma}(\tau)\rangle = a_m^\sigma(\tau)|u_{0,-}(\tau)\rangle + b_m^\sigma(\tau)|u_{0,+}(\tau)\rangle. \tag{22}$$

Substitution of equation (22) into equation (15) and multiplying by $\langle\tilde{u}_{0,\sigma}(\tau)|$ yields with equations (14), (18) for $m \geqslant 1$:

$$\dot{a}_{m-1}^-(\tau) = -\kappa_-(\tau)b_{m-1}(\tau) \tag{23}$$

$$\dot{b}_{m-1}^-(\tau) = -\kappa_+(\tau)a_{m-1}^-(\tau) - \mathrm{i}[E_+(\tau) - E_-(\tau)]b_m^-(\tau), \tag{24}$$

where $\dot{}$ denotes the derivative with respect to τ and

$$\kappa_\sigma(\tau) = \langle\tilde{u}_{0,\sigma}(\tau)|d_\tau|u_{0,-\sigma}(\tau)\rangle \tag{25}$$

are the nonadiabatic coupling functions, responsible for the nonadiabatic transitions. If $\kappa_\sigma(\tau) \equiv 0$, we get from equations (23) and (24)

$$a_m^-(\tau) \equiv a_m^-(\tau_0), \qquad b_m^-(\tau) = \frac{\mathrm{i}}{E_+(\tau) - E_-(\tau)}\dot{b}_{m-1}^-(\tau). \tag{26}$$

Similar equations follow for $a_m^+(\tau), b_m^+(\tau)$, which however will not be needed. Next we fix the initial condition for $|\Psi_\sigma(\tau)\rangle$:

$$|\Psi_\sigma(\tau_0)\rangle = |u_{0,\sigma}(\tau_0)\rangle, \tag{27}$$

i.e., we start in the adiabatic right-eigenstates. From equations (13), (22) we find immediately for $\sigma = -$

$$\begin{aligned} &a_0^-(\tau) \equiv 1, \qquad b_0^-(\tau) \equiv 0 \\ &a_m^-(\tau_0) = 0, \qquad b_m^-(\tau_0) = 0, \qquad m \geqslant 1 \end{aligned} \tag{28}$$

such that equation (26) implies $a_m^-(\tau) \equiv 0, b_m^-(\tau) \equiv 0, m \geqslant 1$ provided $\kappa_\pm(\tau) \equiv 0$. This makes obvious the absence of nonadiabatic transitions.

The next step is the calculation of $\kappa_\sigma(\tau)$. For this we need $e_\sigma^1(\tau)$, which can be determined from (21). As a result we find

$$e_\sigma^1(\tau) = e_\sigma^1(\tau_0)\exp\left[-\sigma\int_{\tau_0}^{\tau} \mathrm{d}\tau' \frac{\dot{\alpha}_\sigma(\tau')}{\alpha_+(\tau') - \alpha_-(\tau')}\right], \tag{29}$$

and taking equation (20) into account we obtain the general result

$$\kappa_\sigma(\tau) = \sigma \frac{e^1_{-\sigma}(\tau_0)}{e^1_\sigma(\tau_0)} \exp\left[\sigma \int_{\tau_0}^{0} \mathrm{d}\tau' \frac{\dot{\alpha}_+(\tau') + \dot{\alpha}_-(\tau')}{\alpha_+(\tau') - \alpha_-(\tau')}\right] \times \frac{\dot{\alpha}_{-\sigma}(\tau)}{\alpha_+(\tau) - \alpha_-(\tau)} \exp\left[\sigma \int_0^\tau \mathrm{d}\tau' \frac{\dot{\alpha}_+(\tau') + \dot{\alpha}_-(\tau')}{\alpha_+(\tau') - \alpha_-(\tau')}\right], \tag{30}$$

where the expression has been split into a τ-independent (first line) and a τ-dependent factor (second line). Following Berry [23] we truncate the series, equation (13), at the nth level

$$|\Psi_{n,\sigma}(\tau)\rangle = \exp\left[-\frac{\mathrm{i}}{\delta}\int_{\tau_0}^{\tau} \mathrm{d}\tau' E_\sigma(\tau')\right] \sum_{m=0}^{n} \delta^m |u_{m,\sigma}(\tau)\rangle. \tag{31}$$

and expand $|\Psi(\tau)\rangle$:

$$|\Psi(\tau)\rangle = \sum_{\sigma=\pm} c_{n,\sigma}(\tau)|\Psi_{n,\sigma}(\tau)\rangle. \tag{32}$$

As an initial condition we choose:

$$|\Psi(\tau_0)\rangle = |\Psi_-(\tau_0)\rangle, \tag{33}$$

which is equivalent to

$$c_{n,-}(\tau_0) = 1, \qquad c_{n,+}(\tau_0) = 0, \quad n \to \infty. \tag{34}$$

Introducing a corresponding truncated state

$$\langle\tilde{\Psi}_{n,\sigma}(\tau)| = f_{n,\sigma}(\tau) \sum_{m=0}^{n} \delta^m \langle\tilde{u}_{m,\sigma}(\tau)|, \tag{35}$$

where the τ-dependent prefactor $f_{n,\sigma}(\tau)$ does not have to be specified we obtain an equation of motion for $c_{n,\sigma}(\tau)$, after equation (32) has been substituted into equation (8):

$$\mathrm{i}\delta\dot{c}_{n,\sigma}(\tau) = \sum_{\sigma'} H_{n;\sigma\sigma'}(\tau) c_{n,\sigma'}(\tau) \tag{36}$$

with

$$\begin{aligned} H_{n;\sigma\sigma'}(\tau) &= \sum_{\sigma''=\pm} \left(\mathcal{L}_n^{-1}(\tau)\right)_{\sigma\sigma''} \mathcal{H}_{n;\sigma''\sigma'}(\tau) \\ \mathcal{L}_{n;\sigma\sigma'}(\tau) &= \langle\tilde{\Psi}_{n,\sigma}(\tau)|\Psi_{n,\sigma'}(\tau)\rangle \\ \mathcal{H}_{n;\sigma\sigma'}(\tau) &= \langle\tilde{\Psi}_{n,\sigma}(\tau)|H(\tau) - \mathrm{i}\delta d_\tau|\Psi_{n,\sigma'}(\tau)\rangle. \end{aligned} \tag{37}$$

Equation (36) can be rewritten as an integral equation

$$c_{n,\sigma}(\tau) = c_{n,\sigma}(\tau_0) + \frac{\mathrm{i}}{\delta}\int_{\tau_0}^{\tau} \mathrm{d}\tau' H_{n;\sigma,-\sigma}(\tau') c_{n,-\sigma}(\tau') \exp\left[-\frac{\mathrm{i}}{\delta}\int_{\tau'}^{\tau} \mathrm{d}\tau'' H_{n;\sigma\sigma}(\tau'')\right]. \tag{38}$$

Apart from the truncation, equation (31), the results are still exact. Equation (38) simplifies in the adiabatic limit $\delta \to 0$. In leading order in δ we get from equations (18), (31) and (35)

$$\mathcal{L}_{n;\sigma\sigma'}(\tau) \cong f_{n,\sigma}(\tau) \exp\left[-\frac{\mathrm{i}}{\delta}\int_{\tau_0}^{\tau} \mathrm{d}\tau' E_\sigma(\tau')\right] \delta_{\sigma\sigma'} \tag{39}$$

$[H(\tau) - \mathrm{i}\delta d_\tau]|\Psi_{n,\sigma'}(\tau)\rangle$ can be found in [22]. Multiplying by $\langle\tilde{\Psi}_{n,\sigma}(\tau)|$ and making use of equations (12), (18), (22) and (35) leads to

$$\mathcal{H}_{n;\sigma\sigma'}(\tau) = -\delta^{n+1} f_{n,\sigma}(\tau)[E_\sigma(\tau) - E_{\sigma'}(\tau')] \times \exp\left[-\frac{\mathrm{i}}{\delta}\int_{\tau_0}^{\tau} \mathrm{d}\tau' E_{\sigma'}(\tau')\right] \left[a^{\sigma'}_{n+1}(\tau)\delta_{\sigma,-} + b^{\sigma'}_{n+1}(\tau)\delta_{\sigma,+}\right] + \mathcal{O}(\delta^{n+2}) \tag{40}$$

from which follows

$$H_{n;\sigma\sigma'}(\tau) = -\delta^{n+1}\big[a^{\sigma'}_{n+1}(\tau)\delta_{\sigma,-} + b^{\sigma'}_{n+1}\delta_{\sigma,+}\big] \times [E_\sigma(\tau) - E_{\sigma'}(\tau)]\exp\left\{\frac{\mathrm{i}}{\delta}\int_{\tau_0}^{\tau} \mathrm{d}\tau'[E_\sigma(\tau') - E_{\sigma'}(\tau')]\right\} + \mathcal{O}(\delta^{n+2}). \tag{41}$$

Note that the prefactor $f_{n,\sigma}(\tau)$ has cancelled. The diagonal elements of $\mathbf{H_n}(\tau)$ are of order δ^{n+2} and the non-diagonal ones of order δ^{n+1}. Therefore it follows from equations (23), (30), (34) and (38)

$$c_{n,+}(\tau) \cong \mathrm{i}\delta^n \frac{e^1_-(\tau_0)}{e^1_+(\tau_0)}\exp\left[\int_{\tau_0}^{0}\mathrm{d}\tau'\frac{\dot\alpha_+(\tau') + \dot\alpha_-(\tau')}{\alpha_+(\tau') - \alpha_-(\tau')}\right] \times \int_{\tau_0}^{\tau}\mathrm{d}\tau'\dot a^-_{n+1}(\tau')\frac{[\alpha_+(\tau') - \alpha_-(\tau')]}{\dot\alpha_+(\tau')}[E_+(\tau') - E_-(\tau')]. \times \exp\left[\int_{0}^{\tau'}\mathrm{d}\tau''\frac{\dot\alpha_+(\tau'') + \dot\alpha_-(\tau'')}{\alpha_+(\tau'') - \alpha_-(\tau'')}\right]\exp\left\{\frac{\mathrm{i}}{\delta}\int_{\tau_0}^{\tau'}\mathrm{d}\tau''[E_+(\tau'') - E_-(\tau'')]\right\}. \tag{42}$$

The time dependence of $H(\tau)$ is chosen such that

$$\begin{aligned} &\lim_{\tau_0\to-\infty}|u_{0,-}(\tau_0)\rangle = |1\rangle, \qquad &&\lim_{\tau_0\to-\infty} u_{0,+}(\tau_0)\rangle = |2\rangle \\ &\lim_{\tau\to\infty}|u_{0,-}(\tau)\rangle \sim |2\rangle, \qquad &&\lim_{\tau\to\infty}|u_{0,+}(\tau)\rangle \sim |1\rangle. \end{aligned} \tag{43}$$

Note that the adiabatic states at initial time τ_0 are normalized. Since equations (27), (33) and (43) imply

$$\lim_{\tau_0\to-\infty}|\Psi(\tau_0)\rangle = |1\rangle \tag{44}$$

we obtain from equation (10) for the survival probability in leading order in δ

$$P(\delta) \cong \left|c_{n,+}(\infty)\langle 1|u_{0,+}(\infty)\rangle\exp\left[-\frac{\mathrm{i}}{\delta}\int_{-\infty}^{\infty}\mathrm{d}\tau' E_+(\tau')\right]\right|^2, \tag{45}$$

where we used $\langle 1|u_{0,-}(\infty)\rangle = 0$, due to equation (43). Note that we used the orthogonality of $|u_{0,+}(\infty)\rangle$ and $|1\rangle$, only. Substituting $c_{n,+}(\infty)$ from equation (42) with $\tau_0 = -\infty$ into equation (45) we get with equations (11), (29) and $\lim_{\tau_0\to-\infty} e^1_-(\tau_0) = 1$ (due to equation (43))

$$P(\delta) \cong \exp\left[-\left(F^{\mathrm{ns}}_g + \frac{1}{\delta}F^{\mathrm{ns}}_d\right)\right]\left|\delta^n\int_{-\infty}^{\infty}\mathrm{d}\tau\,\dot a^-_{n+1}(\tau)\frac{\alpha_+(\tau) - \alpha_-(\tau)}{\dot\alpha_+(\tau)}[E_+(\tau) - E_-(\tau)] \times \exp\left[\int_0^{\tau}\mathrm{d}\tau'\frac{\dot\alpha_+(\tau') + \dot\alpha_-(\tau')}{\alpha_+(\tau') - \alpha_-(\tau')}\right]\exp\left\{\frac{\mathrm{i}}{\delta}\int_0^{\tau}\mathrm{d}\tau'[E_+(\tau') - E_-(\tau')]\right\}\right|^2 \tag{46}$$

with the *nonsingular* ‘geometrical’ and ‘dynamical’ contributions

$$F^{\mathrm{ns}}_g = 2\,\mathrm{Re}\left[\int_0^{\infty}\mathrm{d}\tau\frac{\dot\alpha_+(\tau)}{\alpha_+(\tau) - \alpha_-(\tau)} - \int_{-\infty}^{0}\mathrm{d}\tau\frac{\dot\alpha_-(\tau)}{\alpha_+(\tau) - \alpha_-(\tau)}\right] \tag{47}$$

and

$$F^{\mathrm{ns}}_d = -2\,\mathrm{Im}\left[\int_0^{\infty}\mathrm{d}\tau\,E_+(\tau) + \int_{-\infty}^{0}\mathrm{d}\tau\,E_-(\tau)\right], \tag{48}$$

respectively. Here two comments are in order. First, the integrals in the exponents were split into a τ-dependent and a τ-independent term. The lower limit of the τ-independent integrals has been chosen to be zero, which is a natural choice. Second, the τ-independent contribution, equations (47) and (48), originates from two exponential factors. Taking in equation (45) for $c_{n,+}(\infty)$ the τ-independent part $\int_{\tau_0}^{0} \mathrm{d}\tau'[E_+(\tau') - E_-(\tau')]$ of the second exponential of the third line of equation (42) with $\tau_0 = -\infty$ and multiplying with the exponential factor of equation (45) leads to the result, equation (48). Taking in equation (45) for $c_{n,+}(\infty)$ the τ-independent part (exponential in the first line of equation (42) with $\tau_0 = -\infty$) and substituting for $\langle 1|u_{0,+}(\infty)\rangle = e_+^{(1)}(\infty)$ the exponential in equation (29) with $\tau_0 = -\infty$ and $\tau = \infty$ leads to the result, equation (47). Note that $F_d^{\mathrm{ns}} = 0$, for a Hermitian Hamiltonian, since $E_\sigma(\tau)$ are real. The expressions for F_g^{ns} and F_d^{ns} put some constraints on $H(\tau)$, because both quantities should be larger than or equal to a constant $c > -\infty$, which requires that $\mathrm{Im}\, E_\pm(\tau)$ decays fast enough for $\tau \to \pm\infty$.

The τ-integral in equation (46) is dominated by the singularities of $E_+(\tau) - E_-(\tau)$, for $\delta \to 0$. The adiabatic eigenvalues and $\alpha_\pm(\tau)$ have the form

$$E_\pm(\tau) = \frac{1}{2}[T(\tau) \pm \sqrt{T^2(\tau) - 4D(\tau)}] \tag{49}$$

$$\alpha_\pm(\tau) = \frac{-H_{11}(\tau) + H_{22}(\tau) \pm \sqrt{T^2(\tau) - 4D(\tau)}}{2H_{12}(\tau)}, \tag{50}$$

where T and D are, respectively, the trace and the determinant of the Hamiltonian matrix $H_{\nu\nu'} = \langle\nu|H|\nu'\rangle$. Accordingly, the singularities are the branch points $\tau_c(k)$, $k = 1, 2, \ldots,$ of $E_+(\tau) - E_-(\tau)$. Introducing a new variable [10, 23]

$$z(\tau) = \int_0^\tau \mathrm{d}\tau'[E_+(\tau') - E_-(\tau')] \tag{51}$$

it is shown in the appendix that after taking the limit $n \to \infty$ the survival probability is given by

$$P(\delta) \cong \exp\left[-\left(F_g^{\mathrm{ns}} + \frac{1}{\delta}F_d^{\mathrm{ns}}\right)\right]\left|\sum_k \exp F_g^s(k)\,\mathrm{e}^{\frac{\mathrm{i}}{\delta}z_c(k)}\right|^2 \tag{52}$$

with the *singular* 'geometrical' contribution

$$F_g^s(k) = \int_0^{z_c(k)} \mathrm{d}z \frac{\frac{\mathrm{d}\alpha_+}{\mathrm{d}z}(z) - \frac{\mathrm{d}\alpha_-}{\mathrm{d}z}(z)}{\alpha_+(z) - \alpha_-(z)} \tag{53}$$

and the singular points $z_c(k) = z(\tau_c(k))$, which are *above* the contour $\mathcal{C} = \{z(\tau)| -\infty \leqslant \tau \leqslant \infty\}$. The final result of this section, equation (52), is the generalization of the DDP formula (as it has been rigorously proven for Hermitian TLS Hamiltonians [10]) to non-Hermitian ones, describing dissipative TLS. The reader should note that the use of the superadiabatic basis leads to a pre-exponential factor in equation (52) which is equal to 1, which is identical to the case without dissipation. The result, equation (52), exhibits that the 'dynamical' contributions follow from the adiabatic eigenvalues and their branch points, whereas the 'geometrical' contributions involve $\alpha_\pm(\tau)$, only. If we parametrize for a TLS with Hermitian Hamiltonian the external field components B_j, equation (6), as it has been done in [11], one recovers that $F_g^{\mathrm{ns}} = 0$ and that equation (53) becomes:

$$F_g^s = \int_0^{\tau_c(k)} \mathrm{d}\tau\, \dot{\phi}(\tau) \cos\Theta(\tau) \tag{54}$$

in agreement with the result in [11].

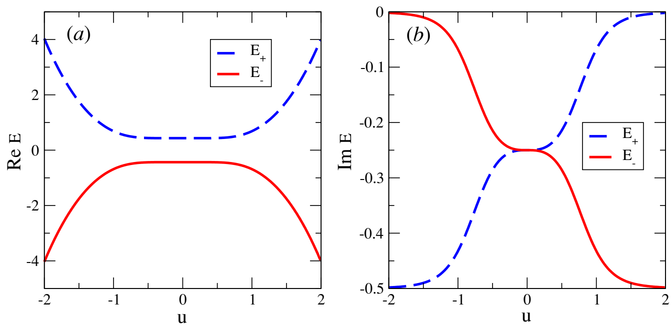

Figure 1. u-dependence of the adiabatic eigenvalues for a power law sweep $\tilde{w}(u) = u^3$ and $\tilde{\gamma} = 0.5 < \tilde{\gamma}_c = 1$ (a) real part of $E_\pm(u)$, and (b) imaginary part of $E_\pm(u)$.

3. Application to the Akulin–Schleich model

The AS model is given by [20]

$$H(t) = -\tfrac{1}{2}[W(t)\sigma_z + \Delta\sigma_x + \mathrm{i}\gamma(\sigma_z - \sigma_0)] \tag{55}$$

with the external field $W(t)$, the tunnelling matrix element Δ and the damping constant $\gamma \geqslant 0$ of level $|2\rangle \mathrel{\hat{=}} |\uparrow\rangle$. σ_0 is the 2×2 unit matrix. Let us introduce dimensionless quantities:

$$\tilde{w}(u) = \frac{W(t)}{\Delta}, \qquad u = \frac{\upsilon t}{\Delta}, \qquad \tilde{\gamma} = \frac{\gamma}{\Delta}, \qquad \tilde{\epsilon} = \frac{\Delta^2}{\hbar\upsilon} \tag{56}$$

where υ is the sweep rate. The t-dependence of W is given by $\tilde{w}(\upsilon t/\Delta)$, so that the sweep rate is defined for a general time-nonlinear sweep. Note that the time variable τ of the previous section is not dimensionless. After the replacement of τ by u, equation (1) takes the form of equation (8) with

$$\delta = \tilde{\epsilon}^{-1}. \tag{57}$$

From equations (49) and (50) it follows immediately

$$E_\pm(u) = \tfrac{1}{2}\left[-\mathrm{i}\tilde{\gamma} \pm \sqrt{(\tilde{w}(u) + \mathrm{i}\tilde{\gamma})^2 + 1}\right] \tag{58}$$

$$\alpha_\pm(u) = -(\tilde{w}(u) + \mathrm{i}\tilde{\gamma}) \pm \sqrt{(\tilde{w}(u) + \mathrm{i}\tilde{\gamma})^2 + 1}, \tag{59}$$

where the branch of the square root has been chosen such that $\sqrt{x} \geqslant 0$, for $x \geqslant 0$. Figures 1(a) and (b) exhibit Re $E_\pm(u)$, and Im $E_\pm(u)$, respectively, for an analytical power law sweep $\tilde{w}(u) = u^3$ and for $\tilde{\gamma} < 1$. The corresponding result for $\tilde{\gamma} > 1$ is shown in figures 2(a) and (b). In the following we will consider crossing sweeps only. For those it is

$$\lim_{u\to\pm\infty} \tilde{w}(u) = \pm\infty. \tag{60}$$

Returning sweeps for which $\lim_{u\to\pm\infty} \tilde{w}(u) = -\infty$ (or $+\infty$) can be treated analogously. It is easy to prove that

$$E_\pm(u) = \frac{1}{2}\left[\tilde{w}(u) + \frac{1}{2\tilde{w}(u)} - \frac{\mathrm{i}\tilde{\gamma}}{2\tilde{w}^2(u)} + \mathcal{O}(\tilde{w}^{-3}(u))\right] \tag{61}$$

for $u \to \pm\infty$ and

$$E_\pm(u) = \frac{1}{2}\left[-\tilde{w}(u) - 2\mathrm{i}\tilde{\gamma} - \frac{1}{2\tilde{w}(u)} + \mathcal{O}(\tilde{w}^{-2}(u))\right] \tag{62}$$

for $u \to \mp\infty$, everywhere with upper or lower sign, consistently.

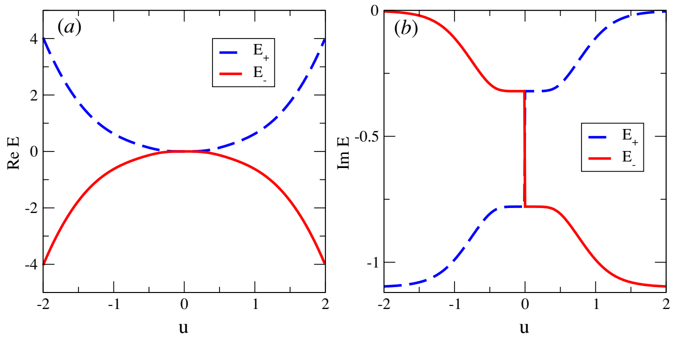

Figure 2. Same as figure 1, but for $\tilde{\gamma} = 1.1 > \tilde{\gamma}_c$.

From equations (61) and (48) it follows that $F_d^{\rm ns}$ is finite provided $\int^u du' \tilde{w}^{-3}(u')$ exists for $u \to \pm\infty$. This is fulfilled if $\tilde{w}(u)$ decays faster than $u^{-1/3}$. Otherwise $F_d^{\rm ns} = \infty$ which makes $P(\delta)$ vanish. Figures 1 and 2 demonstrate that there exists a critical value for $\tilde{\gamma}_c$. For $0 \leqslant \tilde{\gamma} < \tilde{\gamma}_c = 1$ we have $\mathrm{Re}[E_+(u) - E_-(u)] > 0$ for all u and $\mathrm{Im}\, E_\sigma(u)$ is continuous whereas $\mathrm{Re}[E_+(u) - E_-(u)]$ vanishes if $\tilde{w}(u) = 0$ and $\mathrm{Im}\, E_\sigma(u)$ becomes discontinuous for $\tilde{\gamma} > \tilde{\gamma}_c$, provided $E_\pm(u)$ are defined by equation (58). Accordingly, the critical value $\tilde{\gamma}_c$ has the property that the real parts of E_+ and E_- are crossing at $u = 0$ for $\tilde{\gamma} \geqslant \tilde{\gamma}_c$.

The nonsingular geometrical part, equation (47), can be calculated without specifying the u-dependence of $\tilde{w}$. Substituting $\alpha_\pm(u)$ and $\dot{\alpha}_\pm(u)$ from equation (59) into equation (47), both integrals in equation (47) become a sum of two integrals. One of them can be calculated by the introduction of a new integration variable $\zeta = \tilde{w} + \mathrm{i}\tilde{\gamma}$ and the other by noting that its integrand can be rewritten as a derivative of a logarithm with respect to u. Without restricting generality we assume that $\tilde{w}(0) = 0$. Then we obtain with equation (60)

$$F_g^{\rm ns}(\tilde{\gamma}) = 2\,\mathrm{Re}\ln\left(\mathrm{i}\tilde{\gamma} + \sqrt{1-\tilde{\gamma}^2}\right). \tag{63}$$

The nonsingular 'dynamical' and both singular contributions require the explicit u-dependence of $\tilde{w}$. As said above we will consider crossing sweeps only. Therefore we restrict ourselves to power law sweeps $\tilde{w}(u) = u^n$ with $n > 0$ and n *odd*. n should not be confused with the truncation number n in the previous section. Since $\tilde{w}(-u) = -\tilde{w}(u)$ we can rewrite $F_d^{\rm ns}$ as follows:

$$F_d^{\rm ns}(\tilde{\gamma}) = 2\int_0^\infty du\left[\tilde{\gamma} - \mathrm{Im}\sqrt{(\tilde{w}(u) + \mathrm{i}\tilde{\gamma})^2 + 1}\right]. \tag{64}$$

It is easy to see that

$$F_g^{\rm ns}(0) = 0, \qquad F_d^{\rm ns}(0) = 0, \tag{65}$$

for $\tilde{\gamma} = 0$. Hence, the nonsingular contributions to the survival probability vanish if there is no dissipation. In this case the result (52) reduces to that found by Berry [11] for Hermitian Hamiltonians and for a single complex crossing point contributing to equation (52). What remains is the determination of the singular points $u_c(k)$, $k = 1, 2, \ldots$ and the calculation of $z_c(k)$ and $F_g^s(k)$. These singular points are the branch points of $E_+(u) - E_-(u)$. Their location depends on whether $0 \leqslant \tilde{\gamma} < \tilde{\gamma}_c$ or $\tilde{\gamma} > \tilde{\gamma}_c = 1$. Let us start with the *first* case $0 \leqslant \tilde{\gamma} < \tilde{\gamma}_c$. From $(u^n + \mathrm{i}\tilde{\gamma})^2 + 1 = 0$, n odd, we find

$$u_c^\pm(k) = \pm(1 \mp \tilde{\gamma})^{1/n}\exp\left[\mathrm{i}\left(\frac{\pi}{2n} + k\frac{2\pi}{n}\right)\right] \tag{66}$$

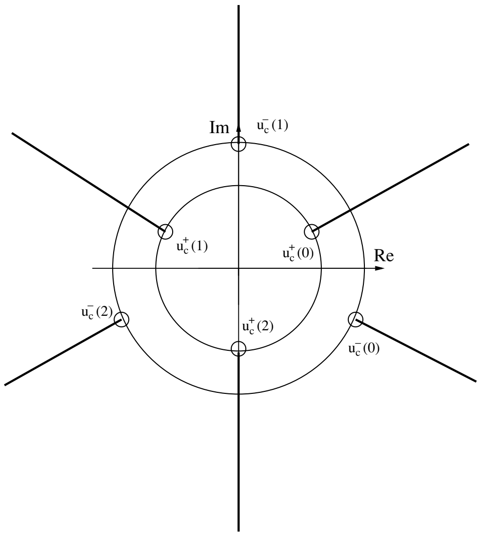

Figure 3. Branch points (open circles) $u_c^{\pm}(k)$ of $E_+(u) - E_-(u)$ for a power law sweep $\tilde{w}(u) = u^3$ and $\tilde{\gamma} < \tilde{\gamma}_c$. The thick solid lines are the branch cuts. The radii of the inner and outer circles are $(1-\tilde{\gamma})^{1/3}$ and $(1+\tilde{\gamma})^{1/3}$, respectively.

for $k = 0, 1, \ldots, n-1$, which are shown together with the branch cuts in figure 3 for $n = 3$. From equations (51) and (66) we obtain the corresponding singular points in the complex z-plane:

$$z_c^{\pm}(k) = \pm h_n^{\pm}(\tilde{\gamma}) \exp\left[\mathrm{i}\left(\frac{\pi}{2n} + k\frac{2\pi}{n}\right)\right] \tag{67}$$

where

$$h_n^{\pm}(\tilde{\gamma}) = \int_0^{(1\mp\tilde{\gamma})^{1/n}} \mathrm{d}x \sqrt{1 - (\tilde{\gamma} \pm x^n)^2}. \tag{68}$$

Since the mapping $z(u)$ is analytic in the complex u-plane, except at the branch lines, it is conformal. Accordingly, for those $u_c^{\pm}(k)$ which are in the upper u-plane the corresponding $z_c^{\pm}(k)$ will be above the integration contour $\mathcal{C}$ and therefore will contribute to P (see end of the second section). After the determination of the singular points we can proceed to calculate their 'geometrical' and 'dynamical' contributions to P. From equations (53) and (59) it follows:

$$\begin{aligned} F_g^s(k) &= \int_0^{u_c^{\pm}(k)} \mathrm{d}u\, \frac{\dot{\alpha}_+(u) - \dot{\alpha}_-(u)}{\alpha_+(u) - \alpha_-(u)} \\ &= -\int_{\tilde{w}(0)+\mathrm{i}\tilde{\gamma}}^{\tilde{w}(u_c^{\pm}(k))+\mathrm{i}\tilde{\gamma}} \mathrm{d}\zeta\, \frac{1}{\sqrt{\zeta^2+1}} \\ &= -\ln\left[-\alpha_-\left(u_c^{\pm}(k)\right)\right] + \ln\left(\mathrm{i}\tilde{\gamma} + \sqrt{1-\tilde{\gamma}^2}\right). \end{aligned} \tag{69}$$

Because $\left(\tilde{w}\left(u_c^{\pm}(k)\right) + \mathrm{i}\tilde{\gamma}\right) + 1 = 0$ we get from equation (59) that $\alpha_-\left(u_c^{\pm}(k)\right) = 1$ such that

$$F_g^s(k) = \ln\left(\mathrm{i}\tilde{\gamma} + \sqrt{1-\tilde{\gamma}^2}\right) + \mathrm{i}\pi \equiv F_g^s(\tilde{\gamma}). \tag{70}$$

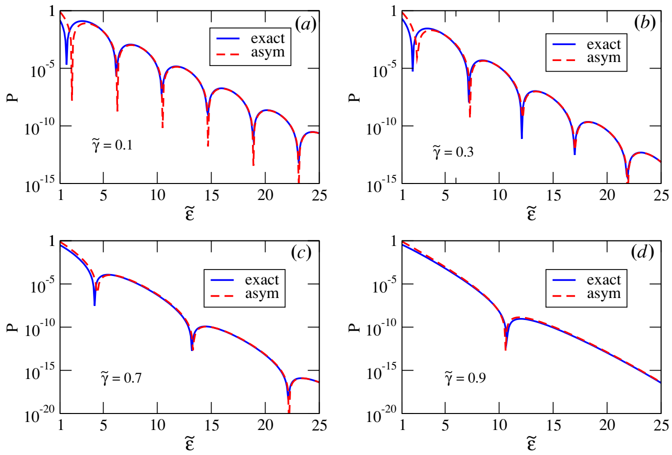

Figure 4. Comparison of the numerical exact (solid line) and the asymptotic result, equation (71), (dashed line) for $P(\tilde{\epsilon}, \tilde{\gamma})$ and a power law sweep $\tilde{w}(u) = u^3$. (*a*) $\tilde{\gamma} = 0.1$, (*b*) $\tilde{\gamma} = 0.3$, (*c*) $\tilde{\gamma} = 0.7$ and (*d*) $\tilde{\gamma} = 0.9$.

The reader should note that F_g^s is independent of k. Consequently, it can be taken in front of the sum in equation (52) which yields $\exp\left(2\,\mathrm{Re}\,F_g^s\right)$ and just cancels the non-singular 'geometrical' factor $\exp\left(-2\,\mathrm{Re}\,F_g^{\mathrm{ns}}\right)$, due to equation (63). Therefore we find that no 'geometrical' factor occurs for the AS model. This will change if we apply an additional *time-dependent* field in the x- and y-direction. What remains is the calculation of the singular 'dynamical' factor. Because we are interested in the adiabatic limit $\delta \to 0$, we have to take into account in equation (52) those singularities in the upper z-plane with smallest imaginary part. These are $z_c^+(k=0)$ and $z_c^+(k=(n-1)/2)$, for which $\mathrm{Re}\,z_c^+(0) = -\mathrm{Re}\,z_c^+((n-1)/2)$ and (of course) $\mathrm{Im}\,z_c^+(0) = \mathrm{Im}\,z_c^+((n-1)/2)$. Using equation (67) with $k=0$ and $k=(n-1)/2$ we obtain finally

$$P \cong 4\cos^2\left(\tilde{\epsilon} h_n^+(\tilde{\gamma})\cos\frac{\pi}{2n}\right)\exp\left[-\tilde{\epsilon}F_d^{\mathrm{ns}}(\tilde{\gamma})\right]\exp\left[-2\tilde{\epsilon}h_n^+(\tilde{\gamma})\right]\sin\frac{\pi}{2n}. \qquad (71)$$

Let us consider linear sweeps, i.e. $n = 1$. Then there exists only one singularity $u_c^+(0) = \mathrm{i}(1-\tilde{\gamma})$ in the upper u-plane and equation (52) reduces to

$$P(\delta) \cong \exp\left[-\frac{1}{\delta}\left(F_d^{\mathrm{ns}} + 2\,\mathrm{Im}\,z_c^+(0)\right)\right]. \qquad (72)$$

The exponent can be calculated analytically by using $u + \mathrm{i}\tilde{\gamma}$ as an integration variable. As a consequence one finds that the $\tilde{\gamma}$-dependence drops out from the exponent. With $\delta = \tilde{\epsilon}^{-1}$ one obtains

$$P \cong e^{-\epsilon}, \qquad \epsilon \equiv \frac{\pi}{2}\tilde{\epsilon} = \frac{\pi\Delta^2}{2\hbar v}, \qquad (73)$$

consistent with the finding in [20]. In order to check the validity of equation (71), we have solved numerically the time-dependent Schrödinger equation in order to determine P. A comparison between the numerically exact and the asymptotic result, equation (71), is shown in figure 4 for $n = 3$ and four different $\tilde{\gamma}$-values. We observe that the deviation between both results, e.g., for $\tilde{\epsilon} = 5$ and $\tilde{\gamma} = 0.3$, is about 1.6% only. Similarly good agreement

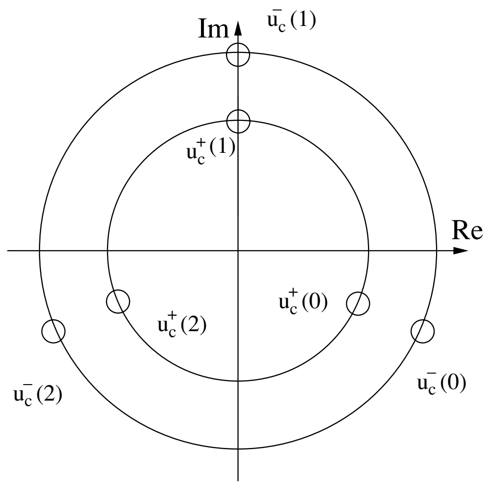

Figure 5. Same as figure 3 but for $\tilde{\gamma} > \tilde{\gamma}_c$ and without branch cuts. The radii of the inner and outer circles are $(\tilde{\gamma} - 1)^{1/3}$ and $(\tilde{\gamma} + 1)^{1/3}$.

has been found for $n > 3$. From equation (71) it follows that there exist an infinite number of critical values $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$, $\nu = 1, 2, 3, \ldots$ at which the oscillatory prefactor in equation (71) vanishes. From this we can conclude that these Stückelberg oscillations, proven to exist for TLS without dissipation [10] and discussed later in [9, 14, 24] for $\tilde{\gamma} = 0$, survive even in the presence of dissipation, provided $\tilde{\gamma} < \tilde{\gamma}_c = 1$. Indeed, we will see below that they disappear for $\tilde{\gamma} > \tilde{\gamma}_c$. It is not only the survival of the oscillations, but also the survival of the *complete* transitions from state $|1\rangle \hat{=} |\downarrow\rangle$ to state $|2\rangle \hat{=} |\uparrow\rangle$ found in [9, 14, 24] for $\tilde{\gamma} = 0$, as long as $\tilde{\gamma} < \tilde{\gamma}_c$.

Now, we turn to the *second* case $\tilde{\gamma} > \tilde{\gamma}_c$. For this case we find:

$$u_c^{\pm}(k) = -(\tilde{\gamma} \mp 1)^{1/n} \exp\left[\mathrm{i}\left(\frac{\pi}{2n} + k\frac{2\pi}{n}\right)\right] \tag{74}$$

for $k = 0, 1, \ldots, n-1$, which are shown in figure 5 for $n = 3$. The main difference to the case $0 \leqslant \tilde{\gamma} < \tilde{\gamma}_c$ is that there is exactly one singular point among $u_c^{\pm}(k)$ denoted by u_c^0 for which $z_c^0 = z\big(u_c^0\big)$ is on the real axis in the complex z-plane. Using the definition, equation (58), of $E_{\pm}(u)$, figure 2 demonstrates that $E_{\pm}(u)$ is discontinuous on the real u-axis. There seem to exist two possibilities to deal with this problem. First, after having chosen the branch cuts in the complex u-plane one has to deform the integration contour along the real u-axis such that $u = 0$ is above that contour and that no branch cut is crossed. This kind of reasoning was used by Moyer in [21]. Second, one could define $E_{\pm}(u)$ such that they are analytic in a strip around the real u-axis. This can be done by interchanging $E_+(u)$ and $E_-(u)$ for $u \leqslant 0$. This has the consequence that the contour $z(u)$ for u real is in the right complex z-plane, starting e.g. above the positive real axis for $u = -\infty$, going through $z = 0$ for $u = 0$ and then continuing below the positive real axis for $u \to +\infty$. This contour would enclose z_0 if $\mathrm{Re}\, z_0 > 0$. Whether it can be closed such that the closure does not make a contribution is not obvious. Since we are not sure how to solve this problem in a rigorous manner, we have assumed that z_0 is the leading contribution to P, equation (52), for $\delta \to 0$. Since $|\mathrm{e}^{\mathrm{i}z_c^0/\delta}| = 1$ and due to the absence of a 'geometrical' contribution we obtain:

$$P \cong \exp\left[-\tilde{\epsilon} F_d^{\mathrm{ns}}(\tilde{\gamma})\right], \tag{75}$$

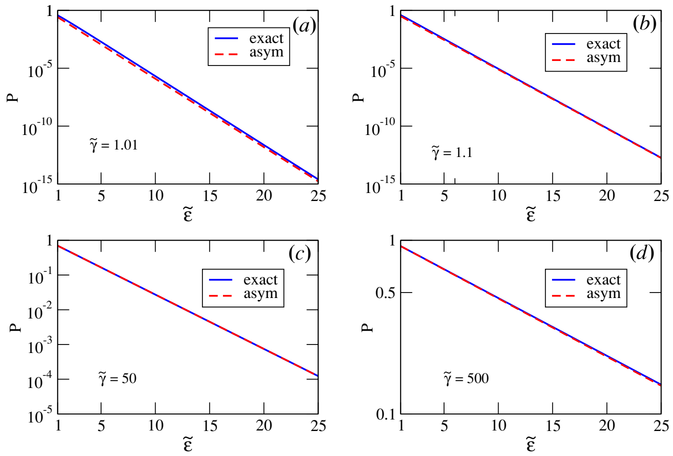

Figure 6. Same as figure 4, however for $\tilde{\gamma} > \tilde{\gamma}_c$ and with the asymptotic result, equation (75). (*a*) $\tilde{\gamma} = 1.01$, (*b*) $\tilde{\gamma} = 1.1$, (*c*) $\tilde{\gamma} = 50$ and (*d*) $\tilde{\gamma} = 500$.

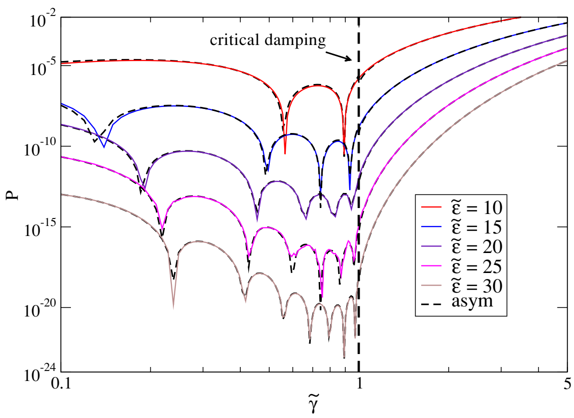

Figure 7. $\tilde{\gamma}$-dependence of $P(\tilde{\epsilon}, \tilde{\gamma})$ for $\tilde{w}(u) = u^3$ and $\tilde{\epsilon} = 10, 15, 20, 25, 30$ (from top to bottom). Numerical exact result (solid line) and the asymptotic one (dashed line).

with $F_d^{\text{ns}}(\tilde{\gamma})$ given by equation (64). A comparison between the $\tilde{\epsilon}$-dependence of the numerically exact and the asymptotic result, equation (75), is presented in figure 6. Again we find a very good agreement already for $\tilde{\epsilon} \geqslant 1$. This strongly supports the correctness of our assumption that z_0 is the most important singularity. Equation (75) reveals that the Stückelberg oscillations as a function of $\tilde{\epsilon}$ have disappeared. We stress that both asymptotic results, equation (71) and (75), are valid for all $\tilde{\gamma}$ with $0 \leqslant \tilde{\gamma} < \tilde{\gamma}_c$ and for all $\tilde{\gamma}$ larger than $\tilde{\gamma}_c$, respectively, provided $\tilde{\epsilon}$ is large enough. This is demonstrated in figure 7 for different $\tilde{\epsilon}$.

4. Interpretation by a damped harmonic oscillator

In this section we will give an intuitive explanation of the Stückelberg oscillations and will present an approximate calculation for the critical values $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$ for power law crossing sweeps $\tilde{w}(u) = u^n$, n odd. Close to the resonance at $u = 0$ we may neglect $\tilde{w}(u)$. Then the time-dependent Schrödinger equation for the amplitude of state $|1\rangle$

$$\tilde{c}_1(u) = c_1(u)\exp\left[\mathrm{i}\int_{-\infty}^{u} \mathrm{d}u'\tilde{w}(u')\right] \tag{76}$$

becomes

$$\ddot{\tilde{c}}_1 + 2\mu\dot{\tilde{c}}_1(u) + \omega_0^2\tilde{c}_1(u) \cong 0 \tag{77}$$

with

$$\mu = \frac{\tilde{\epsilon}\tilde{\gamma}}{2}, \qquad \omega_0 = \frac{\tilde{\epsilon}}{2}. \tag{78}$$

Let $t_{\rm trans}$ be the Landau–Zener transition time. In the adiabatic limit it is well known that $t_{\rm trans} = \Delta/v$. Equation (56) yields $u_{\rm trans} = 1$. Therefore we will require as initial conditions:

$$\tilde{c}_1(-u_{\rm trans} = -1) = 1 \qquad \dot{\tilde{c}}_1(-u_{\rm trans} = -1) = 0. \tag{79}$$

Equation (77) is the equation of motion for a damped harmonic oscillator which can easily be solved. The special solutions are $\exp[\mathrm{i}\omega_\pm(\tilde{\epsilon},\tilde{\gamma})u]$ with

$$\omega(\tilde{\epsilon},\tilde{\gamma}) = \frac{\tilde{\epsilon}}{2}\big[\mathrm{i}\tilde{\gamma} \pm \sqrt{1-\tilde{\gamma}^2}\big]. \tag{80}$$

This result makes obvious the existence of a critical damping $\tilde{\gamma}_c = 1$. For $0 \leqslant \tilde{\gamma} < \tilde{\gamma}_c$ and $\tilde{\gamma} > \tilde{\gamma}_c$ the oscillator is underdamped and overdamped, respectively. This qualitative different behaviour is the origin of the different $\tilde{\epsilon}$-dependence of P for $0 \leqslant \tilde{\gamma} < \tilde{\gamma}_c$ and $\tilde{\gamma} > \tilde{\gamma}_c$, found in the third section. This relationship can be deepened more by calculating $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$. Having solved equation (77) with initial conditions, equation (79) we approximate P by:

$$P \cong |c_1(+u_{\rm trans}) = +1|^2 = |\tilde{c}_1(+u_{\rm trans} = +1)|^2. \tag{81}$$

The zeros (with respect to $\tilde{\epsilon}$) of P yield $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$. A numerical solution of the corresponding transcendental equation leads to the results shown in figure 8 for $\tilde{w}(u) = u^n$ with $n = 5$ and $n = 51$ and $\tilde{\gamma} < \tilde{\gamma}_c$. Figure 8 also contains the result from a numerically exact solution of the time-dependent Schrödinger equation. Comparing both results we observe that the agreement for $n = 5$ is qualitatively good, but quantitatively less satisfactory. However, increasing n more and more leads even to a rather good quantitative agreement, as can be seen for $n = 51$. This behaviour is easily understood, since $\tilde{w}(u)$ within the transition range $(-1, 1)$ becomes practically zero for n large enough. Figure 8 also demonstrates that $\tilde{\epsilon}_c^{(\nu)}$ increases monotonically with $\tilde{\gamma}$ which is related to the decrease of $\mathrm{Re}\,\omega(\tilde{\epsilon},\tilde{\gamma})$ for increasing $\tilde{\gamma}$. The oscillator model can also be used to determine a lower bound for $\tilde{\epsilon}_c^{(1)}(\tilde{\gamma} = 0)$. For $u_{\rm trans} = 1$ one gets

$$\tilde{\epsilon}_c^{(1)}(\tilde{\gamma} = 0) \geqslant \frac{\pi}{2} \tag{82}$$

such that $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma}) \geqslant \tilde{\epsilon}_c^{(1)}(\tilde{\gamma}) > \tilde{\epsilon}_c^{(1)}(\tilde{\gamma} = 0) \geqslant \pi/2$, for all $\tilde{\gamma}$. It is interesting that the lower bound (82) for $\tilde{\epsilon}$ is similar to that obtained from the *inverse* Landau–Zener problem [26]. There, the t-dependent survival probability $P(t;\tilde{\epsilon})$ is given and $W(t;\tilde{\epsilon})$ is determined analytically from $P(t;\tilde{\epsilon})$. If $P(t;\tilde{\epsilon})$ varies from one (for $t = -\infty$) to zero (for $t = +\infty$), it is found that a solution $W(t;\tilde{\epsilon})$ of the inverse problem only exists, if

$$\tilde{\epsilon} > 1. \tag{83}$$

The latter inequality, as well as inequality (82) implies that the ratio $t_{\rm trans}/t_{\rm tunnel}$ of the transit time $t_{\rm trans} = \Delta/v$ and the time period of coherent tunnelling $t_{\rm tunnel} = \hbar/\Delta$, which equals $\tilde{\epsilon}$, is of order one. It is obvious that *complete* transitions cannot occur if $t_{\rm trans}$ is too small compared to $t_{\rm tunnel}$, i.e. for $\tilde{\epsilon} \ll 1$. In that case the quantum system does not have enough time to tunnel from the initial state $|1\rangle$ to state $|2\rangle$.

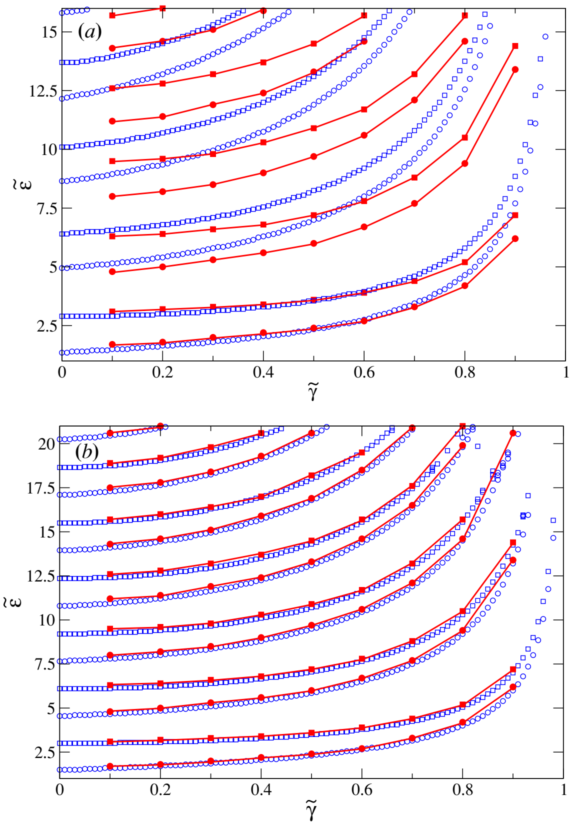

Figure 8. Comparison of the critical values $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$ for (a) $\tilde{w}(u) = u^5$ and (*b*) $\tilde{w}(u) = u^{51}$. The numerically exact result is shown by the open circles and the result obtained for the oscillator model is depicted by the full circles. The solid lines are a guide for the eye.

5. Summary and conclusions

Our main focus has been on the derivation of the survival probability $P(\tilde{\epsilon})$ for a dissipative two-level system modelled by a *general* non-Hermitian Hamiltonian, depending analytically on time. Following for the Hermitian case Berry's approach by use of a superadiabatic basis we have found a generalization of the DDP formula. Besides a 'geometrical' and a 'dynamical' factor, completely determined by the crossing points in the complex time plane, we also have found a non-universal 'geometrical' and 'dynamical' contribution to P. The latter require the knowledge of the Hamiltonian's full time dependence and are identical to zero in the absence of dissipation. Without specification of the TLS Hamiltonian, we have shown that both 'geometrical' contributions can be expressed by $\alpha_\pm(\tau)$, the ratio of the components of each adiabatic states $|u_{0,\pm}(\tau)\rangle$ in the basis $|\nu\rangle$, $\nu = 1, 2$, and both 'dynamical' ones by the adiabatic eigenvalues $E_\pm(\tau)$, only. In this respect our result for $P(\tilde{\epsilon})$ is independent of a special parametrization of the Hamiltonian matrix. Although the result in [21] is not in such an explicit form like equation (46) the existence of this nonsingular 'dynamical' contribution has already been stated there. However, the nonsingular 'geometrical' part, equation (47), has not been found in that paper.

As a physical application we have studied the AS model [20]. This model describes a dissipative TLS where the initial upper level is damped. In [20], it has been shown that the probability P for a linear time dependence of the bias does not depend on the damping constant $\tilde{\gamma}$ for all $\tilde{\epsilon}$. Our results demonstrate that this is not generic. For instance, nonlinear power law crossing sweeps generate a $\tilde{\gamma}$-dependence of P. For such sweeps a critical value $\tilde{\gamma}_c = 1$ exists. Below $\tilde{\gamma}_c$ the survival probability oscillates and vanishes at critical values $\tilde{\epsilon}_c^{(\nu)}(\tilde{\gamma})$, and for $\tilde{\gamma} > \tilde{\gamma}_c$ the oscillations are absent. Hence, the existence of complete transitions at an infinite set of critical sweep rates still holds for all $\tilde{\gamma}$ below $\tilde{\gamma}_c$. In section 4 we have shown how the oscillations and their disappearance for $\tilde{\gamma} > \tilde{\gamma}_c$ can be qualitatively explained by a damped harmonic oscillator. For power law sweeps with rather large exponent, e.g. $n = 51$, this description becomes even quantitatively correct. No doubt, it would be interesting to study a microscopic model of a TLS coupled to phonons, e.g. a spin–boson–Hamiltonian as in [13], in order to check whether the $\tilde{\epsilon}$-dependence of P exhibits oscillations for power law sweeps with $n > 1$ and small enough spin–phonon coupling. For $n = 2$ (a returning sweep) it was shown [14] for a spin–phonon model that the Stückelberg oscillations exist, but are reduced. This has been achieved for fast sweeps (well-separated resonances), weak spin–phonon coupling and high enough temperature. Since weak spin–phonon coupling corresponds to small $\tilde{\gamma}$ the survival of the oscillations found in [14] is consistent with our result. However, whereas the AS model still exhibits complete transitions for $\tilde{\gamma} \leqslant \tilde{\gamma}_c$, they do not occur for the spin–boson Hamiltonian, provided the dephasing time τ_ϕ is nonzero (cf equation (3.19) of [14]). The reason for this discrepancy is not quite obvious. The oscillations in [14] are due to phase changes between the two real crossing of the diabatic levels. Since we consider crossing sweeps only, this kind of phase effect is absent. In our case the oscillations occur due to coherent tunnelling and they do not occur for fast sweeps. Another question concerns the interaction between the TLS which have been completely neglected in our present work. That they can play a crucial role has been shown recently [27]. Whether the oscillations still exist in the presence of interactions between the TLS is not obvious.

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Appendix

In this appendix we will describe how the asymptotic result, equation (52), has been derived from (46). Although we follow Berry's approach [11, 23] we repeat the most important steps since the non-Hermitian property of H does not allow the simple parametrization used in [11] and is not of the form of equation (A.1) or equation (A.4) of [23]. Nevertheless, we will recover the same universal recursion relation for the coefficients $a_m^-(\tau)$ as found by Berry [23]. In order to show how equation (52) can be obtained from equation (46) we have to calculate the three pre-exponential factors $E_+(\tau) - E_-(\tau), [\alpha_+(\tau) - \alpha_-(\tau)]/\dot{\alpha}_+(\tau)$ and $\dot{a}_{n+1}^-(\tau)$ in equation (46). We assume that the Hamiltonian $H(\tau)$ is analytic in τ. Let τ_c be one of the branch points of $E_+(\tau) - E_-(\tau)$. Close to τ_c we get:

$$E_+(\tau) - E_-(\tau) \cong c(\tau - \tau_c)^{1/2} \tag{A.1}$$

with c a constant, depending on τ_c. Equation (51) implies

$$z - z_c \cong \tfrac{2}{3}c(\tau - \tau_c)^{3/2}, \tag{A.2}$$

where $z_c = z(\tau_c)$. In the adiabatic limit $\delta \to 0$ the main contribution to the integral (equation (46)) comes from the singular points τ_c and z_c, respectively. Consequently we have to calculate the pre-exponential factors (first line of equation (46)) close to the singularities only. Let us start with $[\alpha_+(\tau)-\alpha_-(\tau)]/\dot{\alpha}_+(\tau)$. Using equation (50) it follows with $\alpha_\pm(z) = \alpha_\pm(\tau(z))$ close to z_c

$$[\alpha_+(z) - \alpha_-(z)]/\alpha'_+(z) \cong 6(z - z_c), \tag{A.3}$$

where '$'$' denotes derivative with respect to z. Note that H_{11}, H_{12} and H_{22} do not enter in equation (A.3). The calculation of $\dot{a}^-_{n+1}(\tau)$ is more evolved. As a first step we eliminate $\dot{b}^-_{m-1}(\tau), b^-_{m-1}(\tau)$ and $b^-_m(\tau)$ from equations (23), (24) which yields a recursion relation for $a^-_m(\tau)$:

$$\dot{a}^-_m(\tau) = \frac{\mathrm{i}}{E_+(\tau) - E_-(\tau)}\left[\ddot{a}^-_{m-1}(\tau) - \frac{\dot{\kappa}_-(\tau)}{\kappa_-(\tau)}\dot{a}^-_{m-1}(\tau) - \kappa_-(\tau)\kappa_+(\tau)a^-_{m-1}(\tau)\right]. \tag{A.4}$$

Next we calculate the various terms close to τ_c. From equations (30) and (50) we get:

$$\frac{\dot{\kappa}_-(\tau)}{\kappa_-(\tau)} \cong (\tau - \tau_c)^{-1} \tag{A.5}$$

and

$$\kappa_-(\tau)\kappa_+(\tau) \cong \tfrac{1}{16}(\tau - \tau_c)^{-2}. \tag{A.6}$$

Expressing the τ-derivatives of a^-_m and a^-_{m-1} by derivatives with respect to z:

$$\dot{a}^-_m(\tau) \cong c(\tau - \tau_c)^{1/2}a^{-'}_m(z) \tag{A.7}$$

and

$$\ddot{a}_m(\tau) \cong c^2(\tau - \tau_c)a^{-''}_m(z) + \frac{c}{2}(\tau - \tau_c)^{-1/2}a^{-'}_m(z), \tag{A.8}$$

where $\mathrm{d}z/\mathrm{d}\tau = E_+(\tau) - E_-(\tau)$ and (A.1) was used, we get from equation (A.4) with equations (A.5), (A.6):

$$a^{-''}_m(z) \cong (-\mathrm{i})\left[\frac{a^-_{m-1}(z)}{36(z - z_c)^2} - \frac{a^{-'}_{m-1}(z)}{(z - z_c)} - a^{-''}_{m-1}(z)\right] \tag{A.9}$$

with initial condition (cf equation (28)):

$$a^-_0(z) \equiv 1. \tag{A.10}$$

The recursion relation is identical to equation (30) in [23], except the different sign in front of the square bracket. The sign change is irrelevant. The exact solution of equations (A.9), (A.10) can be taken from [23]:

$$a^-_m(z) \cong B_m(z - z_c)^{-m} \tag{A.11}$$

with

$$B_m = \mathrm{i}^m\frac{\left(m - \frac{7}{6}\right)!\left(m - \frac{5}{6}\right)!}{m!\left(-\frac{7}{6}\right)!\left(-\frac{5}{6}\right)!}. \tag{A.12}$$

Then we get from equation (46) with (A.1)–(A.3) and (A.11), (A.12)

$$\begin{aligned}
&\int_{-\infty}^{\infty}\mathrm{d}\tau\,\dot{a}^-_{n+1}(\tau)\frac{\alpha_+(\tau) - \alpha_-(\tau)}{\dot{\alpha}_+(\tau)}[E_+(\tau) - E_-(\tau)]I(\tau)\\
&\quad= \int_{\mathcal{C}}\mathrm{d}z\,a^{-'}_{n+1}(z)\frac{\alpha_+(z) - \alpha_-(z)}{\alpha'_+(z)}I(z)\\
&\quad= -6(n + 1)B_{n+1}\sum_k\int_{\mathcal{C}}\mathrm{d}z\frac{1}{(z - z_c(k))^{n+1}}I(z)\\
&\quad= -6(n + 1)2\pi\mathrm{i}\left(\frac{\mathrm{i}}{\delta}\right)^n B_{n+1}\frac{1}{n!}\sum_k I(z_c(k)) + O(1/\delta^{n-1}),
\end{aligned} \tag{A.13}$$

where the sum over k is restricted to all singular points $z_c(k)$ above the contour $\mathcal{C} = \{z = z(\tau) | -\infty \leqslant \tau \leqslant \infty\}$. Here we used that $I(z)$ is of the form $I(z) = \mathrm{e}^{\frac{\mathrm{i}}{\delta} z} f(z)$ where $f(z)$ is an exponential factor, independent of δ. Application of Cauchy's formula requires the calculation of $\mathrm{d}^n I(z)/\mathrm{d}z^n$. With $I(z)$ from above one obtains $\mathrm{d}^n I(z)/\mathrm{d}z^n = (\mathrm{i}/\delta)^n I(z) + O(1/\delta^{n-1})$. Since we consider the adiabatic limit, $O(1/\delta^{n-1})$ can be neglected. Since

$$-6 \cdot 2\pi(n+1) B_{n+1}/n! \longrightarrow \mathrm{i}^{n+1}, \quad n \to \infty, \tag{A.14}$$

the prefactor in front of $\sum_k$ in equation (A.13) equals $(-1)^{n+1}$. Substituting (A.13) into equation (46) δ^n cancels and one obtains the result (52).

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