Precise coupling terms in adiabatic quantum evolution

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Abstract

It is known that for multi-level time-dependent quantum systems one can construct superadiabatic representations in which the coupling between separated levels is exponentially small in the adiabatic limit. For a family of two-state systems with real-symmetric Hamiltonian we construct such a superadiabatic representation and explicitly determine the asymptotic behavior of the exponentially small coupling term. First order perturbation theory in the superadiabatic representation then allows us to describe the time-development of exponentially small adiabatic transitions. The latter result rigorously confirms the predictions of Sir Michael Berry for our family of Hamiltonians and slightly generalizes a recent mathematical result of George Hagedorn and Alain Joye.

1 Introduction and main result

The decoupling of slow and fast degrees of freedom in the adiabatic limit is at the basis of many important approximations in physics, as, e.g., the Born-Oppenheimer approximation in molecular dynamics and the Peierls substitution in solid state physics. We refer to [BMKNZ, Te] for recent reviews. Generically the decoupling is not exact and a coupling which is exponentially small in the adiabatic parameter remains. However, this small coupling has important physical consequences, as it makes possible, e.g., non-radiative decay to the ground state in molecules. Since Kato's proof from 1950 [Ka] the adiabatic limit of quantum mechanics was considered also as a mathematical problem, with increased activity during the last 20 years. Some of the landmarks are [Ne_1, ASY, JoPf_1, Ne_2, HaJo].

We consider a two-state time-dependent quantum system described by the Schrödinger equation

$$\big(\mathrm{i}\varepsilon\partial_t - H(t)\,\big)\psi(t) = 0 \tag{1}$$

in the *adiabatic limit* $\varepsilon \to 0$. For the moment we take the Hamiltonian $H(t)$ to be the real-symmetric 2×2-matrix

$$H(t) = \rho(t)\begin{pmatrix} \cos\theta(t) & \sin\theta(t) \\ \sin\theta(t) & -\cos\theta(t) \end{pmatrix}.$$

The eigenvalues of $H(t)$ are $\pm\,\rho(t)$ and we assume that the gap between them does not close, i.e. that $2\rho(t) \geq g > 0$ for all $t \in \mathbb{R}$.

As to be explained, even for this simple but prototypic problem there are open mathematical questions. In order to explain the concern of our work, namely the time-development of the exponentially small adiabatic transitions, let us briefly recall some important facts about (1). Let $U_0(t)$ be the orthogonal matrix that diagonalizes $H(t)$, i.e.

$$U_0(t) = \begin{pmatrix} \cos(\theta(t)/2) & \sin(\theta(t)/2) \\ \sin(\theta(t)/2) & -\cos(\theta(t)/2) \end{pmatrix}. \tag{2}$$

Then the Schrödinger equation in the *adiabatic representation* becomes

$$U_0(t)\ \big(\mathrm{i}\varepsilon\partial_t - H(t)\,\big)\,U_0^*(t)\,U_0(t)\psi(t) =:\ \big(\mathrm{i}\varepsilon\partial_t - H^{\mathrm{a}}_\varepsilon(t)\,\big)\psi^{\mathrm{a}}(t) = 0$$

with

$$H^{\mathrm{a}}_\varepsilon(t) = \begin{pmatrix} \rho(t) & \frac{\mathrm{i}\varepsilon}{2}\theta'(t) \\ -\,\frac{\mathrm{i}\varepsilon}{2}\theta'(t) & -\,\rho(t) \end{pmatrix} \qquad \text{and} \qquad \psi^{\mathrm{a}}(t) = U_0(t)\psi(t)\,.$$

Here and henceforth, primes denote time derivatives. First order perturbation theory in the adiabatic representation (cf. proof of Corollary 1) and integration by parts yields the adiabatic theorem [BoFo, Ka]: The off-diagonal elements of the unitary propagator $K^{\mathrm{a}}(t,s)$ in the adiabatic basis, i.e. the solution of

$$\mathrm{i}\varepsilon\partial_t K^{\mathrm{a}}_\varepsilon(t,s) = H^{\mathrm{a}}_\varepsilon(t)K^{\mathrm{a}}_\varepsilon(t,s)\,, \qquad K^{\mathrm{a}}_\varepsilon(s,s) = \mathrm{id}\,,$$

vanish in the limit $\varepsilon \to 0$. More precisely, let

$$P_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad P_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3}$$

which project onto the adiabatic subspaces in the adiabatic representation. Then

$$\|\,P_-\,K^{\mathrm{a}}_\varepsilon(t,s)\,P_+\| = \mathcal{O}(\varepsilon)\,. \tag{4}$$

Therefore the transitions between the adiabatic subspaces are $\mathcal{O}(\varepsilon)$. This bound is optimal in the sense that in regions where $\theta(t)$ is not constant the leading order term in the asymptotic expansion of $P_- \, K_\varepsilon^{\mathrm{a}}(t,s)\, P_+$ in powers of ε is proportional to ε.

However, if $\lim_{t\to\pm\infty} \theta'(t) = 0$ then in the scattering limit the transitions between the adiabatic subspaces are much smaller: if the derivatives of $\theta \in C^\infty(\mathbb{R})$ decay sufficiently fast, then for any $n \in \mathbb{N}$

$$\mathcal{A}(\varepsilon) := \lim_{t\to\infty} \| \, P_- \, K_\varepsilon^{\mathrm{a}}(t,-t)\, P_+ \| = \mathcal{O}(\varepsilon^n)\,. \tag{5}$$

If θ is analytic in a suitable neighborhood of the real axis, then transition amplitudes are even exponentially small, $\mathcal{A}(\varepsilon) = \mathcal{O}(\mathrm{e}^{-c/\varepsilon})$ for some constant c depending on the width of the strip of analyticity, see [JoPf$_1$, Ma].

It is well understood, see [Le, Ga, Ne$_1$], how to reconcile the apparent contrariety between the smallness of the final amplitudes in (5) and the optimality of (4): the adiabatic basis is not the optimal basis for monitoring the transition process. For any $n \in \mathbb{N}$ there exist unitary transformations $U_\varepsilon^n(t)$ such that the Hamiltonian in this n^{th} superadiabatic representation takes the form

$$H_\varepsilon^n(t) = \left(\begin{array}{cc} \rho_\varepsilon^n(t) & c_\varepsilon^n(t) \\ \overline{c}_\varepsilon^n(t) & -\,\rho_\varepsilon^n(t) \end{array} \right) \ \text{ with } \ \rho_\varepsilon^n(t) = \rho(t) + \mathcal{O}(\varepsilon^2) \ \text{ and } \ |c_\varepsilon^n(t)| = \mathcal{O}(\varepsilon^{n+1})\,. \tag{6}$$

In the n^{th} superadiabatic basis the off-diagonal components of the propagator and hence also the transitions are of order $\mathcal{O}(\varepsilon^n)$, i.e. there are constants C_n such that

$$\| \, P_- \, K_\varepsilon^n(t,s)\, P_+ \| \leq C_n \varepsilon^n\,. \tag{7}$$

In the scattering regime, where $\theta(t)$ becomes constant, the superadiabatic bases agree with the adiabatic basis, i.e. $\lim_{t\to\pm\infty} U_\varepsilon^n(t) = U_0(t)$, and therefore the bound in (7) basically yields (5). Typically $\lim_{n\to\infty} C_n \varepsilon^n = \infty$ for all $\varepsilon > 0$, i.e. choosing n larger while keeping ε fixed does not necessarily decrease the bound in (7). However, one can choose $n_\varepsilon = n(\varepsilon)$ in such a way that $C_{n_\varepsilon} \varepsilon^{n_\varepsilon}$ is minimal. If θ is analytic, one obtains the improved estimate

$$\| \, P_- \, K_\varepsilon^{n_\varepsilon}(t,s)\, P_+ \| = \mathcal{O}(\mathrm{e}^{-c/\varepsilon})$$

in the optimal superadiabatic basis n_ε, see [Ne$_2$, JoPf$_2$].

More interesting than bounds on $\mathcal{A}(\varepsilon)$ is its actual value. Since $\mathcal{A}(\varepsilon)$ is asymptotically smaller than any power of ε, this question is beyond standard perturbation theory. For the case of analytic coupling θ, asymptotic formulas of the type

$$\mathcal{A}(\varepsilon) = C\, \mathrm{e}^{-\frac{t_{\mathrm{c}}}{\varepsilon}}\, (1 + \mathcal{O}(\varepsilon)) \tag{8}$$

have been established, see e.g. [JKP, Jo], where the constants C and t_{c} depend on the type and location of the complex singularities of $\theta'(t)/\rho(t)$. However, these results are not obtained by solving (1) along the real axis; instead, (1) is investigated in the complex plane along a Stokes line subject to certain conditions, except in the neighborhood of singular points where a comparison equation is solved. As a consequence, the method gives no information at all about the way in which the exponentially small final transition amplitude $\mathcal{A}(\varepsilon)$ is built up in real time. This question of adiabatic transition histories is the concern of our paper. Berry [Be] and, in a refined way Berry and Lim [BeLi, LiBe], gave an answer on a non-rigorous level and explicitly left a mathematically rigorous treatment as an interesting open problem. Only very recently Hagedorn and Joye [HaJo] succeeded and confirmed Berry's results rigorously for a specific Hamiltonian.

Although our work has been strongly motivated by the findings of Berry, our approach is slightly different. Let us first state our main result before we discuss its relation to the earlier ones. Without loss of generality we assume that $\rho(t) \equiv \frac{1}{2}$. It was observed in [Be], that this can always be achieved by transforming (1) to the natural time scale

$$\tau(t) = 2\int_0^t \varrho(s)\,\mathrm{d}s\,.$$

However, we can only treat a rather special class of Hamiltonians, since we must assume that in the natural time scale the coupling has the form

$$\theta'(t) = \mathrm{i}\gamma\left(\frac{1}{t+\mathrm{i}t_\mathrm{c}} - \frac{1}{t-\mathrm{i}t_\mathrm{c}}\right) = \frac{\gamma t_\mathrm{c}}{t^2+t_\mathrm{c}^2} \tag{9}$$

with $\gamma \in \mathbb{R}$ and $t_\mathrm{c} > 0$. In other words we assume

$$H(t) = \frac{1}{2}\begin{pmatrix} \cos\theta(t) & \sin\theta(t) \\ \sin\theta(t) & -\cos\theta(t)\end{pmatrix} \qquad \text{with} \qquad \theta(t) = 2\,\gamma\arctan\left(\frac{t}{t_\mathrm{c}}\right)\,. \tag{10}$$

We shall comment below on the meaning of this special choice and remark here that the Hamiltonian in [HaJo] is (10) with $\gamma = \frac{1}{2}$.

Our main result is the construction of an optimal superadiabatic basis in which the coupling term in the Hamiltonian is exponentially small and can be computed explicitly at leading order. This optimal basis is given as the $n_\varepsilon^{\mathrm{th}}$ superadiabatic basis where $0 \leq \sigma_\varepsilon < 2$ is such that

$$n_\varepsilon = \frac{t_\mathrm{c}}{\varepsilon} - 1 + \sigma_\varepsilon \qquad \text{is an even integer.} \tag{11}$$

Theorem 1. *Let $H(t)$ be as in (10) and n_ε as in (11), and let $\varepsilon_0 > 0$ be sufficiently small. Then for every $\varepsilon \in (0, \varepsilon_0]$ one can construct a family of unitary matrices $U_\varepsilon^{n_\varepsilon}(t) \in \mathbb{C}^{2\times 2}$, depending smoothly on $t \in \mathbb{R}$, such that*

$$\|U_\varepsilon^{n_\varepsilon}(t) - U_0(t)\| = \mathcal{O}\left(\frac{\varepsilon^2}{1+t^2}\right) \tag{12}$$

and

$$U_\varepsilon^{n_\varepsilon}(t)\,\Big(\mathrm{i}\varepsilon\partial_t - H(t)\Big)\,U_\varepsilon^{n_\varepsilon *}(t) = \mathrm{i}\varepsilon\partial_t - \underbrace{\begin{pmatrix} \rho_\varepsilon^{n_\varepsilon}(t) & c_\varepsilon^{n_\varepsilon}(t) \\ \overline{c}_\varepsilon^{n_\varepsilon}(t) & -\rho_\varepsilon^{n_\varepsilon}(t)\end{pmatrix}}_{=:\,H_\varepsilon^{n_\varepsilon}(t)}\,. \tag{13}$$

Here

$$\rho_\varepsilon^{n_\varepsilon}(t) = \frac{1}{2} + \mathcal{O}\left(\frac{\varepsilon^2}{1+t^2}\right) ,$$

and for every $\alpha < \frac{3}{2}$

$$c_\varepsilon^{n_\varepsilon}(t) = 2\mathrm{i}\sqrt{\frac{2\varepsilon}{\pi t_\mathrm{c}}}\,\sin\left(\frac{\pi\gamma}{2}\right)\,\mathrm{e}^{-\frac{t_\mathrm{c}}{\varepsilon}}\,\mathrm{e}^{-\frac{t^2}{2\varepsilon t_\mathrm{c}}}\,\cos\left(\frac{t}{\varepsilon}-\frac{t^3}{3\varepsilon t_\mathrm{c}^2}+\frac{\sigma_\varepsilon t}{t_\mathrm{c}}\right) + \mathcal{O}\left(\phi^\alpha(\varepsilon,t)\right) , \tag{14}$$

with

$$\phi^\alpha(\varepsilon,t) = \begin{cases} \varepsilon^\alpha \exp\left(-\frac{t_\mathrm{c}}{\varepsilon}\left(1+\frac{t^2}{4t_\mathrm{c}^2}\right)\right) & \textit{if } |t| < t_\mathrm{c}, \\ \dfrac{1}{1+t^2}\exp\Big(-\frac{t_\mathrm{c}}{\varepsilon}\left(1+\frac{\ln 2}{2}\right)\Big) & \textit{if } |t| \geq t_\mathrm{c}. \end{cases} \tag{15}$$

Remark 1. The explicit term in $c_\varepsilon^{n_\varepsilon}$ is of order $\mathcal{O}(\mathrm{e}^{-t_\mathrm{c}/\varepsilon})$ only for times $|t| = \mathcal{O}(\sqrt{\varepsilon})$. For larger times all terms in $c_\varepsilon^{n_\varepsilon}$ are exponentially small compared to the leading exponential $\mathrm{e}^{-t_\mathrm{c}/\varepsilon}$. As a consequence, Taylor expansion of the cosine in $c_\varepsilon^{n_\varepsilon}$ around t/ε for $|t| = \mathcal{O}(\sqrt{\varepsilon})$ shows that it can be replaced by $\cos(t/\varepsilon)$ at the cost of lowering α to $\alpha < 1$: for every $\alpha < 1$

$$c_\varepsilon^{n_\varepsilon}(t) = 2\mathrm{i}\sqrt{\frac{2\varepsilon}{\pi t_\mathrm{c}}}\,\sin\left(\frac{\pi\gamma}{2}\right)\,\mathrm{e}^{-\frac{t_\mathrm{c}}{\varepsilon}}\,\mathrm{e}^{-\frac{t^2}{2\varepsilon t_\mathrm{c}}}\,\cos\left(\frac{t}{\varepsilon}\right) + \mathcal{O}\left(\phi^\alpha(\varepsilon,t)\right) .$$

Remark 2. The slow time decay of the error in (15) for large times is due to the fact that n_ε is optimal for t near 0, but not for large t.

Remark 3. Taking n_ε defined in (11) odd instead of even would yield slightly different off-diagonal elements in the effective Hamiltonian $H_\varepsilon^{n_\varepsilon}(t)$. However, the resulting unitary propagator, cf. Corollary 1, would be the same at leading order. See the end of Section 5 for a discussion of this somewhat surprising fact.

Let us shortly explain the idea of the proof of Theorem 1 and at the same time the structure of our paper. First we construct the n^{th} order superadiabatic basis as in (6) in two steps: in Section 2 we construct the projectors on the superadiabatic basis vectors and in Section 3 we construct the unitary basis transformation $U_\varepsilon^n(t)$. We cannot use existing results here, e.g. [Ga, Ne$_2$], since we need to keep careful track of the exact form of the off-diagonal terms $c_\varepsilon^n(t)$ of the superadiabatic Hamiltonian, and since we aim at a scalar recurrence relation instead of a matrix recurrence relation for the $c_\varepsilon^n(t)$'s. The main mathematical challenge is the asymptotic analysis of the resulting recurrence relation, which is done in Section 4. This is also the only part where we have to assume the special form (9) for θ'. Theorem 1 then follows by choosing the order n of the superadiabatic basis as in (11), a choice which minimizes $c_\varepsilon^n(t)$ near $t = 0$. The details of this optimal truncation procedure and the proper proof of Theorem 1 are given in Section 5. Finally in Section 6 we use first order perturbation theory in the optimal superadiabatic basis in order to obtain the following Corollary, in which we abbreviate

$$\Delta(t,s) := \arctan(t) - \arctan(s)\,.$$

Also recall that $\mathrm{erf} : \mathbb{R} \to (-1,1)$ with $\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x \mathrm{e}^{-x^2}\mathrm{d}x$ switches smoothly and monotonically from $\mathrm{erf}(-\infty) = -1$ to $\mathrm{erf}(\infty) = 1$.

Corollary 1. *The unitary propagator in the optimal superadiabatic basis*

$$K_\varepsilon^{n_\varepsilon}(t,s) = \begin{pmatrix} k_\varepsilon^+(t,s) & k_\varepsilon(t,s) \\ \overline{k}_\varepsilon(t,s) & k_\varepsilon^-(t,s) \end{pmatrix},$$

i.e. the solution of

$$\mathrm{i}\varepsilon\partial_t K_\varepsilon^{n_\varepsilon}(t,s) = H_\varepsilon^{n_\varepsilon}(t)K_\varepsilon^{n_\varepsilon}(t,s)\,, \qquad K_\varepsilon^{n_\varepsilon}(s,s) = \mathrm{id}\,,$$

satisfies

$$k_\varepsilon^\pm(t,s) = \mathrm{e}^{\mp\frac{\mathrm{i}(t-s)}{2\varepsilon}} + \mathcal{O}(\varepsilon\Delta(t,s)) \tag{16}$$

and

$$\begin{aligned} k_\varepsilon(t,s) \;&=\; \sin\left(\frac{\pi\gamma}{2}\right)\mathrm{e}^{-\frac{t_c}{\varepsilon}}\mathrm{e}^{-\frac{\mathrm{i}(t+s)}{2\varepsilon}}\left(\mathrm{erf}\left(\frac{t}{\sqrt{2\varepsilon t_c}}\right) - \mathrm{erf}\left(\frac{s}{\sqrt{2\varepsilon t_c}}\right)\right) \\ &\quad + \mathcal{O}\left(\sqrt{\varepsilon}\mathrm{e}^{-\frac{t_c}{\varepsilon}}\Delta(t,s)\right)\,. \end{aligned} \tag{17}$$

Outside the transition region, more precisely for $|t| > \varepsilon^\beta$ and $|s| > \varepsilon^\beta$ for some $\beta < \frac{1}{2}$, (17) holds with the error term replaced by $\mathcal{O}(\varepsilon^\alpha\mathrm{e}^{-\frac{t_c}{\varepsilon}}\Delta(t,s))$ for every $\alpha < 1$.

Corollary 1 immediately implies the existence of solutions to (1) of the form

$$\psi(t) = U_\varepsilon^*(t)\begin{pmatrix} \mathrm{e}^{-\frac{\mathrm{i}t}{2\varepsilon}} \\ \sin\left(\frac{\pi\gamma}{2}\right)\mathrm{e}^{-\frac{t_c}{\varepsilon}}\mathrm{e}^{\frac{\mathrm{i}t}{2\varepsilon}}\left(\mathrm{erf}\left(\frac{t}{\sqrt{2\varepsilon t_c}}\right)+1\right)\end{pmatrix} + \mathcal{O}\left(\sqrt{\varepsilon}\mathrm{e}^{-\frac{t_c}{\varepsilon}}\right). \tag{18}$$

They start at large negative times in the positive energy adiabatic subspace and smoothly and monotonically develop the exponentially small component in the negative energy adiabatic subspace in a $\sqrt{\varepsilon}$-neighborhood of $t = 0$. Berry and Lim [Be, BeLi] argue that this behavior is universal: whenever θ' has the form

$$\theta'(t) = \frac{\pm\mathrm{i}\gamma}{t \pm \mathrm{i}t_c} + \mathcal{O}(|t \pm \mathrm{i}t_c|^\alpha) \qquad \text{for some } \alpha > -1$$

near its singularities $\pm\,\mathrm{i}t_c$ closest to the real axis, then (18) should hold. For the Landau-Zener Hamiltonian, which describes the generic situation, one finds $\gamma = \frac{1}{3}$ and $\alpha = -\frac{1}{3}$. Hagedorn and Joye [HaJo] proved (18) for the Hamiltonian (10) with

$\gamma = \frac{1}{2}$. In the approach of Berry and, slightly modified, of Hagedorn and Joye, the optimal superadiabatic basis vectors are obtained through optimal truncation of an asymptotic expansion of the true solution of (1) in powers of ε.

In contrast, in our approach the optimal superadiabatic basis is constructed by approximately diagonalizing the Hamiltonian. The main advantage of "transforming the Hamiltonian" over "expanding the solutions" is that the former approach can be applied, at least heuristically, to more general adiabatic problems, cf. [Te], as for example the Born-Oppenheimer approximation. While we cannot control the asymptotics for the Born-Oppenheimer model rigorously yet, the heuristic application of the idea yields new physical insight into adiabatic transition histories and new expressions for the exponentially small off-diagonal elements of the S-matrix for simple Born-Oppenheimer type models, cf. [BeTe]. Therefore we see the rigorous results obtained in this paper also as a first attempt to justify the application of analogous ideas to more complicated but also more relevant systems. Furthermore, the concept of an adiabatically renormalized Hamiltonian was used to derive a criterion for selecting possible transition sequences in multi-level problems [WiMo].

For the specific problem (1) the knowledge of two linearly independent solutions is of course equivalent to the knowledge of the propagator and the effective Hamiltonian in the optimal superadiabatic basis. Therefore we shortly explain which aspects of our result constitute an improvement compared to [HaJo]: Most importantly, our proof does not rely on the a priori knowledge of the scattering amplitude $\mathcal{A}(\varepsilon)$. Indeed, our result yields for the first time a proof of (8) based on superadiabatic evolution, as expressed in Corollary 2. Moreover, we allow for a slightly larger class of Hamiltonians and obtain more detailed error estimates, which, in particular, give rise to close to optimal error bounds in the expansion of the S-matrix, cf. Corollary 2. Finally, we also get explicitly the next order correction in (17) resp. (18), cf. Section 6. It should be noted, however, that the improved error estimates and the next order corrections could have been obtained also based on the proof in [HaJo].

We finally turn to the scattering limit. Let $K^0_\varepsilon(t,s)$ denote the propagator in the original basis and define the scattering matrix in the adiabatic basis by

$$S^{\mathrm{a}}_\varepsilon := \lim_{t\to\infty} \mathrm{e}^{\frac{\mathrm{i}H_0 t}{\varepsilon}}\, U_0(t)\, K^0_\varepsilon(t,-t)\, U_0^*(-t)\, \mathrm{e}^{\frac{\mathrm{i}H_0 t}{\varepsilon}}\,, \quad \text{where } H_0 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}.$$

Since, according to (12), for large negative and positive times the optimal superadiabatic basis agrees with the adiabatic basis, $S^{\mathrm{a}}_\varepsilon$ can be computed with help of the optimal superadiabatic propagator from Corollary 1.

Corollary 2. *For $\beta < 1$ we have*

$$S^{\mathrm{a}}_\varepsilon = \begin{pmatrix} 1+\mathcal{O}(\varepsilon) & 2\sin\left(\frac{\pi\gamma}{2}\right)\mathrm{e}^{-\frac{t_c}{\varepsilon}}\,(1+\mathcal{O}(\varepsilon^\beta)) \\ 2\sin\left(\frac{\pi\gamma}{2}\right)\mathrm{e}^{-\frac{t_c}{\varepsilon}}\,(1+\mathcal{O}(\varepsilon^\beta)) & 1+\mathcal{O}(\varepsilon) \end{pmatrix}.$$

Proof. According to (12) we have

$$S^{\mathrm{a}}_\varepsilon = \lim_{t\to\infty} \mathrm{e}^{\frac{\mathrm{i}H_0 t}{\varepsilon}}\, U^{n_\varepsilon}_\varepsilon(t)\, K^0_\varepsilon(t,-t)\, U^{n_\varepsilon\,*}_\varepsilon(-t)\, \mathrm{e}^{\frac{\mathrm{i}H_0 t}{\varepsilon}} = \lim_{t\to\infty} \mathrm{e}^{\frac{\mathrm{i}H_0 t}{\varepsilon}}\, K^{n_\varepsilon}_\varepsilon(t,-t)\, \mathrm{e}^{\frac{\mathrm{i}H_0 t}{\varepsilon}}\,.$$

Now the claim follows from inserting (16) and (17) with the improved error estimate outside of the transition region. □

From Corollary 2 we conclude that the transition amplitude is given by

$$\mathcal{A}(\varepsilon) = \|P_- S^{\mathrm{a}}_\varepsilon P_+\| = 2\,\sin\left(\frac{\pi\gamma}{2}\right)\, \mathrm{e}^{-\frac{t_c}{\varepsilon}}\, \left(1 + \mathcal{O}(\varepsilon^\beta)\right)\,, \qquad \text{for any } \beta < 1\,,$$

which agrees with the results of [Jo], as explained in [BeLi].

We conclude the introduction with two recommendations for further reading: The numerical results of Berry and Lim [LiBe] beautifully illustrate the idea of optimal superadiabatic bases and universal adiabatic transition histories. The introduction of the paper of Hagedorn and Joye [HaJo] gives a slightly different viewpoint on the problem and, in particular, a short discussion on how exponential asymptotics for the Schrödinger equation (1) fit into the broader field of exponential asymptotics for ordinary differential equations.

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2 Superadiabatic projections

For the present and the following section we assume that $H(t)$ has the form (10), but with some arbitrary $\theta \in C^\infty(\mathbb{R})$. The first aim is to construct time-dependent matrices $\pi^{(n)} \in \mathbb{R}^{2\times 2}$ with

$$(\pi^{(n)})^2 - \pi^{(n)} = \mathcal{O}(\varepsilon^{n+1}), \tag{19}$$

$$\left[\mathrm{i}\varepsilon\partial_t - H, \pi^{(n)}\right] = \mathcal{O}(\varepsilon^{n+1}). \tag{20}$$

Here, $[A,B] = AB - BA$ denotes the commutator two operators A and B. Likewise, we will later use $[A,B]_+ = AB + BA$ to denote the anti-commutator of A and B. Equation (19) says that $\pi^{(n)}$ is a projection up to errors of order ε^{n+1}, while (20) implies that $\pi^{(n)}(t)$ is approximately equivariant, i.e.

$$K^0_\varepsilon(t,s)\, \pi^{(n)}(s) = \pi^{(n)}(t)\, K^0_\varepsilon(t,s) + \mathcal{O}(\varepsilon^n)\,.$$

Recall the $K^0_\varepsilon(t,s)$ is the unitary propagator for (1). Hence $\pi^{(n)}(t)$ is an almost projector onto an almost equivariant subspace.

We construct $\pi^{(n)}$ inductively starting from the Ansatz

$$\pi^{(n)} = \sum_{k=0}^{n} \pi_k \varepsilon^k\,. \tag{21}$$

By (10), H has two eigenvalues $\pm 1/2$. Let π_0 be the projection onto the eigenspace corresponding to $+1/2$, and $\pi^{(0)} = \pi_0$ according to (21). It is easily checked that (19) and (20) are fulfilled for $n = 0$. In order to construct π_n for $n > 0$, let us write $G_n(t)$ for the term of order ε^{n+1} in (19), i.e.

$$(\pi^{(n)})^2 - \pi^{(n)} = \varepsilon^{n+1} G_{n+1} + \mathcal{O}(\varepsilon^{n+2}) \,. \tag{22}$$

Obviously,

$$G_{n+1} = \sum_{j=1}^{n} \pi_j \pi_{n+1-j}. \tag{23}$$

Proposition 1. *Assume that $\pi^{(n)}$ given by (21) fulfills (19) and (20). Then a unique matrix π_{n+1} exists such that $\pi^{(n+1)}$ defined as in (21) fulfills (19) and (20). π_{n+1} is given by*

$$\pi_{n+1} = G_{n+1} - \pi_0 G_{n+1} - G_{n+1}\pi_0 - \mathrm{i}\,[\pi_n', \pi_0] \,. \tag{24}$$

Furthermore π_n' is off-diagonal with respect to π_0, i.e.

$$\pi_0 \pi_n' \pi_0 = (1 - \pi_0)\pi_n'(1 - \pi_0) = 0, \tag{25}$$

and G_n is diagonal with respect to π_0, i.e.

$$\pi_0 G_{n+1}(1 - \pi_0) = (1 - \pi_0) G_{n+1} \pi_0 = 0. \tag{26}$$

Remark 4. The fact that the superadiabatic projections are unique answers the question raised in [Be] to which extend the superadiabatic basis constructed there is uniquely determined.

Remark 5. Our construction can be seen as a special case of the construction in [EmWe]. It was applied in the same context in [PST, Te]. The role and the importance of the superadiabatic subspaces as opposed to the superadiabatic evolution have been emphasized by Nenciu [Ne$_2$]. He constructs the superadiabatic projections for much more general time-dependent Hamiltonians. However, Nenciu's construction is less suitable for the explicit computations we need to perform. For a pseudo differential calculus point of view cf. [Sj].

Proof. Let $\pi^{(n+1)}$ be given by (21) and suppose $\pi^{(n)}$ fulfills (19) and (20). Let $\tilde{\pi}_{n+1}$ be an arbitrary matrix, and define $\tilde{\pi}^{(n+1)} = \pi^{(n)} + \varepsilon^{n+1}\tilde{\pi}_{n+1}$. Then

$$(\tilde{\pi}^{(n+1)})^2 - \tilde{\pi}^{(n+1)} = (\pi^{(n)})^2 - \pi^{(n)} + \varepsilon^{n+1}\left(\left[\tilde{\pi}^{(n+1)}, \tilde{\pi}_{n+1}\right]_+ - \tilde{\pi}_{n+1}\right).$$

Using (22), we see that terms of order ε^{n+1} vanish if and only if

$$G_{n+1} = \tilde{\pi}_{n+1} - [\pi_0, \tilde{\pi}_{n+1}]_+ = (1 - \pi_0)\tilde{\pi}_{n+1}(1 - \pi_0) - \pi_0 \tilde{\pi}_{n+1} \pi_0. \tag{27}$$

Multiplying (27) with $(1-\pi_0)$ and with π_0 on both sides and subtracting the results, we find that $\tilde{\pi}_{n+1}$ must fulfill

$$(1-\pi_0)\tilde{\pi}_{n+1}(1-\pi_0)+\pi_0\tilde{\pi}_{n+1}\pi_0 = G_{n+1}-[G_{n+1},\pi_0]_+ \,. \tag{28}$$

Similarly

$$\left[\mathrm{i}\varepsilon\partial_t - H, \tilde{\pi}^{(n+1)}\right] = \left[\mathrm{i}\varepsilon\partial_t - H, \pi^{(n)}\right] + \varepsilon^{n+1}\left[\mathrm{i}\varepsilon\partial_t - H, \tilde{\pi}_{n+1}\right].$$

Again terms of order ε^{n+1} vanish if and only if

$$\mathrm{i}\pi_n' = [H, \tilde{\pi}_{n+1}]\,. \tag{29}$$

Since π_0 is the projector onto the eigenspace of H, we have $\pi_0 H = H\pi_0 = E\pi_0$, where $E = 1/2$ is the positive eigenvalue of H, and similarly $(1-\pi_0)H = H(1-\pi_0) = -E(1-\pi_0)$. When we multiply (29) first with with π_0 from the left and with $1-\pi_0$ from the right, then the other way round, and finally subtract the second result from the first, we get

$$2E(\pi_0\tilde{\pi}_{n+1}(1-\pi_0)+(1-\pi_0)\tilde{\pi}_{n+1}\pi_0) = -\mathrm{i}\,[\pi_n', \pi_0]\,. \tag{30}$$

Now we divide (30) by $2E$ and add (28) to find

$$\tilde{\pi}_{n+1} = G_{n+1} - [G_{n+1},\pi_0]_+ - \frac{\mathrm{i}}{2E}\,[\pi_n',\pi_0]\,. \tag{31}$$

Thus $\tilde{\pi}_{n+1}$ is uniquely determined by the requirement that $\tilde{\pi}^{(n+1)}$ should fulfill (19) and (20). On the other hand, $\left[H, G_{n+1} - [G_{n+1},\pi_0]_+\right] = 0$ and

$$\pi_0\,[\pi_n',\pi_0]\,\pi_0 = (1-\pi_0)\,[\pi_n',\pi_0]\,(1-\pi_0) = 0\,,$$

and thus π_{n+1} given by the right hand side of (31) indeed fulfills (28) and (29). This shows existence. (26) and (25) now follow directly from (27) and (29). □

The calculation of $\pi^{(n)}$ via the matrix recurrence relation (24) and (23) is now possible in principle, but extremely cumbersome. In order to make more explicit calculations possible, we introduce a special basis of $\mathbb{R}^{2\times 2}$. Recall that $U_0(t)$ as defined in (2) is the unitary transformation into the basis consisting of the eigenvectors of H, i.e. the adiabatic basis, and let $V_0(t) = \frac{2}{\theta'(t)}U_0'(t)$. With $P = P_+$ as in (3) we then have $U_0^2 = V_0^2 = \mathrm{id}$ and $PU_0V_0P = PV_0U_0P = 0$, and $\pi_0 = U_0PU_0$. Moreover, since $G_1 = 0$ by (23), (24) implies

$$\pi_1 = -\frac{\mathrm{i}}{2}\theta'(V_0PU_0 - U_0PV_0). \tag{32}$$

Motivated by this, we put

$$\begin{aligned} X &= V_0PU_0 - U_0PV_0\,, & Y &= V_0PV_0 - U_0PU_0\,,\\ Z &= V_0PU_0 + U_0PV_0\,, & W &= V_0PV_0 + U_0PU_0\,. \end{aligned}$$

It is immediate that this is a basis of $\mathbb{R}^{2\times 2}$ for all t, and in fact

$$X = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad W = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad Y = -2H, \quad Z = \frac{-1}{\theta'} Y'.$$

Our reason for representing X through Z via U_0 and V_0 is that the following important relations now follow without effort:

$$X' = 0, \quad Y' = -\theta' Z, \quad Z' = \theta' Y, \tag{33}$$
$$[X,Y]_+ = [X,Z]_+ = [Y,Z]_+ = 0, \quad -X^2 = Y^2 = Z^2 = W, \tag{34}$$
$$[X,\pi_0] = Z, \quad [Y,\pi_0] = 0, \quad [Z,\pi_0] = X, \tag{35}$$
$$W - [W,\pi_0]_+ = Y. \tag{36}$$

These relations show that this basis behaves extremely well under the operations involved in the recursion (24). This enables us to obtain

Proposition 2. *For all $n \in \mathbb{N}$, π_n is of the form*

$$\pi_n = x_n X + y_n Y + z_n Z, \tag{37}$$

where the functions x_n, y_n and z_n satisfy the differential equations

$$x_n' = \mathrm{i} z_{n+1}, \tag{38}$$
$$y_n' = -\theta' z_n, \tag{39}$$
$$z_n' = \mathrm{i} x_{n+1} + \theta' y_n. \tag{40}$$

Moreover,

$$x_1(t) = -\frac{\mathrm{i}}{2}\theta'(t), \quad y_1(t) = z_1(t) = 0. \tag{41}$$

Remark 6. Hence, for all even n, $x_n = 0$, while for all odd n, $y_n = z_n = 0$.

Proof. (41) was already noticed in (32), or alternatively follows from $\pi_0 = (W - Y)/2$, (33) and (35). Now suppose π_n is given by (37). By (34) and (36), $G_{n+1} - [G_{n+1}, \pi_0]_+$ is proportional to Y with a prefactor given through (23), and by (24), (33) and (35),

$$\pi_{n+1} = \sum_{j=1}^{n} (-x_j x_{n+1-j} + y_j y_{n+1-j} + z_j z_{n+1-j}) Y + \mathrm{i}(\theta' y_n - z_n') X - \mathrm{i} x_n' Z. \tag{42}$$

Comparing with (37) shows (38) and (40). To show (39), we use (25). This gives

$$0 = \pi_0 \pi_n' \pi_0 = (y_n' + \theta' z_n) \pi_0 Y \pi_0 + (z_n' - \theta' y_n) \pi_0 Z \pi_0 + x_n' \pi_0 X \pi_0.$$

Since $\pi_0 Z \pi_0 = \pi_0 X \pi_0 = 0$ and $\pi_0 Y \pi_0 = -\pi_0$, the claim follows. □

Remark 7. From (38) through (40) we may derive recursions for calculating x_n or z_n, e.g.

$$z_{n+2}(t) = -\frac{\mathrm{d}}{\mathrm{d}t}\left(z_n'(t) + \theta'(t)\left(\int \theta'(t) z_n(t)\,\mathrm{d}t + C\right)\right). \tag{43}$$

The constant of integration C must (and in some cases can) be determined by comparison with (42). In the case where θ' is given by (9), this strategy will lead to fairly explicit expressions of the coefficient functions x_n, y_n and z_n, cf. Proposition 5; from these we will extract the asymptotic behaviour of x_n, y_n and z_n, cf. Theorem 3.

Using (38)–(40), we can give very simple expressions for the quantities appearing in (19) and (20). As for (20), we use (33) and the differential equations to find

$$\begin{aligned}\left[\mathrm{i}\varepsilon\partial_t - H, \pi^{(n)}\right] &= \mathrm{i}\varepsilon^{n+1}\pi_n' = \mathrm{i}\varepsilon^{n+1}\left(x_n'X + (y_n' + \theta' z_n)Y + (z_n' - \theta' y_n)Z\right) = \\ &= -\varepsilon^{n+1}(z_{n+1}X + x_{n+1}Z). \end{aligned}\tag{44}$$

Now we turn to $(\pi^{(n)})^2 - \pi^{(n)}$, the term by which $\pi^{(n)}$ fails to be a projector. Let us write

$$(\pi^{(n)})^2 - \pi^{(n)} = \sum_{k=1}^{n} \varepsilon^{n+k} G_{n+1,k}. \tag{45}$$

With our earlier convention, $G_{n+1,1} = G_{n+1}$. Explicitly, (21) and (45) give

$$G_{n+1,k} = [\pi_k, \pi_n]_+ + [\pi_{k+1}, \pi_{n-1}]_+ + \ldots = \sum_{j=0}^{n-k} \pi_{j+k}\pi_{n-j}. \tag{46}$$

Proposition 3. *For each $n \in \mathbb{N}$, there exist functions $g_{n+1,k}, k \leq n$ with*

$$((\pi^{(n)})^2 - \pi^{(n)})(t) = \left(\sum_{k=1}^{n} \varepsilon^{n+k} g_{n+1,k}(t)\right) W. \tag{47}$$

For each $k \leq n$,

$$g_{n+1,k}' = 2\mathrm{i}(x_k z_{n+1} - z_k x_{n+1}).$$

Proof. By (34), each $G_{n+1,k}$ is proportional to W. Using (37) additionally, we find $[\pi_k, \pi_m]_+ = 2(-x_k x_m + y_k y_m + z_k z_m)W$, and thus (46) yields

$$g_{n+1,k} = \sum_{j=0}^{n-k} -x_{j+k}x_{n-j} + y_{j+k}y_{n-j} + z_{j+k}z_{n-j}.$$

Thus by using Proposition 2,

$$\begin{aligned}
g'_{n+1,k} &= \sum_{j=0}^{n-k} \mathrm{i}(z_{j+k+1}x_{n-j} + x_{j+k}z_{n-j+1}) - (\theta' z_{j+k}y_{n-j} + \theta' y_{j+k}z_{n-j}) + \\
&\quad +\theta y_{j+k}z_{n-j} + \theta' y_{j+k}z_{n-j} - \mathrm{i}(x_{j+k+1}z_{n-j} + z_{j+k}x_{n-j+1}) = \\
&= \mathrm{i}\sum_{j=0}^{n-k}((z_{j+k+1}x_{n-j} - z_{j+k}x_{n-j+1}) + (x_{j+k}z_{n-j+1} - x_{j+k+1}z_{n-j}) = \\
&= 2\mathrm{i}(x_k z_{n+1} - z_k x_{n+1}).
\end{aligned}$$

The last equality follows because the sum is a telescopic sum. □

Since $W = \mathrm{id}$ is independent of t, Proposition 3 gives the derivative of the correction $(\pi^{(n)})^2 - \pi^{(n)}$ to a projector. As above, this gives an easy way for estimating the correction itself provided we have some clue how to choose the constant of integration.

3 Construction of the unitary

We now proceed to construct the unitary transformation U_ε^n into the n^{th} superadiabatic basis. By (21) and (24), $\pi^{(n)}$ is self-adjoint. Thus it has two orthonormal eigenvectors v_n and w_n. Let

$$v_0 = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix}, \quad w_0 = \begin{pmatrix} \sin(\theta/2) \\ -\cos(\theta/2) \end{pmatrix}$$

be the eigenvectors of π_0, and write

$$v_n = \alpha v_0 + \beta w_0, \quad w_n = \overline{\alpha} w_0 - \overline{\beta} v_0 \qquad (\alpha, \beta \in \mathbb{C}). \tag{48}$$

We make this representation unique by requiring $0 \le \alpha \in \mathbb{R}$. Let U_ε^n be the unitary operator taking (v_n, w_n) to the standard basis (e_1, e_2) of $\mathbb{R}^2$, i.e.

$$U_\varepsilon^n = e_1 v_n^* + e_2 w_n^*, \tag{49}$$

where all vectors are column vectors. Note that the definition (2) of U_0 is consistent with (49) for $n = 0$. U_ε^n diagonalizes $\pi^{(n)}$, thus

$$U_\varepsilon^n \pi^{(n)} U_\varepsilon^{n\,*} = D \equiv \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \tag{50}$$

where $\lambda_{1,2}$ are the eigenvalues of $\pi^{(n)}$. Although α, β and $\lambda_{1,2}$ depend on n, ε and t, we suppress this from the notation.

Lemma 1.

$$U_0 U_\varepsilon^{n\,*} = \begin{pmatrix} \alpha & -\overline{\beta} \\ \beta & \alpha \end{pmatrix}, \quad \textit{and} \quad U_0 U_\varepsilon^{n\,*\,'} = \begin{pmatrix} \alpha' + \beta & \alpha - \overline{\beta}' \\ \beta' - \alpha & \alpha' + \overline{\beta} \end{pmatrix}.$$

Proof. The calculations are straightforward and we only show the second equality. First note that $v_0' = -w_0$ and $w_0' = v_0$. Thus

$$U_\varepsilon^{n\,*\,'} = ((\alpha' + \beta)v_0 + (\beta' - \alpha)w_0)e_1^* + ((\alpha - \overline{\beta}')v_0 + (\alpha' + \overline{\beta})w_0)e_2^*,$$

and using the orthogonality of v_0 and w_0 yields the claim,

$$U_0 U_\varepsilon^{n\,*\,'} = e_1(\alpha' + \beta)e_1^* + e_1(\alpha - \overline{\beta}')e_2^* + e_2(\beta' - \alpha)e_1^* + e_2(\alpha' + \overline{\beta})e_2^*\,.$$

$\square$

It will turn out that $\beta, \alpha'\alpha$, and β' are small quantities, λ_1', λ_2', and λ_2 are even much smaller, while α^2 and λ_1 are large, i.e. of order $1 + \mathcal{O}(\varepsilon)$. This motivates the form in which we present the following result.

Proposition 4. *Suppose $\lambda_1 \neq \lambda_2$. Then for each $n \in \mathbb{N}$,*

$$U_\varepsilon^n(\mathrm{i}\varepsilon\partial_t - H)U_\varepsilon^{n\,*} = \mathrm{i}\varepsilon\partial_t - \begin{pmatrix} \frac{1}{2} & \frac{\alpha^2\varepsilon^{n+1}}{\lambda_1 - \lambda_2}(x_{n+1} - z_{n+1}) \\ \frac{\alpha^2\varepsilon^{n+1}}{\lambda_1 - \lambda_2}(-x_{n+1} - z_{n+1}) & -\frac{1}{2} \end{pmatrix} + R,$$

with

$$R = \begin{pmatrix} \varepsilon\mathrm{Im}(\overline{\beta}(2\alpha + \beta')) + |\beta|^2 & -\frac{\varepsilon^{n+1}\overline{\beta}^2}{\lambda_1 - \lambda_2}(x_{n+1} + z_{n+1}) \\ \frac{\varepsilon^{n+1}\beta^2}{\lambda_1 - \lambda_2}(x_{n+1} - z_{n+1}) & -\varepsilon\mathrm{Im}(\overline{\beta}(2\alpha + \beta')) - |\beta|^2 \end{pmatrix}.$$

Proof. Let us write $U_\varepsilon^n(\mathrm{i}\varepsilon\partial_t - H)U_\varepsilon^{n\,*} = (M_{i,j})$, $i,j \in \{1,2\}$. $M_{1,1}$ and $M_{2,2}$ are calculated in a straightforward manner, using Lemma 1 together with the fact $U_0 H U_0^* = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}$:

$$\begin{aligned} U_\varepsilon^n(\mathrm{i}\varepsilon\partial_t - H)U_\varepsilon^{n\,*} &= \mathrm{i}\varepsilon\partial_t + \mathrm{i}\varepsilon U_\varepsilon^n U_0^* U_0 U_\varepsilon^{n\,*\,'} - U_\varepsilon^n U_0^* U_0 H U_0^* U_0 U_\varepsilon^{n\,*} = \\ &= \mathrm{i}\varepsilon\partial_t + \mathrm{i}\varepsilon \begin{pmatrix} \alpha & \overline{\beta} \\ -\beta & \alpha \end{pmatrix} \begin{pmatrix} \alpha' + \beta & \alpha - \overline{\beta}' \\ \beta' - \alpha & \alpha' + \overline{\beta} \end{pmatrix} \\ &\quad -\frac{1}{2} \begin{pmatrix} \alpha & \overline{\beta} \\ -\beta & \alpha \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha & -\overline{\beta} \\ \beta & \alpha \end{pmatrix}. \end{aligned}$$

Carrying out the matrix multiplication yields

$$M_{1,1} = -M_{2,2} = \mathrm{i}\varepsilon\partial_t + \mathrm{i}\varepsilon((\alpha(\alpha' + \beta) + \overline{\beta}(\beta' - \alpha)) - \frac{1}{2}(\alpha^2 - |\beta|^2). \tag{51}$$

We now use $\alpha^2 + |\beta|^2 = 1$ to obtain $0 = 2\alpha\alpha' + \beta'\overline{\beta} + \overline{\beta}'\beta = 2\mathrm{Re}(\alpha\alpha' + \overline{\beta}\beta')$ and $\alpha^2 - |\beta|^2 = 1 - 2|\beta|^2$. Plugging these into (51) gives the diagonal coefficients of M. Although we could get expressions for the off-diagonal coefficients by the same method, these would not be useful later on. Instead we use (50), i.e. $U_\varepsilon^{n\,*}D = \pi^{(n)}U_\varepsilon^{n\,*}$ together with (44) and obtain

$$U_\varepsilon^n(\mathrm{i}\varepsilon\partial_t - H)U_\varepsilon^{n\,*}D = DU_\varepsilon^n(\mathrm{i}\varepsilon\partial_t - H)U_\varepsilon^{n\,*} - \varepsilon^{n+1}U_\varepsilon^n(z_{n+1}X + x_{n+1}Z)U_\varepsilon^{n\,*}. \quad (52)$$

By multiplying (52) with $e_je_j^*$ from the left and by $e_ke_k^*$ from the right ($j,k \in \{1,2\}$) and rearranging, we obtain

$$\begin{aligned}(\lambda_k - \lambda_j)\, e_j\, e_j^*\, U_\varepsilon^n(\mathrm{i}\varepsilon\partial_t - H)\, U_\varepsilon^{n\,*}e_k\, e_k^* = & \qquad (53)\\ = \quad -\varepsilon^{n+1}e_j\, e_j^*\, U_\varepsilon^n(z_{n+1}X + x_{n+1}Z)\, U_\varepsilon^{n\,*}e_k\, e_k^* - \mathrm{i}\delta_{k,j}\,\varepsilon\,\lambda_j'\, e_j\, e_j^*\,. &\end{aligned}$$

From the equalities $U_0XU_0^* = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, $U_0ZU_0^* = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$ and Lemma 1 we obtain

$$U_\varepsilon^n X U_\varepsilon^{n\,*} = \begin{pmatrix} \alpha(\beta - \overline{\beta}) & \alpha^2 + \overline{\beta}^2 \\ -(\alpha^2 + \beta^2) & -\alpha(\beta - \overline{\beta}) \end{pmatrix},$$

$$U_\varepsilon^n Z U_\varepsilon^{n\,*} = \begin{pmatrix} -\alpha(\beta + \overline{\beta}) & -(\alpha^2 - \overline{\beta}^2) \\ -(\alpha^2 - \beta^2) & \alpha(\beta + \overline{\beta}) \end{pmatrix}.$$

The expressions for $M_{1,2}$ and $M_{2,1}$ follow by taking $k \neq j$ in (53). $\square$

We now use our results from the previous section to express α, β and $\lambda_{1,2}$ in terms of x_k, y_k and z_k, $k \leq n$. Let us define

$$\xi \;\equiv\; \xi(n,\varepsilon,t) = \textstyle\sum_{k=1}^n \varepsilon^k x_k(t), \quad (54)$$
$$\eta \;\equiv\; \eta(n,\varepsilon,t) = \textstyle\sum_{k=1}^n \varepsilon^k y_k(t), \quad (55)$$
$$\zeta \;\equiv\; \zeta(n,\varepsilon,t) = \textstyle\sum_{k=1}^n \varepsilon^k z_k(t). \quad (56)$$

Moreover, let

$$g \equiv g(n,\varepsilon,t) = \textstyle\sum_{k=1}^n \varepsilon^{n+k} g_{n+1,k}(t) \quad (57)$$

be the quantity appearing in (47).

Lemma 2. *The eigenvalues of $\pi^{(n)}$ solve the quadratic equation*

$$\lambda_{1,2}^2 - \lambda_{1,2} - g = 0.$$

Proof. By (50) and Proposition 3 we obtain

$$\begin{pmatrix} \lambda_1^2 - \lambda_1 & 0 \\ 0 & \lambda_2^2 - \lambda_2 \end{pmatrix} = U_\varepsilon^n((\pi^{(n)})^2 - \pi^{(n)})\, U_\varepsilon^{n\,*} = U_\varepsilon^n gW U_\varepsilon^{n\,*} = \begin{pmatrix} g & 0 \\ 0 & g \end{pmatrix}.$$

$\square$

Lemma 3.

$$\alpha^2(\lambda_1 - \lambda_2) = 1 - \eta - \lambda_2, \qquad \textit{and} \qquad \alpha\beta(\lambda_1 - \lambda_2) = -\xi - \zeta.$$

Proof. We have

$$\pi^{(n)} = \lambda_1 v_n v_n^* + \lambda_2 w_n w_n^*. \tag{58}$$

Plugging in (48), we obtain

$$\begin{aligned} \pi^{(n)} v_0 &= \lambda_1 \alpha v_n - \lambda_2 \beta w_n = (\lambda_1 \alpha^2 + \lambda_2 |\beta|^2) v_0 + (\lambda_1 - \lambda_2)\alpha\beta w_0 = \\ &= (\alpha^2(\lambda_1 - \lambda_2) + \lambda_2) v_0 + (\lambda_1 - \lambda_2)\alpha\beta w_0. \end{aligned}$$

In the last step, we used $|\beta|^2 + \alpha^2 = 1$. On the other hand, from (21) and (24) we have

$$\pi^{(n)} = \pi_0 + \sum_{k=1}^{n} \varepsilon^k (x_k X + y_k Y + z_k Z)\,, \tag{59}$$

and since $X v_0 = Z v_0 = -w_0$, $\pi_0 v_0 = v_0$ and $Y v_0 = -v_0$, we find

$$\pi^{(n)} v_0 = (1 - \eta) v_0 - (\xi + \zeta) w_0.$$

Comparing coefficients finishes the proof. □

Theorem 2. *Let $\varepsilon_0 > 0$ be sufficiently small. For $\varepsilon \in (0, \varepsilon_0]$ assume there is a bounded function q on $\mathbb{R}$ such that $\xi(t)$, $\eta(t)$, $\zeta(t)$ and their derivatives $\xi'(t), \eta'(t), \zeta'(t)$ are all bounded in norm by $\varepsilon q(t)$. Then*

$$\begin{aligned} &U_\varepsilon^n (\mathrm{i}\varepsilon\partial_t - H) U_\varepsilon^{n\,*} = \\ &= \mathrm{i}\varepsilon\partial_t - \begin{pmatrix} \frac{1}{2} + \mathcal{O}(\varepsilon^2 q) & \varepsilon^{n+1}(x_{n+1} - z_{n+1})\,(1 + \mathcal{O}(\varepsilon q)) \\ \varepsilon^{n+1}(-x_{n+1} - z_{n+1})\,(1 + \mathcal{O}(\varepsilon q)) & -\frac{1}{2} + \mathcal{O}(\varepsilon^2 q) \end{pmatrix}. \end{aligned} \tag{60}$$

Proof. From (59) and our assumptions it follows that $\pi^{(n)} - \pi_0 = \mathcal{O}(\varepsilon q)$. Thus $\lambda_1 = 1 + \mathcal{O}(\varepsilon q)$ and $\lambda_2 = \mathcal{O}(\varepsilon q)$, and from Lemma 2 we infer $g = \mathcal{O}(\varepsilon)$ and

$$\lambda_1 = \tfrac{1}{2}\left(1 + \sqrt{1 + 4g}\right), \qquad \lambda_2 = \tfrac{1}{2}\left(1 - \sqrt{1 + 4g}\right).$$

Since $\lambda_1 - \lambda_2 \neq 0$, Lemma 3 yields

$$\alpha^2 = \frac{1 + \sqrt{1 + 4g} - 2\eta}{2\sqrt{1 + 4g}}, \quad \beta = \frac{-\xi - \zeta}{\sqrt{1 + 4g}\alpha}.$$

Hence $\alpha^2 = 1 + \mathcal{O}(\varepsilon q)$, and β, β' and $\alpha\alpha' = (\alpha^2)'/2$ are all $\mathcal{O}(\varepsilon q)$. Plugging these into the matrix R in Proposition 4 shows the claim. □

4 Solving the recursion: a pair of simple poles

In order to make further progress, we need to understand the asymptotic behavior of the off-diagonal elements of the effective Hamiltonian in the n^{th} superadiabatic basis for large n. According to (60) this amounts to the asymptotics of x_n and z_n as given by the recursion from Proposition 2. It is clear that the function θ' alone determines the behavior of this recursion. We will study here the special case

$$\theta'(t) = \frac{\mathrm{i}\gamma}{t + \mathrm{i}t_{\mathrm{c}}} - \frac{\mathrm{i}\gamma}{t - \mathrm{i}t_{\mathrm{c}}} = \frac{\gamma t_{\mathrm{c}}}{t^2 + t_{\mathrm{c}}^2}\,. \tag{61}$$

The reason lies in the intuition that the poles of θ' closest to the real axis determine the superadiabatic transitions, and that these transitions are of universal form whenever these poles are of order one, see [Be, BeLi] for details. As in [HaJo], we have to restrict to the special case that θ' has no contribution besides these poles in order to solve the recursion. We now have two parameters left in θ'. The distance t_{c} of the poles from the real axis determines the exponential decay rate in the in the off-diagonal elements of the Hamiltonian and the strength of the residue γ determines the pre-factor in front of the exponential. As is done in [HaJo], we could get rid of the parameter t_{c} by rescaling time, but we choose not to do so because t_{c} plays a nontrivial role in optimal truncation and the error bounds obtained therein, and keeping this parameter will make things more transparent.

We use (43) in order to determine the asymptotics of z_n. From Proposition 2 together with (42) it is clear that y_n must go to zero as $t \to \pm\infty$. This fixes the constant of integration in (43), and we arrive at the linear two-step recursion

$$z_{n+2}(t) = -\frac{\mathrm{d}}{\mathrm{d}t}\left(z_n'(t) + \theta'(t) \int_{-\infty}^{t} \theta'(s) z_n(s)\,\mathrm{d}s \right). \tag{62}$$

The fact that the recursion is linear will make its analysis simpler than the one of the nonlinear recursion in [HaJo]. We rewrite θ' as

$$\theta'(t) = \frac{\gamma}{t_{\mathrm{c}}}(f + \overline{f}) \qquad \text{with} \qquad f(t) = \frac{\mathrm{i}t_{\mathrm{c}}}{t + \mathrm{i}t_{\mathrm{c}}}\,.$$

For z_n, we will make an Ansatz as a sum of powers of f and $\overline{f}$. The reason for the success of this approach is the fact that this representation is stable under differentiation and integration, and also under multiplication with θ' through the partial fraction expansion. More explicitly, the following identities hold for the m-th power f^m of f:

Lemma 4. *For each $m \geq 1$,*

$$\theta' \mathrm{Im}(f^m) \quad = \quad \frac{\gamma}{t_{\mathrm{c}}} \sum_{k=0}^{m-1} 2^{-k} \mathrm{Im}(f^{m+1-k}), \tag{63}$$

$$\theta' \mathrm{Re}(f^m) = \frac{\gamma}{t_c}\left(\sum_{k=0}^{m-1} 2^{-k}\mathrm{Re}(f^{m+1-k}) + 2^{-m}\theta'\right), \tag{64}$$

$$\mathrm{Im}(f^m)' = -\frac{m}{t_c}\mathrm{Re}(f^{m+1}), \tag{65}$$

$$\mathrm{Re}(f^m)' = \frac{m}{t_c}\mathrm{Im}(f^{m+1}). \tag{66}$$

Proof. We have $f + \overline{f} = \frac{2t_c^2}{t^2+t_c^2} = 2f\overline{f}$, and thus

$$f^k\overline{f} = \frac{1}{2}f^{k-1}(f+\overline{f}) = \frac{1}{2}(f^k + f^{k-1}\overline{f})$$

and

$$\theta' f^{n-j} = \frac{\gamma}{t_c}\left(\sum_{k=0}^{n-j} 2^{-k} f^{n+1-(j+k)} + 2^{-n+j}\overline{f}\right). \tag{67}$$

Taking the complex conjugate of (67) and adding it to resp. subtracting it from (67), we arrive at (63) and (64). To prove (65) and (66), it suffices to use that $(f^k)' = kf^{k+1}/(\mathrm{i}t_c)$ along with the complex conjugate equation. □

Proposition 5. *For each even $n \in \mathbb{N}$ and $j = 0, \ldots, n-1$, let the numbers $a_j^{(n)}$ be recursively defined through*

$$a_0^{(2)} = 1, \qquad a_1^{(2)} = 0, \tag{68}$$

$$a_j^{(n+2)} = \frac{n+1-j}{(n+1)\,n}\left((n-j)\,a_j^{(n)} - \gamma^2\sum_{k=0}^{j}\frac{1}{n-k}\sum_{m=0}^{k}a_m^{(n)}\right) \quad (j<n), \tag{69}$$

$$a_n^{(n+2)} = a_{n-1}^{(n+2)}, \qquad a_{n+1}^{(n+2)} = 0.$$

Then

$$z_n = -\gamma\frac{(n-1)!}{t_c^n}\sum_{j=0}^{n-1}2^{-j}a_j^{(n)}\mathrm{Im}(f^{n-j}) \quad (n\ \mathit{even}), \tag{70}$$

$$y_n = \gamma^2\frac{(n-1)!}{t_c^n}\sum_{j=0}^{n-1}2^{-j}\left(\frac{1}{n-j}\sum_{k=0}^{j}a_k^{(n)}\right)\mathrm{Re}(f^{n-j}) \quad (n\ \mathit{even}), \tag{71}$$

$$x_n = \mathrm{i}\gamma\frac{(n-1)!}{t_c^n}\sum_{j=0}^{n-1}2^{-j}\left(\frac{n}{n-j}a_j^{(n+1)}\right)\mathrm{Re}(f^{n-j}) \quad (n\ \mathit{odd}), \tag{72}$$

Proof. We proceed by induction. We have $x_1 = \mathrm{i}\theta'/2 = \frac{\mathrm{i}\gamma}{t_c}\mathrm{Re}(f)$, and thus by (38) and (66),

$$z_2 = \frac{\mathrm{i}}{t_c}x_1' = -\frac{\gamma}{t_c^2}\mathrm{Im}(f^2).$$

This proves (70) for $n = 2$. Now suppose that (70) holds for some even $n \in \mathbb{N}$. Then by (38) and (66), (72) holds for $n-1$. To prove (71) for the given n, we want to use (39). (63) and the induction hypothesis on z_n yield

$$\begin{aligned} \theta' z_n &= -\gamma^2 \frac{(n-1)!}{t_{\mathrm{c}}^{n+1}} \sum_{j=0}^{n-1} a_j^{(n)} \sum_{k=0}^{n-j-1} 2^{-(k+j)} \mathrm{Im}(f^{n+1-(j+k)}) = \\ &= -\gamma^2 \frac{(n-1)!}{t_{\mathrm{c}}^{n+1}} \sum_{m=0}^{n-1} 2^{-m} \left(\sum_{j=0}^{m} a_j^{(n)} \right) \mathrm{Im}(f^{n+1-m}). \end{aligned} \tag{73}$$

Since (73) only contains second or higher order powers of f, it is easy to integrate using (66). Let us write

$$b_m^{(n)} = \frac{1}{n-m} \sum_{j=0}^{m} a_j^{(n)}. \tag{74}$$

Then by (66) we obtain

$$y_n = -\int_{-\infty}^{t} \theta'(s) z_n(s)\, \mathrm{d}s = r^2 \frac{(n-1)!}{t_{\mathrm{c}}^{n-1}} \sum_{m=0}^{n-1} 2^{-m} b_m^{(n)} \mathrm{Re}(f^{n-m}),$$

proving (71) for n. It remains to prove (70) for $n+2$. We want to use (62), and therefore we employ (64) and our above calculations in order to get

$$\begin{aligned} &\theta'(t) \int_{-\infty}^{t} \theta'(s) z_n(s)\, \mathrm{d}s = \\ &= -\gamma^3 \frac{(n-1)!}{t_{\mathrm{c}}^{n+1}} \sum_{j=0}^{n-1} b_j \left(\sum_{k=0}^{n-j+1} 2^{-(k+j)} \mathrm{Re}(f^{n+1-(k+j)}) + 2^{-n}\theta' \right) = \\ &= -\gamma^3 \frac{(n-1)!}{t_{\mathrm{c}}^{n+1}} \left(\left(\sum_{j=0}^{n-1} 2^{-j} \left(\sum_{k=0}^{j} b_k \right) \mathrm{Re}(f^{n+1-j}) \right) + 2^{-n+1} \left(\sum_{k=0}^{n-1} b_k \right) \mathrm{Re}(f) \right). \end{aligned}$$

By (65),

$$z_n' = \gamma \frac{(n-1)!}{t_{\mathrm{c}}^{n+1}} \sum_{j=0}^{n-1} 2^{-j} a_j^{(n)} (n-j) \mathrm{Re}(f^{n+1-j}).$$

Now we sum the last two expressions, differentiate again and obtain

$$\begin{aligned} z_{n+2} &= -\gamma \frac{(n-1)!}{t_{\mathrm{c}}^{n+2}} \left(\sum_{j=0}^{n-1} 2^{-j} (n+1-j) \left((n-j) a_j^{(n)} - \gamma^2 \sum_{k=0}^{j} b_k \right) \mathrm{Im}(f^{n+2-j}) \right. \\ &\qquad \left. -2\gamma^2 2^{-n} \left(\sum_{k=0}^{n-1} b_k \right) \mathrm{Im}(f^2) \right). \end{aligned}$$

Comparing coefficients, this proves (70) for $n+2$. □

We now investigate the behavior of the coefficients $a_j^{(n)}$ as $n \to \infty$.

Proposition 6. *Let $a_j^{(n)}$ be defined as in Proposition 5.*

(a) $a_0^{(n)} = \dfrac{\sin(\gamma\pi/2)}{\gamma\pi/2}\left(1 + \mathcal{O}\left(\frac{\gamma^2}{n^2}\right)\right).$

(b) *There exists $C_1 > 0$ such that for all $n \in \mathbb{N}$*

$$|a_1^{(n)}| \le C_1 \frac{\ln n}{n-1}\,.$$

(c) *For each $p > 1$ there exists $C_2 > 0$ such that for all $n \in \mathbb{N}$*

$$\sup_{j\ge 2} p^{-j}|a_j^{(n)}| \le \frac{C_2}{n-1}\,.$$

Proof. (a) By (68), $a_0^{(2)} = 1$, and

$$a_0^{(n+2)} = a_0^{(n)}\left(1 - \frac{\gamma^2}{n^2}\right).$$

Comparing with the product representation of the sine function ([AbSt], 4.3.89)

$$\sin(\pi x) = \pi x \prod_{n=1}^{\infty}\left(1 - \frac{x^2}{n^2}\right),$$

we arrive at (a).
(b) Put $\alpha_n = (n-1)a_1^{(n)}$. Then by (69),

$$\alpha_{n+2} = \alpha_n\left(1 - \frac{\gamma^2}{(n-1)^2}\right) - \gamma^2\left(\frac{1}{n} + \frac{1}{n-1}\right)a_0^{(n)}.$$

thus for $n-1 > \gamma$, we have

$$|\alpha_{n+2}| \le |\alpha_n| + \gamma^2\left(\frac{1}{n} + \frac{1}{n-1}\right)\max_{m\in\mathbb{N}}|a_0^{(m)}|,$$

which shows (b).
(c) Put $c_j^{(n)} = (n-1)p^{-j}a_j^{(n)}$, and $c^{(n)} = \max_{j\ge 2}|c_j^{(n)}|$. We will show that the sequence $c^{(n)}$ is bounded. We have

$$\begin{aligned} c_j^{(n+2)} \quad &= \quad \frac{n+1-j}{n(n-1)}\left((n-j)c_j^{(n)} - \gamma^2\sum_{k=2}^{j}\frac{1}{n-k}\sum_{m=2}^{k}p^{-j+m}c_m^{(n)} - \right.\\ &\left. -(n-1)p^{-j}\gamma^2\left(a_0^{(n)}\sum_{k=0}^{j}\frac{1}{n-k} + a_1^{(n)}\sum_{k=1}^{j}\frac{1}{n-k}\right)\right). \end{aligned} \tag{75}$$

Now

$$\left| \sum_{k=2}^{j} \frac{1}{n-k} \sum_{m=2}^{k} p^{-j+m} c_m^{(n)} \right| \leq c^{(n)} \frac{1}{n-j} \frac{p^2}{(p-1)^2}, \tag{76}$$

and

$$p^{-j} \sum_{k=0}^{j} \frac{1}{n-k} \leq \frac{(j+1)p^{-j}}{n-j} \leq \frac{1}{(n-j)\ln p}. \tag{77}$$

We plug these results into (75) and obtain

$$\begin{aligned} |c_j^{(n+2)}| \quad &\leq \quad c^{(n)} \left(\frac{(n+1-j)(n-j)}{n(n-1)} + \frac{(n+1-j)\,\gamma^2 p^2}{(n-j)(p-1)^2} \frac{1}{n(n-1)} \right) + \\ &+ \frac{1}{n} \frac{(n+1-j)\, p^2\, \gamma^2}{(n-j)(p-1)^2 \ln p} (|a_0^{(n)}| + |a_1^{(n)}|). \end{aligned}$$

By (a) and (b), $a_0^{(n)}$ and $a_1^{(n)}$ are bounded. Taking the supremum over $j \geq 2$ above, we see that there exist constants B_1 and B_2 with

$$c^{(n+2)} \leq c^{(n)} \left(\frac{n-2}{n} + \frac{B_1}{n(n-1)} \right) + \frac{B_2}{n},$$

hence

$$c^{(n+2)} - c^{(n)} \leq \frac{1}{n} \left(\left(-2 + \frac{B_1}{n-1} \right) c^{(n)} + B_2 \right).$$

Now let $n-1 > B_1$. Then for $c^{(n)} > B_2$, the above inequality shows $c^{(n+2)} < c^{(n)}$, while for $c^{(n)} \leq B_2$, $c^{(n+2)} \leq c^{(n)} + B_2/n \leq B_2(1+1/n)$. Thus $c^{(n)}$ is a bounded sequence. □

Remark 8. We will make no use of the fact that the logarithmic correction to the $1/n$-decay of the higher coefficients occurs only in the coefficient $a_1^{(n)}$. We chose to include this in the statement of the preceding theorem anyway, because this gives some insight into the nature of the recursion and is not hard to prove.

Remark 9. Numerical calculations of the first few thousand $a_j^{(n)}$ suggest that (c) above continues to be true if we choose $p = 1$, but this seems to be much harder to prove. However, the estimate above is more than good enough for us.

Remark 10. The constants appearing in the proof of Proposition 6 (b) and (c) are not optimal, and could be improved by more careful arguments. This is unimportant for our purposes, and for the sake of brevity and readability we chose to use the simple estimates given.

Corollary 3. *Let $b_j^{(n)}$ be given by (74). Then for each $p > 1$, there exists $C_3 > 0$ such that*

$$\sup_{j \geq 0} p^{-j} b_j^{(n)} \leq \frac{C_3}{n-1}.$$

Proof. For $j \leq n-1$, we have $n-1 \leq j(n-j)$, and thus Proposition 6 (c) gives

$$\begin{aligned} p^{-j} b_j^{(n)} &\leq \frac{p^{-j}}{n-j}\left((a_0^{(n)}+a_1^{(n)})+\frac{C_2}{n-1}\frac{p^2}{p-1}(p^{j-1}-1)\right) \leq \\ &\leq p^{-j}\frac{j(a_0^{(n)}+a_1^{(n)})}{n-1}+\frac{p\,C_2}{p-1}\frac{1}{n-1} \leq \frac{C_3}{n-1}\,. \end{aligned}$$

$\square$

Having good control over the coefficients $a_j^{(n)}$, we can now derive relatively sharp estimates on the functions x_n, y_n and z_n. Let us fix $\alpha < 1$ and define

$$R_n^\alpha(t) = \frac{1}{(n-1)^\alpha}\max\left\{\left|\frac{t_{\mathrm{c}}}{t+\mathrm{i}t_{\mathrm{c}}}\right|^n, \left(\frac{1}{\sqrt{2}}\right)^{n-2}\left|\frac{t_{\mathrm{c}}}{t+\mathrm{i}t_{\mathrm{c}}}\right|^2\right\}.$$

Obviously, for $t \leq t_{\mathrm{c}}$ the first function in the maximum above dominates, for $t > t_{\mathrm{c}}$ the second one does.

For families of functions $g_n(t), G_n(t)$ we write

$$g_n(t) = \mathcal{O}(G_n(t))$$

if there exists $C > 0$ such that $|g_n(t)| \leq C|G_n(t)|$ for all $n \in \mathbb{N}$ and all $t \in \mathbb{R}$.

Theorem 3. *For $n > 1$ and $\alpha < 1$, we have*

$$x_n(t) = \mathrm{i}\frac{(n-1)!}{t_{\mathrm{c}}^n}\left(\frac{2\sin(\gamma\pi/2)}{\pi}\mathrm{Re}\left(\left(1-\mathrm{i}\frac{t}{t_{\mathrm{c}}}\right)^{-n}\right)+\mathcal{O}(R_n^\alpha(t))\right), \quad (78)$$

$$y_n(t) = \frac{(n-1)!}{t_{\mathrm{c}}^n}\,\mathcal{O}(R_n^\alpha(t)), \quad (79)$$

$$z_n(t) = -\frac{(n-1)!}{t_{\mathrm{c}}^n}\left(\frac{2\sin(\gamma\pi/2)}{\pi}\mathrm{Im}\left(\left(1-\mathrm{i}\frac{t}{t_{\mathrm{c}}}\right)^{-n}\right)+\mathcal{O}(R_n^\alpha(t))\right), \quad (80)$$

Proof. With the definition of f and Proposition 6 (a) we get

$$a_0^{(n)}\mathrm{Im}(f^n) = \frac{2\sin(\gamma\pi/2)}{\pi\gamma}\mathrm{Im}\left(\left(1-\mathrm{i}\frac{t}{t_{\mathrm{c}}}\right)^{-n}\right)+O\left(\frac{1}{n^2}\left|\frac{t_{\mathrm{c}}}{t+\mathrm{i}t_{\mathrm{c}}}\right|^n\right)$$

when n is even, and a similar formula for $a_0^{(n+1)}\mathrm{Re}(f^n)$ when n is odd. This covers the $j=0$ terms in (72) and (70). For the remaining terms, let

$$c_j^{(n)} = \begin{cases} a_j^{(n)} & \text{if } n \text{ is even,} \\ n a_j^{(n)}/(n-j) & \text{if } n \text{ is odd.} \end{cases}$$

Now $n/(n-j) \leq j$ for $j < n$, and thus by Proposition 6 (b) and (c) for each $p > 1$ we can find $C > 0$ such that

$$c_j^{(n)} \leq jp^j \frac{C}{(n-1)^\alpha}$$

for all $j \geq 1$. (For $j \geq 2$, we may even choose $\alpha = 1$, but we will not exploit this.) For $|t| \leq t_\mathrm{c}$, we have $|t_\mathrm{c}/(t + \mathrm{i}t_\mathrm{c})|^{-j} \leq 2^{j/2}$, so we get

$$\left| \sum_{j=2}^{n-1} \frac{c_j^{(n)}}{2^j} \left(\frac{\mathrm{i}t_\mathrm{c}}{t + \mathrm{i}t_\mathrm{c}} \right)^{n-j} \right| \leq \left(\frac{C}{(n-1)^\alpha} \sum_{j=2}^{n-1} j \left(\frac{p}{\sqrt{2}} \right)^j \right) \left| \frac{t_\mathrm{c}}{t + \mathrm{i}t_\mathrm{c}} \right|^n .$$

If we choose $p < \sqrt{2}$, the sum on the right hand sided is bounded uniformly in n. Combining this with our above calculations, (78) and (80) are proved for $|t| < t_\mathrm{c}$. For $|t| > t_\mathrm{c}$, we have $|t_\mathrm{c}/(t + \mathrm{i}t_\mathrm{c})| \leq 1/\sqrt{2}$, and thus

$$\left| \sum_{j=2}^{n-2} \frac{c_j^{(n)}}{2^j} \left(\frac{\mathrm{i}t_\mathrm{c}}{t + \mathrm{i}t_\mathrm{c}} \right)^{n-j} \right| \leq \frac{C}{(n-1)^\alpha} \left| \frac{t_\mathrm{c}}{t + \mathrm{i}t_\mathrm{c}} \right|^2 \sum_{j=2}^{n-2} j \left(\frac{p}{2} \right)^j \left(\frac{1}{\sqrt{2}} \right)^{n-2-j} .$$

If we choose again $p < \sqrt{2}$, the sum on the right hand side is bounded by $\tilde{C}(1/\sqrt{2})^{n-2}$ uniformly in n. For the term with $j = n-1$, this does not work since then $n - 2 - j < 0$. But for n even, this term vanishes since then $c_{n-1}^{(n)} = 0$, and for n odd, it equals

$$\frac{c_{n-1}^{(n)}}{2^n} \mathrm{Re} \left(\frac{\mathrm{i}t_\mathrm{c}}{t + \mathrm{i}t_\mathrm{c}} \right) = \frac{n a_{n-1}^{(n+1)}}{2^n} \frac{t_\mathrm{c}^2}{t^2 + t_\mathrm{c}^2} \leq \frac{\tilde{C}}{n-1} \left(\frac{1}{\sqrt{2}} \right)^{n-2} \left| \frac{t_\mathrm{c}}{t + \mathrm{i}t_\mathrm{c}} \right|^2 .$$

This proves (78) and (80) for $|t| \geq t_\mathrm{c}$. The proof of (79) is similar and uses Corollary 3. □

5 Optimal truncation

By the results of the previous section π_k grows like $(k-1)!/t_\mathrm{c}^k$. Hence, the sum $\pi^{(n)} = \sum_{k=0}^n \varepsilon^k \pi_k$ does not converge to an exactly equivariant projection $\pi^{(\infty)}$ as $n \to \infty$. This is the reason why we see exponentially small transitions. The basis in which these transitions develop smoothly is the optimal superadiabatic basis: since we cannot go all the way to infinity with n, we fix ε and choose $n = n(\varepsilon)$ such that the off-diagonal elements in (2) become minimal. Using Stirling's formula and (78) resp. (80), it is easy to see that the place to truncate is at $n(\varepsilon) = t_\mathrm{c}/\varepsilon$. This $n(\varepsilon)$ is in general not a natural number, but we will find that a change of n which is of order one does not change the results. Before we go into more details, we need a preliminary result.

Lemma 5. *Uniformly in $x \in [0,1]$ and for $k > 0$, we have*

$$(1+x)^{-k} = \mathrm{e}^{-kx} + \mathrm{e}^{-kx/2}\mathcal{O}\big(\tfrac{1}{k}\big).$$

Proof. We start with the equality

$$(1+x)^{-k} - \mathrm{e}^{-kx} = \mathrm{e}^{-kx}\left(\mathrm{e}^{k(x-\ln(1+x))} - 1\right). \tag{81}$$

At first consider $x > \sqrt{1/k}$. There we use the inequality $(x - \ln(1+x)) \le x/3$, valid for $0 \le x \le 1$, in (81) and obtain

$$|(1+x)^{-k} - \mathrm{e}^{-kx}| \le \mathrm{e}^{-kx}\left(\mathrm{e}^{kx/3} - 1\right) = \mathrm{e}^{-kx/2}\left(\mathrm{e}^{-kx/6} - \mathrm{e}^{-kx/2}\right).$$

For $x > \sqrt{1/k}$, the term in the last bracket above is $\mathcal{O}(1/k)$, and we are done in this case. For $x \le \sqrt{1/k}$, we use $(x - \ln(1+x)) \le x^2/2$ and rearrange (81) to get

$$\mathrm{e}^{kx/2}((1+x)^{-k} - \mathrm{e}^{-kx}) = \mathrm{e}^{-kx/2}\left(\mathrm{e}^{kx^2/2} - 1\right) =: f(x,k).$$

To find out where $f(x,k)$ is maximal, we calculate

$$\frac{\mathrm{d}}{\mathrm{d}x} f(x,k) = \frac{k}{2}\mathrm{e}^{-kx/2}\left(1 + \mathrm{e}^{kx^2/2}(2x-1)\right).$$

The derivative is zero exactly at the solutions of the equation

$$\ln(1-2x)/x^2 = -k/2. \tag{82}$$

Now $\ln(1-2x)/x^2 = -2/x + R(x)$, where $R(x)$ is a power series in x, convergent for $x < 1/2$. Thus for $x < \sqrt{1/k}$ and k sufficiently large, there exists exactly one solution $x^*(k)$ of (82), and $x^*(k) < C/k$ uniformly in k for some $C > 0$. Since $\frac{\mathrm{d}}{\mathrm{d}x} f(x,k) > 0$ for $x < 1/k^2$, $f(x,k)$ has a maximum at $x^*(k)$. Thus

$$f(x,k) \le f(x^*(k),k) \le \mathrm{e}^{-C/2k} - 1 = \mathcal{O}(1/k)$$

for $x < \sqrt{1/k}$, and the claim is proved. $\square$

Lemma 5 immediately yields

$$\left(1 + \frac{a}{k}\right)^{-k} = \mathrm{e}^{-a}\,\left(1 + \mathcal{O}\left(\tfrac{1}{k}\right)\right) \tag{83}$$

uniformly on compact intervals of a by taking $x = a/k$.

We now turn to the proof of Theorem 1, which we deduce from Theorems 2 and 3. As stated already in (11), we will use

$$n_\varepsilon = \frac{t_{\mathrm{c}}}{\varepsilon} - 1 + \sigma_\varepsilon, \tag{84}$$

where $\sigma_\varepsilon \in [0,2[$ is such that n_ε is an even integer. The advantage of this convention about σ_ε is that now the off-diagonal components in (60) are always given by $\varepsilon^{n_\varepsilon+1}x_{n_\varepsilon+1}$ since $z_{n+1}=0$ for even n. Of course we could as well consider the asymptotic behavior of $\varepsilon^{n+1}z_{n+1}$ for odd n and one would expect to end up with the same result. However, it is obvious from (78) and (80) that x_{n+1} is purely imaginary and z_{n+1} is real at leading order. Thus the large n asymptotics of the off-diagonal component of the effective Hamiltonian do depend on whether we consider even or odd superadiabatic bases. On the other hand, the asymptotics of the propagator must be independent of the exact choice of basis. We will discuss this point after giving the proof of Theorem 1 based on the above convention.

Proof of Theorem 1. We want to apply Theorem 2 and thus have to check that ξ, η and ζ defined in (54)–(56) together with their derivatives are $\mathcal{O}(\varepsilon\theta')$. From Proposition 5 together with Proposition 6 we infer that there exists $C>0$ such that $|x_k(t)| \le C\theta'(t)(k-1)!/t_{\mathrm{c}}^k$ for each k. The same is true for y_n and z_n. Using the differential equations (38)–(40), we find that there is $C'>0$ with $|x_n'(t)| \le C'\theta'(t)n!/t_{\mathrm{c}}^{n+1}$. This means that

$$|\xi'(t)| \le \varepsilon C'\theta'(t)\sum_{k=1}^{n}\varepsilon^k t_{\mathrm{c}}^{-k-1}k!\,\varepsilon^{k-1},$$

with similar expressions for the other quantities. Now taking $\varepsilon = t_{\mathrm{c}}/(n_\varepsilon-\sigma_\varepsilon)$, we find

$$\sum_{k=0}^{n_\varepsilon} t_{\mathrm{c}}^{-k}\varepsilon^k(k+1)! = \sum_{k=0}^{n_\varepsilon}\frac{(k+1)!}{(n_\varepsilon-\sigma_\varepsilon)^k} = \left(1+\frac{2}{n_\varepsilon-\sigma_\varepsilon}+\frac{3!}{(n_\varepsilon-\sigma_\varepsilon)^2}+\dots\right).$$

Each of the $n_\varepsilon+1$ terms in the sum above is bounded by $\mathrm{const}/(n_\varepsilon-\sigma_\varepsilon)$ except the first which is 1. This shows

$$|\xi'(t)| \le \varepsilon\theta' C'\left(1+\tfrac{n_\varepsilon}{n_\varepsilon-\sigma_\varepsilon}\right),$$

and Theorem 2 gives (13) with $c_\varepsilon^{n_\varepsilon}(t) = \varepsilon^{n_\varepsilon+1}x_{n_\varepsilon+1}(t)(1+\mathcal{O}(\varepsilon\theta'(t)))$. Recall that $z_{n_\varepsilon+1}(t)=0$ due to our convention. It remains to determine the leading order asymptotics of $\varepsilon^{n_\varepsilon+1}x_{n_\varepsilon+1}$. For convenience of the reader let us rewrite (78) as

$$\varepsilon^{n_\varepsilon+1}x_{n_\varepsilon+1}(t) = \mathrm{i}\frac{\varepsilon^{n_\varepsilon+1}n_\varepsilon!}{t_{\mathrm{c}}^{n_\varepsilon+1}}\left[\tfrac{2\sin(\gamma\pi/2)}{\pi}\,\mathrm{Re}\left(\left(1-\mathrm{i}\tfrac{t}{t_{\mathrm{c}}}\right)^{-(n_\varepsilon+1)}\right)+\mathcal{O}\left(R^\beta_{n_\varepsilon+1}(t)\right)\right]. \tag{85}$$

Lemma 6. *With (84), we have*

$$\frac{\varepsilon^{n_\varepsilon+1}n_\varepsilon!}{t_{\mathrm{c}}^{n_\varepsilon+1}} = \sqrt{\frac{2\pi\varepsilon}{t_{\mathrm{c}}}}\mathrm{e}^{-\frac{t_{\mathrm{c}}}{\varepsilon}}(1+\mathcal{O}(\varepsilon)).$$

Proof. Stirling's formula for $(n+1)!$ implies

$$n! = \frac{1}{n+1}\left(\frac{n+1}{\mathrm{e}}\right)^{n+1}\sqrt{n+1}\sqrt{2\pi}\,\left(1+\mathcal{O}\left(\tfrac{1}{n+1}\right)\right).$$

Together with (83) this yields

$$\begin{aligned}\varepsilon^{n_\varepsilon+1}n_\varepsilon! &= t_{\mathrm{c}}^{n_\varepsilon+1}\,\mathrm{e}^{-(n_\varepsilon+1)}\left(1-\frac{\sigma_\varepsilon}{n_\varepsilon+1}\right)^{-(n_\varepsilon+1)}\sqrt{\frac{2\pi}{n_\varepsilon+1}}\,\left(1+\mathcal{O}\left(\tfrac{1}{n_\varepsilon+1}\right)\right) = \\ &= t_{\mathrm{c}}^{n_\varepsilon+1}\,\mathrm{e}^{-(n_\varepsilon+1)}\,\mathrm{e}^{\sigma_\varepsilon}\sqrt{\frac{2\pi}{n_\varepsilon+1}}\,\left(1+\mathcal{O}\left(\tfrac{1}{n_\varepsilon+1}\right)\right) = \\ &= t_{\mathrm{c}}^{n_\varepsilon+1}\,\mathrm{e}^{-\frac{t_{\mathrm{c}}}{\varepsilon}}\sqrt{\frac{2\pi\varepsilon}{t_{\mathrm{c}}+\varepsilon\sigma_\varepsilon}}\,(1+\mathcal{O}(\varepsilon)).\end{aligned}$$

Finally,

$$\sqrt{\frac{2\pi\varepsilon}{t_{\mathrm{c}}+\varepsilon\sigma_\varepsilon}} = \sqrt{\frac{2\pi\varepsilon}{t_{\mathrm{c}}}}\left(1+\frac{\varepsilon\sigma_\varepsilon}{t_{\mathrm{c}}}\right)^{-1/2} = \sqrt{\frac{2\pi\varepsilon}{t_{\mathrm{c}}}}\,(1+\mathcal{O}(\varepsilon))\,.$$

□

Lemma 6 takes care of the first factor in (85). Turning to the terms inside the square brackets in (85), let us first note that for $|t| \geq t_c$, both terms are

$$\mathcal{O}(2^{-(n_\varepsilon-1)/2}/(1+t^2)) = \mathcal{O}(\exp(-t_{\mathrm{c}}\ln 2/(2\varepsilon))/(1+t^2))\,,$$

proving the theorem in this case. For $|t| < t_c$, we investigate the modulus and the phase separately. Let $0 < \beta < 1$. From Lemma 5 it follows that

$$\left|1+\mathrm{i}\tfrac{t}{t_{\mathrm{c}}}\right|^{n_\varepsilon+1} = \left(1+\tfrac{t^2}{t_{\mathrm{c}}^2}\right)^{(t_{\mathrm{c}}/\varepsilon+\sigma_\varepsilon)/2} = \left(1+\tfrac{t^2}{t_{\mathrm{c}}^2}\right)^{\sigma_\varepsilon/2}\left(\mathrm{e}^{-\frac{t^2}{2t_{\mathrm{c}}\varepsilon}}+\mathcal{O}\left(\varepsilon\mathrm{e}^{-\frac{t^2}{4t_{\mathrm{c}}\varepsilon}}\right)\right).$$

For $|t| \geq \varepsilon^{\beta/2}$, $\exp(-t^2/(2t_{\mathrm{c}}\varepsilon)) = \mathcal{O}(\varepsilon\exp(-t^2/(4t_{\mathrm{c}}\varepsilon)))$. Thus neither the prefactor involving σ_ε above nor the phase play any role in this region. For $|t| < \varepsilon^{\beta/2}$, $(1+t^2/t_{\mathrm{c}}^2)^{\sigma_\varepsilon/2} = 1+\mathcal{O}(\sigma_\varepsilon\varepsilon^\beta)$ and therefore

$$\left|1+\mathrm{i}\tfrac{t}{t_{\mathrm{c}}}\right|^{n_\varepsilon+1} = \mathrm{e}^{-\frac{t^2}{2t_{\mathrm{c}}\varepsilon}}+\mathcal{O}\left(\varepsilon^\beta\mathrm{e}^{-\frac{t^2}{4t_{\mathrm{c}}\varepsilon}}\right).$$

The same reasoning applies to $R^\beta_{n_\varepsilon+1}$ and gives

$$R^\beta_{n_\varepsilon+1}(t) \leq \varepsilon^\beta\left(\mathrm{e}^{-\frac{t^2}{2t_{\mathrm{c}}\varepsilon}}+\mathcal{O}\left(\varepsilon^\beta\mathrm{e}^{-\frac{t^2}{4t_{\mathrm{c}}\varepsilon}}\right)\right).$$

Turning to the phase in the region $|t| < \varepsilon^{\beta/2}$, we find

$$\begin{aligned}\mathrm{e}^{\mathrm{i}(n_\varepsilon+1)\arctan(t/t_{\mathrm{c}})} &= \exp\left(\mathrm{i}\left(\tfrac{t_{\mathrm{c}}}{\varepsilon}+\sigma_\varepsilon\right)\left((t/t_{\mathrm{c}})-\tfrac{1}{3}(t/t_{\mathrm{c}})^3+\mathcal{O}((t/t_{\mathrm{c}})^5)\right)\right) = \\ &= \exp\left(\mathrm{i}\left(\tfrac{t}{\varepsilon}-\tfrac{t^3}{3\varepsilon t_{\mathrm{c}}^2}+\tfrac{\sigma_\varepsilon t}{t_{\mathrm{c}}}\right)+\mathcal{O}(t_{\mathrm{c}}(t/t_{\mathrm{c}})^5/\varepsilon)+\mathcal{O}(\sigma_\varepsilon(t/t_{\mathrm{c}})^3)\right) \\ &= \exp\left(\mathrm{i}\left(\tfrac{t}{\varepsilon}-\tfrac{t^3}{3\varepsilon t_{\mathrm{c}}^2}+\tfrac{\sigma_\varepsilon t}{t_{\mathrm{c}}}\right)\right)\left(1+\mathcal{O}(\varepsilon^{5\beta/2-1})+\mathcal{O}(\varepsilon^{3\beta/2})\right).\end{aligned}$$

Now we just have to collect all the pieces and add the complex conjugate. □

Let us now see what of the above would have changed for n_ε odd. Then $x_{n_\varepsilon+1} = 0$, and (80) together with Lemma 5 and 6 yields

$$\begin{aligned} c_\varepsilon^{n_\varepsilon}(t) &= -\varepsilon^{n_\varepsilon+1} z_{n_\varepsilon+1}(t)\,(1+\mathcal{O}(\varepsilon\theta')) \qquad (86)\\ &= 2\sqrt{\frac{2\varepsilon}{\pi t_c}}\,\sin\left(\frac{\pi\gamma}{2}\right)\,\mathrm{e}^{-\frac{t_c}{\varepsilon}}\,\mathrm{e}^{-\frac{t^2}{2\varepsilon t_c}}\,\sin\left(\frac{t}{\varepsilon}-\frac{t^3}{3\varepsilon t_c^2}+\frac{\sigma_\varepsilon t}{t_c}\right)+\mathcal{O}\left(\phi^\alpha(\varepsilon,t)\right)\,. \end{aligned}$$

At first, this looks like an important difference, since now the off-diagonal elements in the transformed Hamiltonian are purely real-valued in leading order, while in the other case they were purely imaginary. However, in the computation of the propagator, another factor of $\exp(\pm\mathrm{i}t/\varepsilon)$ from the dynamical phase appears, cf. (87). At leading order only the resonant term of the Hamiltonian survives, which is the same for odd and even n_ε.

6 First order perturbation in the optimal superadiabatic basis

In this section we prove Corollary 1. Since we use standard first order perturbation theory, we stay sketchy in some parts. After splitting $H_\varepsilon^{n_\varepsilon}(t)$, see (13), as

$$H_\varepsilon^{n_\varepsilon}(t) = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} + V_\varepsilon(t) =: H_0 + V_\varepsilon(t)\,,$$

Dyson expansion in the interaction picture (cf. [ReSi], Thm. X.69) yields

$$\begin{aligned} K_\varepsilon^{n_\varepsilon}(t,s) &= \mathrm{e}^{-\frac{\mathrm{i}tH_0}{\varepsilon}}\left(\mathrm{id}-\frac{\mathrm{i}}{\varepsilon}\int_s^t \mathrm{e}^{\frac{\mathrm{i}\tau H_0}{\varepsilon}}\,V_\varepsilon(\tau)\,\mathrm{e}^{-\frac{\mathrm{i}\tau H_0}{\varepsilon}}\,\mathrm{d}\tau\right)\mathrm{e}^{\frac{\mathrm{i}sH_0}{\varepsilon}}\\ &\quad+\begin{pmatrix} \mathcal{O}(\varepsilon^2) & \mathcal{O}(\varepsilon\mathrm{e}^{-\frac{t_c}{\varepsilon}}) \\ \mathcal{O}(\varepsilon\mathrm{e}^{-\frac{t_c}{\varepsilon}}) & \mathcal{O}(\varepsilon^2) \end{pmatrix}\Delta(t,s)\,. \end{aligned}$$

Thus we only need to evaluate the integral

$$\begin{aligned} -\frac{\mathrm{i}}{\varepsilon}\int_s^t \mathrm{e}^{\frac{\mathrm{i}\tau H_0}{\varepsilon}}\,V_\varepsilon(\tau)\,\mathrm{e}^{-\frac{\mathrm{i}\tau H_0}{\varepsilon}}\,\mathrm{d}\tau &= -\frac{\mathrm{i}}{\varepsilon}\int_s^t \begin{pmatrix} 0 & \mathrm{e}^{\frac{\mathrm{i}\tau}{\varepsilon}}c_\varepsilon^{n_\varepsilon}(\tau) \\ \mathrm{e}^{-\frac{\mathrm{i}\tau}{\varepsilon}}\overline{c}_\varepsilon^{n_\varepsilon}(\tau) & 0 \end{pmatrix}\mathrm{d}\tau\\ &\quad+\begin{pmatrix} \mathcal{O}(\varepsilon) & 0 \\ 0 & \mathcal{O}(\varepsilon) \end{pmatrix}\Delta(t,s)\,. \end{aligned}$$

Inserting (14) and using (15) gives

$$\begin{aligned} &-\frac{\mathrm{i}}{\varepsilon}\int_s^t \mathrm{e}^{\frac{\mathrm{i}\tau}{\varepsilon}}c_\varepsilon^{n_\varepsilon}(\tau)\mathrm{d}\tau =\\ &= \sqrt{\frac{2}{\varepsilon\pi t_c}}\,\sin\left(\frac{\pi\gamma}{2}\right)\,\mathrm{e}^{-\frac{t_c}{\varepsilon}}\int_s^t \mathrm{e}^{\frac{\mathrm{i}\tau}{\varepsilon}}\,\mathrm{e}^{-\frac{\tau^2}{2\varepsilon t_c}}\left(\mathrm{e}^{-\frac{\mathrm{i}\tau}{\varepsilon}+\frac{\mathrm{i}\tau^3}{3\varepsilon t_c^2}-\frac{\mathrm{i}\sigma\tau}{t_c}}+\mathrm{e}^{\frac{\mathrm{i}\tau}{\varepsilon}-\frac{\mathrm{i}\tau^3}{3\varepsilon t_c^2}+\frac{\mathrm{i}\sigma\tau}{t_c}}\right)\mathrm{d}\tau\\ &\quad+\mathcal{O}\left(\varepsilon^\alpha\mathrm{e}^{-\frac{t_c}{\varepsilon}}\,\Delta(t,s)\right) = (*)\,, \qquad (87) \end{aligned}$$

for each $\alpha < 1$. Now we replace the exponentials $\mathrm{e}^{\pm(\frac{\mathrm{i}\tau^3}{3\varepsilon t_\mathrm{c}^2} - \frac{\mathrm{i}\sigma\tau}{t_\mathrm{c}})}$ by $1 \pm (\frac{\mathrm{i}\tau^3}{3\varepsilon t_\mathrm{c}^2} - \frac{\mathrm{i}\sigma\tau}{t_\mathrm{c}})$. Using $|\mathrm{e}^{\mathrm{i}\varphi} - 1 - \mathrm{i}\varphi| \leq \varphi^2$, we conclude that the resulting error is bounded by a constant times

$$\varepsilon^{-\frac{1}{2}}\mathrm{e}^{-\frac{t_\mathrm{c}}{\varepsilon}} \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{\tau^2}{2\varepsilon t_\mathrm{c}}} \left(\frac{\tau^6}{\varepsilon^2} + \frac{\tau^4}{\varepsilon} + \tau^2\right) \mathrm{d}\tau = \mathcal{O}(\varepsilon \mathrm{e}^{-\frac{t_\mathrm{c}}{\varepsilon}})\,.$$

Hence we obtain

$$\begin{aligned}(*) \quad = \; & \sqrt{\tfrac{2}{\varepsilon\pi t_\mathrm{c}}}\,\sin\left(\tfrac{\pi\gamma}{2}\right)\mathrm{e}^{-\frac{t_\mathrm{c}}{\varepsilon}} \int_s^t \mathrm{e}^{-\frac{\tau^2}{2\varepsilon t_\mathrm{c}}} \left(1 + \tfrac{\mathrm{i}\tau^3}{3\varepsilon t_\mathrm{c}^2} - \tfrac{\mathrm{i}\sigma\tau}{t_\mathrm{c}} + \mathrm{e}^{\frac{2\mathrm{i}\tau}{\varepsilon}}\left(1 - \tfrac{\mathrm{i}\tau^3}{3\varepsilon t_\mathrm{c}^2} + \tfrac{\mathrm{i}\sigma\tau}{t_\mathrm{c}}\right)\right)\mathrm{d}\tau \\ & + \mathcal{O}\left(\varepsilon^\alpha \mathrm{e}^{-\frac{t_\mathrm{c}}{\varepsilon}}\Delta(t,s)\right) \qquad (88)\end{aligned}$$

with $\alpha < 1$, where the first summand in the integrand gives rise to the explicit term in (17). The remaining terms can be integrated explicitly as well, most conveniently using Maple or Mathematica. They are all of order $\mathcal{O}(\sqrt{\varepsilon}\mathrm{e}^{-\frac{t_\mathrm{c}}{\varepsilon}}\Delta(t,s))$ uniformly in t and s resp. of order $\mathcal{O}(\varepsilon^\alpha \mathrm{e}^{-\frac{t_\mathrm{c}}{\varepsilon}}\Delta(t,s))$ for $|t|$ and $|s|$ larger than ε^β for some $\beta < \frac{1}{2}$. To illustrate the reasoning note that

$$\int_s^t \mathrm{e}^{-\frac{\tau^2}{2\varepsilon t_\mathrm{c}}}\,\tau\,\mathrm{d}\tau = \varepsilon t_\mathrm{c}\left(\mathrm{e}^{-\frac{s^2}{2\varepsilon t_\mathrm{c}}} - \mathrm{e}^{-\frac{t^2}{2\varepsilon t_\mathrm{c}}}\right)\,.$$

This is uniformly of order $\mathcal{O}(\varepsilon)$, but of order $\mathcal{O}(\mathrm{e}^{-\varepsilon^{2\beta-1}})$ for $|t|$ and $|s|$ larger than ε^β. Finally we emphasize that we could get the next order corrections to (17) explicitly by evaluating (88).

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