Precise coupling terms in adiabatic quantum evolution: The generic case.

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Abstract

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. Based on results from [BeTe$_1$] for special Hamiltonians we explicitly determine the asymptotic behavior of the exponentially small coupling term for generic two-state systems with real-symmetric Hamiltonian. The superadiabatic coupling term takes a universal form and depends only on the location and the strength of the complex singularities of the adiabatic coupling function.

As shown in [BeTe$_1$], first order perturbation theory in the superadiabatic representation then allows to describe the time-development of exponentially small adiabatic transitions and thus to rigorously confirm Michael Berry's [Ber] predictions on the universal form of adiabatic transition histories.
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1 Introduction and the main result

We consider the dynamics of a two-state time-dependent quantum system with state vector $\psi \in \mathbb{C}^2$ described by the Schrödinger equation

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

in the *adiabatic limit* $\varepsilon \to 0$. The Hamiltonian $H(t)$, $t \in \mathbb{R}$, takes values in the real-symmetric traceless 2×2-matrices of the form

$$H(t) = \tfrac{1}{2} \begin{pmatrix} \cos\theta(t) & \sin\theta(t) \\ \sin\theta(t) & -\cos\theta(t) \end{pmatrix}. \tag{2}$$

This is the prototype of all adiabatic problems in quantum mechanics and the "Adiabatic Theorem" states that if $H(\cdot) \in C^2(\mathbb{R})$ the system (1) can be decomposed into two scalar equations which are decoupled up to errors of order ε. Under further regularity assumptions on $H(t)$ the error bound can be improved and for suitable real analytic $H(t)$ it is even exponentially small in $\frac{1}{\varepsilon}$. This adiabatic decoupling is at the basis of understanding a large number of physical phenomena related to the separation of time scales, ranging from the classical Stern-Gerlach experiment for the measurement of spin to the dynamics of molecules; see [PST, Te] for recent reviews. Despite its asymptotic smallness, the exponentially small coupling that generically remains has itself important physical consequences such as the non-radiative decay in molecules. In the scattering limit the exponentially small non-adiabatic transitions are quantified by the Landau-Zener formula and its generalizations, with rigorous justification given in [JKP, Jo]. In this work we treat the problem of explicitly determining the exponentially small non-adiabatic coupling for arbitrary finite times t in order to obtain a complete understanding of the nature and the time-development of non-adiabatic transitions. Our main result is the construction of a family of unitary maps $U^{n_\varepsilon}_\varepsilon(t)$ that brings (1) into almost diagonal form (6) with off-diagonal elements $c^{n_\varepsilon}_\varepsilon(t)$ that are exponentially small in ε and are explicitly given at leading order. The construction works under assumptions satisfied for "generic" Hamiltonians in a sense to be made precise. Our work was motivated by results of Berry [Ber] (see also [BerLi, LiBe]). He argues that the time-development of non-adiabatic transitions is determined solely by the complex singularities of $\theta'(t)$ closest to the real axis, which are "generically" first order poles. For such generic poles the transition histories then have the universal form of an error function. Despite substantial progress in adiabatic theory during the last decade, e.g. [JoPf, Ne, Sj, Ma], a rigorous justification of Berry's conjecture for the generic case remained an open problem until now. We are aware only of two results [HaJo, BeTe$_1$], which both deal with special and "non-generic" Hamiltonians. However, the present work is a continuation of [BeTe$_1$] and relies on techniques and results developed there. We also refer to [BeTe$_1$] for a more detailed introduction and a guide to the literature on adiabatic theory in quantum mechanics.

Before we describe our result in detail let us shortly comment on the special form of the Hamiltonian (2), whose eigenvalues are equal to $\pm\frac{1}{2}$ independent of t. Berry and Lim [BerLi] observed that the Schrödinger equation

$$(\mathrm{i}\varepsilon\partial_s - \widetilde{H}(s))\psi(s) = 0 \tag{3}$$

for any traceless real-symmetric Hamiltonian $\widetilde{H}(s)$,

$$\widetilde{H}(s) = \begin{pmatrix} Z(s) & X(s) \\ X(s) & -Z(s) \end{pmatrix} = \rho(s) \begin{pmatrix} \cos\tilde{\theta}(s) & \sin\tilde{\theta}(s) \\ \sin\tilde{\theta}(s) & -\cos\tilde{\theta}(s) \end{pmatrix}, \tag{4}$$

with eigenvalues $\rho_\pm(s) = \pm\rho(s) = \pm\sqrt{X^2(t) + Z^2(t)}$ that satisfy $\rho_+(s) - \rho_-(s) = 2\rho(s) \geq g > 0$ for all $s \in \mathbb{R}$, can be brought into the form (1) & (2) through the invertible transformation to the natural time variable

$$t(s) = 2\int_0^s \rho(u)\,\mathrm{d}u\,. \tag{5}$$

While our main result is formulated for (1) and (2), the difficulty of the problem stems in parts from the fact that our assumptions must be general enough to be satisfied by Hamiltonians (2) that arise from generic analytic Hamiltonians of the form (4) through the transformation (5). E.g., it turns out that these assumptions prevent the use of standard Cauchy estimates. Note that, as was observed by Berry [Ber], Equation (1) with a complex-hermitian Hamiltonian is unitarily equivalent to a similar equation with a real-symmetric but ε-dependent Hamiltonian. Our results on (1) & (2) are sufficiently uniform to also apply to this case and thus cover generic analytic self-adjoint 2×2-Hamiltonians, cf. [BeTe$_2$].

It is well known (see [BeTe$_1$] for details and references) that for all $n \in \mathbb{N}_0$ there is basis transformation such that in the n^{th} *superadiabatic basis* the off-diagonal elements of the Hamiltonian are of order ε^{n+1}, i.e. there is a unitary $U^n_\varepsilon(t)$ such that

$$U^n_\varepsilon(t)\,(\mathrm{i}\varepsilon\partial_t - H(t))\,U^n_\varepsilon(t)^*\,U^n_\varepsilon(t)\psi(t) =: (\mathrm{i}\varepsilon\partial_t - H^n_\varepsilon(t))\psi^n(t) = 0$$

with

$$H^n_\varepsilon(t) = \begin{pmatrix} \rho^n_\varepsilon(t) & c^n_\varepsilon(t) \\ \bar{c}^n_\varepsilon(t) & -\rho^n_\varepsilon(t) \end{pmatrix}, \quad c^n_\varepsilon(t) = \mathcal{O}(\varepsilon^{n+1}), \quad \text{and} \quad \psi^n(t) = U^n_\varepsilon(t)\psi(t)\,. \tag{6}$$

Here $\rho^n_\varepsilon(t) = \frac{1}{2} + \mathcal{O}(\varepsilon^2)$. Note that $U^0_\varepsilon(t) =: U_0(t)$ is the orthogonal transformation that diagonalizes the symmetric matrix $H(t)$. It is independent of ε and maps to the *adiabatic basis*. However, in general, $\lim_{n\to\infty}|c^n_\varepsilon(t)| = \infty$ for all $\varepsilon > 0$ and the coupling can not be eliminated completely for fixed ε by going to higher and higher superadiabatic bases. Instead, for each $\varepsilon > 0$ there exists an optimal $n_\varepsilon = n(\varepsilon)$ for which $n \mapsto |c^n_\varepsilon(t)|$ attains it minimum $|c^{n_\varepsilon}_\varepsilon(t)|$. This defines the *optimal superadiabatic basis*. In order to determine n_ε and $c^{n_\varepsilon}_\varepsilon(t)$ it is necessary to understand precisely the asymptotic behavior of the coupling $c^n_\varepsilon(t)$ as $n\to\infty$.

As in the case of Berry's non-adiabatic transition histories one expects that for large n the superadiabatic coupling function $c^n_\varepsilon(t)$ is determined by the singularities of the adiabatic coupling function $c^0_\varepsilon(t) = \frac{\mathrm{i}\varepsilon}{2}\theta'(t)$ and thus has a universal form. From the abstract asymptotic analysis point of view this universality is just another manifestation of Darboux' Principle, which in its original form says that the late coefficients in the Taylor series of an analytic function are determined by the convergence limiting singularities, see Theorem 5. Dingle [Di] realized that the same idea also applies to various divergent series arising for example from asymptotic expansions of integrals. In our case the coefficients $c^n_\varepsilon(t)$ are determined by a non-linear system of recurrence relations starting with $\frac{\mathrm{i}}{2}\theta'(t)$ and involving differentiation, integration and multiplication of terms. We show that Darboux' Principle can be applied also to this system of recurrence relations, i.e. that the large n asymptotics of the coefficients $c^n_\varepsilon(t)$ depend solely on the convergence limiting singularities of θ'. As to be discussed in Section 2, our system of recurrence relations can be interpreted as the formal asymptotic expansion of the solutions to a system of ODEs. It might well be that established techniques of asymptotic analysis can be used to determine the asymptotic behavior of $c^n_\varepsilon(t)$ as $n\to\infty$ by studying this system of ODEs, but this is far from obvious. Instead, our proof is based on a direct analysis of the recurrence relation using a family of norms tailored to Darboux' Principle and introduced in Definition 1 below. One merit of our approach is that, in principle, it can be applied also to more complicated recurrences as arising, e.g., in the context of constructing precise coupling terms between different electronic levels in molecular dynamics, see [BeTe3].

We now describe our main result in detail. Since our construction is local in time, we can restrict our attention to a compact interval $I \subset \mathbb{R}$. A sufficient condition for our main theorem is that the singularities of the analytic continuation of θ' are of the form

$$\theta'(z - z_0) = \frac{-\mathrm{i}\gamma}{z - z_0} + \sum_{j=1}^{N} (z - z_0)^{-\alpha_j} h_j(z - z_0) \tag{7}$$

where $|\mathrm{Im} z_0| > 0$, $\gamma \in \mathbb{R}$, $\alpha_j < 1$ and h_j is analytic in a neighborhood of 0 for $j = 1, \dots, N$. Following arguments of Berry and Lim [BerLi] we show in Section 4 that this condition is fulfilled for generic Hamiltonians of the form (4). However, in all but a few non-generic cases, $-\alpha_j \notin \mathbb{N}$ for at least one j. The technical problem arising from this fact is that by removing the leading singularity one does not obtain a function which is analytic in a larger region. As a consequence, it is not sufficient to use standard Cauchy estimates to show that the remainder terms are asymptotically smaller than the contribution from the leading singularity. Instead we introduce the following norms tailored to Darboux' Principle.

Definition 1. Let $t_c > 0$, $\alpha > 0$ and $I \subset \mathbb{R}$ be an interval. For $f \in C^\infty(I)$ we define

$$\|f\|_{(I,\alpha,t_c)} := \sup_{t \in I} \sup_{k \geq 0} \left| \partial^k f(t) \right| \frac{{t_c}^{\alpha+k}}{\Gamma(\alpha + k)} \leq \infty \tag{8}$$

and

$$F_{\alpha,t_c}(I) = \left\{ f \in C^\infty(I) : \|f\|_{(I,\alpha,t_c)} < \infty \right\}.$$

The connection of Definition 1 with (7) is given by Darboux' Principle, Theorem 5, which allows to translate the information about the complex singularities of θ' into information about the late coefficients of the Taylor expansion of θ' on the real line. Taking $I = \{t\}$ we obtain

$$\|f\|_{(\{t\},\alpha,t_c)} = C < \infty \quad \Rightarrow \quad |f^{(k)}(t)| \leq C \, \frac{\Gamma(\alpha + k)}{{t_c}^{\alpha+k}} \quad \forall k \in \mathbb{N}. \tag{9}$$

Consequently $\|f\|_{(\{t\},\alpha,t_c)} < \infty$ for some $\alpha > 0$ implies that f is analytic at t and that the Taylor series at t converges at least inside the disk $D_{t_c}(t)$ of radius t_c. Suppose that the Taylor series has finitely many singularities on $\partial D_{t_c}(t)$, all of them being of the form $(z - z_0)^{-\alpha_k} h_k(z - z_0)$, h_k analytic near the origin, $\alpha_k > 0$, then Theorem 5 implies

$$\|f\|_{(\{t\},\beta,t_c)} < \infty \quad \Leftrightarrow \quad \beta \geq \max_k \alpha_k .$$

Remark 1. One might be tempted to think that for functions f that are analytic in $D_{t_c}(t)$ the norm $\|f\|_{(\{t\},\alpha,t_c)}$ is equivalent to

$$\|f\|^{\mathrm{Cauchy}}_{(\{t\},\alpha,t_c)} := \sup_{|z| < t_c} |f(t + z)| \, \frac{(t_c - |z|)^\alpha}{\Gamma(\alpha)} .$$

However, standard Cauchy estimates only yield

$$\|f\|^{\mathrm{Cauchy}}_{(\{t\},\alpha,t_{\mathrm{c}})} < \infty \quad \Rightarrow \quad \exists C > 0 : |f^{(k)}(t)| \leq C \, \frac{\Gamma(\alpha+k+1)}{{t_{\mathrm{c}}}^{\alpha+k}} \quad \forall k \in \mathbb{N}, \tag{10}$$

which is larger than (9) by a factor of $k+\alpha$. There may be ways to improve, but not up to equivalence of the norms: for the elliptic theta function $\theta_3(z) = \sum_{n=0}^{\infty} z^{n^2}$, obviously $\|\theta_3\|_{(0,\alpha,1)} < \infty$ if and only if $\alpha \geq 1$. On the other hand, an elementary estimate shows that $\|\theta_3\|^{\mathrm{Cauchy}}_{(0,\frac{1}{2},1)} < \infty$. The reason of the discrepancy is that the Taylor coefficients of functions with a dense set of singularities on the boundary of the disk of convergence (as θ_3 has) have worse asymptotics than those of functions with isolated singularities. In many problems of asymptotic analysis this lack of preciseness of $\|\cdot\|^{\mathrm{Cauchy}}_{(\{t\},\alpha,t_{\mathrm{c}})}$ plays no role, since the leading singularity is isolated. Then one can subtract the leading singularity and the remainder is analytic on a slightly larger domain. In that case Cauchy estimates applied to the larger domain yield sufficiently small error terms. However, in our case the form (7) of the function near the singularity requires the use of the precise norms $\|f\|_{(I,\alpha,t_{\mathrm{c}})}$, since subtracting the leading singularity does not increase the domain of analyticity.

The norms $\|\cdot\|_{(I,\alpha,t_{\mathrm{c}})}$ have very convenient mapping properties under differentiation, integration and multiplication of functions, which are summarized in Proposition 1 and Proposition 2. These mapping properties are the key ingredient for our analysis of the recurrence relations defining $c^n_\varepsilon(t)$, of which we will now give precise assumptions and results. For γ, t_{r}, $t_{\mathrm{c}} \in \mathbb{R}$ let

$$\theta_0'(t) = \mathrm{i}\,\gamma \left(\frac{1}{t - t_{\mathrm{r}} + \mathrm{i} t_{\mathrm{c}}} - \frac{1}{t - t_{\mathrm{r}} - \mathrm{i} t_{\mathrm{c}}} \right)$$

be the sum of two complex conjugate first order poles located at $t_{\mathrm{r}} \pm \mathrm{i} t_{\mathrm{c}}$ with residues $\mp \mathrm{i}\gamma$. Then, as to be discussed in Section 4, for $z_0 = t_{\mathrm{r}} + \mathrm{i} t_{\mathrm{c}}$ condition (7) generalizes to

Assumption 1: *On a compact interval $I \subset [t_{\mathrm{r}} - t_{\mathrm{c}}, t_{\mathrm{r}} + t_{\mathrm{c}}]$ with $t_{\mathrm{r}} \in I$ let*

$$\theta'(t) = \theta_0'(t) + \theta_{\mathrm{r}}'(t) \quad \textit{with} \quad \theta_{\mathrm{r}}'(t) \in F_{\alpha,t_{\mathrm{c}}}(I) \tag{11}$$

for some γ, $t_{\mathrm{c}}, t_{\mathrm{r}} \in \mathbb{R}$, $0 < \alpha < 1$.

It turns out that under Assumption 1 the optimal superadiabatic basis is given as the $n_\varepsilon^{\mathrm{th}}$ superadiabatic basis where $0 \leq \sigma_\varepsilon < 2$ is such that

$$n_\varepsilon = \frac{t_{\mathrm{c}}}{\varepsilon} - 1 + \sigma_\varepsilon \qquad \text{is an even integer.} \tag{12}$$

Our main result is the leading order asymptotics of $c^{n_\varepsilon}_\varepsilon(t)$ for $t \in I$. For times t that do not belong to an interval satisfying Assumption 1 we establish bounds on $c^{n_\varepsilon}_\varepsilon(t)$ which are exponentially smaller than the exponentially small leading order terms near the singularities. For this we assume

Assumption 2: *For a compact interval I and some $\tau \geq t_c$ let $\theta'(t) \in F_{1,\tau}(I)$.*

The case of degenerate $I = \{t\}$, $t \in \mathbb{R}$, is explicitly allowed. Assumptions 1 and 2 are formulated in such a way that, in principle, θ' need only be known on the real axis. However, in practice we will check these assumptions by analyzing the complex singularities of the analytic continuation of θ', cf. Section 4.

In our main theorem we do not only control the asymptotic behavior of the Hamiltonian in the optimal superadiabatic basis, but we also obtain constants which are uniform on compact intervals of the other parameters t_c, α and γ. This makes the formulation somewhat involved, but is necessary, e.g., for the study of hermitian but not symmetric Hamiltonians and for the study of the scattering regime.

Theorem 1. *Let $J_{t_c} \subset (0,\infty)$, $J_\alpha \subset (0,1)$ and $J_\gamma \subset (0,\infty)$ be compact intervals.*

(i) *There exists $\varepsilon_0 > 0$ and a locally bounded function $\phi_2 : \mathbb{R}^+ \to \mathbb{R}^+$ with $\phi_2(x) = \mathcal{O}(x)$ as $x \to 0$, such that for all $H(t)$ as in (2) satisfying Assumption 2 with $t_c \in J_{t_c}$, for all $\varepsilon \in (0, \varepsilon_0]$ and all $t \in I$ the elements of the optimal superadiabatic Hamiltonian (6) and the unitary $U_n^{n_\varepsilon}(t)$ with n_ε as in (12) satisfy*

$$\left|\rho_\varepsilon^{n_\varepsilon}(t) - \frac{1}{2}\right| \leq \varepsilon^2 \phi_2\Big(\|\theta'\|_{(I,1,\tau)}\Big)\,, \quad |c_\varepsilon^{n_\varepsilon}(t)| \leq \sqrt{\varepsilon}\, \mathrm{e}^{-\frac{t_c}{\varepsilon}(1+\ln\frac{\tau}{t_c})}\phi_2\Big(\|\theta'\|_{(I,1,\tau)}\Big) \quad (13)$$

and

$$\|U_\varepsilon^{n_\varepsilon}(t) - U_0(t)\| \leq \varepsilon\phi_2\Big(\|\theta'\|_{(I,1,\tau)}\Big)\,. \quad (14)$$

(ii) *Define*

$$c_\varepsilon(t) = 2\mathrm{i}\sqrt{\tfrac{2\varepsilon}{\pi t_c}}\,\sin\left(\tfrac{\pi\gamma}{2}\right)\,\mathrm{e}^{-\frac{t_c}{\varepsilon}}\,\mathrm{e}^{-\frac{(t-t_r)^2}{2\varepsilon t_c}}\,\cos\left(\tfrac{t-t_r}{\varepsilon} - \tfrac{(t-t_r)^3}{3\varepsilon t_c{}^2} + \tfrac{\sigma_\varepsilon t}{t_c}\right).$$

There exists $\varepsilon_0 > 0$ and a locally bounded function $\phi_1 : \mathbb{R}^+ \to \mathbb{R}^+$ with $\phi_1(x) = \mathcal{O}(x)$ as $x \to 0$, such that for all $H(t)$ as in (2) satisfying Assumption 1 with $t_c \in J_{t_c}$, $\alpha \in J_\alpha$, $\gamma \in J_\gamma$, for all $\varepsilon \in (0,\varepsilon_0]$ and all $t \in I$

$$|c_\varepsilon^{n_\varepsilon}(t) - c_\varepsilon(t)| \leq \varepsilon^{\frac{3}{2}-\alpha}\mathrm{e}^{-\frac{t_c}{\varepsilon}}\phi_1(M), \quad (15)$$

where $M = \max\left\{\|\theta'\|_{(I,1,t_c)}\,, \|\theta_r'\|_{(I,\alpha,t_c)}\right\}$.

Remark 2. Assumption 1 implies Assumption 2 on the same interval I with $\tau = t_c$. Hence, Assumption 1 implies also (13) and (14) with $\tau = t_c$. Furthermore this shows that in this case the bound on $c_\varepsilon^{n_\varepsilon}$ in (13) is optimal with respect to the dependence on ε. Again, this is only possible since we use the precise norms $\|f\|_{(I,\alpha,t_c)}$ instead of standard Cauchy estimates.

Remark 3. Note that the explicit term in (15) is asymptotically dominant only if $|t-t_r| = \mathcal{O}(\sqrt{\varepsilon})$. Since typically $\tau > t_c$ in Assumption 2, for all other times t the bound given in (13) is asymptotically smaller than the error term in (15).

Remark 4. It was shown in [BeTe_1] how to derive from Theorem 1, using first order perturbation theory in the optimal superadiabatic basis, the universal transition histories predicted by Berry [Ber].

For generic analytic Hamiltonians the whole real line can be covered by intervals satisfying either Assumption 1 or Assumption 2. Under additional conditions on the location of the singularities of θ', we can also consider the scattering problem and recover the well known Landau-Zener formulas for the adiabatic transition amplitudes. Then the decay of the exponentially small coupling for large times can come either from $\|\theta'\|_{(I,1,t_c)}$ or from the τ-dependence of the exponent in (13).

Our paper consist of two parts. The main part and the key mathematical point of our work is the proof of Theorem 1. Our proof relies on our previous results in [BeTe_1], where we established Theorem 1 assuming $\theta'(t) = \theta_0'(t)$. In Section 2 we recall the necessary tools and results from [BeTe_1] and prove Theorem 1, postponing the proofs of the key inequalities to Section 3. The main mathematical challenge is to determine the asymptotic behavior of the solutions of a system of recurrence relation, which, as shown in [BeTe_1], yield the couplings $c_\varepsilon^n(t)$. This is done in Section 3 and the analysis heavily relies on mapping properties of the norms $\|\cdot\|_{(I,\alpha,t_c)}$, which we believe are of independent mathematical interest. In Section 3 we also use a combinatorial lemma, whose rather involved proof is postponed to the Appendix. In Section 4 we finally discuss several issues concerned with the transformation (5). In particular we present the argument of Berry and Lim [BerLi] showing that Assumption 1 is "generically" satisfied. A more detailed analysis of this point as well as an analysis of interesting non-generic cases and of the scattering problem are postponed to [BeTe_2]. This is because the mathematical problems involved are of a completely different type from the main problem solved in this paper.

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2 Superadiabatic representations and optimal truncation

In this section we prove Theorem 1. The mathematical object to control is the Hamiltonian (6) in the superadiabatic representation. This can be achieved by studying superadiabatic projections. In the simple model at hand, our understanding of these projections and their relation to the unitary is rather complete and has been described in [BeTe_1]. For the convenience of the reader, we give a synopsis here.

The n^{th} superadiabatic projection

$$\pi^{(n)} = \sum_{k=0}^{n} \pi_k \varepsilon^k \tag{16}$$

is the unique operator (which is a 2×2 matrix in our case) with

$$(\pi^{(n)})^2 - \pi^{(n)} = \mathcal{O}(\varepsilon^{n+1}) \qquad \text{and} \tag{17}$$

$$\left[\mathrm{i}\varepsilon\partial_t - H, \pi^{(n)}\right] = \mathcal{O}(\varepsilon^{n+1}) \tag{18}$$

for all $n \in \mathbb{N}$. Here, $[A, B]$ denotes the commutator of the matrices A and B; π_0 is the adiabatic projection, i.e. the projection onto the eigenspaces of H. π_k can be constructed recursively by using the basis

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

of $\mathbb{R}^{2\times 2}$ and making the Ansatz

$$\pi_k = x_k X + y_k Y + z_k Z + w_k W \,.$$

It turns out that $w_k = 0$ for all k, while the remaining coefficients fulfill the recursive differential equations

$$x_1 = -\frac{\mathrm{i}}{2}\theta', \quad y_1 = z_1 = 0 \tag{19}$$

and

$$x_n = -\mathrm{i}(z'_{n-1} - \theta' y_{n-1}), \tag{20}$$

$$y_n = \sum_{j=1}^{n-1}(-x_j x_{n-j} + y_j y_{n-j} + z_j z_{n-j}), \tag{21}$$

$$z_n = -\mathrm{i}x'_{n-1}. \tag{22}$$

In addition, the differential equation

$$y'_n = -\theta' z_n \tag{23}$$

holds for each $n \in \mathbb{N}$.

In [BeTe$_1$] we construct a unitary matrix $U^n_\varepsilon(t)$ which diagonalizes the self-adjoint matrix $\pi^{(n)}(t)$ and achieves

$$U^n_\varepsilon(t)\,(\mathrm{i}\varepsilon\partial_t - H(t))\,U^{n\,*}_\varepsilon(t) = \mathrm{i}\varepsilon\partial_t - \begin{pmatrix} \rho^n_\varepsilon(t) & c^n_\varepsilon(t) \\ \bar{c}^n_\varepsilon(t) & -\rho^n_\varepsilon(t) \end{pmatrix}$$

with

$$\rho^n_\varepsilon(t) = 1/2 + \mathcal{O}(\varepsilon^2) \quad \text{and} \quad c^n_\varepsilon(t) = \varepsilon^{n+1}(x_{n+1}(t) - z_{n+1}(t))\,(1 + \mathcal{O}(\varepsilon)). \tag{24}$$

In Theorem 3 we will prove that under Assumption 2,

$$|x_{n+1}(t)|\,,\,|z_{n+1}(t)| \le \frac{n!}{\tau^{n+1}}\left\|\theta'\right\|_{(1)}\left(\exp(42\left\|\theta'\right\|^2_{(1)}) - \frac{1}{2}\right) \tag{25}$$

where $\|\theta'\|_{(1)} = \|\theta'\|_{(I,1,\tau)}$. Note that the right hand side above is $\mathcal{O}(\|\theta'\|_{(1)})$ as $\|\theta'\|_{(1)} \to 0$ uniformly in $\tau \geq t_c \geq \inf J_{t_c} > 0$. Using (25) and the corresponding inequality for y_{n+1} from Theorem 3 in the explicit formulas given in Section 3 of [BeTe$_1$], it is not difficult to see that (14) holds, and that (24) can be sharpened: there exists a locally bounded function ϕ with $\phi(x) = \mathcal{O}(x)$ as $x \to 0$, such that for all $H(t)$ as in (2) satisfying Assumption 2 with $t_c \in J_{t_c}$ and for all $t \in I$

$$|\rho_\varepsilon^n(t) - 1/2| \leq \varepsilon^2 \phi(\|\theta'\|_{(1)}) \tag{26}$$

and

$$\left|c_\varepsilon^n(t) - \varepsilon^{n+1}(x_{n+1}(t) - z_{n+1}(t))\right| \leq \varepsilon^{n+2}(|x_{n+1}(t)| + |z_{n+1}(t)|)\, \phi(\|\theta'\|_{(1)}). \tag{27}$$

Combining (25) and (27), we obtain

$$|c_\varepsilon^n(t)| \leq \varepsilon^{n+1} \frac{n!}{\tau^{n+1}} \tilde{\phi}(\|\theta'\|_{(I,1,\tau)}),$$

where $\tilde{\phi}$ has the same properties as ϕ, uniformly in the class of Hamiltonians just discussed. To arrive at (13), we take $n_\varepsilon = t_c/\varepsilon$, use Stirling's formula and analyze the asymptotics of the terms involved. The procedure is performed in detail in [BeTe$_1$], and from the calculations there it is again obvious that uniformity in the Hamiltonians is not lost. The only trivial difference is that since we do not truncate at the optimal value τ/ε of n but rather at t_c/ε, we obtain in (13) only a factor of $\exp\left(-\frac{t_c}{\varepsilon}(1 + \ln\frac{\tau}{t_c})\right)$ instead of $\exp\left(-\frac{\tau}{\varepsilon}\right)$. Thus we have shown part (i) of Theorem 1.

As for part (ii), let M be defined as in Theorem 1. In Theorem 4 we will show that there exists a locally bounded function ϕ_1 with $\phi_1(x) = \mathcal{O}(x)$ as $x \to 0$, such that for all $H(t)$ as in (2) satisfying Assumption 1 with $t_c \in J_{t_c}$, $\alpha \in J_\alpha$, $\gamma \in J_\gamma$, and for all $t \in I$

$$\left| x_{n+1}(t) - \mathrm{i}\frac{n!}{t_c^{n+1}} \frac{2\sin(\gamma\pi/2)}{\pi} \mathrm{Re}\left(1 + \mathrm{i}\frac{t - t_r}{t_c}\right)^{-n-1} \right| \leq \frac{n^{-1+\alpha} n!}{t_c^{n+1}} \phi_1(M) \tag{28}$$

provided θ' fulfills Assumption 1 and n is even; $z_{n+1} = 0$ in that case. Now (27), (28) and optimal truncation show (15), and the proof of Theorem 1 is finished.

Remark 5. In [BeTe$_1$], we used (23) and converted the nonlinear recursion into the linear but nonlocal recursive integro-differential equation

$$-z_{n+2} = z_n'' + (\theta')^2 z_n + \theta'' \int_{-\infty}^t \theta' z_n \, \mathrm{d}s. \tag{29}$$

Since we treated the special case where $\theta_r' = 0$ in Assumption 1, the calculations were rather explicit and we obtained the analogue of Theorem 1 with even better error bounds. In the general situation, there is no way to avoid the nonlinear recursion (but even so, (29) will be useful). As an added bonus of not resorting to (29), all our results are local.

Remark 6. As pointed out to us by Vassili Gelfreich, (19)–(22) is connected to the set of singularly perturbed algebraic-differential equations

$$\begin{aligned}
\partial_t X(\varepsilon,t) &= \mathrm{i}\varepsilon Z(\varepsilon,t),\\
\partial_t Z(\varepsilon,t) &= \mathrm{i}\varepsilon X(\varepsilon,t) - \theta'(t)Y(\varepsilon,t),\\
Y(\varepsilon,t) &= \varepsilon(-X^2(\varepsilon,t)+Y^2(\varepsilon,t)+Z^2(\varepsilon,t))
\end{aligned}$$

with the initial condition $X(0,t)=\theta'(t), Y(0,t)=Z(0,t)=0$. Indeed, consider the formal series expansion for X, Y and Z, i.e.

$$X(\varepsilon,t)=\sum_{k=0}^{\infty}\varepsilon^k x_{k+1},$$

with similar expressions for Y and Z. Then (19)–(22) are just the equations for the coefficients of the expansion. This opens the possibility to treat the problem using e.g. Borel summation, but it is not clear to us whether this would be successful. On the other hand, given the connection above, it may well be that our approach, to be presented in the following section, can be used successfully in the theory of singularly perturbed ODE.

3 Solving the functional recursion

In this section we examine the recursion (19)–(22) and prove, in particular, the estimates (25) and (28). The main ingredient to our proofs is the family of norms from Definition 1. Recall that for $t_\mathrm{c}>0$, $\alpha>0$ and a compact interval I we defined

$$\|f\|_{(I,\alpha,t_\mathrm{c})} := \sup_{t\in I}\sup_{k\geq 0}\left|\partial^k f(t)\right|\frac{t_c^{\alpha+k}}{\Gamma(\alpha+k)} \leq \infty \tag{30}$$

and

$$F_{\alpha,t_c}(I)=\left\{f\in C^\infty(I):\|f\|_{(I,\alpha,t_\mathrm{c})}<\infty\right\}.$$

Often t_c and I will be fixed, and then we will simply write $\|.\|_{(\alpha)}$ and F_α. The following mapping properties of $\|.\|_{(\alpha)}$ are crucial.

Proposition 1. *Let $t_\mathrm{c}>0$ be fixed, $\alpha,\beta>0$ and $t\in\mathbb{R}$. Then*

a) $\sup_{t\in I}\left|\partial^k f(t)\right| \leq \frac{\Gamma(\alpha+k)}{t_c^{\alpha+k}}\|f\|_{(I,\alpha,t_\mathrm{c})} \quad \forall k\geq 0.$

b) $\|f'\|_{(I,\alpha+1,t_\mathrm{c})} \leq \|f\|_{(I,\alpha,t_\mathrm{c})}.$

c) Let $B(\alpha,\beta)=\Gamma(\alpha)\Gamma(\beta)/\Gamma(\alpha+\beta)$ denote the Beta function. Then

$$\|fg\|_{(I,\alpha+\beta,t_\mathrm{c})} \leq B(\alpha,\beta)\|f\|_{(I,\alpha,t_\mathrm{c})}\|g\|_{(I,\beta,t_\mathrm{c})}.$$

Proof. a) and b) follow directly from the definitions. Turning to c), for $k \geq 0$ we have

$$\begin{aligned}\left|(\partial^k fg)(t)\right| &\leq \sum_{l=0}^{k} \binom{k}{l} \left|\partial^l f(t)\right| \left|\partial^{k-l} g(t)\right| \leq \\ &\leq \frac{\|f\|_{(\alpha)} \|g\|_{(\beta)}}{t_c^{\alpha+\beta+k}} \sum_{l=0}^{k} \binom{k}{l} \Gamma(\alpha+l)\Gamma(\beta+k-l).\end{aligned}$$

We thus have to investigate the sum in the last line above and relate it to $\Gamma(\alpha+\beta+k)$. To do so, we use a nice trick, which is presumably well known. For $-1/2 < t < 1/2$ let

$$h_\beta(t) := \Gamma(\beta) \left(\frac{1}{1-t}\right)^\beta. \tag{31}$$

Then $\partial^n h_\beta = h_{\beta+n}$. Now consider $\partial^k(h_\alpha h_\beta)$. Then on the one hand,

$$\partial^k(h_\alpha h_\beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)} \partial^k \underbrace{\left(\Gamma(\alpha+\beta)\left(\frac{1}{1-t}\right)^{\alpha+\beta}\right)}_{=h_{\alpha+\beta}} = B(\alpha,\beta) h_{\alpha+\beta+k}.$$

On the other hand, of course

$$\partial^k(h_\alpha h_\beta) = \sum_{l=0}^{k} \binom{k}{l} \partial^l h_\alpha \partial^{k-l} h_\beta = \sum_{l=0}^{k} \binom{k}{l} h_{\alpha+l} h_{\beta+k-l}.$$

Now we take $t = 0$ and use $h_\beta(0) = \Gamma(\beta)$. Then the above calculations give

$$B(\alpha,\beta)\Gamma(\alpha+\beta+k) = \sum_{l=0}^{k} \binom{k}{l} \Gamma(\alpha+l)\Gamma(\beta+k-l).$$

Inserting this in the calculations from the beginning of the proof of d), we find

$$\left|(\partial^k fg)(t)\right| \leq \|f\|_{(\alpha)} \|g\|_{(\beta)} \frac{\Gamma(\alpha+\beta+k)}{t_c^{\alpha+\beta+k}} B(\alpha,\beta)$$

for each $k \geq 0$, and consequently

$$\|fg\|_{(\alpha+\beta)} \leq B(\alpha,\beta) \|f\|_{(\alpha)} \|g\|_{(\beta)}.$$

□

By taking $g = 1$ in c) we arrive at

$$\|f\|_{(I,\alpha+\beta,t_c)} \leq t_c^\beta \frac{\Gamma(\alpha)}{\Gamma(\alpha+\beta)} \|f\|_{(I,\alpha,t_c)}. \tag{32}$$

We will also need the following somewhat more special property of the norms:

Proposition 2. *Let $s \in I$ and $\alpha > 1$. If $f \in F_{\alpha,t_c}(I)$, then $t \mapsto \int_s^t f(r)\,\mathrm{d}r \in F_{\alpha-1,t_c}(I)$, and*

$$\left\| \int_s^t f(r)\,\mathrm{d}r \right\|_{(\alpha-1)} \leq \max\left\{ \frac{(\alpha-1)|t|}{t_c}, 1 \right\} \|f\|_{(\alpha)} .$$

In case $\alpha > 2$ and $|t-s| \leq t_c$ this simplifies to

$$\left\| \int_s^t f(r)\,\mathrm{d}r \right\|_{(\alpha-1)} \leq (\alpha-1) \|f\|_{(\alpha)} .$$

Proof. We have

$$\left\| \int_s^t f(r)\,\mathrm{d}r \right\|_{\infty} \leq |t-s| \, \|f\|_{\infty} \leq |t-s| \, \|f\|_{(\alpha)} \frac{\Gamma(\alpha)}{t_c^{\alpha}},$$

and for $k \geq 1$

$$\sup_{k\geq 1} \left\| \partial^k \int_0^x f(s)\,\mathrm{d}s \right\|_{\infty} \frac{t_c^{(\alpha-1)+k}}{\Gamma(\alpha-1+k)} = \sup_{k\geq 0} \left\| \partial^k f \right\|_{\infty} \frac{t_c^{\alpha+k}}{\Gamma(\alpha+k)} = \|f\|_{(\alpha)} .$$

The claim now follows from the definition of $\|\cdot\|_{(\alpha-1)}$ and the fact $\Gamma(\alpha) = (\alpha-1)\Gamma(\alpha-1)$. ∎

Remark 7. The intuition behind the norm $\|f\|_{(I,\alpha,t_c)}$ is that when it is finite, the function f behaves equally good or better than the function $t \mapsto \frac{1}{(\mathrm{i}t_c+t)^\alpha}$ when taking derivatives. The amazing and useful fact stated in Proposition 1 c) is that multiplication not only leaves this property intact, but even furnishes a factor that becomes small when either α or β become large. It is this property that gets all our estimates going.

Theorem 2. *Suppose that Assumption 2 holds, and write*

$$\|\theta'\|_{(1)} := \|\theta'\|_{(I,1,\tau)} < \infty.$$

Then for each $n \in \mathbb{N}$,

$$\|x_n\|_{(I,n,\tau)} \leq \|\theta'\|_{(1)} \left(\exp(42 \|\theta'\|_{(1)}^2) - \frac{1}{2} \right), \tag{33}$$

$$\|z_n\|_{(I,n,\tau)} \leq \|\theta'\|_{(1)} \left(\exp(42 \|\theta'\|_{(1)}^2) - \frac{1}{2} \right), \tag{34}$$

$$\|y_n\|_{(I,n,\tau)} \leq \frac{1}{n-1} \left(\exp(42 \|\theta'\|_{(1)}^2) - 1 \right). \tag{35}$$

Remark 8. The Douglas-Adams-constant $M = 42$ comes out of our proof in a natural way. Numerical calculations suggest that Theorem 2 holds with $M = 1$, but this is probably much harder to prove. There is also numerical evidence that the asymptotic behavior for large $\|\theta'\|_{(1)}$ is not optimal. It appears that $\exp(M \|\theta'\|_{(1)}^{3/2})$ is still an upper bound, while $\exp(M \|\theta'\|_{(1)})$ is not.

Proof of Theorem 2. We define C_n and D_n recursively through $C_1 = \|\theta'\|_{(1)}/2$, $D_1 = 0$ and

$$C_n = \begin{cases} C_{n-1} & \text{for } n \text{ even}, \\ C_{n-1} + \frac{\|\theta'\|_{(1)}}{(n-1)} D_{n-1} & \text{for } n \text{ odd}, \end{cases} \tag{36}$$

$$D_n = \begin{cases} \sum_{k=1}^{n-1} B(k, n-k)(C_k C_{n-k} + D_k D_{n-k}) & \text{for } n \text{ even}, \\ 0 & \text{for } n \text{ odd}. \end{cases} \tag{37}$$

We now show that for each $n \in \mathbb{N}$,

$$\|x_n\|_{(I,n,\tau)} \leq C_n, \tag{38}$$

$$\|z_n\|_{(I,n,\tau)} \leq C_n, \tag{39}$$

$$\|y_n\|_{(I,n,\tau)} \leq D_n. \tag{40}$$

This is checked directly for $n = 1$ and $n = 2$. Suppose it holds for $n - 1$. If n is even, then $x_n = 0$ so (38) trivially holds, and (22) implies

$$\|z_n\|_{(n)} = \left\|x'_{n-1}\right\|_{(n)} = \|x_{n-1}\|_{(n-1)} \leq C_{n-1} = C_n.$$

Proposition 1 c), (21) and the fact that either $x_n = 0$ or $z_n = 0$ at any given $n \in \mathbb{N}$ yield

$$\begin{aligned} \|y_n\|_{(n)} &\leq \sum_{k=1}^{n-1} \Big(\|x_k x_{n-k}\|_{(n)} + \|y_k y_{n-k}\|_{(n)} + \|z_k z_{n-k}\|_{(n)} \Big) \leq \\ &\leq \sum_{k=1}^{n-1} B(k, n-k)(C_k C_{n-k} + D_k D_{n-k}). \end{aligned}$$

If n is odd, it follows from (20) that $y_n = z_n = 0$, and

$$\begin{aligned} \|x_n\|_{(n)} &\leq \left\|z'_{n-1}\right\|_{(n)} + \left\|\theta' y_{n-1}\right\|_{(n)} \leq \\ &\leq \|z_{n-1}\|_{(n-1)} + \frac{1}{n-1} \left\|\theta'\right\|_{(1)} \|y_{n-1}\|_{(n-1)} \leq C_{n-1} + \frac{\|\theta'\|_{(1)}}{n-1} D_{n-1}. \end{aligned}$$

This proves (38)–(40). From (36) it follows immediately that

$$\begin{aligned} C_n &= C_{n-1} + \frac{\|\theta'\|_{(1)}}{n-1} D_{n-1} = C_{n-2} + \frac{\|\theta'\|_{(1)}}{n-1} D_{n-1} + \frac{\|\theta'\|_{(1)}}{n-2} D_{n-2} = \\ &= \ldots = C_1 + \left\|\theta'\right\|_{(1)} \sum_{j=2}^{n-1} \frac{D_j}{j} = \left\|\theta'\right\|_{(1)} \left(\frac{1}{2} + \sum_{j=2}^{n-1} \frac{D_j}{j} \right). \end{aligned} \tag{41}$$

Thus it is sufficient to control the D_j. We claim:

Lemma 1. *For $M \geq 42$ and all even $n \in \mathbb{N}$,*

$$D_n \leq \frac{1}{n-1} \sum_{j=1}^{n/2} \frac{\|\theta'\|_{(1)}^{2j} M^j}{j!}. \tag{42}$$

The proof of this purely combinatorial fact is somewhat involved and deferred to the appendix. From (42) and (40) it now follows immediately that

$$\|y_n\|_{(n)} \le D_n \le \frac{\exp(M\,\|\theta'\|_{(1)}^2) - 1}{n-1}$$

for all $n \in \mathbb{N}$. Using (38) and (41) we obtain

$$\begin{aligned}\|x_n\|_{(n)} \;&\le\; C_n \le \|\theta'\|_{(1)} \left(\frac{1}{2} + (\exp(M\,\|\theta'\|_{(1)}^2) - 1) \sum_{j=2}^{n-1} \frac{1}{j(j-1)}\right) \le \\ &\le\; \|\theta'\|_{(1)} \left(\exp(M\,\|\theta'\|_{(1)}^2) - \frac{1}{2}\right),\end{aligned}$$

and the same estimate applies to $\|z_n\|_{(n)}$. The proof is finished. □

Proposition 1 a) now immediately implies

Theorem 3. *Suppose that Assumption 2 holds and write*

$$\|\theta'\|_{(1)} = \|\theta'\|_{(I,1,\tau)}.$$

Then for each $n \in \mathbb{N}$ and each $t \in \mathbb{R}$, we have

$$\begin{aligned}\sup_{t\in I} |x_n(t)| \;&\le\; \frac{(n-1)!}{\tau^n} \|\theta'\|_{(1)} \left(\exp(42\,\|\theta'\|_{(1)}^2) - \frac{1}{2}\right), \\ \sup_{t\in I} |z_n(t)| \;&\le\; \frac{(n-1)!}{\tau^n} \|\theta'\|_{(1)} \left(\exp(42\,\|\theta'\|_{(1)}^2) - \frac{1}{2}\right), \\ \sup_{t\in I} |y_n(t)| \;&\le\; \frac{(n-2)!}{\tau^n} \left(\exp(42\,\|\theta'\|_{(1)}^2) - 1\right).\end{aligned}$$

It is interesting that although the inequalities in Theorem 3 were derived using some seemingly rather crude estimates, they are optimal up to constants in the two most important asymptotic regimes: For large n and each $\|\theta'\|_{(1)}$ as well as for small $\|\theta'\|_{(1)}$ and each n the results in [BeTe$_1$] are an example that displays exactly the asymptotic behavior predicted by Theorem 3.

Surprisingly, the accurate asymptotics of the recursion (19)–(22) under Assumption 1 are not difficult to obtain from the results of [BeTe$_1$] once we have the uniform bounds of Theorem 3 and use our norms.

Theorem 4. *Let $J_{t_c} \subset (0,\infty)$, $J_\alpha \subset (0,1)$ and $J_\gamma \subset (0,\infty)$ be compact intervals. There exists a locally bounded function $\phi_1 : \mathbb{R}^+ \to \mathbb{R}^+$ with $\phi_1(x) = \mathcal{O}(x)$ as $x \to 0$, such that for all $H(t)$ as in (2) satisfying Assumption 1 with $t_c \in J_{t_c}$, $\alpha \in J_\alpha$, $\gamma \in J_\gamma$ and all $t \in I$ we have*

$$\left| x_n(t) - \mathrm{i} c_\gamma \frac{(n-1)!}{t_c^n} \mathrm{Re}\left(\left(1 - \mathrm{i}\frac{t - t_r}{t_c}\right)^{-n}\right)\right| \le \frac{(n-1)!}{t_c^n} n^{-1+\alpha} \phi_1(M), \tag{43}$$

$$\left| z_n(t) + c_\gamma \frac{(n-1)!}{t_c^n} \mathrm{Im}\left(\left(1 - \mathrm{i}\frac{t - t_r}{t_c}\right)^{-n}\right)\right| \le \frac{(n-1)!}{t_c^n} n^{-1+\alpha} \phi_1(M), \tag{44}$$

where $M = \max\left\{\|\theta'\|_{(I,1,t_c)}, \|\theta'_r\|_{(I,\alpha,t_c)}\right\}$ and $c_\gamma = \frac{2\sin(\gamma\pi/2)}{\pi}$.

Proof. Let $x_{n,0}$, $y_{n,0}$ and $z_{n,0}$ be defined via the recursion (20) - (22) started with $x_{1,0} = \mathrm{i}\theta'_0/2$. This is the situation where θ' just consists of a pair of simple poles, and Theorem 3 of [BeTe$_1$] implies (43) and (44) for $x_{n,0}$, $y_{n,0}$ and $z_{n,0}$ and any $\alpha < 1$. Uniformity in the parameters γ and t_c is not spelled out there, but again it is easy to derive from the estimates given. Let us now write

$$\xi_n = x_n - x_{n,0}, \quad \eta_n = y_n - y_{n,0} \quad \text{and} \quad \zeta_n = z_n - z_{n,0}.$$

The proof will be done as soon as we show

$$|\xi_n|, |\zeta_n| \leq \frac{(n-1)!}{t_c^n} n^{-1+\alpha} \phi_1(M) \tag{45}$$

for some ϕ with the properties given in the Theorem, uniformly in the parameters α and t_c. Without loss we assume $t_r = 0$, and we write F_k instead of $F_{k,t_c}(I)$ etc. The main step is

Lemma 2. *$\xi_n \in F_{n-1+\alpha}$ and $\zeta_n \in F_{n-1+\alpha}$ for each $n \in \mathbb{N}$, and there exists $\phi : \mathbb{R}^+ \to \mathbb{R}^+$ with $\phi(x) = \mathcal{O}(x)$ as $x \to 0$ such that*

$$\|\zeta_n\|_{(n-1+\alpha)} \leq \phi(M) \quad \textit{and} \quad \|\xi_n\|_{(n-1+\alpha)} \leq \phi(M)$$

for all $n \in \mathbb{N}$, uniformly in $\alpha \in J_\alpha$, $t_c \in J_{t_c}$.

Proof of Lemma 2. We first prove the assertion for the ζ_n. For odd n, $\zeta_n = 0$ and there is nothing to prove, so let n be even. Since $\zeta_2 = \theta''_r/2$, the assertion is true for $n = 2$. Using (23) along with the recursion, we find

$$-z_{n+2} = z''_n + (\theta')^2 z_n + \theta''\left(\int_0^t \theta' z_n \,\mathrm{d}s + y_n(0)\right), \tag{46}$$

which is obviously just another way to write (29). We decompose (46) into terms which contribute to $z_{n+2,0}$ and those that do not, with the result

$$z_{n+2} = \underbrace{z''_{n,0} + (\theta'_0)^2 z_{n,0} + \theta''_0\left(\int_0^t \theta'_0 z_{n,0}\,ds + y_{n,0}(0)\right)}_{=z_{n+2,0}} + \tag{47}$$

$$+\zeta''_n + (\theta')^2\zeta_n + (2\theta'_0\theta'_r + (\theta'_r)^2) z_{n,0} + \tag{48}$$

$$+\theta''\int_0^t \theta'\zeta_n\,ds + \theta''_0\int_0^t \theta'_r z_{n,0}\,ds + \theta''_r\int_0^t \theta' z_{n,0}\,ds + \theta'' y_n(0) - \theta''_0 y_{n,0}(0). \tag{49}$$

The terms in (48) and (49) contribute to ζ_{n+2}, and we are going to estimate the $\|.\|_{(n+1+\alpha)}$-norm of each of them, using Propositions 1 and 2. Starting with (48), we have

$$\begin{aligned}\left\|\zeta''\right\|_{(n+1+\alpha)} &\leq \|\zeta\|_{(n-1+\alpha)}, & (50)\\ \left\|(\theta')^2\zeta_n\right\|_{(n+1+\alpha)} &\leq B(2, n-1+\alpha)\left\|(\theta')^2\right\|_{(2)}\|\zeta\|_{(n-1+\alpha)} \leq \\ &\leq \frac{1}{(n+\alpha)(n-1+\alpha)}\left\|\theta'\right\|_{(1)}^2\|\zeta\|_{(n-1+\alpha)}, & (51)\end{aligned}$$

and

$$\begin{aligned}\left\|(2\theta_0'\theta_{\rm r}' + (\theta_{\rm r}')^2) z_{n,0}\right\|_{(n+1+\alpha)} &\leq B(1+\alpha, n) \left\|\theta_{\rm r}'(\theta_0' + \theta')\right\|_{(1+\alpha)} \|z_{n,0}\|_{(n)} \\ &\leq \frac{\Gamma(\alpha)\Gamma(n)}{\Gamma(n+\alpha+1)} \left\|\theta_{\rm r}'\right\|_{(\alpha)} \left(\left\|\theta_0'\right\|_{(1)} + \left\|\theta'\right\|_{(1)}\right) \|z_{n,0}\|_{(n)} . \qquad (52)\end{aligned}$$

Turning to (49), let us first note that

$$\left\|\int_0^t \theta' \zeta_n \, ds\right\|_{(n-1+\alpha)} \leq (n-1+\alpha) \left\|\theta' \zeta_n\right\|_{(n+\alpha)} \leq \left\|\theta'\right\|_{(1)} \|\zeta_n\|_{(n-1+\alpha)} .$$

Similarly,

$$\begin{aligned}\left\|\int_0^t \theta_{\rm r}' z_{n,0} \, ds\right\|_{(n-1+\alpha)} &\leq (n-1+\alpha) B(\alpha, n) \left\|\theta_{\rm r}'\right\|_{(\alpha)} \|z_{n,0}\|_{(n)} = \\ &= \frac{\Gamma(\alpha)\Gamma(n)}{\Gamma(n-1+\alpha)} \left\|\theta_{\rm r}'\right\|_{(\alpha)} \|z_{n,0}\|_{(n)}\end{aligned}$$

and

$$\left\|\int_0^t \theta' z_{n,0} \, ds\right\|_{(n)} \leq \left\|\theta'\right\|_{(1)} \|z_{n,0}\|_{(n)} .$$

With these estimates we obtain

$$\left\|\theta'' \int_0^t \theta' \zeta_n \, ds\right\|_{(n+1+\alpha)} \leq \frac{1}{(n+\alpha)(n+\alpha-1)} \left\|\theta'\right\|_{(1)}^2 \|\zeta_n\|_{(n-1+\alpha)} , \qquad (53)$$

$$\left\|\theta_0'' \int_0^t \theta_{\rm r}' z_{n,0} \, ds\right\|_{(n+1+\alpha)} \leq \frac{\Gamma(\alpha)\Gamma(n)}{\Gamma(n+1+\alpha)} \left\|\theta_0'\right\|_{(1)} \left\|\theta_{\rm r}'\right\|_{(\alpha)} \|z_{n,0}\|_{(n)} , \qquad (54)$$

$$\left\|\theta_{\rm r}'' \int_0^t \theta' z_{n,0} \, ds\right\|_{(n+1+\alpha)} \leq B(1+\alpha, n) \left\|\theta_{\rm r}'\right\|_{(\alpha)} \left\|\theta'\right\|_{(1)} \|z_{n,0}\|_{(n)} . \qquad (55)$$

Finally,

$$\begin{aligned}\left\|\theta'' y_n(0)\right\|_{(n+1+\alpha)} &\leq |y_n(0)| \frac{{t_{\rm c}}^{n-1+\alpha}}{\Gamma(n+1+\alpha)} \left\|\theta''\right\|_{(2)} \\ &\leq {t_{\rm c}}^{-1+\alpha} \frac{\Gamma(n)}{\Gamma(n+1+\alpha)} \left\|\theta'\right\|_{(1)} \|y_n\|_{(n)} , \qquad (56)\end{aligned}$$

and

$$\left\|\theta_0'' y_{n,0}(0)\right\|_{(n+1+\alpha)} \leq {t_{\rm c}}^{-1+\alpha} \frac{\Gamma(n)}{\Gamma(n+1+\alpha)} \left\|\theta_0'\right\|_{(1)} \|y_{n,0}\|_{(n)} . \qquad (57)$$

Now we collect all the estimates from (50) through (57) and obtain

$$\begin{aligned}\|\zeta_{n+2}\|_{(n+1+\alpha)} \leq &\left(1 + \frac{\left\|\theta'\right\|_{(1)}^2}{(n+\alpha)(n-1+\alpha)}\right) \|\zeta_n\|_{(n-1+\alpha)} + \\ &+ \frac{\left\|\theta_{\rm r}'\right\|_{(\alpha)} \Gamma(n)}{\Gamma(n+1+\alpha)} \left(2\Gamma(\alpha) \left\|\theta_0'\right\|_{(1)} + (\Gamma(\alpha) + \Gamma(1+\alpha)) \left\|\theta'\right\|_{(1)}\right) \|z_{n,0}\|_{(n)} + \\ &+ \frac{{t_{\rm c}}^{1+\alpha}\Gamma(n)}{\Gamma(n+1+\alpha)} \left(\left\|\theta'\right\|_{(1)} \|y_n\|_{(n)} + \left\|\theta_0'\right\|_{(1)} \|y_{n,0}\|_{(n)}\right) .\end{aligned}$$

This shows $\zeta_{n+2} \in F_{n+1+\alpha}$. The above calculations and the bounds from Theorem 2 now imply the existence of a locally bounded function $\phi : \mathbb{R}^+ \to \mathbb{R}^+$ with $\phi(x) = \mathcal{O}(x)$ as $x \to 0$, such that with $M = \max\{\|\theta'\|_{(1)}, \|\theta_{\mathrm{r}}'\|_{(\alpha)}\}$ and $Q = \phi(M)$ we have

$$\|\zeta_{n+2}\|_{(n+1+\alpha)} \leq \left(1 + \frac{Q}{n(n-1)}\right) \|\zeta_n\|_{(n-1+\alpha)} + \frac{\Gamma(n)}{\Gamma(n+1+\alpha)} Q.$$

Moreover, since

$$\lim_{n\to\infty} n^\beta \frac{\Gamma(n)}{\Gamma(n+\beta)} = 1 \tag{58}$$

for each $\beta > 0$ and $n^\beta \frac{\Gamma(n)}{\Gamma(n+\beta)} \leq 1$ for each $n \in \mathbb{N}$ and $\beta \geq 1$ (cf. [AbSt], 6.1.46 and 6.1.47), the sequence $(\|\zeta_n\|_{(n+\alpha-1)})_{n\in\mathbb{N}}$ is bounded by the sequence $(a_n)_{n\in\mathbb{N}}$ defined through

$$a_{n+2} = a_n \left(1 + \frac{2Q}{n^2}\right) + \frac{Q}{n^{1+\alpha}}$$

with $a_2 = \|\zeta_2\|_{(1+\alpha)} \leq \|\theta_{\mathrm{r}}'\|_{(\alpha)}$. a_n is increasing, and so either $(Q+1)a_n \leq Q$ for all n (then $a_n \leq Q$), or eventually $\frac{Q}{n^{1+\alpha}} \leq \frac{a_n(Q+1)}{n^{1+\alpha}}$, and then

$$a_{n+2} \leq a_n \left(1 + \frac{2Q}{n^2} + \frac{Q+1}{n^{1+\alpha}}\right) \leq a_n \left(1 + \frac{3(Q+1)}{n^{1+\alpha}}\right).$$

This shows

$$a_{n+2} \leq a_2 \prod_{k=1}^{n/2} \left(1 + \frac{3(Q+1)}{(2k)^{1+\alpha}}\right) \leq \|\theta_{\mathrm{r}}'\|_{(\alpha)} \exp\left(3(Q+1) \sum_{k=1}^{\infty} \frac{1}{(2k)^{1+\alpha}}\right)$$

where the infinite sum is bounded uniformly in $\alpha > \inf J_\alpha > 0$. The last inequality above follows by taking the logarithm of the product above and using $\ln(1 + |x|) < |x|$ in the resulting sum. Thus we obtain

$$\|\zeta_{n+2}\|_{(n+1+\alpha)} \leq \max\left\{\phi(M), \|\theta_{\mathrm{r}}'\|_{(\alpha)} \exp\left(3(\phi(M)+1) \sum_{k=1}^{\infty} \frac{1}{(2k)^{1+\alpha}}\right)\right\},$$

and the claim for ζ_n is shown.

Turning now to the ξ_n, (20) implies

$$\xi_n = -\mathrm{i}(\zeta_{n-1}' - \theta_0' \eta_{n-1} - \theta_{\mathrm{r}}' y_{n-1}), \tag{59}$$

and (23) gives

$$\eta_{n-1} = -\int_0^t (\theta_{\mathrm{r}}' z_{n-1} + \theta_0' \zeta_{n-1})\, ds - y_{n-1}(0) + y_{n-1,0}(0). \tag{60}$$

The claim now follows in a very similar way as above from Propositions 1 and 2. □

By the Lemma and Proposition 1 a),

$$\|\zeta_n\|_\infty \leq \|\zeta_n\|_{(n-1+\alpha)} \frac{\Gamma(n+1-\alpha)}{{t_\mathrm{c}}^{n+1-\alpha}} \leq \phi(M)\frac{(n-1)!}{{t_\mathrm{c}}^n}\left(\frac{\Gamma(n+1-\alpha)}{{t_\mathrm{c}}^{1-\alpha}\Gamma(n)}\right).$$

Now (58) implies

$$\|\zeta_n\|_\infty \leq c\phi(M)\frac{(n-1)!}{{t_\mathrm{c}}^n} n^{-1+\alpha},$$

with

$$c = \sup_{n\in\mathbb{N},\alpha\in J_\alpha} \frac{\Gamma(n+1-\alpha)}{{t_\mathrm{c}}^{1-\alpha}\Gamma(n)} n^{1-\alpha} < \infty,$$

and (44) is shown. The same reasoning applies to ξ_n, showing (43) and finishing the proof.

□

4 General Hamiltonians

Our main result Theorem 1 is formulated for Hamiltonians (2) with constant eigenvalues satisfying Assumptions 1 or 2. In this section we show that these assumptions are satisfied for a large class of Hamiltonians after transformation to the natural time scale.

Let us consider

$$(\mathrm{i}\varepsilon\partial_s - \widetilde{H}(s))\psi(s) = 0 \tag{61}$$

for the traceless real-symmetric Hamiltonian

$$\widetilde{H}(s) = \begin{pmatrix} Z(s) & X(s) \\ X(s) & -Z(s) \end{pmatrix} = \rho(s)\begin{pmatrix} \cos\tilde{\theta}(s) & \sin\tilde{\theta}(s) \\ \sin\tilde{\theta}(s) & -\cos\tilde{\theta}(s) \end{pmatrix}. \tag{62}$$

If $X^2 + Z^2 > 0$, then for each $s_\mathrm{r} \in \mathbb{R}$ the transformation

$$\tau(s) = 2\int_{s_\mathrm{r}}^{s} \sqrt{\rho^2(u)}\,\mathrm{d}u \tag{63}$$

takes the equation (61) with Hamiltonian (62) into equation (1) with Hamiltonian (2) with $\theta = \tilde{\theta}\circ\tau^{-1}$. Berry and Lim [BerLi] found that under very general conditions on X and Z the singularities of θ' have the form of a first order pole plus lower order singularities. Then, as to be explained, by the Darboux' Principle Assumption 1 resp. Assumption 2 are satisfied pointwise on the real line. More precisely, the n^{th} derivative of θ' at $t \in \mathbb{R}$ behaves like $\Gamma(n)r^{-n}$ as $n \to \infty$, where r is the distance from t to the nearest pole; the corrections have derivatives going like $\Gamma(n-\alpha)r^{-n}$ as $n \to \infty$ for some $\alpha > 0$, and thus are in $F_{1-\alpha,r}$.

The task is now to make this discussion rigorous, and we start with giving a version of Darboux' Theorem. While this theorem in various forms is certainly well known [He, Bo, Di], we were unable to find a statement in the precision and generality we need in the literature. The proof given in the Appendix uses Cauchy's formula and explicit integration near the singularities. This strategy was suggested to us by Vassili Gelfreich.

Theorem 5 (Darboux' Principle). *Let f be analytic on $D_R = \{z \in \mathbb{C} : |z| < R\}$, and assume that f is analytic also on ∂D_R except for finitely many points. Assume that there exists $N \in \mathbb{N}$ and $(z_j, \alpha_j, g_j)_{j \le N}$ with the properties:*

(i) For each j, z_j is one of the singularities of f on ∂D_R;

(ii) $\alpha_j \in \mathbb{R} \setminus \{0, -1, -2, \dots\}$;

(iii) the function g_j is analytic in a neighborhood U_j of $z = 0$;

(iv) When z_0 is a singularity of f on ∂D_R and $A_{z_0} := \{j : z_j = z_0\}$, then

$$f(z) = \sum_{j \in A_{z_0}} (z - z_0)^{-\alpha_j} \, g_j(z - z_0) \quad \text{on} \quad \bigcap_{j \in A_{z_0}} (U_j + z_0) \cap D_R \, . \tag{64}$$

Then

$$\frac{f^{(n)}(0)}{n!} = \sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}\pi\alpha_j} \frac{g_j(0)}{\Gamma(\alpha_j)} \frac{n^{\alpha_j - 1}}{z_j^{n+\alpha_j}} \left(1 + \mathcal{O}\left(\tfrac{1}{n}\right)\right) . \tag{65}$$

In words, Darboux' Theorem says that when f has finitely many algebraic convergence-limiting singularities, each of those contributes to the growth of the derivatives of f with a term of absolute value $|g(0)|\Gamma(n+\alpha)/R^{n+\alpha}$ depending on the strength $g(0)$, order α and distance R of the singularity, and a phase depending on its strength and location. It is now clear that any function fulfilling the assumptions of Theorem 5 is in $F_{\alpha,R}(\{0\})$, where $\alpha = \max_j \alpha_j$. We have to prove this for the analytic continuation of θ', and for this purpose put the following assumptions on the Hamiltonian $\widetilde{H}$:

Assumption XZ: *X and Z are meromorphic in an open set $U \subset \mathbb{C}$ containing some point s_r on the real axis. X and Z fulfill*

$$\rho^2(s) := X^2(s) + Z^2(s) \ge c > 0 \qquad \forall s \in \mathbb{R} \cap U. \tag{66}$$

By convention, we do not lift removable singularities of ρ^2, so the critical points of ρ^2 consist of its zeros and the poles of X and Z. For s close to such a critical point s_0 of ρ^2, we require

$$\begin{aligned} X(s) &= (s - s_0)^m f(s - s_0) \left[1 + (s - s_0)^n g_X(s - s_0)\right], \\ Z(s) &= \pm\mathrm{i}(s - s_0)^m f(s - s_0) \left[1 + (s - s_0)^n g_Z(s - s_0).\right] \end{aligned} \tag{67}$$

where $0 < n \in \mathbb{N}$, $m \in \mathbb{Z}$ and $\frac{2m+n}{2} > -1$; the functions f, g_X and g_Z are analytic in a neighborhood of s_0, and $K := |f^2(0)(g_X(0) - g_Z(0))| > 0$. The set of critical points has no accumulation points in U.

The class of X and Z fulfilling Assumption XZ is smaller than the universality class considered in [BerLi]. It is not our ambition here to investigate just how large we can take our class while still giving a mathematically rigorous proof; but note that (67) does

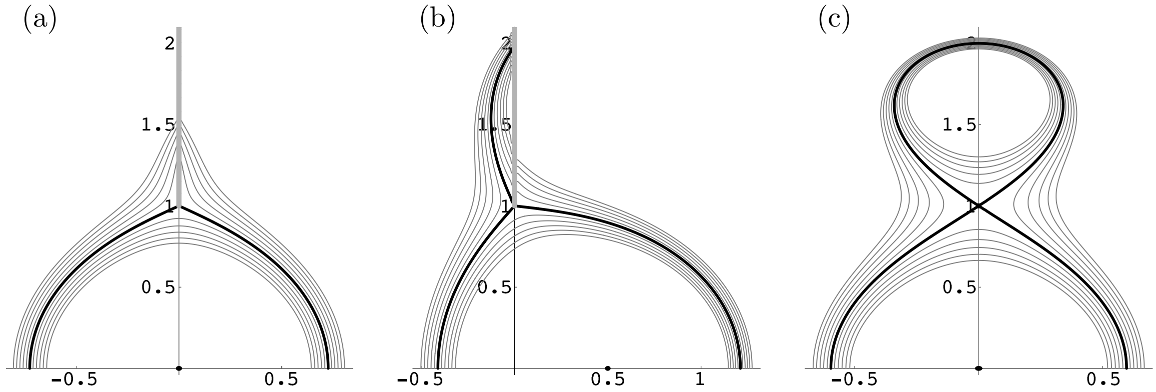

Figure 1: *The boundaries of the sets C_r for various situations; the black line is the boundary of C_R. In (a) and (b), $\rho^2 = 1 + s^2$, and $s_\mathrm{r} = 0$ in (a) while $s_\mathrm{r} = 0.5$ in (b). The branch cuts are on the imaginary axis. In (c), $\rho^2 = (1 + s^2)^2$ and $s_\mathrm{r} = 0$; examples (b) and (c) show why it is necessary to consider the connected components.*

contain the generic case of analytic X and Z and a simple zero of ρ^2, i.e. $m = 0$ and $n = 1$, along with many others.

By (66), the map $s \mapsto \sqrt{\rho(s)^2}$ is analytic and invertible on $U \cap \mathbb{R}$, but may have critical points in the complex plane. For each such critical point s_0 for which a branch cut B_{s_0} of $\sqrt{\rho^2}$ is needed, we choose the branch cut such that it points away from s_r, and define U_0 to be the connected component of $U \setminus \bigcup_{s_0} B_{s_0}$ containing s_r. Then τ as given in (63) is well-defined and analytic in U_0. We define

$$C_r(s_\mathrm{r}) := \{s \in U_0 : |\tau(s) - \tau(s_\mathrm{r})| < r\},$$

denote by $C_{r,0}$ the connected component of C_r containing s_r and put

$$R = R(s_\mathrm{r}) := \sup\{r > 0 : \overline{C_{r,0}(s_\mathrm{r})} \subset U_0\}.$$

Figure 1 shows some typical cases.

We restrict the discussion to the case where $C_r(s_\mathrm{r})$ hits the boundary of U_0 at critical points of ρ^2 as r grows to R. When U is large enough, this is the generic case, provided one has put the branch points B_{s_0} in a sensible way. We distinguish two cases corresponding to our Assumptions 1 and 2 on θ':

Assumption R1: *Let $s_\mathrm{r} \in \mathbb{R}$ be a point where a Stokes line of τ, i.e. a level line of $Re(\tau(s))$, emanating from a critical point s_0 of ρ^2 crosses the real axis. Assume that $\partial C_R(s_\mathrm{r}) \cap \partial U_0 = \{s_0, \overline{s_0}\}$, which means that $\tau(s_0)$ is closer to $\tau(s_\mathrm{r})$ than the τ-image of any other critical point of ρ^2.*

Assumption R2: $\partial C_R(s_\mathrm{r}) \cap \partial U_0 = \{s_1, \dots s_k\}$, *where the s_j are critical points of ρ^2.*

Theorem 6. *Let $\tilde{H}$, ρ and $\tilde{\theta}$ be defined as in (61) with X and Z fulfilling Assumption XZ. Define $\theta = \tilde{\theta} \circ \tau^{-1}$ with τ given by (63), and $t_0 = \tau(s_0)$.*

(i) *If Assumption R2 holds, then $\theta' \in F_{1,R}(\{t_\mathrm{r}\})$, i.e. Assumption 2 is fulfilled at t_r.*

(ii) *Suppose that Assumption R1 holds, and that X and Y are given by (67) at s_0. Then with $\gamma = \frac{\pm n}{2m+n+2}$ there exists a closed interval $I \ni s_{\mathrm{r}}$ such that on I,*

$$\theta'(t) = \mathrm{i}\gamma \left(\frac{1}{t-t_0} - \frac{1}{t-\overline{t_0}} \right) + \theta'_{\mathrm{r}}(t) .$$

where $\theta'_{\mathrm{r}} \in F_{\alpha,R}(I)$ for each $\alpha \in (0,1)$ with $\alpha \geq \frac{2m+n}{2m+n+2}$.

Proof. Let Assumption 2 hold; without loss we assume $s_{\mathrm{r}} = 0$. Then τ is analytic on C_R, while on ∂C_R there are finitely many singularities. Let s_0 be a singularity, and let A_0 be the class of functions h which are analytic in a neighborhood of 0 with $h(0) = 0$. Then for s close to s_0,

$$\rho^2(s) = 2K(s-s_0)^{2m+n}(1 + h_1(s-s_0))$$

with $h_1 \in A_0$. Consequently

$$\begin{aligned} \tau(s) - \tau(s_0) &= 2\int_{s_0}^{s} (r-s_0)^{(2m+n)/2} \sqrt{2K(1+h_1(r-s_0))}\, dr = \\ &= \frac{4\sqrt{2K}}{2m+n+2}(s-s_0)^{\frac{2m+n+2}{2}}(1+h_2(s-s_0)) \end{aligned} \tag{68}$$

with $h_2 \in A_0$.

Since by construction τ has no critical points inside C_R, it is locally analytically invertible there. Since $D_R := \tau(C_R)$ is the disc with radius R and center $\tau(s_{\mathrm{r}})$, global invertibility follows. Thus τ is one-to-one from C_R onto D_R with analytic inverse.

We have

$$\theta'(\tau(s)) = \frac{\tilde{\theta}'(s)}{2\rho(s)} = \frac{1}{2\rho(s)}\frac{\mathrm{d}}{\mathrm{d}s} \arctan\left(\frac{X}{Z}\right)(s) = \frac{X'Z - Z'X}{2\rho^3}(s),$$

and taking $s = \tau^{-1}(t)$, $t \in D_R$, shows that θ' is analytic on the circle D_R, fulfilling the first assumption of Darboux' theorem. Note in particular that $X'Z - Z'X$ is non-singular on D_R by our convention of not lifting removable singularities of ρ^2. For the behavior of θ' near a singularity s_0 at the boundary of D_R, we revisit the calculation of Berry and Lim [BerLi], paying special attention to the error terms that arise. We have

$$(X'Z - Z'X)(s) = \pm \mathrm{i}nK(s-s_0)^{2m+n-1}(1 + h_3(s-s_0)),$$

with $h_3 \in A_0$, A_0 as above. Writing $\sigma = s - s_0$ we now obtain

$$\begin{aligned} \theta'(\tau(s)) &= \frac{\pm \mathrm{i}nK\sigma^{2m+n-1}(1+h_3(\sigma))}{2(2K\sigma^{2m+n})^{3/2}(1+h_1(\sigma))^{3/2}} = \frac{\pm \mathrm{i}n(1+h_3(\sigma))}{4\sqrt{2K}\sigma^{(2m+n+2)/2}(1+h_1(\sigma))^{3/2}} \\ &= \frac{\pm \mathrm{i}n}{(2m+n+2)(\tau(s)-\tau(s_0))} \frac{(1+h_3(\sigma))(1+h_2(\sigma))}{(1+h_1(\sigma))^{3/2}} \\ &= \frac{\pm \mathrm{i}n}{(2m+n+2)(\tau(s)-\tau(s_0))}(1+h_4(\sigma)), \end{aligned}$$

with $h_4 \in A_0$, where we used (68) in the second line. It remains to find the form of τ^{-1} near the singularity $\tau(s_0)$. First note that since τ is an integral, $\tau(s)-\tau(s_0) = \tau(\sigma)$. From (68), $\tau(\sigma) = \tilde{K}\sigma^\alpha(1 + h_2(\sigma))$ with the obvious $\tilde{K}$ and α. The function

$$\sigma \mapsto \sigma\tilde{K}^{1/\alpha}(1 + h_2(\sigma))^{1/\alpha}$$

is invertible in a neighborhood of $\sigma = 0$, and the inverse function $h_5(\sigma)$ is an element of A_0. We then find

$$h_4(\sigma) = h_4 \circ h_5\left(\tau(\sigma)^{2/(2m+n+2)}\right) = \sum_{j=1}^{2m+n+2} \tau(\sigma)^{\frac{2j}{2m+n+2}} g_j(\tau(\sigma))$$

with analytic functions g_j. Putting things together and writing $t = \tau(s)$, $t_0 = \tau(s_0)$ we obtain

$$\theta'(t) = \frac{\pm\mathrm{i}n}{(2m+n+2)(t-t_0)}\left(1 + \sum_{j=1}^{2m+n+2} (t-t_0)^{\frac{2j}{2m+n+2}} g_j(t-t_0)\right) \tag{69}$$

in a neighborhood of t_0. This has exactly the form (64), and thus Darboux' Theorem shows (i). As for (ii), note that when Assumption R1 is fulfilled, by continuity of τ still $\partial C_R(s) \cap \partial U_0 = \{s_0, \overline{s_0}\}$ for all s in a real neighborhood of s_{r}. All the above calculations only need information from the singularities, so they are valid without change, and the proof is finished. □

Example 1. (Landau Zener transitions): In the Landau-Zener model, $X(s) = s$, $Z(s) = \delta$ and consequently $\rho(s) = \sqrt{\delta^2 + s^2}$. The critical points of ρ are at $\pm\mathrm{i}\delta$, and

$$R(0) = \tau(\mathrm{i}\delta) = 2\int_0^\delta \sqrt{\delta^2 - s^2}\,\mathrm{d}s = \frac{\pi\delta^{3/2}}{2}.$$

Moreover, at $s = \pm\mathrm{i}\delta$ the functions X and Z have the form (67) with $m = 0$, $n = 1$, $f = \pm\mathrm{i}\delta$, $g_X = \mp\mathrm{i}/\delta$ and $g_Z = 0$. Thus

$$\theta'(t) = \pm\frac{\mathrm{i}}{3(t \mp \mathrm{i}\delta)}\left(1 + (t \mp \mathrm{i}\delta)^{2/3} g_1(t \mp \mathrm{i}\delta) + (t \mp \mathrm{i}\delta)^{4/3} g_2(t \mp \mathrm{i}\delta)\right),$$

where g_1 and g_2 are analytic near $\pm\mathrm{i}\delta$. Thus

$$\theta_0' := \frac{\mathrm{i}}{3t - \mathrm{i}\delta} - \frac{\mathrm{i}}{3t + \mathrm{i}\delta}$$

and $\theta_{\mathrm{r}} = \theta' - \theta_0' \in F_{1/3,\delta}(I)$ for some $I \supset \{0\}$. In the simple situation at hand, it is easy to see that in fact $\theta_{\mathrm{r}}' \in F_{1/3,\delta}(I)$ for every finite interval I. When ρ^2 has more that one critical point on each side of the real axis, the situation is more involved and we refer to [BeTe$_2$].

Appendix

Proof of Lemma 1

We start by converting (36) and (37) to a recursion for the D_n alone by plugging (41) into (37). The result, in a somewhat expanded form, is

$$\begin{aligned} D_n &= \frac{\|\theta'\|^2_{(1)}}{4}\sum_{k=1}^{n-1} B(k,n-k)+ && (70)\\ &+\frac{\|\theta'\|^2_{(1)}}{2}\sum_{k=2}^{n-1} B(k,n-k)\left(\sum_{j=1}^{k-1}\frac{D_j}{j}+\sum_{j=1}^{n-k-1}\frac{D_j}{j}\right)+ && (71)\\ &+\|\theta'\|^2_{(1)}\sum_{k=2}^{n-1} B(k,n-k)\sum_{j=1}^{k-1}\frac{D_j}{j}\sum_{l=1}^{n-k-1}\frac{D_l}{l}+ && (72)\\ &+\sum_{k=2}^{n-2} B(k,n-k)D_kD_{n-k}. && (73)\end{aligned}$$

To show (42), we will of course proceed inductively. Direct calculation yields that (42) is true up to $n = 10$ (even for $M = 1$). Let us now suppose that $n \in \mathbb{N}$ is an even number and that (42) holds up to $n-2$. We will show that (42) also holds for n and for this purpose treat each line of (70) through (73) separately. We start with (73). Using the induction hypothesis, we get

$$\begin{aligned}(73) &\leq \sum_{k=2}^{n-2} B(k,n-k)\left(\tfrac{1}{k-1}\sum_{j=1}^{\lfloor k/2\rfloor}\tfrac{\|\theta'\|^{2j}_{(1)}M^j}{j!}\right)\left(\tfrac{1}{n-k-1}\sum_{l=1}^{\lfloor (n-k)/2\rfloor}\tfrac{\|\theta'\|^{2l}_{(1)}M^l}{l!}\right)=\\ &= \tfrac{1}{(n-1)(n-2)}\sum_{k=2}^{n-2} B(k-1,n-k-1)\sum_{j=1}^{\lfloor k/2\rfloor}\tfrac{\|\theta'\|^{2j}_{(1)}M^j}{j!}\sum_{l=1}^{\lfloor (n-k)/2\rfloor}\tfrac{\|\theta'\|^{2l}_{(1)}M^l}{l!} = (*_1).\end{aligned}$$

We sort this triple sum by powers p of $\|\theta'\|^2_{(1)}$, i.e. take $p = j + l$. The scheme is the following:

$$\begin{array}{lllll} p=2: & j=1 & \Rightarrow & l=1, & k=2,3,\dots,n-2.\\ p=3: & j=1 & \Rightarrow & l=2, & k=2,3,\dots,n-4\\ & j=2 & \Rightarrow & l=1, & k=4,5,\dots,n-2\\ \vdots & & & & \end{array}$$

so for given $p \leq n/2$ (which is the highest power of $\|\theta'\|^2_{(1)}$ that occurs) we have j running form 1 through $p-1$, and for this j we have $l = p-j$ and $k = 2j, 2j+1, \dots, n-2(p-j)$. This gives

$$(*_1) = \tfrac{1}{(n-1)(n-2)}\sum_{p=2}^{n/2}\|\theta'\|^{2p}_{(1)} M^p\left(\sum_{j=1}^{p-1}\tfrac{1}{j!(p-j)!}\sum_{k=2j}^{n-2p+2j} B(k-1,n-k-1)\right) =$$

$$= \frac{1}{(n-1)(n-2)} \sum_{p=2}^{n/2} \frac{\|\theta'\|_{(1)}^{2p} M^p}{p!} \underbrace{\left(\sum_{j=1}^{p-1} \sum_{k=0}^{n-2p} \binom{p}{j} \frac{B(2j+k-1, n-2j-k-1)}{j!(p-j)!} \right)}_{\psi(n,p)}.$$

We will prove that $\psi(n,p)$ is bounded uniformly in n and $p \leq n/2$. We use the integral representation

$$B(n,m) = \int_0^1 u^{m-1}(1-u)^{n-1} \, \mathrm{d}u \tag{74}$$

of the Beta function, and obtain

$$\begin{aligned} \psi(n,p) &= \int_0^1 \sum_{j=1}^{p-1} \sum_{k=0}^{n-2p} \binom{p}{j} u^{2j+k-2}(1-u)^{n-2j-k-2} \, \mathrm{d}u = \\ &= \int_0^1 \left(\sum_{j=1}^{p-1} \binom{p}{j} u^{2j-2}(1-u)^{2(p-j)-2} \right) \left(\sum_{k=0}^{n-2p} u^k (1-u)^{n-2p-k} \right) \mathrm{d}u. \end{aligned}$$

The sum in the second bracket above is bounded by 2 uniformly on $[0,1]$, and thus $\psi(n,p)$ is shown to be bounded provided we are able to prove

$$\int_0^1 \sum_{j=1}^{p-1} \binom{p}{j} u^{2j-2}(1-u)^{2(p-j)-2} \mathrm{d}u \leq 5. \tag{75}$$

To see (75), first note that the terms with $j=1$ and $j=p-1$ are equal to $p/(2p-3)$ and thus bounded by 2 since $p \geq 2$. For the remaining terms, we use $u^{2j-2} \leq u^j$ and $(1-u)^{2(p-j)-2} \leq (1-u)^{p-j}$.We then obtain

$$\sum_{j=2}^{p-2} \binom{p}{j} u^{2j-2}(1-u)^{2(p-j)-2} \leq \sum_{j=0}^{p} \binom{p}{j} u^j (1-u)^{p-j} = 1$$

by the binomial theorem. This proves (75), and we obtain

$$(73) \leq \frac{5}{(n-1)(n-2)} \sum_{p=2}^{n/2} \frac{\|\theta'\|_{(1)}^{2p} M^p}{p!} \leq \frac{1}{2(n-1)} \sum_{p=2}^{n/2} \frac{\|\theta'\|_{(1)}^{2p} M^p}{p!} \tag{76}$$

since $n \geq 12$. We now turn to (72), and start by proving

Lemma 3. *For $m < n$ we have*

$$\sum_{j=1}^{m} \frac{D_j}{j} \leq \frac{1}{m} \sum_{l=1}^{\lfloor m/2 \rfloor} \frac{(m-2l+1) \, \|\theta'\|_{(1)}^{2l} \, M^l}{(2l-1)l!}. \tag{77}$$

Proof. We use the induction hypothesis to calculate

$$\sum_{j=1}^{m} \frac{D_j}{j} \leq \sum_{j=2}^{m} \frac{1}{j(j-1)} \sum_{l=1}^{\lfloor j/2 \rfloor} \frac{\|\theta'\|_{(1)}^{2l} M^l}{l!} = \sum_{l=1}^{\lfloor m/2 \rfloor} \frac{\|\theta'\|_{(1)}^{2l} M^l}{l!} \sum_{j=2l}^{m} \frac{1}{j(j-1)}.$$

The claim now follows from

$$\sum_{k=j}^{m} \frac{1}{k(k-1)} = \frac{1}{j-1} - \frac{1}{m} = \frac{m-j+1}{m(j-1)}. \tag{78}$$

□

Using (77) we get

$$\begin{aligned}(72) \quad \leq \quad & \|\theta'\|_{(1)}^2 \sum_{k=2}^{n-1} \frac{B(k,n-k)}{(k-1)(n-k-1)} \sum_{j=1}^{\lfloor \frac{k-1}{2} \rfloor} \frac{(k-2j)\,\|\theta'\|_{(1)}^{2j} M^j}{(2j-1)j!} \times \\ & \times \sum_{l=1}^{\lfloor \frac{n-k-1}{2} \rfloor} \frac{(n-k-2l)\,\|\theta'\|_{(1)}^{2l} M^l}{(2l-1)l!} =: (*_2).\end{aligned}$$

Again we sort this by powers p of $\|\theta'\|_{(1)}^2$, leaving the leading $\|\theta'\|_{(1)}^2$ out. The scheme is

$$\begin{array}{lllll} p=2: & j=1 & \Rightarrow & l=1, & k=3,4,\ldots,n-3. \\ p=3 & j=1 & \Rightarrow & l=2, & k=3,4,\ldots,n-5 \\ & j=2 & \Rightarrow & l=1, & k=5,6,\ldots,n-3, \\ \vdots & & & & \end{array}$$

and this time the general term is $j=1,\ldots,p-1$, $l=p-j$, $k=2j+1,\ldots,n-2(p-j)-1$. We use $\frac{B(k,n-k)}{(k-1)(n-k-1)} = \frac{B(k-1,n-k-1)}{(n-1)(n-2)}$ and obtain

$$(*_2) = \frac{\|\theta'\|_{(1)}^2}{(n-1)(n-2)} \sum_{p=2}^{n/2-1} \frac{\|\theta'\|_{(1)}^{2p} M^p}{p!} \phi(n,p) \tag{79}$$

with

$$\begin{aligned}\phi(n,p) &= \sum_{j=1}^{p-1} \sum_{k=2j+1}^{n-2p+2j-1} \binom{p}{j} \frac{(k-2j)(n-k-2(p-j))}{(2j-1)(2(p-j)-1)} B(k-1,n-k-1) = \\ &= \sum_{j=1}^{p-1} \sum_{k=1}^{n-2p-1} \binom{p}{j} \frac{k(n-k-2p)}{(2j-1)(2(p-j)-1)} B(2j+k-1,n-2j-k-1) = \\ &= \int_0^1 \sum_{j=1}^{p} \binom{p}{j} \frac{u^{2j-1}(1-u)^{2(p-j)-1}}{(2j-1)(2(p-j)-1)} \sum_{k=1}^{n-2p-1} k(n-2p-k)u^{k-1}(1-u)^{n-2p-k-1}\,\mathrm{d}u.\end{aligned}$$

The second sum above is obviously bounded by $(n-2p-1)\sum_{k=1}^{\infty} ku^{k-1} \leq 4(n-2p-1)$ on $[0,1/2]$, and since it is symmetric around $u=1/2$, this bound is also valid on $[0,1]$. On the other hand, the integral representation of the Beta function yields

$$\int_0^1 \sum_{j=1}^{p} \binom{p}{j} \frac{u^{2j-1}(1-u)^{2(p-j)-1}}{(2j-1)(2(p-j)-1)} \,\mathrm{d}u = \sum_{j=1}^{p-1} \binom{p}{j} \frac{B(2j, 2(p-j)}{(2j-1)(2(p-j)-1)} =$$

$$= \frac{1}{(2p-1)(2p-2)} \sum_{j=1}^{p-1} \binom{p}{j} B(2j-1, 2(p-j-1)) =$$

$$= \frac{1}{(2p-1)(2p-2)} \int_0^1 \sum_{j=1}^{p-1} \binom{p}{j} u^{2j-2}(1-u)^{2(p-j)-2} \,\mathrm{d}u.$$

The last integral is bounded by 5 due to (75), and thus $\phi(n,p) \leq \frac{20(n-2p-1)}{(2p-1)(2p-2)} \leq \frac{5(n-2)}{(p+1)}$. Inserting in (79) yields

$$(72) \leq \frac{5}{M(n-1)} \sum_{p=2}^{n/2-1} \frac{\|\theta'\|_{(1)}^{2(p+1)} M^{p+1}}{(p+1)!}. \tag{80}$$

Turning to (71), note first that for $j < n-1$, we have

$$\begin{aligned} \sum_{k=j+1}^{n-1} B(k, n-k) &= B(j+1, n-j-1) + \\ &\quad + B(j+2, n-j-2) + \ldots + B(n-1, 1) = \\ &= \sum_{k=1}^{n-j-1} B(k, n-k). \end{aligned}$$

Moreover, $B(1, n-1) = 1/(n-1)$ and $B(k, n-k) \leq 2/((n-1)(n-2))$ for $2 \leq k \leq n-2$, and thus

$$\sum_{k=1}^{n-1} B(k, n-k) \leq 4/(n-1).$$

By symmetry,

$$\begin{aligned} (71) &= 2\left\|\theta'\right\|_{(1)}^2 \sum_{k=2}^{n-1} B(k, n-k) \sum_{j=1}^{k-1} \frac{D_j}{j} = 2\left\|\theta'\right\|_{(1)}^2 \sum_{j=1}^{n-2} \frac{D_j}{j} \sum_{k=j+1}^{n-1} B(k, n-k) \leq \\ &\leq \frac{8\left\|\theta'\right\|_{(1)}^2}{n-1} \sum_{j=1}^{n-2} \frac{D_j}{j} \leq \frac{8\left\|\theta'\right\|_{(1)}^2}{(n-1)(n-2)} \sum_{l=1}^{n/2-1} \frac{(n-2l)\left\|\theta'\right\|_{(1)}^{2l} M^l}{(2l-1)l!} \end{aligned}$$

where the last inequality is (77). Thus

$$(71) \leq \frac{16}{M(n-1)} \sum_{p=2}^{n/2} \frac{\|\theta'\|_{(1)}^{2p} M^p}{p!}. \tag{81}$$

Finally

$$(70) = \frac{1}{4}\left\|\theta'\right\|_{(1)}^{2}\sum_{k=1}^{n-1}B(k,n-k) \leq \frac{\|\theta'\|_{(1)}^{2}}{n-1}. \tag{82}$$

Combining (76), (80), (81) and (82) we arrive at

$$D_n \leq \frac{1}{n-1}\left(\left\|\theta'\right\|_{(1)}^{2} + \left(\frac{1}{2}+\frac{5}{M}\right)\frac{\|\theta'\|_{(1)}^{4}M^2}{2!} + \sum_{p=3}^{n/2}\left(\frac{1}{2}+\frac{21}{M}\right)\frac{\|\theta'\|_{(1)}^{2p}M^p}{p!}\right).$$

Choosing $M \geq 42$, the proof of Lemma 1 is finished.

Proof of Theorem 5

Let z_0 be a singularity of f and write $U_{z_0} = \bigcap_{j\in A_{z_0}}(U_j)$. From (64) it is clear that the function $z \mapsto \sum_{j\in A_{z_0}}(z-z_0)^{-\alpha_j}\, g_j(z-z_0)$ is the unique analytic continuation of f from $(U_{z_0}+z_0)\cap D_R$ to $(U_{z_0}+z_0)\setminus B_{z_0}$, where $B_{z_0} := \{z \in \mathbb{C} : z = az_0,\, a > 1\}$ is the branch cut (if necessary). Moreover f is analytic on the closed set $\overline{D_R}\setminus\bigcup_j(U_j+z_j)$, and therefore analytic in a neighborhood of that set. Putting this continuation together with the continuations near each singularity, we conclude that there exists $\delta > 0$ such that the analytic continuation of f to $D_{R+2\delta}\setminus\bigcup_j B_j$ exists and is bounded on $(\partial D_{R+\delta})\setminus\bigcup_j B_j$. Here we may choose $\delta < 1$ and sufficiently small to guarantee $D_\delta \in U_j$ and $D_{\delta R} \in U_j$ for all j. Let $\Gamma = \partial D_{R+\delta}\cup\bigcup_{j=1}^{N} C_j$ be the piecewise smooth path that encircles 0 anticlockwise along the boundary of the disk with radius $R+\delta$ and avoids the branch cuts B_{z_0} by encircling clockwise the singularities at z_j with a circle C_j of radius δ. Then

$$\frac{f^{(n)}(0)}{n!} = \frac{1}{2\pi \mathrm{i}}\oint_{\Gamma}\frac{f(z)}{z^{n+1}}\,\mathrm{d}z = \frac{1}{2\pi \mathrm{i}}\int_{\partial D_{R+\delta}}\frac{f(z)}{z^{n+1}}\,\mathrm{d}z + \frac{1}{2\pi \mathrm{i}}\sum_{j=1}^{N}\int_{C_j}\frac{f(z)}{z^{n+1}}\,\mathrm{d}z\,.$$

The first integral is easily estimated through

$$\left|\frac{1}{2\pi \mathrm{i}}\int_{\partial D_{R+\delta}}\frac{f(z)}{z^{n+1}}\,\mathrm{d}z\right| \leq \frac{\sup_{|z|=R+\delta}|f(z)|}{(R+\delta)^n} = R^{-n}\mathcal{O}(n^{-k}) \quad \forall\, k\in\mathbb{N}\,.$$

For the contribution of the poles, first note that by (64) we may treat each $j \leq N$ separately, even if they belong to the same pole. If $\alpha_j \in \mathbb{N}$, a straightforward computation shows that

$$\mathrm{Res}_{z=z_j}\left(\frac{f(z)}{z^{n+1}}\right) = (-1)^{\alpha_j-1}\frac{g_j(0)}{\Gamma(\alpha_j)}\frac{n^{\alpha_j-1}}{z_j^{n+\alpha_j}}\left(1+\mathcal{O}\left(\tfrac{1}{n}\right)\right)\,.$$

Noting that C_j is negatively oriented, we conclude that the contribution from poles is the one claimed in (65).

For the remaining terms let $g_j(z-z_j) = \sum_{k=0}^{\infty} b_k(z-z_j)^k$. Then

$$\frac{1}{2\pi \mathrm{i}}\int_{C_j}\frac{f(z)}{z^{n+1}}\,\mathrm{d}z \quad = \quad \frac{1}{2\pi \mathrm{i}}\sum_{k=0}^{\infty} b_k\int_{C_j}\frac{(z-z_j)^{k-\alpha_j}}{z^{n+1}}\,\mathrm{d}z =$$

$$= \frac{1}{2\pi i}\sum_{k=0}^{\infty} b_k z_j^{k-\alpha_j-n} \int\limits_{C_j/z_j} \frac{(\zeta-1)^{k-\alpha_j}}{\zeta^{n+1}}\,d\zeta\,, \tag{83}$$

where we substituted $z = z_j\,\zeta$. The remaining integral is shifted to the origin and can then be solved explicitly in terms of the hypergeometric function F,

$$\begin{aligned}
\int\limits_{C_j/z_j} \frac{(\zeta-1)^{k-\alpha_j}}{\zeta^{n+1}}\,d\zeta &= \int\limits_{C_j/z_j-1} \frac{\zeta^{k-\alpha_j}}{(\zeta+1)^{n+1}}\,d\zeta \\
&= \frac{F\left(\begin{matrix} 1+n, k-\alpha_j+1 \\ k-\alpha_j+2 \end{matrix} ; -\delta\right)}{k-\alpha_j+1}\left[z^{k-\alpha_j+1}\right]_{\delta-0i}^{\delta+0i} \\
&= \frac{F\left(\begin{matrix} 1+n, k-\alpha_j+1 \\ k-\alpha_j+2 \end{matrix} ; -\delta\right)}{k-\alpha_j+1}\delta^{k-\alpha_j+1}\left(1-e^{-2\pi i\alpha_j}\right) .
\end{aligned}$$

In the second line above we used the power series expansion

$$\frac{1}{(1+\zeta)^{n+1}} = \sum_{j=0}^{\infty}(-\zeta)^j \binom{n+j}{j} ,$$

valid for $|\zeta| = \delta < 1$. Note also that the branch cut was moved to the positive real axis through the two changes of variables.

For $k \le \max(a, 2-a)$ we use the asymptotic expansion of the hypergeometric function (cf. [AbSt], 15.7.2)

$$F\left(\begin{matrix} 1+n, k-\alpha_j+1 \\ k-\alpha_j+2 \end{matrix} ; -\delta\right) = (\delta n)^{-(k-\alpha_j+1)}\Gamma(k-\alpha_j+2)\left(1+\mathcal{O}\left(\tfrac{1}{n}\right)\right) ,$$

which shows that from the first $\lfloor\max(a, 2-a)\rfloor + 1$ terms in each sum only the $k = 0$ terms contribute to the leading order in (65) with

$$b_0 \frac{n^{\alpha_j-1}}{z_j^{n+\alpha_j}} \frac{\Gamma(2-\alpha_j)}{1-\alpha_j} \frac{e^{-i\pi\alpha_j}\sin((1-\alpha_j)\pi)}{\pi} = g_j(0)\frac{n^{\alpha_j-1}}{z_j^{n+\alpha_j}}\frac{e^{-i\pi\alpha_j}}{\Gamma(\alpha_j)} .$$

As to be shown, for $k > \max(a, 2-a)$ we have

$$F\left(\begin{matrix} 1+n, k-\alpha_j+1 \\ k-\alpha_j+2 \end{matrix} ; -\delta\right) = \mathcal{O}\left(\frac{k-\alpha_j+1}{n^{1+\frac{k-\alpha_j}{2}}}\right) = \mathcal{O}\left(\frac{k-\alpha_j+1}{n^{2-\alpha_j}}\right) . \tag{84}$$

Hence, these terms do no contribute to the leading order in (65). Note that the sum over k in (83) converges since $D_{\delta|z_j|} \in U_j$.

To check (84) we use the integral representation of the hypergeometric function,

$$F\left(\begin{matrix} 1+n, k-\alpha_j+1 \\ k-\alpha_j+2 \end{matrix} ; -\delta\right) = \frac{\Gamma(2-\alpha_j+k)}{\Gamma(1-\alpha_j+k)\Gamma(1)}\int_0^1 dt\, \frac{t^{k-\alpha_j}}{(1+\delta t)^{n+1}}$$

$$
\begin{aligned}
&= (k-\alpha_j+1)\left(\int_0^s \mathrm{d}t\,\frac{t^{k-\alpha_j}}{(1+\delta t)^{n+1}} + \int_s^1 \mathrm{d}t\,\frac{t^{k-\alpha_j}}{(1+\delta t)^{n+1}}\right)\\
&\leq (k-\alpha_j+1)\left(-\frac{s^{k-\alpha_j}}{n\delta}\frac{1}{(1+\delta t)^n}\bigg|_0^s + \frac{1}{(1+\delta s)^{n+1}}\frac{1}{k-\alpha_j+1}\,t^{k-\alpha_j+1}\bigg|_s^1\right)\\
&\leq (k-\alpha_j+1)\frac{s^{k-\alpha_j}}{n\delta} + \frac{1}{(1+\delta s)^{n+1}}\\
&\overset{s=\frac{1}{\sqrt{n}}}{=} \frac{(k-\alpha_j+1)}{\delta}\frac{1}{n^{1+\frac{k-\alpha_j}{2}}} + \frac{1}{(1+\frac{\delta\sqrt{n}}{n})^{n+1}} = \mathcal{O}\left(\frac{k-\alpha_j+1}{n^{1+\frac{k-\alpha_j}{2}}}\right).
\end{aligned}
$$

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