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Time Development of Exponentially Small Non-Adiabatic Transitions

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Abstract: Optimal truncations of asymptotic expansions are known to yield approximations to adiabatic quantum evolutions that are accurate up to exponentially small errors. In this paper, we rigorously determine the leading order non–adiabatic corrections to these approximations for a particular family of two–level analytic Hamiltonian functions. Our results capture the time development of the exponentially small transition that takes place between optimal states by means of a particular switching function. Our results confirm the physics predictions of Sir Michael Berry in the sense that the switching function for this family of Hamiltonians has the form that he argues is universal.

1. Introduction

The adiabatic approximation in quantum mechanics asymptotically describes solutions to the time dependent Schrödinger equation when the Hamiltonian of the system is a slowly varying function time. After a rescaling of the time variable, the adiabatic approximation describes the small ϵ behavior of solutions to the Schrödinger equation

$$i\,\epsilon\,\frac{\partial\psi}{\partial t} \;=\; H(t)\,\psi. \tag{1.1}$$

In the simplest non-trivial situation, $\{H(t)\}_{t\in\mathbb{R}}$ is a family of 2×2 Hermitian matrices that depends smoothly on t, and whose eigenvalues $E_1(t)$ and $E_2(t)$ are separated by a minimal gap $E_2(t)-E_1(t) \,>\, g \,>\, 0$ for all $t\,\in\,\mathbb{R}$.

To discuss scattering transition amplitudes, we also assume that $H(t)$ approaches limits as t tends to plus or minus infinity. We let $\Phi_j(t)$, $j\,=\,1,2$ be smooth normalized instantaneous eigenstates associated with $E_j(t)$, respectively. Then the transition amplitude $\mathcal{A}(\epsilon)$ across the gap between the asymptotic eigenstates is defined as

$$\mathcal{A}(\epsilon) \;=\; \lim_{\substack{t_0\to-\infty\\ t_1\to+\infty}}\;|\,\langle\,\Phi_2(t_1),\;U_\epsilon(t_1,\,t_0)\,\Phi_1(t_0)\,\rangle\,|, \tag{1.2}$$

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where $U_\epsilon(t_1,\ t_0)$ denotes the evolution operator corresponding to (1.1). The adiabatic theorem of quantum mechanics, [6], asserts that $\mathcal{A}(\epsilon) = O(\epsilon)$, so the transition probability $\mathcal{A}(\epsilon)^2$ is of order $O(\epsilon^2)$.

If the Hamiltonian is an analytic function of time, the transition amplitude is much smaller. Long ago, Zener [34] considered a specific real symmetric two-level system, that had an exponentially small transition $\mathcal{A}(\epsilon)$ as $\epsilon \to 0$. Generalizations of Zener's result to analytic real symmetric two-level Hamiltonians with gaps in their spectra were then proposed in the physics literature. Formulas for $\mathcal{A}(\epsilon)$ of the form

$$\mathcal{A}(\epsilon) \simeq e^{-\gamma/\epsilon}, \quad \text{as} \quad \epsilon \to 0, \tag{1.3}$$

with $\gamma > 0$ that applied more generally were obtained, *e.g.*, in [24, 9, 13]. The decay rate γ was essentially determined by complex crossing points, *i.e.*, the points in the complex t–plane where the analytic continuations of the eigenvalues coincided. Later on, papers [4] and [18] recognized independently that non-trivial prefactors G, with $|G| \neq 1$ could be present for general Hermitian two-level Hamiltonians to yield the general formula

$$\mathcal{A}(\epsilon) \simeq |G|\, e^{-\gamma/\epsilon}, \quad \text{as} \quad \epsilon \to 0. \tag{1.4}$$

Also, [5] and [15] pointed out independently that certain complex degeneracies could lead to the same formula in the real symmetric case. Formulas (1.3) and (1.4) are variants of the well–known Landau-Zener formula that has been widely used in many areas of atomic and molecular physics.

The goal of this paper is to obtain more precise results for a family of two–level systems. For all times t, we construct an approximate solution to (1.1) that is accurate up to errors of order $\exp(-\gamma/\epsilon)\,\epsilon^{\mu}$, for some $\mu > 0$. This captures the transition process which is of order $\exp(-\gamma/\epsilon)$.

Explicitly, let $E > 0$ and $\delta > 0$, and consider the Hamiltonian function

$$H(t) = \frac{E}{2\sqrt{t^2+\delta^2}} \begin{pmatrix} \delta & t \\ t & -\delta \end{pmatrix} \tag{1.5}$$

whose eigenvalues are $\pm E/2$ for every t. This Hamiltonian can be viewed as the familiar Landau-Zener Hamiltonian modified to keep its eigenvalues constant. In our case, the notion of eigenvalue crossing point is replaced by the singularities of the Hamiltonian itself at $t = \pm i\,\delta$. These points govern the transitions between the two levels. Let $\Phi_1(t)$ and $\Phi_2(t)$ be smooth, normalized real eigenvectors corresponding to $-E/2$ and $E/2$ respectively.

Theorem 1.1. *Let $H(t)$ be given by (1.5) and let $0 < \mu < 1/2$. Then:*

1) There exist vectors $\chi_1(\epsilon,\ t)$ and $\chi_2(\epsilon,\ t)$ that satisfy the Schrödinger equation (1.1) up to errors of order $e^{-E\,\delta/\epsilon}$ and correspond to the eigenstates $\Phi_1(t)$, and $\Phi_2(t)$ in the sense that

$$\lim_{|t|\to\infty} |\langle \Phi_j(t),\ \chi_j(\epsilon,\ t)\rangle| = 1 + O\left(e^{-E\,\delta/\epsilon}\left(\frac{\epsilon}{E\delta}\right)^{\mu}\right). \tag{1.6}$$

Moreover, the set $\{\chi_j(\epsilon,\ t)\}_{j=1,2}$ is orthonormal up to errors of order $e^{-E\,\delta/\epsilon}\,\epsilon^{\mu}$.

2) The Schrödinger equation has solutions $\Psi_j(\epsilon,\ t)$, $j = 1, 2$ such that uniformly in $t \in \mathbb{R}$ as $\epsilon \to 0$,

$$\Psi_1(\epsilon, t) = \chi_1(\epsilon, t) - \sqrt{2}\, e^{-E\,\delta/\epsilon} \frac{1}{2} \left\{ \mathrm{erf}\left(\sqrt{\frac{E}{2\,\delta\,\epsilon}}\, t \right) + 1 \right\} \chi_2(\epsilon, t) + O\left(e^{-E\,\delta/\epsilon} \left(\frac{\epsilon}{E\delta}\right)^{\mu} \right),$$

and

$$\Psi_2(\epsilon, t) = \chi_2(\epsilon, t) + \sqrt{2}\, e^{-E\,\delta/\epsilon} \frac{1}{2} \left\{ \mathrm{erf}\left(\sqrt{\frac{E}{2\,\delta\,\epsilon}}\, t \right) + 1 \right\} \chi_1(\epsilon, t) + O\left(e^{-E\,\delta/\epsilon} \left(\frac{\epsilon}{E\delta}\right)^{\mu} \right).$$

Remarks.

0. Recall that the function erf is defined by

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2}\, dy = \frac{2}{\sqrt{\pi}} \int_{-\infty}^x e^{-y^2}\, dy - 1 \in [-1, 1]. \tag{1.7}$$

1. The vectors $\chi_j(\epsilon, t)$, $j = 1, 2$, are constructed as approximate solutions to (1.1) obtained by means of optimal truncation of asymptotic expansions of actual solutions. As $t \to -\infty$ they are asymptotic to the instantaneous eigenvectors $\Phi_j(t)$ of $H(t)$, up to a phase. We call them optimal adiabatic states. See (4.10), (4.11) and (6.9).

2. The transition mechanism between optimal adiabatic states takes place from the value zero to the value $\sqrt{2}\, e^{-E\,\delta/\epsilon}$ in a smooth monotonic way described by the switching function (erf+1)/2, on a time scale of order $\sqrt{\epsilon}$. By contrast, the transition between instantaneous eigenstates of the Hamiltonian displays oscillations of order ϵ for any finite time to eventually reach its exponentially small value only at $t = \infty$. In that sense also, the vectors $\chi_j(\epsilon, t)$ are optimal.

3. As the optimal adiabatic states and eigenstates essentially coincide at $t = \pm\infty$, the transition amplitude equals $\mathcal{A}(\epsilon) \simeq \sqrt{2}\, e^{-E\,\delta/\epsilon}$, up to errors of order $e^{-E\,\delta/\epsilon} \left(\frac{\epsilon}{E\delta}\right)^{\mu}$.

4. The parameters E and δ play somewhat different roles. If we fix E and decrease δ, the singularity of $H(t)$ approaches the real axis. The transition amplitude $\sqrt{2}\, e^{-E\,\delta/\epsilon}$ increases whereas the time it takes to accomplish the transition decreases as $\sqrt{2\,\delta\,\epsilon/E}$. If instead we fix δ and let E decrease, the gap between the eigenvalues decreases. The transition amplitude increases as well, whereas the typical time of the transition now increases.

5. Our results allow us to control the evolution operator $U_\epsilon(t, s)$ associated with (1.1) up to errors of order $e^{-E\,\delta/\epsilon} \left(\frac{\epsilon}{E\delta}\right)^{\mu}$, for any time interval $[s, t]$.

6. Further comments concerning the relevance of the Hamiltonian (1.5) are presented at the end of this section.

We now put our results in perspective by describing previous work on exponential asymptotics for the adiabatic approximation.

Rigorous computations of the behavior of the exponentially small quantity $\mathcal{A}(\epsilon)$ for two-level systems, or generalizations of this typical setting, were provided relatively late in [18, 20, 15, 16, 21, 17, 23]. Although we shall not use the technique in this paper, let us briefly describe the mechanism that is typically used to get the asymptotics leading to the exponentially small quantity $\mathcal{A}(\epsilon)$ in these papers. It involves deforming integration paths from the real axis to the complex plane t–plane until they reach a (non–real) crossing point. Crossing points provide singularities where significant transitions take place, but their lying away in the complex plane makes these transitions exponentially small due to the presence of dynamical phases $\exp(-i\int_0^t E_j(s)\,ds/\epsilon)$ whose exponents acquire a non–zero real part along the path. With this approach, the link with the initial problem posed on the real axis is possible only at infinity. One does not learn about the dynamics of the transition. We note that in a more general framework where $\mathcal{A}(\epsilon)$ represents the transition between two isolated bands of the spectrum for general (unbounded) analytic Hamiltonians, exponential bounds on $\mathcal{A}(\epsilon)$ were obtained by suitable adaptations of this method in [19, 14]. See also [26, 33] for similar results using the pseudo-differential operator machinery.

The other successful method used to construct precise approximations of solutions to (1.1) uses optimal truncation of asymptotic expansions. With sufficiently sharp estimates of the errors, one can prove exponential accuracy. Under appropriate analyticity assumptions, one typically proves that the error committed by retaining n terms in the asymptotic expansion is of order $n!\,\epsilon^n$. This error is minimized by choosing $n \simeq 1/\epsilon$. By virtue of Stirling's formula, it is of order $\exp(-1/\epsilon)/\sqrt{\epsilon}$ as $\epsilon \to 0$. The optimal truncation method was first used for the adiabatic approximation by Berry in [3]. He constructed approximate solutions to (1.1) and gave heuristic arguments concerning their exponential accuracy and the determination of the exponentially small transition mechanism between asymptotic eigenstates. In particular, the switching function (erf+1)/2 in Theorem 1.1 first appeared in [3]. Berry further claimed that this function was universal, *i.e.*, the time development of non–adiabatic transitions in all systems governed by one crossing point (and its conjugate) were described by this switching function. His formal arguments were supported by beautiful numerical investigations of Lim and Berry [25].

Berry's paper [3] is the main inspiration for the present work.

Mathematically rigorous exponential bounds for solutions to (1.1) (and of $\mathcal{A}(\epsilon)$) using optimal truncation were first obtained in the general situations by Nenciu in [31]. They were refined later in [20]. See [11] for an elementary derivation of such results.

Although these rigorous results prove the exponential accuracy of the optimal truncation technique, their estimates are not accurate enough to capture the exponentially smaller non–adiabatic transitions. An exponentially small bound on $\mathcal{A}(\epsilon)$ is an easy corollary, but the estimates do not provide the asymptotic leading term (1.4) for $\mathcal{A}(\epsilon)$.

We refer the reader to two fairly recent reviews, [22] and [1], for more details and many other aspects of the adiabatic approximation in quantum mechanics.

We also note that in the broader context of singular perturbations of linear ODE's, Theorem 1.1 can be interpreted as the smooth crossing of a Stokes line that emanates from some eigenvalue crossing point or singularity. See *e.g.*, [2, 27, 32, 12, 8] and references therein. However, from our perspective, in all rigorous work that has dealt with such issues, the crossing of a Stokes line is performed on a very small circle around the point responsible for the transition. In this paper all estimates are performed on the real axis, and the two conjugate points responsible for the transition are fixed and away from the real axis.

Another angle of attack for such problems uses Borel summation ideas. This is done for certain singularly perturbed ODE's *e.g.*, in [7]. The method consists of writing the solution as a Laplace transform evaluated at $1/\epsilon$, *i.e.*, as $\displaystyle\int_0^\infty F(t,\ p)\,e^{p/\epsilon}\,dp$. One then derives a PDE for F. The PDE is roughly what one obtains from the original equation by replacing $1/\epsilon$ by the symbol $\partial/\partial p$. To get exponentially precise information about the solution to the original problem, it is enough to study the location and nature of complex singularities of F.

We tried to implement the Borel summation technique for our problem, but failed to obtain sufficiently detailed information on the nature of the singularities.

To the best of our knowledge, no rigorous results that address the issue we describe in Theorem 1.1 are available in the literature.

Before we turn to the proof of Theorem 1.1, let us briefly discuss our choice of Hamiltonian (1.5). This choice belongs to the family of real–symmetric time–dependent 2×2 Hamiltonians with non–degenerate eigenvalues $E_2(t) > E_1(t)$. For any member of that family, we can assume without loss of generality that $E_1(t) = -E_2(t)$, because we can subtract a time–dependent multiple of the identity from $H(t)$, which only changes the solutions by a trivial phase. If we change the time variable from t to $t' = 2 \int_0^t E_2(s)\, ds/E$ and drop the prime on t', we obtain a Schrödinger equation (1.1) with a new Hamiltonian $h(t)$ of the form

$$h(t) = \frac{E}{2} \begin{pmatrix} \cos(\alpha(t)) & \sin(\alpha(t)) \\ \sin(\alpha(t)) & -\cos(\alpha(t)) \end{pmatrix} \tag{1.8}$$

whose eigenvalues are $\pm E/2$ for every t. The angle α is given by some function of time. We choose

$$\Phi_1(t) = \begin{pmatrix} -\sin(\alpha(t)/2) \\ \cos(\alpha((t)/2) \end{pmatrix}, \qquad \text{and} \qquad \Phi_2(t) = \begin{pmatrix} \cos(\alpha(t)/2) \\ \sin(\alpha((t)/2) \end{pmatrix},$$

as the normalized real eigenvectors of $h(t)$. Then the coupling $f(t)$ that drives transitions between the instantaneous eigenvectors is given by

$$f(t) = \langle\, \Phi_2(t),\, \Phi_1'(t)\, \rangle = -\, \langle\, \Phi_1(t),\, \Phi_2'(t)\, \rangle = -\, \frac{\alpha'(t)}{2}.$$

Our choice of Hamiltonian (1.5) corresponds to

$$f(t) = \frac{1}{2(t^2 + \delta^2)} \qquad \Leftrightarrow \qquad \alpha(t) = -\, \frac{1}{\delta} \arctan(t/\delta),$$

where $\delta > 0$ is a parameter monitoring the strength of the coupling. This choice of coupling presents the simplest non-trivial singularities in the complex t-plane.

From another point of view, our choice of Hamiltonian is motivated by the Landau–Zener Hamiltonian, $\begin{pmatrix} \delta & t \\ t & -\delta \end{pmatrix}$, which has the local structure of a generic avoided crossing [10]. Physically, one expects the transition to take place in a neighborhood of $t = 0$, and one expects that only the form of the Hamiltonian for small t should determine the transition dynamics. To first order near $t = 0$, our Hamiltonian agrees with the Landau–Zener Hamiltonian.

However, quantum transitions have a more global character. The presence of the square root factor in (1.5), gives rise to the nontrivial prefactor $\sqrt{2}$ in the transition amplitude. Indeed, it is shown in [15] that a change of variable allows one to transform Eq. (1.1) with Hamiltonian (1.5) into an equivalent Schrödinger equation driven by a Hamiltonian that behaves locally near $t = 0$ as a Landau–Zener type Hamiltonian, but with a non-generic complex crossing point. This non-generic structure is responsible for the nontrivial prefactor $\sqrt{2}$ in the transition amplitude. It follows from [15], Sect. 4, that the leading order transition amplitude for our Hamiltonian (1.5) is

$$\mathcal{A}(\epsilon) \simeq \sqrt{2} e^{-E\,\delta/\epsilon}. \tag{1.9}$$

The rest of the paper is organized as follows. In the next section we develop perturbation expansions for solutions to the time–dependent Schrödinger equation (1.1) with Hamiltonian (1.5). In Sect. 3 we analyze the behavior of the high order terms of this expansion that are required for precise optimal truncation. In Sect. 4 we study the error term obtained from optimal truncation and define optimal adiabatic states. Section 5 is devoted to the study of two integrals that arise in the error term and give rise to the switching function. Theorem 1.1 is then proven in Sect. 6.

2. The Formal Perturbation Expansion

We begin by converting our time–dependent Schrödinger equation (1.1) with Hamiltonian (1.5) into a parameter free equation.

Changing variables from t to s with $s = t/\delta$, we obtain

$$i\,\epsilon\,\frac{\partial\psi}{\partial s} \;=\; \frac{E\,\delta}{2\sqrt{1+s^2}}\begin{pmatrix} 1 & s \\ s & -1 \end{pmatrix}\psi.$$

Thus, without loss of generality, by changing ϵ into $\epsilon' = \epsilon/(E\delta)$, we can study the parameter free model

$$i\,\epsilon'\,\frac{\partial\psi}{\partial s} \;=\; \frac{1}{2\sqrt{1+s^2}}\begin{pmatrix} 1 & s \\ s & -1 \end{pmatrix}\psi.$$

In this way, we see that it is sufficient to consider (1.1) with $\delta = E = 1$, which corresponds to the coupling

$$f(t) = \frac{1}{2\,(1+t^2)}. \tag{2.1}$$

The general results are recovered by making the substitutions $\epsilon \to \dfrac{\epsilon}{E\delta}$ and $t \to \dfrac{t}{\delta}$.

We now develop a formal asymptotic expansion to solutions of (1.1).

We concentrate on constructing a formal perturbation expansion of the solution to (1.1) that corresponds to the negative eigenvalue $-1/2$ for small ϵ. We make the unusual ansatz that (1.1) has a formal solution of the form

$$\psi(\epsilon,\,t) \;=\; e^{it/(2\epsilon)}\; e^{\int_0^t f(s)\,g(\epsilon,\,s)\,ds}\;\left(\,\Phi_1(t) \;+\; g(\epsilon,\,t)\,\Phi_2(t)\,\right), \tag{2.2}$$

where $g(\epsilon,\,t) \;=\; \displaystyle\sum_{j=1}^{\infty} g_j(t)\,\epsilon^j$.

Remarks.

1. We arrived at this ansatz by attempting a formal solution of the form

$$\psi(\epsilon,\,t) \;=\; e^{it/(2\epsilon)}\; e^{z(\epsilon,\,t)}\;\left(\,\Phi_1(t) \;+\; g(\epsilon,\,t)\,\Phi_2(t)\,\right),$$

with $z(\epsilon,\,t) \;=\; \displaystyle\sum_{j=1}^{\infty} z_j(t)\,\epsilon^j$. We then realized that this required

$$z(\epsilon,\,t) \;=\; \int_0^t f(s) g(\epsilon,\,s)\,ds.$$

2. There are more standard ansätze for the perturbation expansion [3, 4, 11, 16, 18–20, 22, 26, 28–31, 33], but we were unable to get sufficient control of their n^{th} terms to prove the estimates that we required.
3. If we do not expand $g(\epsilon,\, t)$, then we find that it must satisfy

$$i\,\epsilon\, g'(\epsilon,\, t) \;=\; g(\epsilon,\, t) \;-\; i\,\epsilon\, f(t)\,\Big(1 \,+\, g(\epsilon,\, t)^2\Big).$$

However, we will not use this equation.
4. For normalization purposes, we later consider (2.2) with $\int_{-\infty}^{t} f(s)g(\epsilon, s)\,ds$ in the exponent, instead of $\int_0^t f(s)g(\epsilon, s)\,ds$.
5. When seeking a solution that corresponds to the positive eigenvalue for small ϵ, one makes the similar ansatz

$$\psi(\epsilon,\, t) \;=\; e^{-it/(2\epsilon)}\; e^{-\int_0^t f(s)\,\tilde{g}(\epsilon,\, s)\,ds}\;\left(\,\Phi_2(t) \,+\, \tilde{g}(\epsilon,\, t)\,\Phi_1(t)\,\right), \tag{2.3}$$

where $\tilde{g}(\epsilon,\, t) \;=\; \sum_{j=1}^{\infty} \tilde{g}_j(t)\,\epsilon^j$ satisfies

$$i\,\epsilon\, \tilde{g}'(\epsilon,\, t) \;=\; -\,\tilde{g}(\epsilon,\, t) \,+\, i\,\epsilon\, f(t)\,\Big(1 \,+\, \tilde{g}(\epsilon,\, t)^2\Big).$$

Hence, for any $j \in \mathbf{N}$, we have $\tilde{g}_j(t) = g_j(-t)$.

We substitute (2.2) into (1.1) and formally solve the resulting equation order by order in powers of ϵ.

First Order. The terms of order ϵ require

$$g_1(t) \;=\; i\, f(t). \tag{2.4}$$

Second Order. The terms of order ϵ^2 require

$$g_2(t) \;=\; i\, g_1'(t). \tag{2.5}$$

Third and Higher Order. The terms of order ϵ^{n+1} for $n \geq 2$ require

$$g_{n+1}(t) \;=\; i\,\left(g_n'(t) \,+\, f(t)\sum_{j=1}^{n-1} g_j(t)\, g_{n-j}(t)\right). \tag{2.6}$$

Using (2.1) for the coupling f, and an easy induction using partial fractions decompositions, we see that $g_n(t)$ can be written as

$$g_n(t) \;=\; \sum_{j=1}^{2n} c_{n,j}\, e_j(t), \quad \text{where} \quad e_{2j-1}(t) \;=\; (1+it)^{-j}, \;\; e_{2j}(t) \;=\; (1-it)^{-j}. \tag{2.7}$$

Thus, for each n, we can associate g_n with a unique element of l^1, the space of absolutely summable sequences.

Following the intuition of Michael Berry [3, 4], we isolate the highest order poles of $g_n(t)$ by decomposing $g_n(t) \;=\; G_n(t) \,+\, h_n(t)$, where $G_n(t) \;=\; c_{n,2n-1}\, e_{2n-1}(t) \,+\, c_{n,2n}\, e_{2n}(t)$.

Proof of our results now depends on an analysis of the behavior of $G_n(t)$ and $h_n(t)$ for large n.

3. Analysis of the Recurrence Relation

The main goals of this section are summarized in the following proposition.

Proposition 3.1. *There exists C, such that for all real t and each $n \geq 1$,*

$$|G_n(t)| \leq (n-1)!, \tag{3.1}$$

$$|G_n'(t)| \leq n!, \tag{3.2}$$

$$|h_n(t)| \leq C\,(n-2)!\,\log(n-2), \tag{3.3}$$

$$|h_n'(t)| \leq C\,(n-1)!\,\log(n-2). \tag{3.4}$$

We prove this result using the recurrence formulas (2.4)–(2.6) and the following amazing fact that we use to control the nonlinear terms in the recurrence relation.

Lemma 3.1. *For each k and m,* $e_k(t)\, e_m(t) \;=\; \sum_{j=1}^{k+m+1} d_{k,m,j}\, e_j(t).$

Every $d_{k,m,j}$ *is a non-negative real number, and* $\sum_{j=1}^{k+m+1} d_{k,m,j} \;=\; 1.$

Remark. This lemma implies that we have a Banach algebra structure on l^1, where the product of $\{a_n\}$ and $\{b_n\}$ is determined by formally multiplying $\sum_n a_n\, e_n(t)$ times $\sum_n b_n\, e_n(t)$ and then taking the coordinates of the result in the $\{e_j(t)\}$ basis.

Proof of Lemma 3.1. We first remark that by keeping track of the orders of the poles, it is easy to see that $j \leq k+m+1$ in the sums in the lemma.

Next, we observe that there are many trivial situations. If k and m are both odd, then $e_k(t)\, e_m(t) = e_{k+m+1}(t)$. If k and m are both even, then $e_k(t)\, e_m(t) = e_{k+m}(t)$.

Thus, the only non-trivial cases are when one is odd and the other is even. To prove these cases, we do inductions on odd k and even m.

For $k = 1$ and $m = 2$, the lemma follows immediately from

$$(1+it)^{-1}\,(1-it)^{-1} \;=\; \frac{1}{2}\,(1+it)^{-1} \;+\; \frac{1}{2}\,(1-it)^{-1}. \tag{3.5}$$

Next, we fix $m = 2$ and assume inductively that the lemma has been proven for $k = 2K-1$. Then using (3.5) again, we have

$$\begin{aligned} e_{k+2}(t)\, e_m(t) &= (1+it)^{-K-1}\,(1-it)^{-1} \\ &= (1+it)^{-K}\left[\frac{1}{2}\,(1+it)^{-1} \;+\; \frac{1}{2}\,(1-it)^{-1}\right] \\ &= \frac{1}{2}\left[\, e_{k+2}(t) \;+ e_k(t) e_2(t)\,\right]. \end{aligned} \tag{3.6}$$

The result now follows from our induction hypothesis.

Thus, the lemma is true for all k and $m = 2$.

Finally, we fix an odd k, and assume inductively that the lemma has been proven for this k and an even m. Then

$$\begin{aligned} e_k(t)\, e_{m+2}(t) &= (e_k(t)\, e_m(t))\, e_2(t) \\ &= \sum_j d_{k,m,j}\, e_j(t)\, e_2(t) \\ &= \sum_j d_{k,m,j} \sum_{j'} d_{j,2,j'}\, e_{j'}(t). \end{aligned}$$

The lemma now follows since $\sum_{j'} d_{j,2,j'} = 1, \quad \sum_j d_{k,m,j} = 1$, and all the d's that occur here are non-negative. □

We also need the following technical result.

Lemma 3.2. *For each $n \geq 1$, we have*

$$\sum_{j=0}^{n} \frac{(n-j)!\, j!}{n!} \leq \frac{8}{3}, \tag{3.7}$$

$$\sum_{j=0}^{n-1} \frac{(n-j)!\, j!}{n!} \leq \frac{5}{3}, \quad \textit{and}$$

$$\sum_{j=1}^{n-1} \frac{(n-j)!\, j!}{n!} \leq \frac{2}{3}.$$

Proof. The first inequality trivially implies the other two.

We observe by direct computation that the result is true for the first few values of n, and that the sum equals $8/3$ when $n = 3$ and $n = 4$.

For $n \geq 5$, we separate the first two terms and last two terms to see that the sum equals

$$2 + \frac{2}{n} + \sum_{j=2}^{n-2} \frac{(n-j)!\, j!}{n!}.$$

The largest terms in the sum over j in this expression come from $j = 2$ and $j = n-2$. Those terms equal $\dfrac{2}{n(n-1)}$, and there are $(n-3)$ terms. Thus, the left-hand side of (3.7) is bounded by

$$2 + \frac{2}{n} + \frac{2(n-3)}{n(n-1)} \leq 2 + \frac{2}{5} + \frac{1}{5} < \frac{8}{3}.$$

This last step relies on the observation that $\frac{2(n-3)}{n(n-1)}$ takes the value $1/5$ when $n = 5$ and $n = 6$, and that it is decreasing for $n \geq 6$. □

For any $y(t) = \sum_j y_j e_j(t)$, with $\{y_j\} \in l^1$, we define $\|y\| = \sum_j |y_j|$. We note that for $t \in \mathbb{R}$, $|y(t)| \leq \|y\|$. Since G_n is obtained from g_n by dropping components in the $e_j(t)$ basis, we note that $\|G_n\| \leq \|g_n\|$. Thus, the following lemma implies (3.1) and (3.2) since $\frac{d}{dt}(1 \pm it)^{-j} = \mp i\, j\, (1 \pm it)^{-j-1}$.

Lemma 3.3. $\|g_n\| \leq (n-1)!$.

Proof. We prove that the sequence $a_n = \|g_n\|/(n-1)!$ is bounded above by 1.

By (2.6), Lemmas 3.1 and 3.2, we see that $n \geq 2$ implies

$$a_{n+1} \leq a_n + \frac{4\,a_{n-1}^2}{3n(n-1)}. \tag{3.8}$$

From (2.4) and (2.5) we have $a_1 = a_2 = 1/2$. By explicit computation, we observe that $a_3 = \frac{17}{32} \leq 1 - \frac{4}{9}$, and $a_4 = \frac{197}{384} \leq 1 - \frac{4}{12}$.

The lemma now follows by induction (starting at $n = 4$) and the following statement: If $n \geq 4$, $a_{n-1} \leq 1 - \frac{4}{3(n-1)}$ and $a_n \leq 1 - \frac{4}{3n}$, then $a_{n+1} \leq 1 - \frac{4}{3(n+1)}$.

To prove this statement, we use (3.8) to see that for $n \geq 4$,

$$\begin{aligned} a_{n+1} &\leq 1 - \frac{4}{3n} + \frac{4}{3n(n-1)}\left(1 - \frac{4}{3(n-1)}\right)^2 \\ &= 1 - \frac{4}{3(n+1)} - \frac{8(3n^2+10n-29)}{27(n+1)n(n-1)^3} \\ &\leq 1 - \frac{4}{3(n+1)}. \end{aligned}$$

□

Lemma 3.1 is now proven by the comments before Lemma 3.3 and the following lemma.

Lemma 3.4. *There exists C, such that* $\|h_n\| \leq C\,(n-2)!\,\log(n-2)$ *and* $\|h_n'\| \leq C\,(n-1)!\,\log(n-2)$.

Proof. The first estimate implies the second since h_n is in the span of $e_j(t)$ with $j \leq 2n-2$.

Define $b_n = \|h_n\|/((n-2)!)$. Since h_n is obtained from g_n by dropping components in the $e_j(t)$ basis, we have $\|h_n\| \leq \|g_n\|$. Thus, by Lemma 3.3, $b_n \leq n-1$.

We rewrite (2.6), using $g_n = G_n + h_n$:

$$\begin{aligned} &G_{n+1} + h_{n+1} \\ &\quad = i\left(\frac{dG_n}{dt} + \frac{dh_n}{dt} + f\sum_{j=1}^{n-1} G_j\,G_{n-j} + 2f\sum_{j=1}^{n-1} G_j\,h_{n-j} + f\sum_{j=1}^{n-1} h_j\,h_{n-j}\right). \end{aligned}$$

We then drop the $e_{2n+1}(t)$ and $e_{2n+2}(t)$ components of this expression to obtain an expression for h_{n+1}. This involves dropping the entire term $i\,\dfrac{dG_n}{dt}$, as well as parts of other terms. Since the norm decreases when we drop components, we see that

$$\|h_{n+1}\| \leq \left(\left\| \frac{dh_n}{dt} \right\| + \left\| f \sum_{j=1}^{n-1} G_j\, G_{n-j} \right\| + 2 \left\| f \sum_{j=1}^{n-1} G_j\, h_{n-j} \right\| + \left\| f \sum_{j=1}^{n-1} h_j\, h_{n-j} \right\| \right).$$

Since h_n is in the span of $\{e_j(t)\}$ for $j \leq 2n-2$, $\left\| \frac{dh_n}{dt} \right\| \leq (n-1)\,\|h_n\|$. Thus, by $\|f\| \leq 1/2$, $\|G_n\| \leq (n-1)!$, $h_1 = h_2 = 0$, Lemmas 3.1, and 3.2, we have

$$b_{n+1} \leq b_n + \frac{4/3}{n-1} + \frac{5/3}{(n-1)(n-2)}\, b_{n-1} + \frac{1/3}{(n-1)(n-2)(n-3)}\, b_{n-3}^2.$$

Since we already have $b_n \leq n-1$ and $b_1 = b_2 = 0$, this implies

$$b_{n+1} \leq b_n + \frac{4/3}{n-1} + \frac{5/3}{n-1} + \frac{1/3}{n-1} = b_n + \frac{10/3}{(n-1)},$$

for $n \geq 2$. Thus,

$$b_n = \sum_{k=2}^{n-1} (b_{k+1} - b_k) = \sum_{k=2}^{n-1} \frac{10/3}{k-1} \leq \frac{10}{3}\,(1 + \log(n-2)).$$

This implies the lemma and completes the proof of Proposition 3.1. □

The functions $e_j(t)$ are in $L^1(\mathbb{R})$ for $j \geq 3$. The functions $e_1(t)$ and $e_2(t)$ are not in $L^1(\mathbb{R})$, but $e_1(t) + e_2(t)$ is. The following lemma facilitates getting L^1 information about the functions g_n.

Lemma 3.5. *For every n, the $e_1(t)$ and $e_2(t)$ coefficients in $g_n(t)$ are equal. Furthermore, the $L^1(\mathbb{R})$ norm of g_n is bounded by $\pi\ \|g_n\|$. These results are also true for h_n.*

Proof. We prove the first statement by induction on n. It is clearly true for $n = 1$. Suppose it is true for all $n < N$. The function $i\, g'_{N-1}$ contains no $e_1(t)$ or $e_2(t)$ component. Since the g_n are bounded, $f\, \sum_{j=1}^{N-2} g_j\, g_{N-j-1}$ is in $L^1(\mathbb{R})$ since f is. The only way this function can be in L^1 is if its $e_1(t)$ and $e_2(t)$ components are equal. This implies the result for g_N, and the induction can proceed.

The second statement follows from the first because the absolute values of $(e_1(t) + e_2(t))$ and $e_j(t)$ for $j \geq 3$ are dominated by $(1+t^2)^{-1}$ which has integral π.

The third statement follows since h_n is obtained from g_n by removal of the n^{th} order pole terms. □

We now examine G_n more closely. We note that highest order pole terms in g_n at $t = \pm i$ satisfy the recurrence relation

$$G_{n+1}^{\pm}(t) = \left(i\, \frac{dG_n^{\pm}}{dt}(t) \pm \frac{1/4}{t \mp i} \sum_{j=1}^{n-1} G_j^{\pm}(t)\, G_{n-j}^{\pm}(t) \right),$$

with $G_1^{\pm}(t) = \pm \frac{1}{4} \frac{1}{t \mp i}$ and $G_2^{\pm}(t) = \frac{\mp i}{4} \frac{1}{(t \mp i)^2}$. From this it follows that

$$G_n(t) = i\,\gamma_n \left(e_{2n-1}(t) + (-1)^{n-1}\, e_{2n}(t) \right), \tag{3.9}$$

where γ_n satisfies the real numerical recurrence relation

$$\gamma_{n+1} = n\,\gamma_n - \frac{1}{4} \sum_{j=1}^{n-1} \gamma_j\, \gamma_{n-j}, \tag{3.10}$$

with $\gamma_1 = \gamma_2 = 1/4$.

By Lemma 3.1, the quantity $\beta_n = \gamma_n/(n-1)!$ is bounded. It satisfies

$$\beta_{n+1} = \beta_n - \frac{1}{4} \sum_{j=1}^{n-1} \frac{((j-1)!)((n-j-1)!)}{n!}\, \beta_j\, \beta_{n-j}, \tag{3.11}$$

with $\beta_1 = \beta_2 = 1/4$. From this relation and Lemma 3.2, it follows that β_n has a limit β^* as n tends to infinity. To see this, suppose that the sequence β_m is positive and strictly decreasing for $m \leq n$. Then,

$$0 < \sum_{j=1}^{n-1} \frac{((j-1)!)((n-j-1)!)}{n!}\, \beta_j\, \beta_{n-j} < \frac{8}{3} \frac{\beta_1^2}{n(n-1)}. \tag{3.12}$$

Thus, iterating and using $\beta_1 = \beta_2 = 1/4$, we have

$$\begin{aligned} \beta_{n+1} > \beta_n - \frac{2}{3} \frac{\beta_1^2}{n(n-1)} &> \beta_2 - \frac{2\beta_1^2}{3} \sum_{j=2}^{n} \frac{1}{j(j-1)} \\ &= \beta_2 - \frac{2\beta_1^2}{3} \left(1 - \frac{1}{n}\right) > \frac{5}{24}. \end{aligned} \tag{3.13}$$

Therefore, the sequence $\{\beta_n\}$ is positive, strictly decreasing and bounded below.

Similarly, for some constant $C > 0$ and any $p > 0$, we have

$$\beta_n - \beta_{n+p} \leq C \left(\frac{1}{n-1} - \frac{1}{n+p-1} \right), \tag{3.14}$$

so that,

$$\beta_n = \beta^* \,(1 + O(n^{-1})). \tag{3.15}$$

Remark. Later, we will see that $\beta^* = \frac{1}{\pi\sqrt{2}}$.

4. Optimal Truncation

We begin this section by studying

$$\zeta_n(\epsilon,\, t) \;=\; i\,\epsilon\,\frac{\partial\psi}{\partial t} \;-\; H(t)\,\psi, \tag{4.1}$$

where ψ is given by (2.2) with $g(\epsilon,\, t) \;=\; \sum_{j=1}^{n} g_j(t)\,\epsilon^j$. We ultimately choose $n \;=\; [\![1/\epsilon]\!] - 1$, where $[\![k]\!]$ denotes the greatest integer less than or equal to k.

By explicit calculation, $\zeta_n(\epsilon,\, t)$ equals $e^{it/(2\epsilon)}\; e^{\int_0^t (f(s)\,\sum_{j=1}^n\, g_j(s)\,\epsilon^j)\,ds}\;\Phi_2(t)$ times

$$i\,\epsilon^{n+1}\,G_n' \;+\; i\,\epsilon^{n+1}\,h_n' \;+\; i\,\epsilon^{n+1}\,f\,\sum_{j=1}^{n-1} g_j\,g_{n-j} \;+\; \sum_{k=n+2}^{2n+1} i\,\epsilon^k\,f \sum_{j=k-n-1}^{n} g_j\,g_{k-j-1}. \tag{4.2}$$

Lemma 4.1. *The first term in (4.2) satisfies*

$$\epsilon^{n+1}\,\|G_n'\| \;=\; 2\,\beta_n\,\epsilon^{n+1}\,(n!). \tag{4.3}$$

When n is chosen to be $n \;=\; [\![1/\epsilon]\!] \;-\; 1$, the norm of the remaining terms in (4.2) satisfies

$$\left\|\,\zeta_n(\epsilon,\, t) \;-\; i\,\epsilon^{n+1}\,G_n'\,\right\| \;\le\; C\,\epsilon^{n+1}\,((n-1)!)\,\log(n-2) \tag{4.4}$$

for some C. Thus, as ϵ tends to zero with $n \;=\; [\![1/\epsilon]\!] \;-\; 1$, $\zeta_n(\epsilon,\, t)$ is asymptotic to $i\,\epsilon^{n+1}\,G_n'(t)\;e^{it/(2\epsilon)}\;e^{\int_0^t (f(s)\,\sum_{j=1}^n\, g_j(s)\,\epsilon^j)\,ds}\;\Phi_2(t)$.

Proof. The result (4.3) was proven at the end of the previous section.

By Lemma 3.4, the second term in (4.2) satisfies

$$\epsilon^{n+1}\,\|h_n'\| \;\le\; C'\,\epsilon^{n+1}\,(n-1)!\;\log(n-2). \tag{4.5}$$

By Lemmas 3.1, 3.2, and 3.3, the third term satisfies

$$\epsilon^{n+1}\left\|\,f\sum_{j=1}^{n-1} g_j\,g_{n-j}\,\right\| \;\le\; \epsilon^{n+1}\,\frac{8}{3}\,\frac{1}{2}\,(n-2)! \;=\; \frac{4}{3}\,\epsilon^{n+1}\,(n-2)!. \tag{4.6}$$

We now prove that

$$\left\|\,\sum_{k=n+2}^{2n+1} \epsilon^k\,f \sum_{j=k-n-1}^{n} g_j\,g_{k-j-1}\,\right\| \;\le\; C''\,\epsilon^{n+1}\,(n-1)! \tag{4.7}$$

for some C'' when $n \;=\; [\![1/\epsilon]\!] \;-\; 1$.

We begin the proof of (4.7) with a technical lemma:

Lemma 4.2. *For positive integers $l \le m/2$,*

$$\sum_{p=l}^{m-l} (p!)\,((m-p)!) \;\le\; (m-2l+1)\,(l!)\,((m-l)!).$$

Proof.

$$\sum_{p=l}^{m-l} (p!)\,((m-p)!) = (l!)((m-l)!) \;+\; ((l+1)!)((m-l-1)!) \;+\; \cdots$$

$$+\,((m-l-1)!)((l+1)!) \;+\; ((m-l)!)(l!).$$

The first and last terms are the largest terms in this sum, and they equal $(l!)\,((m-l)!)$. The lemma follows since there are $(m-2l+1)$ terms in the sum. □

We apply Lemma 4.2 with $p = j-1$, $m = k-3$, and $l = k-n-2$, along with Lemmas 3.1, 3.2, and 3.3, to see that the norm of the term $i\,\epsilon^k\, f \displaystyle\sum_{j=k-n-1}^{n} g_j\, g_{k-j-1}$ in (4.2) is bounded by $\epsilon^k\, \dfrac{1}{2} \displaystyle\sum_{p=l}^{m-l} p!\,((m-p)!) \;\le\; \epsilon^k\,(2n-k+2)\,((k-n-2)!)\,((n-1)!)/2$.

To prove (4.7), we now sum this quantity over k:

$$\sum_{k=n+2}^{2n+1} \epsilon^k\,(2n-k+2)\,((k-n-2)!)\,((n-1)!)/2$$

$$= \epsilon^{n+1}\,((n-1)!) \sum_{k=n+2}^{2n+1} \frac{2n-k+2}{2}\,\epsilon^{k-n-1}\,((k-n-2)!)$$

$$= \epsilon^{n+1}\,((n-1)!) \sum_{m=0}^{n-1} \frac{n-m}{2}\,\epsilon^{m+1}\,(m!). \tag{4.8}$$

We now fix $n = [\![1/\epsilon]\!] - 1$ and note that this implies that

$$\sum_{m=0}^{n-1} \frac{n-m}{2}\,\epsilon^{m+1}\,(m!) \le \frac{1}{2} \sum_{m=0}^{n-1} \epsilon^m\,(m!)$$

$$\le \frac{1}{2}\left(1 + \frac{1}{n} + \frac{2!}{n^2} + \cdots + \frac{(n-1)!}{n^{n-1}}\right).$$

By Stirling's formula, $j!/n^j \;\le\; C\,(j/n)^j\,e^{-j}\,\sqrt{j}$ for some $C > 0$. So, the quantity on the right hand side here is bounded. This and (4.8) imply (4.7), which proves the lemma. □

We note that our choice of $n = [\![1/\epsilon]\!] - 1$ implies that there exists a $C > 0$ such that

$$\left| \int \sum_{j=1}^{n} g_j(t)\,\epsilon^j\,dt \right| \;\le\; C\,\epsilon. \tag{4.9}$$

This follows from Lemmas 3.3 and 3.5, since the left hand side of (4.9) is bounded by

$$\pi \sum_{j=1}^{n} \|g_j\|\,\epsilon^j \;\le\; \pi \sum_{j=1}^{n} (j-1)!\,\epsilon^j \;\le\; \pi\,\epsilon \sum_{k=0}^{n-1} \epsilon^k\,k! \;\le\; C\,\epsilon.$$

This allows us to define the optimal adiabatic state $\psi_1(\epsilon, t)$ associated with the eigenvalue $-1/2$ by

$$\psi_1(\epsilon,\ t) \ = \ e^{it/(2\epsilon)}\ e^{\int_{-\infty}^t\ f(s)\,g(\epsilon,\,s)\,ds}\ \ (\,\Phi_1(t)\ +\ g(\epsilon,\ t)\,\Phi_2(t)\,)\,, \qquad (4.10)$$

where $g(\epsilon,\ t)\ =\ \sum_{j=1}^{[\![1/\epsilon]\!]-1}\ g_j(t)\,\epsilon^j$, with the $g_j(t)$'s defined in Sect. 2. By construction, $\psi_1(\epsilon, t)$ is normalized as $t\to-\infty$. The optimal adiabatic state $\psi_2(\epsilon, t)$ associated with the eigenvalue $1/2$ is defined similarly, according to (2.3),

$$\psi_2(\epsilon,\ t) \ = \ e^{-it/(2\epsilon)}\ e^{-\int_{-\infty}^t\ f(s)\,\tilde{g}(\epsilon,\,s)\,ds}\ \ (\,\Phi_2(t)\ +\ \tilde{g}(\epsilon,\ t)\,\Phi_1(t)\,)\,, \qquad (4.11)$$

where $\tilde{g}(\epsilon,\ t)\ =\ \sum_{j=1}^{[\![1/\epsilon]\!]-1}\ \tilde{g}_j(t)\,\epsilon^j$. Since the entire analysis of the g_j's above does not depend on the sign of t, it holds for the $\tilde{g}_j(t)$ as well. See Remark 5 of Sect. 2.

5. Analysis of Some Integrals

The main goal of this section is to analyze the two (quite different) integrals

$$\int_{-\infty}^t \frac{e^{is/\epsilon}}{(1\pm is)^m}\,ds,$$

where $\epsilon>0$ is a small parameter, and $m=[\![1/\epsilon]\!]$. By taking conjugates, we obtain the analogous results for

$$\int_{-\infty}^t \frac{e^{-is/\epsilon}}{(1\mp is)^m}\,ds.$$

Remark. As we see below, the reason the two integrals have different behavior is that in one case, there is a cancellation of rapidly oscillating phases, while in the other, the phases reinforce one another.

Lemma 5.1. *For small* $\epsilon>0$, $m=[\![1/\epsilon]\!]$ *and any* $\gamma\ \in\ (1/2,\ 1)$, *we have*

$$\int_{-\infty}^t \frac{e^{is/\epsilon}}{(1+is)^m}\,ds \ = \ \sqrt{\frac{\pi}{2\,m}}\left\{\operatorname{erf}\left(\sqrt{\frac{m}{2}}\,t\right)\ +\ 1\right\}\ +\ O(m^{-\gamma}), \qquad (5.1)$$

and

$$\int_{-\infty}^t \frac{e^{is/\epsilon}}{(1-is)^m}\,ds \ = \ O(m^{-\gamma}). \qquad (5.2)$$

Proof. We begin with some preliminary estimates that apply to both integrals. We note that for real s,

$$\left|\,\frac{e^{is/\epsilon}}{(1\mp is)^m}\,\right| \ = \ (1+s^2)^{-m/2}.$$

When $|s| \geq 1$, this is bounded by $|s|^{-m}$. Since $\int_1^\infty ds/s^m = 1/(m-1)$, we make an $O(m^{-1})$ error in each of the integrals, if we drop the contributions from $|s| \geq 1$.

Next, let $\delta > 0$ be small and $a = m^\delta/\sqrt{m}$. If $a \leq |s| \leq 1$, then $(1+s^2)^{-m/2} \leq (1+a^2)^{-m/2}$. Thus

$$\int_a^1 (1+s^2)^{-m/2}\, ds \;\leq\; (1-a)\,(1+a^2)^{-m/2} \;\leq\; (1+a^2)^{-m/2}. \tag{5.3}$$

Now, if δ is small enough, (5.3) is of the order of

$$e^{-\frac{m}{2}\ln(1+a^2)} = e^{-\frac{m^{2\delta}}{2}+O(1/m^{1-4\delta})} = O(e^{-\frac{m^{2\delta}}{2}}) << O(m^{-1}). \tag{5.4}$$

Therefore, if we let $A_m = \{s\,:\,|s| \leq a = m^\delta/\sqrt{m}\}$, then

$$\int_{-\infty}^t \frac{e^{is/\epsilon}}{(1 \pm is)^m}\, ds \;=\; \int_{-a}^t \frac{e^{is/\epsilon}}{(1 \pm is)^m}\, \chi_{A_m}(s) \;+\; O(m^{-1}). \tag{5.5}$$

We now concentrate on (5.1).

$$(1+is)^{-m} \;=\; (1+s^2)^{-m/2} \left(\frac{1-is}{1+is}\right)^{m/2}.$$

We separately examine the logs of the factors on the right-hand side of this equation.

First,

$$\log\Big((1+s^2)^{-m/2}\Big) \;=\; -\frac{m}{2}\,\log(1+s^2).$$

On the support of χ_{A_m}, this equals

$$-\frac{m}{2}\,\Big(s^2 \,-\, s^4/2 \,+\, \ldots\Big) \;=\; -m\,s^2/2 \,+\, O(m^{-(1-4\delta)}).$$

Exponentiating, we have

$$(1+s^2)^{-m/2} \;=\; e^{-m\,s^2/2} \,+\, O(m^{-(1-4\delta)}) \quad \text{on the support of } \chi_{A_m}. \tag{5.6}$$

Second,

$$\log\left(\left(\frac{1-is}{1+is}\right)^{m/2}\right) \;=\; -\,i\,m\ \arctan(s) = -\,i\,m\ (s + O(s^3)).$$

On the support of χ_{A_m}, this equals

$$-\,i\,m\,s \,+\, O(m^{-(1/2-3\delta)}).$$

Exponentiating, we have

$$\left(\frac{1-is}{1+is}\right)^{m/2} \;=\; e^{-i\,m\,s} \,+\, O(m^{-(1/2-3\delta)}) \quad \text{on the support of } \chi_{A_m}. \tag{5.7}$$

For $m = [\![1/\epsilon]\!]$, we have

$$e^{is/\epsilon} = e^{ims}\, e^{is(1/\epsilon - m)} = e^{ims}\left(1 + O(m^{-(1/2-\delta)})\right) = e^{ims} + O(m^{-(1/2-\delta)}), \tag{5.8}$$

on the support of χ_{A_m}.

The support of the integrand in (5.5) has length $O(m^{-(1/2-\delta)})$. Using this, (5.6), (5.7), and (5.8) in (5.5) we see that for δ small enough,

$$\begin{aligned}\int_{-\infty}^{t} \frac{e^{is/\epsilon}}{(1+is)^m}\, ds &= \int_{-a}^{t} \frac{e^{is/\epsilon}}{(1+is)^m}\, \chi_{A_m}(s)\, ds + O(m^{-1}) \\ &= \int_{-m^{-(1/2-\delta)}}^{t} e^{-ms^2/2}\, \chi_{A_m}(s)\, ds + O(m^{-(1-4\delta)}).\end{aligned}$$

By simple estimates on the tail of the Gaussian, this equals

$$\int_{-\infty}^{t} e^{-ms^2/2}\, ds + O(m^{-(1-4\delta)}),$$

which implies (5.1).

We now turn to (5.2). The analysis is very similar, except that we use the conjugate of (5.7). This leads us to

$$\begin{aligned}\int_{-\infty}^{t} \frac{e^{is/\epsilon}}{(1-is)^m}\, ds &= \int_{-a}^{t} \frac{e^{is/\epsilon}}{(1-is)^m}\, \chi_{A_m}(s)\, ds + O(m^{-1}) \\ &= \int_{-m^{-(1/2-\delta)}}^{t} e^{-ms^2/2}\, e^{2ims} \chi_{A_m}(s)\, ds + O(m^{-(1-4\delta)}).\end{aligned} \tag{5.9}$$

Integrating by parts, we have

$$\int e^{-ms^2/2}\, e^{2ims}\, ds = \frac{1}{2im}\, e^{-ms^2/2}\, e^{2ims} + \frac{1}{2i} \int s\, e^{-ms^2/2}\, e^{2ims}\, ds.$$

Since $\displaystyle\int_{-\infty}^{\infty} |s|\, e^{-ms^2/2}\, ds = \frac{2}{m}$, the integral on the right-hand side of (5.9) is $O(1/m)$ for all t, and (5.2) follows for δ small enough. □

In the following section, we will also need the following trivial estimate for any $m \geq 2$:

$$\int_{-\infty}^{t} \left| \frac{1}{(1 \pm is)^m} \right| ds \leq C. \tag{5.10}$$

6. Proof of the Theorem

The perturbation expansions of Sect. 2 generate formal approximate solutions to (1.1) associated with the energy levels $\mp 1/2$. When truncated at $n = [\![1/\epsilon]\!] - 1$, the expansions define the optimal adiabatic states $\psi_1(\epsilon, t)$ and $\psi_2(\epsilon, t)$ by (4.10) and (4.11).

As we see below, each of these optimal adiabatic states agrees with an exact solution up to an exponentially small error. Since $\psi_1(\epsilon, t)$ and $\psi_2(\epsilon, t)$ are asymptotically normalized for $t \to -\infty$, it follows that they are normalized up to the same exponentially small error for all t. Similarly, the inner product $\langle\, \psi_1(\epsilon, t),\ \psi_2(\epsilon, t)\,\rangle$ is exponentially small for all t.

We compute the asymptotic leading term to the solution of (1.1) that coincides with $\psi_1(\epsilon, t)$ as $t \to -\infty$, using the optimal adiabatic states $\psi_1(\epsilon, t)$ and $\psi_2(\epsilon, t)$ as a basis. This approximation is accurate up to an error of order $e^{-1/\epsilon}\epsilon^{\mu}$, for $0 < \mu < 1/2$, uniformly for $t \in \mathbb{R}$.

We now define $\zeta(\epsilon, t)$ by (4.1) with $n = [\![1/\epsilon]\!] - 1$. We denote the unitary propagator associated with the Schrödinger equation (1.1) by $U_\epsilon(t_1, t_2)$. There is an exact solution $\Psi_1(\epsilon, t)$ to (1.1) that is asymptotic to $\psi_1(\epsilon, t)$ as $t \longrightarrow -\infty$. We compute

$$\Psi_1(\epsilon, t) - \psi_1(\epsilon, t) = \lim_{r \to -\infty} U_\epsilon(t, r)\, \psi_1(\epsilon, r) - \psi_1(\epsilon, t).$$

In this expression, we replace $U_\epsilon(t, r)\, \psi_1(\epsilon, r)$ with the integral of its derivative with respect to r (with the proper constant of integration) to obtain

$$\begin{aligned}
\Psi_1(\epsilon, t) - \psi_1(\epsilon, t) &= \lim_{r \to -\infty} - \int_r^t U_\epsilon(t, s) \left(\frac{i}{\epsilon} H(s)\, \psi_1(\epsilon, s) + \frac{\partial}{\partial s}\, \psi_1(\epsilon, s) \right) ds \\
&= \frac{i}{\epsilon} \int_{-\infty}^t U_\epsilon(t, s)\, \zeta(\epsilon, s)\, ds.
\end{aligned}$$

To bound the difference between $\Psi_1(\epsilon, t)$ and $\psi_1(\epsilon, t)$, we use the unitarity of the evolution operator together with the expression we derived for $\zeta(\epsilon, s)$ in Sect. 4.

This yields

$$\begin{aligned}
&\Psi_1(\epsilon, t) - \psi_1(\epsilon, t) \\
&= -\epsilon^n \int_{-\infty}^t e^{ir/(2\epsilon)}\, e^{\int_{-\infty}^r (f(s) \sum_{j=1}^n g_j(s)\epsilon^j)\, ds} \left(G_n'(r) + F_n(r) \right) U_\epsilon(t, r)\, \Phi_2(r)\, dr \\
&= -\epsilon^n \int_{-\infty}^t e^{ir/(2\epsilon)}\, e^{\int_{-\infty}^r (f(s) \sum_{j=1}^n g_j(s)\epsilon^j)\, ds}\, G_n'(r)\, U_\epsilon(t, r)\, \Phi_2(r)\, dr \qquad (6.1) \\
&\quad - \epsilon^n \int_{-\infty}^t e^{ir/(2\epsilon)}\, e^{\int_{-\infty}^r (f(s) \sum_{j=1}^n g_j(s)\epsilon^j)\, ds}\, F_n(r)\, U_\epsilon(t, r)\, \Phi_2(r)\, dr, \qquad (6.2)
\end{aligned}$$

where $F_n(r)$ is $-i/\epsilon^{n+1}$ times the expression (4.2) with the first term removed.

We now examine (6.1), which, as we shall see, dominates (6.2). Using (5.10), and (4.9) we first see that

$$e^{\int_0^r (f(s) \sum_{j=1}^n g_j(s)\epsilon^j)\, ds} = 1 + O(\epsilon),$$

where the $O(\epsilon)$ is uniform in r.

We also have

$$U_\epsilon(t,\,r)\,\Phi_2(r) \;=\; e^{-i(t-r)/(2\epsilon)}\,\Phi_2(t) \;+\; O(\epsilon) \;=\; e^{ir/(2\epsilon)}\,\psi_2(\epsilon,\,t) \;+\; O(\epsilon),$$

where the $O(\epsilon)$ is uniform in t and r. Using these estimates together with Proposition 3.1 and (5.10), we see that (6.1) equals

$$-\,\epsilon^n\,\psi_2(\epsilon,\,t)\int_{-\infty}^{t} e^{i\,r/\epsilon}\,G_n'(r)\,dr \;+\; O(\epsilon^{n+1}\,n!), \tag{6.3}$$

with the remainder estimate uniform in t. By (3.9), (3.10), (3.11), (3.15), our choice of $n \simeq 1/\epsilon$, and Lemma 5.1 with $m = n+1$, we see that for $1/2 < \gamma < 1$, (6.3) equals

$$-\,\beta^*\,\epsilon^n\,\frac{(n+1)!}{n+1}\sqrt{\frac{\pi}{2\,(n+1)}}\left\{\mathrm{erf}\left(\sqrt{\frac{n+1}{2}}\,t\right) \;+\; 1 \;+\; O(n^{-(\gamma-1/2)})\right\}\psi_2(\epsilon,t)$$
$$+\;O(\epsilon^{n+1}\,n!). \tag{6.4}$$

We deal with the prefactor before the curly bracket using Stirling's Formula

$$k! \;=\; \sqrt{2\,\pi\,k}\,k^k\,e^{-k}\,(1+O(1/k))$$

(applied with $k = n+1$) and with the easily checked asymptotics

$$e^{x-[\![x]\!]}\left(\frac{[\![x]\!]}{x}\right)^{[\![x]\!]-1} \;=\; 1 \;+\; O(1/x) \qquad \text{as } x \to \infty.$$

By the mean value theorem, the erf function satisfies

$$\begin{aligned}\mathrm{erf}\,(\sqrt{x}\tau) &= \mathrm{erf}\,(\sqrt{[\![x]\!]}\,\tau) \;+\; \frac{\tau\sqrt{y}}{2y}\,e^{-\tau^2 y}\,(x-[\![x]\!]), \qquad \text{where}\\ & \qquad y \in (\,[\![x]\!],\; x\,),\;\; \tau \in \mathbb{R},\\ &= \mathrm{erf}\,(\sqrt{[\![x]\!]}\tau) \;+\; O(1/x), \qquad \text{uniformly in } \;\tau.\end{aligned} \tag{6.5}$$

Finally, the remainder term in (6.3) is of order $O(\sqrt{\epsilon}\,e^{-1/\epsilon})$ so that the quantity (6.1) equals

$$-\,\beta^*\,\pi\,e^{-1/\epsilon}\left\{\mathrm{erf}\left(\sqrt{\frac{1}{2\,\epsilon}}\,t\right) \;+\; 1 \;+\; O(\epsilon^\mu)\right\}\psi_2(\epsilon,t) \;+\; O(e^{-1/\epsilon}\,\sqrt{\epsilon}), \tag{6.6}$$

uniformly in t for any $0 < \mu < 1/2$.

Since $F_n \in L^1$, a similar analysis of (6.2) shows that it is uniformly bounded in t and that its absolute value is smaller than the estimate of the absolute value of the integral in (6.3) by a factor of $C\,\dfrac{\sqrt{n+1}\;\log(n-2)}{n}$. This factor arises as the product of $\dfrac{\log(n-2)}{n}$ from Lemma 4.1 and a factor of $\sqrt{n+1}$ that appears in the denominator of (5.1). Therefore, by estimates similar to those above, (6.2) is of order $O(e^{-1/\epsilon}\,\sqrt{\epsilon}\;\ln(1/\epsilon))$, as $\epsilon \to 0$. Hence, for any $0 < \mu < 1/2$,

$$\begin{aligned}\Psi_1(\epsilon,\,t) = \psi_1(\epsilon,t) \;-\; \beta^*\,\pi\,e^{-1/\epsilon}\left\{\mathrm{erf}\left(\sqrt{\frac{1}{2\,\epsilon}}\,t\right) \;+\; 1 \;+\; O(\epsilon^\mu)\right\}\,\psi_2(\epsilon,t)\\ +O(e^{-1/\epsilon}\,\sqrt{\epsilon}\;\ln(1/\epsilon)),\end{aligned} \tag{6.7}$$

uniformly for $t \in \mathbb{R}$.

A similar analysis of the solution $\Psi_2(\epsilon, t)$ of (1.1) that coincides with $\psi_2(\epsilon, t)$ as $t \to -\infty$ leads to the estimate

$$\Psi_2(\epsilon, t) = \psi_2(\epsilon, t) + \beta^* \pi e^{-1/\epsilon} \left\{ \mathrm{erf}\left(\sqrt{\frac{1}{2\epsilon}}\, t \right) + 1 + O(\epsilon^{\mu}) \right\} \psi_1(\epsilon, t) + O(e^{-1/\epsilon} \sqrt{\epsilon} \ln(1/\epsilon)), \tag{6.8}$$

uniformly for $t \in \mathbb{R}$.

For any $0 < \mu < 1/2$, the following estimates follow directly from (6.7), (6.8) and the unitarity of $U_\epsilon(t, r)$:

$$\Psi_j(\epsilon, t) = \psi_j(\epsilon, t) + O(e^{-1/\epsilon}),$$

$$\|\psi_j(\epsilon, t)\| = 1 + O(e^{-1/\epsilon}\,\epsilon^{\mu}), \qquad \text{and}$$

$$\langle\, \psi_1(\epsilon, t),\ \psi_2(\epsilon, t)\,\rangle = O(e^{-2/\epsilon}\,\epsilon^{\mu})$$

for $j = 1, 2$. Thus, by (4.10) and (4.11), we have

$$\lim_{|t|\to\infty} |\langle \Phi_j(t),\ \psi_j(\epsilon, t)\rangle| = \left| e^{(-1)^{j+1} \int_{-\infty}^{\infty} f(s) g(\epsilon, (-1)^{j+1} s)\, ds} \right| = 1 + O(e^{-1/\epsilon}\,\epsilon^{\mu}).$$

We prove that the value of β^* is $1/(\pi\sqrt{2})$ by comparing the asymptotics above as $t \to \infty$ with the transition amplitude (1.9).

This proves Theorem 1.1 with

$$\chi_j(\epsilon, t) = \psi_j(\epsilon, t/\delta) \tag{6.9}$$

when we return to the original notation $\epsilon \mapsto \epsilon/(E\,\delta)$ and original time variable $t \mapsto t/\delta$. □

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