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Random Gap Control in Landau Zener Transitions

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Abstract

The Landau Zener model describes a two level quantum system which undergoes an avoided crossing. In the adiabatic limit, the transition probability $\mathcal{P}_{\text{LZ}}$ vanishes. An auxiliary control field H_{CD} can be reverse-engineered, such that the full Hamiltonian $H + H_{\text{CD}}$ reproduces adiabaticity for all parameter values. Our aim is to construct a single control field H_1 that drives an ensemble of LZ-type Hamiltonians with a distribution of energy gaps. H_1 works best statistically, minimizing the average transition probability. We restrict our attention to a special class of H_1 controls, motivated by H_{CD} . We found a systematic trade-off between instantaneous adiabaticity and the final transition probability. Certain limiting cases with a linear sweep, can be treated analytically, one of them being the LZ system with Dirac $\delta(t)$ function. Comprehensive and systematic numerical simulations support and extend the analytic results.

Zusammenfassung

Das Landau-Zener-Modell beschreibt ein Zwei-Niveau-Quantensystem, das einen vermiedenen Kreuzungspunkt durchläuft. Im adiabatischen Grenzfall verschwindet die Übergangswahrscheinlichkeit $\mathcal{P}_{\text{LZ}}$. Ein zusätzlicher Kontrollterm H_{CD} kann konstruiert werden, sodass der vollständige Hamiltonoperator $H + H_{\text{CD}}$ für alle Parameter adiabatische Entwicklung garantiert. Unser Ziel ist es, ein einziges Kontrollfeld H_1 zu konstruieren, das ein Ensemble von LZ-artigen Hamiltonians mit einer Verteilung von Energielücken kontrolliert. H_1 wirkt statistisch optimal, indem es die mittlere Übergangswahrscheinlichkeit minimiert. Wir beschränken uns auf eine spezielle Klasse von H_1 -Kontrolloperatoren, motiviert durch H_{CD} . Wir fanden einen systematischen Zielkonflikt zwischen instantaner Adiabaticität und der endgültigen Übergangswahrscheinlichkeit. Bestimmte Grenzfälle lassen sich analytisch behandeln, einer davon ist das LZ-System mit Dirac- $\delta(t)$ -Antrieb. Umfassende und systematische numerische Simulationen unterstützen und erweitern die analytischen Ergebnisse.

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Abbreviations

AGP	Adiabatic Gauge Potential
AT	Adiabatic Theorem
CC	Characteristic Curve
CD	Counderdiabatic
GLZS	Generalized Landau Zener System
IVP	Initial Value Problem
LZ	Landau Zener
LZS	Landau Zener System
ONB	Orthonormal Basis
PCF	Parabolic Cylinder Functions
PDF	Probability Density Function
QHO	Quantum Harmonic Oscillator
TLS	Two Level System
σ ($\sigma_1, \sigma_2, \sigma_3$)	Pauli Matrices
$\mathbf{1}(A)$	Indicator function
$\mathbb{1}$	Identity matrix

Chapter 1

Introduction

The Landau Zener system (LZS) was first studied in 1932. It describes a two dimensional (TLS) quantum mechanical system, with a linearly varying time-dependent Hamiltonian, which undergoes an avoided crossing (AC). Although it is time dependent, it is exactly solvable [1, 2]. Due to the explicit time dependence, transitions between the two eigenstates are generated, with the asymptotic transition probability being the famous the Landau Zener formula [3–6].

The transitions are restricted by the (quantum) Adiabatic Theorem (AT) [7]. In the adiabatic regime, the time evolution of the system follows the instantaneous eigenstate and the probability of transition is small. The conditions under which the the system remains in its initially prepared eigenstate, have both theoretical and practical significance [8, 9]. In theory, letting the system evolve slow enough or equivalently long enough, ensures the following of the adiabatic trajectory, but in practice, decoherence effects and technological limitations set an upper limit to the total time evolution of the system.

The need for fast adiabatic evolution created the field "Shortcuts to Adiabaticity" (STA) [10, 11]. STA collectively refers to protocols that reproduce adiabatic evolution, but not necessarily following the adiabatic path. Relevant to this thesis, is the Counterdiabatic Driving (CD), introduced by Demirplak and Rice [12, 13] and Berry [14] independently. An additional control field H_{CD} is added to the initial Hamiltonian H_0 such that the full system $H_0 + H_{\text{CD}}$ drives the eigenstates of H_0 transitionlessly. CD driving is essentially the reverse engineering of adiabaticity. For the TLS, H_{CD} can be found in closed form, and for low dimensional systems various approximation schemes [15, 16] reproduce H_{CD} sufficiently well.

The problem of the current thesis is the construction of a control field H_1 that works for an ensemble of LZS with a distribution of random gaps. In an experimental setup, it is usually the case that we have either uncertainties in the experimentally

control fields or inherent lack of information on the system. Complex interaction can be modeled by simpler systems by allowing randomness in the parameters [17] or in other cases, physical limitations, e.g., on the energy gap of atoms in a thermal equilibrium [18] enforce uncertainties.

A single control field, cannot drive all the systems in the ensemble transitionlessly, and here H_1 is designed to work statistically, minimizing the average transition probability $\langle \mathcal{P} \rangle$. The space of time dependent Hamiltonians even for the TLS is too large to exhaust, without extra constraints. We will restrict our attention to a special family of H_1 fields that is motivated by the form of H_{CD} . This leads to the definition of the Generalized Landau Zener System (GLZS), having exactly one gap parameter and one control parameter.

The GLZS is interesting in its own right and certain limiting cases can be solved analytically. One of them is the LZS with a Dirac $\delta(t)$ function centered at the AC. This is the limit case, of an infinite control parameter, and it is unphysical since the wavefunction becomes discontinuous. Nevertheless, it is an interesting case because it provides insight to our optimization problem and it is analytically solvable. We have calculated the transition probability $\mathcal{P}_{LZD}$ in closed form, as a function of the gap parameter. The other solvable case is the rectangular pulse shape control, which provides a first-order approximation for the whole class H_1 in the GLZS.

One of our main numerical findings is that the minimization of the final transition probability happens at the cost of instantaneous adiabaticity. If we allow the system to deviate from the adiabatic path, we can achieve lower final transition probability, on average. This is encoded as σ_1 vs σ_2 comparison, with σ_i are the Pauli as control operators for our 2 level problem. The advantage of σ_1 over σ_2 is related to the LZS with $\delta(t)$ and the geometric meaning of $\mathcal{P}_{LZD}$. Moreover, the initial Lorentzian pulsed Hamiltonian H_{CD} , is the worst among the class H_1 . This is qualitatively evident since H_{CD} optimizes for adiabaticity and it is supported from the analytic methods.

In Chapter 2, we give an introduction to the LZS, the AT and CD driving. These three elements are required to define the central problem and the GLZS in Chapter 3. In Chapter 4, we summarize the analytic results. Most of the technical details and can be found in the relevant appendix App.(B). In Chapter 5, we present the numerical analysis. Our approach, is mostly independent of the gap distribution. For the numerical part, we have used the Normal distribution for the random gaps.

Appendices App.(A),(B),(C) are complementary to the main text, including more detailed and additional calculations. In App.(D), for convenience, we have collected the properties of special functions that were used in the calculations.

Chapter 2

Theoretical Background

2.1 Landau Zener

We begin with a brief outline of the history of the LZS equations followed by a derivation. Afterwards, we make the connection to the Weber differential equation. The famous LZ formula is derived as the limit of the transition probability. Finally, we present a modified version of the LZS which is more suitable for applications. More technical details can be found in App.(A).

2.1.1 Motivation

The Landau Zener formula was discovered independently by Landau, Zener, Stueckelberg and Majorana, all within the same year in 1932 [3–6]¹. The four authors were concerned with different physical systems and applied various mathematical techniques to establish the result [2, 19]. In the current work, our approach is closer to Zener's and the relation between LZS with the Weber equation. Zener did not provide the full wavefunction and although it is a relatively easy task, it probably appeared for the first time in 1996 [1]².

As noted in [22], any TLS with linear time dependence can be brought into the standard LZS form. Let H_0 be a two dimensional linear Hamiltonian

$$H(t) = (\partial_t H)t + H(0)$$

with $\partial_t H, H(0) \in \text{mat}(2, \mathbb{C})$, Hermitian and trace free³. From our assumptions,

¹Although the correct time ordering would have been MLZS [2], the problem is usually refereed as LZSM or LZ for short.

²Most likely the result was known prior to that. Asymptotic expansions of the time evolution matrix can be found in [20, 21].

³Without loss of generality, for H_0 finite dimensional, we may assume that $\text{tr}(H_0(t)) = 0 \forall t$.

$\partial_t H_0$ is unitary equivalent to $\lambda \sigma_3$ with $\sigma_3 = \text{diag}(1, -1)$ and $\pm\lambda$ the eigenvalues of $\partial_t H_0$. $\exists U \in \text{mat}(2, \mathbb{C})$, $U^{-1} = U^\dagger : U^\dagger \partial_t H_0 U = -\lambda \sigma_3$, with the minus sign being conventional. Applying the similarity transformation we get $U^\dagger H_0(t) U = -\lambda \sigma_3 t + U^\dagger H_0(0) U$, with the new Hamiltonian $H'_0(t) \equiv U^\dagger H_0(t) U$ being physically equivalent to H_0 . The constant matrix $H'(0) \equiv U^\dagger H(0) U$ is again traceless by the cyclic property of trace and thus admits an expansion of the form $H'(0) = \mathbf{a} \cdot \boldsymbol{\sigma}$ with $\mathbf{a} \equiv (a_1, a_2, a_3) \in \mathbb{R}^3$ necessarily real vector due to the Hermiticity of $H'(0)$.

The Schrödinger equation $i\partial_t |\psi\rangle = H_0 |\psi\rangle$ ($\hbar = 1$) transform to

$$i\partial_t |\psi'\rangle = (-\lambda \sigma_3 t + \mathbf{a} \cdot \boldsymbol{\sigma}) |\psi'\rangle$$

with $|\psi'\rangle \equiv U^\dagger |\psi\rangle$. After the change of variables $t \rightarrow t + a_3/\lambda$ followed by $t \rightarrow \sqrt{\lambda} t, a_{1/2} \rightarrow a_{1/2}/\sqrt{\lambda}$ we get

$$i\partial_{t'} |\psi'\rangle = \begin{pmatrix} -t & a_{\mathbb{C}} \\ a_{\mathbb{C}}^* & t \end{pmatrix} |\psi'\rangle$$

with $a_{\mathbb{C}} := a_1 - ia_2$, $a_1, a_2 \in \mathbb{R}$. The complex coupling will be relevant in certain sections but unless stated otherwise, we will restrict to $a \in \mathbb{R}$. Converting back to unprimed notation

$$i\partial_t |\psi\rangle = \begin{pmatrix} -t & a \\ a & t \end{pmatrix} |\psi\rangle, \quad a \in \mathbb{R} \quad (2.1.1)$$

Eq.(2.1.1) in one of the main equations and will be referred to as LZS.

2.1.2 Landau Zener System

Although Eq.(2.1.1) is time dependent, the system is exactly solvable in the sense that the time evolution matrix can be expressed in closed form [1, 2, 23].

Decoupling the two equations, and after the change of variables $z(t) \equiv te^{-i\pi/4}\sqrt{2}$, $\nu(a) \equiv ia^2/2$, the LZS reduces to the second order differential equation, App.(A.1)

$$\varphi''(z) + \left(\nu + \frac{1}{2} - \frac{z^2}{4}\right)\varphi(z) = 0 \quad (2.1.2)$$

with the prime notation denoting $(\cdot)' \equiv d/dz$ and $\varphi(z)$ a complex valued scalar function. Eq.(2.1.2) is known as the Weber equation [24] but also recognized as the Schrödinger equation for a particle trapped in a one dimensional quadratic potential, the Quantum Harmonic Oscillator (QHO) [25]

$$\varphi''(x) + (2E - x^2)\varphi(x) = 0, \quad E \equiv \nu + \frac{1}{2} \quad (2.1.3)$$

with $x \equiv z/\sqrt{2}$ and the difference that $x, \nu \in \mathbb{R}$. For $|x| \rightarrow \infty$, dropping the constant term $2E$, $\varphi''(x) - x^2\varphi(x) = 0 \Rightarrow \varphi(x) \sim e^{\pm x^2/2}$. Therefore, $\varphi(x) \propto e^{\pm x^2/2} H(x)$

and the need for square integrable solutions requires the termination of the series for $H(x)$, which in turn forces $\nu \in \mathbb{N}$. Thus $\varphi(x) \propto e^{-x^2/2} H_n(x)$ with $H_n(x)$ polynomials of order $n \in \mathbb{N}$, known as the Hermite polynomials [26, 27].

In contrast to QHO Eq.(2.1.3), in Eq.(2.1.2) there are two major complications. Firstly, the solution is complex valued and secondly, since $\nu = ia^2/2$ is purely imaginary, the series of $H(z)$ do not terminate, producing a more complicated function. The special functions that solve Eq.(2.1.2) are known as Parabolic Cylinder functions (PCF) denoted by $D_\nu(z)$ and they are related to Whittaker and the Confluent Hypergeometric Functions [24]. Although they are holomorphic in both parameters, their asymptotic behavior, which is relevant to our discussion, is quite cumbersome due to the Stokes phenomenon [28–31] and its the source to many technical complications.

The (unitary) time evolution matrix $\mathcal{U}_0$ connects the initial to the final state $|\psi_f\rangle = \mathcal{U}_0(t_f, t_i) |\psi_i\rangle$, with $|\psi_f\rangle$ being the solution to the IVP $i\partial_t |\psi\rangle = H_0(t) |\psi\rangle$, $|\psi(t_i)\rangle \equiv |\psi_i\rangle$, $t \in [t_i, t_f]$. In general, $\mathcal{U}_0$ is written symbolically as the time order exponential $\mathcal{U}_0(t_f, t_i) \equiv \mathcal{T} e^{-i \int_{t_i}^{t_f} dt H_0(t)}$ [32]. For a TLS it takes the form

$$\mathcal{U}_0 \equiv \begin{pmatrix} \mathcal{A}_0 & \mathcal{B}_0 \\ -\mathcal{B}_0^* & \mathcal{A}_0^* \end{pmatrix} \quad (2.1.4)$$

with $\mathcal{A}_0, \mathcal{B}_0$ complex functions ($\mathbb{C}$) satisfying $\det \mathcal{U}_0 = |\mathcal{A}_0|^2 + |\mathcal{B}_0|^2 \stackrel{!}{=} 1$. The connection between Eq.(2.1.1) and Eq.(2.1.2), allows us to express $\mathcal{A}_0$ and $\mathcal{B}_0$ as products of PCF and Gamma functions [1, 23]. For more details see App.(A.1) and Eq.(A.1.2),(A.1.3).

2.1.3 Landau Zener Formula

The eigenvalues of $H_0(t) = -t\sigma_3 + a\sigma_1$ are easily found to be

$$E_{e/g} = \pm \sqrt{t^2 + a^2} \quad (2.1.5)$$

and for $a > 0$, $\tan 2\theta = a/t$, $\theta \in (0, \pi/2)$, the corresponding eigenvectors are [2]

$$|g; t\rangle = \begin{pmatrix} \cos \theta \\ -\sin \theta \end{pmatrix}, \quad |e; t\rangle = \begin{pmatrix} \sin \theta \\ \cos \theta \end{pmatrix} \quad (2.1.6)$$

For $a = 0$, the two eigenvalues cross at $t = 0$ and for $a > 0$ there is an avoided crossing with minimum gap $\Delta E_{\min} = 2a$. For $a = 0$, the eigenstates $\{|+\rangle \equiv (1\ 0)^T, |-\rangle \equiv (0\ 1)^T\}$ are also called diabatic states whereas for $a > 0$, they are called adiabatic [2], Fig.(2.1) (left).

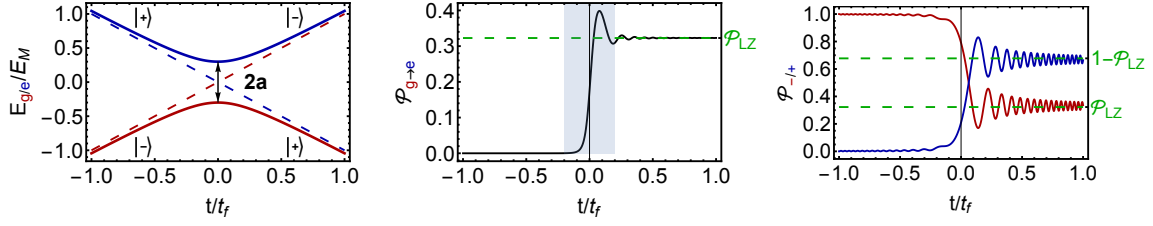


Figure 2.1. (Left) Adiabatic states (solid lines) and diabatic energy levels (dashed lines). Due to the avoided crossing at $t = 0$, the diabatic states exchange roles. The minimum gap is equal to $\Delta E_{\min} = 2a$. (Middle) Transition probability between the two eigenstate for $a = 0.6$, evaluated numerically. The asymptotic value is equal to the LZ formula $\mathcal{P}_{\text{LZ}} \approx 0.32$. For large negative times, the probability stays closed to zero. Around $t = 0$, it jumps to its maximum and afterwards it exhibits oscillatory behavior, decaying to the asymptotic value $\mathcal{P}_{\text{LZ}}$ [33]. Outside the shaded area, the time evolution is approximately trivial (adiabatic impulse approximation) [19, 34]. (Right) Population of the diabatic states defined as $\mathcal{P}_{\pm}(t) = |\langle + | \psi(t) \rangle|^2$.

For simplicity consider the symmetric integration of Eq.(2.1.1) in the interval $[-t_f, t_f]$, $t_f > 0$. Starting from the ground state at $t = -t_f$ the transition probability to the excited state at time $t = t_f$ is given by $\mathcal{P}(t_f) = |\langle e; t_f | \psi; t_f \rangle|^2$, with $|\psi_f\rangle$ being the solution to Eq.(2.1.1). With the help of $\mathcal{U}_0$

$$\mathcal{P}(t_f) = |\langle e; t_f | \mathcal{U}_0(t_f, -t_f) | g; -t_f \rangle|^2 \quad (2.1.7)$$

The asymptotic value of $\mathcal{P}(t_f)$ is defined as the limit

$$\mathcal{P}_{\infty} = \lim_{t \rightarrow \infty} |\langle e; t | \mathcal{U}_0(t, -t) | g; -t \rangle|^2 \quad (2.1.8)$$

and with $\lim_{t \rightarrow \infty} |g, t\rangle = \lim_{t \rightarrow \infty} |e; t\rangle = |-\rangle$ Eq.(2.1.5)

$$\mathcal{P}_{\infty} = |\mathcal{A}_0(+\infty, -\infty)|^2 \quad (2.1.9)$$

From the asymptotic expansions of PCF [24], keeping leading order terms, we are able to compute the limit in Eq.(2.1.9). Using properties of the Gamma function, Eq.(2.1.9) simplifies to

$$\mathcal{P}_{\text{LZ}} = e^{-\pi a^2} \quad (2.1.10)$$

which is known as the Landau Zener formula. See App.(A.1), Eq.(A.1.5) and prior to that.

The behavior of $\mathcal{P}_{\text{LZ}}$ in the two limits $\mathcal{P}_{\text{LZ}} \xrightarrow{a \rightarrow 0} 1$ and $\mathcal{P}_{\text{LZ}} \xrightarrow{a \rightarrow \infty} 0$ can be explained as follows. In the weak coupling limit $a \rightarrow 0$, the diabatic states evolve freely but due to the energy crossing, they exchange roles at $t = 0$ after which the ground state becomes the excited state and vice versa. The strong coupling limit $a \rightarrow \infty$

coincides with the adiabatic limit (see next section) in which $\mathcal{P} \rightarrow 0$. For systems with avoided crossing, the exponential decay is universal in the adiabatic limit [35], and specifically for the LSZ, it describes exactly the transition probability at the full parameter range. The even symmetry $\mathcal{P}_{\text{LZ}}(-a) = \mathcal{P}_{\text{LZ}}(a)$ is the result of time symmetry, see App.(A.2), Eq.(A.2.2).

Post 1932, many alternative derivation have appeared that bypass the solution of Eq.(2.1.1) and the use of special functions. Pioneered by Wittig in [36] and also [37, 38], the formula is extracted via contour integration. In [39] and more recently in [40], $\mathcal{P}_{\text{LZ}}$ is obtained by summing the Dyson series. Other approaches can be found in [41, 42]. See App.(A.3) for a detailed presentation of [39].

A single line derivation is the following. Although the eigenvalues Eq.(2.1.5) do not cross on the real line, they do on the complex plane at $z_c = \pm ia$. The first one who realized the importance of the complex crossing was Landau [3, 43] and the idea was further developed by Dykhne, Davis and Pechukas to what is known today as the DDP formalism [44–46]. According to that, in the adiabatic limit, the asymptotic non adiabatic transition probability is given by

$$\mathcal{P}_{\text{DDP}} \sim \exp\left(-2 \operatorname{Im} \left[\int_0^{z_c} dt E_e(t) - E_g(t) \right]\right) \quad (2.1.11)$$

with $E_{e/g}$ given by Eq.(2.1.5), from which $\mathcal{P}$ is easily calculated

$$\mathcal{P}_{\text{DDP}} = e^{-2 \operatorname{Im} \int_0^{ia} dt \sqrt{a^2 + t^2}} = e^{-4a^2 \int_0^1 dt \sqrt{1-t^2}} = e^{-\pi a^2} \quad (2.1.12)$$

with the last integral being the area of first quadrant of the unit circle. This should only have worked in $a \rightarrow \infty$ (adiabatic limit) but unexpectedly agrees with Eq.(2.1.10) $\forall a$ [22, 47].

2.1.4 Non Linear, Finite Time

In applications, the LZ equation is usually presented in the form

$$i\partial_s |\psi\rangle = T(-\lambda(s)\sigma_3 + a\sigma_1) |\psi\rangle, \quad s \in [0, 1] \quad (2.1.13)$$

with $\lambda(s)$ being a nonlinear sweep function, replacing the linear ramp Tab.(2.1). In contrast to Eq.(2.1.1), the time evolution is restricted in a finite interval $[t_f, -t_f]$ which is mapped to $[0, 1]$ with an appropriate change of variables $t \rightarrow s$. The parameter T is related to t_f and usually called protocol time.

For finite time evolution, Eq.(2.1.10) is corrected by powers of $1/t_f$ [1]. In the large T limit, Eq.(2.1.1), (2.1.13) are equivalent for the linear sweep, Tab.(2.1), with $\mathcal{P}_{\text{LZ}} \approx e^{-\pi T a^2 / \lambda_0}$. Non nonlinearities can typically be treated only in perturbation

Sweep	$\lambda(s), s \in [0, 1]$
Lin	$\lambda_0(s - \frac{1}{2})$
Tan	$\frac{\lambda_0}{2} a \tan(c(2s - 1))$
RC	$\lambda_0(s - \frac{1}{2}) \frac{\sqrt{1-4\eta^2(a)}}{\sqrt{1-16\eta^2(a)(s-1/2)^2}}$
Exp	$\begin{cases} \frac{\lambda_0}{2} \left(\frac{1-e^{-2ns}}{1-e^{-n}} - 1 \right) & s < \frac{1}{2} \\ \frac{\lambda_0}{2} \left(1 - \frac{e^{2n}-e^{2ns}}{e^{2n}-e^n} \right) & s > \frac{1}{2} \end{cases}$

Table 2.1. Example of nonlinear sweeps adapted for Eq.(2.1.13) with $c = \arctan(1/a)$, $\eta(a) = \frac{1}{\sqrt{4+a^2}}$ and n free parameter for the Exp sweep. $s \in [0, 1]$, with $\lambda(\frac{1}{2}) = 0$, $\lambda(0) = -\lambda_0$, $\lambda(1) = \lambda_0$ Fig.(2.2) (Left).

theory or methods like the DDP formalism, in the adiabatic limit [22, 47]. Therefore for the rest of the sweeps in Tab.(2.1) we have to rely on numerics.

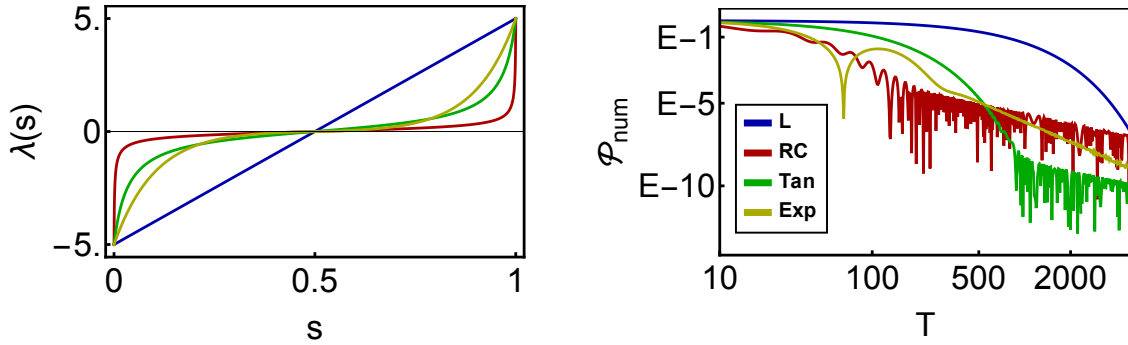


Figure 2.2. (Left) Graphs of NLS in Tab.(2.1). (Right) Log-Log plot of the transition probability as a function of protocol time T . Parameter values: $\lambda_0 = 10, a = 0.1, n = 5$.

Appropriately designed NLS are advantageous over the linear, decreasing the probability by several orders of magnitude Fig.(2.2) (Right). The general principle is to move fast in regions where the energy gap is large and slowly around the avoided crossing, where the gap is small. This can be explained by the Quantum Adiabatic Condition (QAC), see following section, Eq.(2.2.4). A simple condition like $|\lambda'(s)| \propto \Delta E$, leads to Exp in Tab.(2.1), [48]. The other two cases, Tan and RC are instances of Local Adiabatic Drivings (LAD), satisfying (some version of) the so called Local Adiabatic Condition [49, 50]. The RC, adapted to the LZS have been

studied extensively, both theoretically and experimentally [51–53]. There are other methods, e.g. Boundary Cancellation Method (BCM), requiring the derivatives of the Hamiltonian to vanish at the endpoints [53–55], but they are not part of our analysis.

2.2 Adiabatic Theorem

Firstly, we give a short summary of the history of the Adiabatic Theorem (AT) and its importance to contemporary fields. Following to that, we present the standard version of the AT that is found in physics textbooks [25, 56]. We close this section with a brief discussion of the Quantum Adiabatic Conditions (QAC). There is a huge literature on this topic, concerning its validity and generalization and the construction of nonlinear sweeps but a formal discussion is beyond our scope.

2.2.1 History

The Quantum Adiabatic Theorem, successor to the one by Ehrenfest in the old Quantum Theory [57], was stated in its modern form in 1928 by Born and Fock [7, 58, 59], only three years after the formulation of the Schrödinger equation. There are different versions but the qualitative statement is the following: A system prepared in an eigenstate, will approximately follow the instantaneous eigenstate, as long as the Hamiltonian varies sufficiently slowly. Different assumptions about the energy spectrum lead to different error bounds in the time evolution.

In its standard version, the spectrum is assumed to be discrete, non degenerate and without crossings, although in the original version of the theorem [7], crossings were allowed. Kato in 1950 in his influential paper [60], generalized the theorem to degenerate Hamiltonians and since then, it has been further generalized to continuous spectra [61], Hamiltonians without a gap condition [62] and open quantum systems [63]. There are many contemporary rederivations highlighting different aspects [64–66]. For a more mathematical exposition see [67, 68].

The theorem is of high importance in modern research since it has given birth to subjects like Adiabatic Quantum Computing [9, 69], Counterdiabatic driving [12–14] and the notion of geometric phases in quantum mechanics [8, 70, 71], to name a few. In adiabatic computing, a simple initial state is prepared and under the assumption of adiabatic evolution, it is driven to a desired more complicated state. For example, in Eq.(2.1.1) the initial ground state will adiabatically evolve to the antisymmetric superposition at the avoided crossing Eq.(2.1.6). Counterdiabatic

driving essentially is the reverse engineering of the adiabatic evolution with the introduction of external fields and the notion of a geometric phases arise when the system undergoes a cyclic evolution in the parameter space.

2.2.2 Derivation

Consider a non degenerate Hamiltonian with discrete spectrum, $H_0(t) |n(t)\rangle = E_n(t) |n(t)\rangle$. Since $\{|n\rangle\}$ is an ONB $\forall t$, the solution to the IVP $i\partial_t |\psi\rangle = H_0 |\psi\rangle$, $|\psi(0)\rangle = \sum_n a_n(0) |n(0)\rangle$, admits an expansion $|\psi(t)\rangle = \sum_m a_m(t) |m(t)\rangle$. From the Schrödinger equation⁴

$$i \sum_m \left(\dot{a}_m |m\rangle + a_m |\dot{m}\rangle \right) = \sum_m a_m E_m |m\rangle$$

Projecting onto $|n\rangle$ and using the orthonormality conditions $\langle n|m\rangle = \delta_{nm}$

$$\left[\dot{a}_n + (\langle n|\dot{n}\rangle + iE_n)a_n \right] = - \sum_{m \neq n} a_m \langle n|\dot{m}\rangle \quad (2.2.1)$$

Under the QAC, the r.h.s in Eq.(2.2.1) is ignored. The system uncouples and becomes integrable, $a_n(t) = e^{i(\theta_n(t) + \gamma_n(t))} a_n(0)$ and $|\psi\rangle \approx |\psi\rangle_{\text{ad}}$, with

$$|\psi(t)\rangle_{\text{ad}} \equiv \sum_n a_n(0) e^{i(\theta_n(t) + \gamma_n(t))} |n(t)\rangle \quad (2.2.2)$$

The phases θ_n, γ_n are the Dynamic and Geometric phases respectively defined as [25]

$$\theta_n(t) \equiv - \int_0^t dt' E_n(t'), \quad \gamma_n(t) \equiv i \int_0^t dt' \langle n(t') | \partial_t n(t') \rangle^5 \quad (2.2.3)$$

For a time-independent Hamiltonian, $|\dot{n}\rangle = 0 \Rightarrow \gamma_n(t) = 0, \theta_n(t) = E_n t$, Eq.(2.2.2) leads to the familiar expansion of $|\psi(t)\rangle = e^{-iH_0 t} |\psi(0)\rangle$ [25].

2.2.3 Quantum Adiabatic Conditions

The main question is what is the condition QAC that if satisfied $|\psi\rangle \approx |\psi\rangle_{\text{ad}}$ and whether it is necessary or sufficient. Assume that $t \in [0, \tau_{\text{ext}}]$. The physical argument is the following. The minimum spectral gap sets an internal time scale for the system⁶

$$\min_{n, m \in \mathbb{N}, t \in [0, \tau_{\text{ext}}]} |E_n - E_m| \sim 1/\tau_{\text{int}}$$

⁴We drop the time dependence from the notation

⁵Notice that since $\forall t, \langle n|n\rangle = 1 \Rightarrow \langle n|\dot{n}\rangle + \langle \dot{n}|n\rangle = 0 \Rightarrow \text{Re}(\langle n|\dot{n}\rangle) = 0 \Rightarrow \gamma_n(t) \in \mathbb{R}, \forall t$.

⁶We work in units $\hbar = 1$, $[E] = [T]^{-1}$.

Under sufficient regularity conditions, the brackets in the r.h.s of Eq.(2.2.1) are of order ⁷

$$\max_{n,m \in \mathbb{N}, t \in [0, \tau_{\text{ext}}]} |\langle n(t) | \dot{m}(t) \rangle| \sim 1/\tau_{\text{ext}}$$

Therefore, for the ratio

$$\text{QAC} \equiv \left| \frac{\langle n(t) | \dot{m}(t) \rangle}{E_n(t) - E_m(t)} \right| \leq \frac{\max |\langle n | \dot{m} \rangle|}{\min |E_n - E_m|} \sim \tau_{\text{int}}/\tau_{\text{ext}} \quad (2.2.4)$$

For sufficiently large τ_{ext} , $(\text{QAC}) \ll 1 \Rightarrow |\langle n | \partial_t m \rangle| \ll 1$, the r.h.s in Eq.(2.2.1) should be discarded, leading to $|\psi\rangle \approx |\psi\rangle_{\text{ad}}$ given by Eq.(2.2.2).

For a long time $(\text{QAC}) \ll 1$ was considered to be sufficient and necessarily condition for the approximation $|\psi\rangle \approx |\psi\rangle_{\text{ad}}$. In [72], for a TLS, they have showed that although QAC is satisfied, the solution to the Schrödinger equation deviates from the adiabatic evolution. Although initially there was a push back [73–75], the traditional (QAC) is not considered necessary nor sufficient criterion, for adiabatic evolution [76, 77], supported by experimental results [78].

On the other hand, for interpolating Hamiltonians $H_0(s) = H_0^{(0)}s + (1-s)H_0^{(1)}$, like the LZS, it is generally considered to be true and on the contrary to the previous discussion, too strict. Relaxing the so called global QAC to local, leads to the notion of LAD and the construction of the NLS in Tab.(2.1).

Specifically for Eq.(2.1.1), $\langle E_g | \dot{E}_e \rangle = \dot{\theta} = -\frac{a/2}{t^2+a^2}$, $|E_e - E_g| = 2\sqrt{t^2 + a^2}$ and $(\text{QAC}) = \frac{(a/4)}{(t^2+a^2)^{3/2}} \leq \frac{1}{4a}$ which shows that $(\text{QAC})(a) \rightarrow 0 \Rightarrow \mathcal{P}(a) \rightarrow 0$.

2.3 Counterdiabatic Driving

In the following section we will explain the concept of Counterdiabatic Driving, its history and motivation. Next, the main equations are derived, omitting most of the calculations, which can be found in the App.(C.2). Lastly, although it won't be directly relevant to our work, due to its importance, we briefly mention the variational approach and the perturbative series expansion.

⁷Assuming the total time evolution is of order τ_{ext} and the time-dependence of the eigenstates is reasonable, e.g not rapidly oscillating, then

$$|\langle n(t) | m'(t) \rangle|_{t \in [0, \tau_{\text{ext}}]} = \frac{1}{\tau_{\text{ext}}} |\langle n(s) | m'(s) \rangle|_{s \in [0, 1]} \leq \frac{1}{\tau_{\text{ext}}} \|n(s)\|_{s \in [0, 1]} \|m'(s)\|_{s \in [0, 1]} \leq M/\tau_{\text{ext}}$$

with $M > 0$ and upper bound. Thus $|\langle n | \dot{m} \rangle| \sim 1/\tau_{\text{ext}}$.

2.3.1 Introduction

Adiabatic evolution requires long integrations times which are hard to realize experimentally due to decoherence. Counterdiabatic driving is part of the methods collectively called Shortcuts to Adiabaticity. Typically, by introducing external fields and evolving non adiabatically, the adiabatic evolution of a given system is reproduced. Not restricted by adiabatic evolution, the target state can be reached in much faster time [10, 11].

At its core, the idea of CD driving is simple. Consider a time dependent Hamiltonian H and the corresponding time evolution matrix $\mathcal{U}$ that satisfies $i\partial_t\mathcal{U} = H\mathcal{U}$. Solving w.r.t $\mathcal{U}$, $\mathcal{U} = \mathcal{T}e^{-i\int^t H_0}$, is in general a hard problem, if not impossible. On the other hand, solving for H is trivial, $H = i(\partial_t\mathcal{U})\mathcal{U}^\dagger$. Now, given H_0 , the goal is to reverse engineer H , such that $\mathcal{U}$ exactly reproduces the adiabatic evolution of H_0 . H takes the form $H = H_0 + H_{\text{CD}}$, with H_{CD} a correction term which for the TLS can be expressed in closed form. For higher dimensional systems, H_{CD} becomes highly complicated and approximation schemes are employed [15, 16].

The seminal papers are independently by Demirplak and Rice [12, 13] and Berry [14]. For a pedagogical introduction to the topic see [79]. Shortly after, the geometric meaning of H_{CD} as the generator of adiabatic transport was realized [8, 80, 81], thus the name Adiabatic Gauge Potential (AGP). At the same time a variational approach was developed which in contrast to the initial formulation, only requires the knowledge of H_0 and not its spectral properties [16]. The AGP is now the solution to the minimization problem of a certain functional. Based on that, perturbative like expansions were developed [82, 83] that can produce accurate analytic approximations for low dimensional system. Those approaches still require the precise knowledge of the base system which is not feasible for high dimensional problems. Recently there are attempts for the development of a universal, system independent formalism [84, 85].

2.3.2 Main equations

We will mostly follow [14] and [15, 66]. Let H_0 finite dimensional, time dependent, with non degenerate spectrum $H_0 |n\rangle = E_n |n\rangle$. We consider the auxiliary Hamiltonian $H = i(\partial_t\mathcal{U})\mathcal{U}^\dagger$ for which we impose the constraints

$$\mathcal{U} |n_0\rangle = e^{i\varphi_n} |n\rangle \quad (2.3.1)$$

with $|n_0\rangle \equiv |n(0)\rangle$ ⁸. For a given choice of phases, Eq.(2.3.1) is the defining equation of $\mathcal{U}$, and consequently H , since a linear map is sufficiently described by its action on a basis. From the identity $\mathbb{1} = \sum_n |n_0\rangle \langle n_0|$ we get $\mathcal{U} = \sum_n \mathcal{U} |n_0\rangle \langle n_0| = \sum_n e^{i\varphi_n} |n\rangle \langle n_0|$ and

$$H = - \sum_n \partial_t \varphi_n |n\rangle \langle n| + H_{\text{CD}} \quad (2.3.2)$$

with H_{CD} defined as

$$H_{\text{CD}} \equiv i \sum_n |\partial_t n\rangle \langle n| \quad (2.3.3)$$

In order to simplify the notation we define two operators

$$P_n \equiv |n\rangle \langle n|, \quad Q_n \equiv |\partial_t n\rangle \langle n| \quad (2.3.4)$$

with $\sum_n P_n = \mathbb{1}$ and by differentiation, $\sum_n Q_n + Q_n^\dagger = 0 \Rightarrow \sum_n Q_n = -\sum_n Q_n^\dagger$. The last equations shows that $H_{\text{CD}}^\dagger = H_{\text{CD}}$ is well defined. W.l.o.g we may assume that H_{CD} is traceless⁹. Let

$$D \equiv \sum_n \partial_t E_n |n\rangle \langle n| \quad (2.3.5)$$

Differentiating $H_0 = \sum_n E_n |n\rangle \langle n|$, from Eq.(2.3.3,2.3.5) we get

$$\partial_t H_0 = D + \frac{1}{i} [H_{\text{CD}}, H_0] \quad (2.3.6)$$

The operator D is usually hard to compute since it explicitly requires knowledge of the spectral properties of H_0 . D, H_0 share the same eigenstates and thus $[D, H_0] = 0$. The latter is used to eliminate D in Eq.(2.3.6)

$$[H_0, \partial_t H_0 + i[H_{\text{CD}}, H_0]] = 0 \quad (2.3.7)$$

Eq.(2.3.7) and Eq.(2.3.6) are equivalent [81] but as it is evident from Eq.(2.3.7), the spectral quantities $|n\rangle, E_n$ are only indirectly present via H_0 .

Thus far the phases in Eq.(2.3.1,2.3.2) are arbitrary. By choosing $\varphi_n = \theta_n + \gamma_n$ as in AT, Eq.(2.2.2,2.2.3), $\partial_t \varphi_n = -E_n + i \langle n | \partial_t n \rangle$, the Hamiltonian in Eq.(??) simplifies to $H = H_0 + H_{\text{CD}}$ with

$$H_{\text{CD}} = i \sum_{n \neq m} \frac{P_n \partial_t H_0 P_m}{E_m - E_n} \quad (2.3.8)$$

and P_n given by Eq.(2.3.4). With respect to the inner product on operator space, $\langle A, B \rangle = \text{tr}(A^\dagger B)$ [86], H_{CD} satisfies three orthogonality conditions [66]

$$H_{\text{CD}} \perp \mathbb{1}, \quad H_{\text{CD}} \perp H_0, \quad H_{\text{CD}} \perp \partial_t H_0 \quad (2.3.9)$$

⁸Dropping the explicit time dependence in the notation.

⁹ $\text{tr } H_{\text{CD}} = i \sum_n \langle n | \partial_t n \rangle$ can be set to zero by the redefinition of phases $|n\rangle \rightarrow e^{-\int^t \langle n | \partial_t n \rangle} |n\rangle$

For a TLS, the possible Hamiltonians are spanned $\text{span}_{\mathbb{R}}\{\mathbb{1}, \sigma\}$. Eq.(2.3.9) are restrictive enough to fix the direction of H_{CD} . For the LSZ Eq.(2.1.1), $H_{\text{CD}} \parallel \sigma_2$ thus $H_{\text{CD}} = f_{\text{CD}}\sigma_2$ with f_{CD} a scalar real function since the H_0 in Eq.(2.1.1) is also real.

There are multiple ways to find f_{CD} [12, 14]. For Eq.(2.1.1), we can directly calculate f_{CD} via Eq.(2.3.6, 2.3.7), App.(C.2)

$$f_{\text{CD}}(t; a) = \frac{1}{2} \frac{a}{t^2 + a^2} \quad (2.3.10)$$

For Eq.(2.1.13), f_{CD} straightforwardly generalizes to $f_{\text{CD}} = \frac{\partial_t \lambda}{2} \frac{a}{\lambda^2 + a^2}$. Notice that in Eq.(2.3.10), f_{CD} vanished at $|t| \rightarrow \infty$ and therefore H and H_0 have the same asymptotic eigenstates.

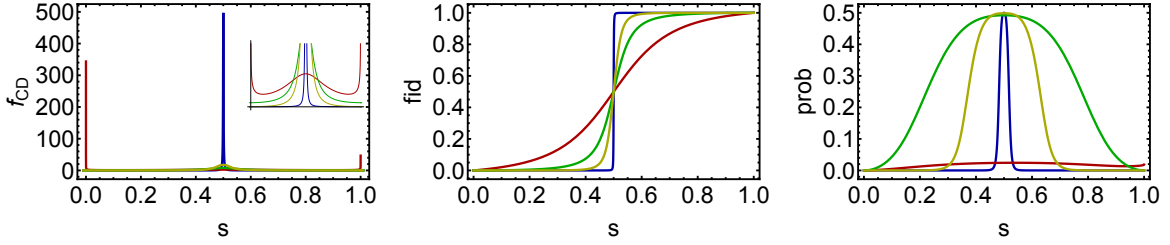


Figure 2.3. The different nonlinear sweep correspond to Tab.(2.1) and colors as in Fig.(2.2). (Left) profile of f_{CD} . Characteristic Lorentzian curve for the linear sweep. (Middle) Fidelity defined $\text{fid}(t) \equiv |\langle + | \psi(t) \rangle|^2$ with i.c $|\psi(0)\rangle = |-\rangle$. For better visualization, we graph the fidelity instead of the probability, which is zero for all times. H drives the ground state $|E_g(0)\rangle = |-\rangle$ transitionlessly to the final state $|E_g(1)\rangle = |+\rangle$. (Right) Transition probability between the eigenstates of the full Hamiltonian $H = H_0 + H_{\text{CD}}$. The evolution of H is not adiabatic. Parameters: $\lambda_0 = 10, a = 0.01, T = 5$ and $n = 5$.

2.3.3 Variational Approach

Eq.(2.3.7) can be recast into a functional minimization form as follows. Isolating D and replacing H_0 with a variable A

$$D(A) = \partial_t H_0 + i[A, H_0] \quad (2.3.11)$$

The idea is to construct a functional $S(A)$ that has H_0 as its minimum. The important observation is that in the basis $\{|n\rangle\}$, the diagonal element of $D(A)$ are independent of A , $\langle n | D | n \rangle = \langle n | \partial_t E_n | n \rangle$. Next, consider the norm induced by the inner product related to Eq.(2.3.9), $\|D\| = \sqrt{\text{tr}(D^\dagger D)}$. Let $\langle n | D | m \rangle \equiv D_{nm}$. From the trace being

basis independent we have

$$\|D\|^2 = \sum_{nm} |D_{nm}|^2 = \sum_n |D_{nn}|^2 + \sum_{n \neq m} |D_{nm}|^2 \geq \sum_n |D_{nn}|^2 = \|D(H_0)\|^2$$

since for H_0 , $D(H_0)$ is diagonal. Thus, H_0 can be defined as the minimum of the functional

$$S(A) \equiv \|D(A)\|^2 \quad (2.3.12)$$

An approximation solution to Eq.(2.3.12) can be obtained by [82]

$$A^{(\ell)}(c_1, \dots, c_\ell) \equiv i \sum_{k=1}^{\ell} c_k \underbrace{[H_0, [H_0, \dots [H_0, \partial_t H_0]]]}_{2k-1} \quad (2.3.13)$$

$A^\ell \equiv A^\ell(c_1, \dots, c_\ell) : \mathbb{R}^\ell \rightarrow \mathbb{R}$. Via Eq.(2.3.11) and Eq.(2.3.12), $S(c_1, \dots, c_\ell)$ becomes a function of $\{c_k\}_{k=1, \dots, \ell}$ and the critical values are given by the condition $\nabla_{\mathbf{c}} S = 0$.[!] In the limit $\ell \rightarrow \infty$, the exact AGP is recovered [82]. For Eq.(2.1.1), the first order expansion, $\ell = 1$, gives the full AGP, Eq.(2.3.10), App.(C.2).

Chapter 3

Random Gap

3.1 Defining the problem

In the following section, we define the Random-Gap LZ problem with generalized CD potential, along with the main quantities and their properties. For the illustration of the definitions, we consider the simplest case scenario before the introduction of the general system GLZS, in the second section of this chapter. In the end of this section, we give a simple toy model example.

3.1.1 Introduction

For fixed gap parameter a , combining Eq.(2.1.1) with Eq.(2.3.10), the full Hamiltonian that generates transitionless driving for the LZS is

$$H(t; a) = H_0(t; a) + H_{\text{CD}}(t; a) = -t\sigma_3 + a\sigma_1 + \frac{1}{2} \frac{a}{a^2 + t^2} \sigma_2 \quad (3.1.1)$$

In our case the parameter a , with $2a$ being the minimum gap, is promoted to a random variable $a \sim f_{\text{PDF}}$. The problem is to find the appropriate correction term H_1 such that the full Hamiltonian $H = H_0 + H_1$ minimizes the average transition probability $\langle \mathcal{P} \rangle$. With one external field, is not possible to drive transitionlessly all the systems in the ensemble and for particular realizations, the evolution may deviate significantly from the adiabatic path. We are interested in the minimization of the final transition probability Fig.(3.1).

The default option, is to choose for H_1 the same functional form with the original H_{CD} , $H_{1,\text{CD}}(t; b) = \frac{b}{b^2 t^2 + 1} \sigma_2$ ¹ The full Hamiltonian $H(t; a, b) = H_0(t; a) + H_{1,\text{CD}}(t; b)$

¹The use of $1/b$ instead of b is conventional. We will conflate the notation H_{CD} with $H_{1,\text{CD}}$ and it will be understood from context whether we are referring to Eq.(3.1.1) or to Eq.(3.1.2).

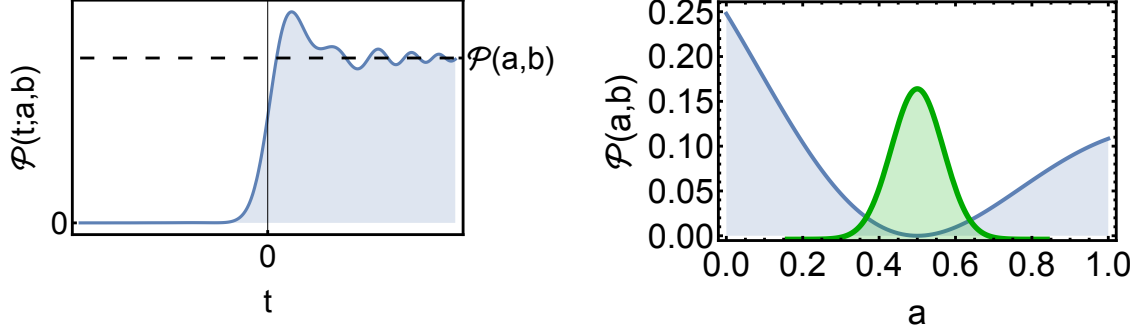


Figure 3.1. (Left) For unrelated parameter a, b , the time dependence of $\mathcal{P}$ in Eq.(3.1.2) is similar to the LZS, Fig.(2.1) (Middle). (Right) Final $\mathcal{P}(a, b)$ as a function of a for $b = 2$. Green curve is a gaussian distribution centered at $\mu = 0.5$ (not in scale). The average probability corresponds to the shaded area, amplified by the gaussian, Eq.(3.1.3).

is

$$H(t; a, b) = -t\sigma_3 + a\sigma_1 + \frac{1}{2} \frac{b}{b^2 t^2 + 1} \sigma_2 \quad (3.1.2)$$

and generates probability $\mathcal{P}(a, b)$. With $\mathcal{P}$, we are referring to the final, or in the case of Eq.(2.1.1), the asymptotic transition probability, Fig.(3.1), in the same sense that the LZ formula arises Eq.(2.1.10).

Given the PDF $a \sim f_{\text{PDF}}$, we define the quantities $b^*, \mathcal{P}^*$ as the minimum, and the minimum value of $\langle \mathcal{P}(a, b) \rangle$

$$\langle \mathcal{P}(a, b) \rangle = \int_{\mathbb{R}} da \mathcal{P}(a, b) f_{\text{PDF}}(a) \quad (3.1.3)$$

$$b^* \equiv \min_{b>0} \langle \mathcal{P}(a, b) \rangle, \quad \mathcal{P}^* \equiv \langle \mathcal{P}(a, b^*) \rangle \quad (3.1.4)$$

We will assume that the PDF is sufficiently regular and unimodal (single peaked). Our analysis won't depend on the particular shape of PDF and for simplicity we will choose the Normal distribution $a \sim \mathcal{N}(\mu, \sigma)$ in the numerical part. Every PDF is characterized uniquely by its cumulants. For the Normal distribution, only the first two are non zero, which makes our analysis simpler. Note that there is no straightforward way to systematically account for higher cumulants. It is a known result in probability theory that only the Normal distribution has a polynomial generating function (of order 2), meaning for any other PDF, there are infinite number of non vanishing cumulants [87].

3.1.2 General properties

We will assume that $b^*, \mathcal{P}^*$ in Eq.(3.1.4) are well defined. This is qualitatively evident. As a probability, $\mathcal{P}$ is bounded, $\mathcal{P}(a, b) \in [0, 1], \forall a, b$. Moreover, for large

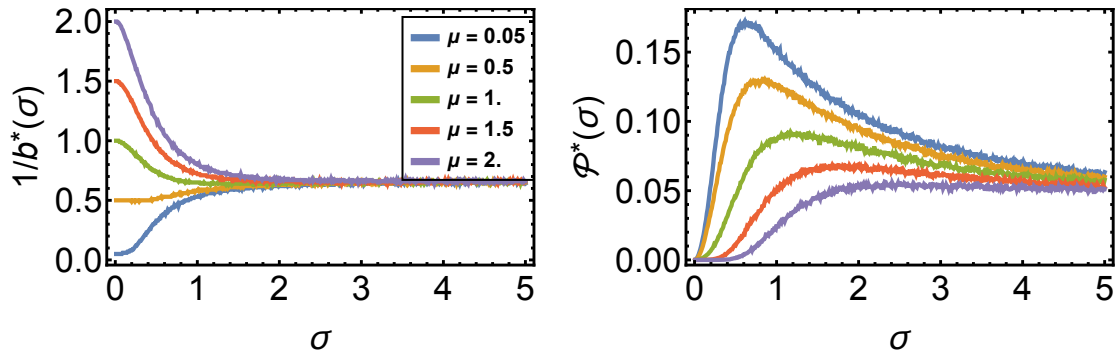


Figure 3.2. b^* and $\mathcal{P}^*$ Eq.(3.1.4) for Eq.(3.1.2) as a function of σ , for different values of μ . The two limit $b^* \xrightarrow{\sigma \rightarrow 0} b_0(\mu) = 1/\mu$ and $\mathcal{P}^* \xrightarrow{\sigma \rightarrow \infty} 0$ are verified. The limit on the right appears to be finite and moreover numerically coinciding with the value obtained from the uniform distribution. This is an artifact of the simulation. On a finite interval $a \in [-L, L]$, in the limit $\sigma \rightarrow \infty$, the truncated Normal distribution, uniformly converges to the uniform distribution $f_{\text{unif}}(a) \equiv \frac{1}{2L} \forall a \in [-L, L]$. The even symmetry of b^* is indirectly verifiable due to the faster convergence on the left.

a , the last term in Eq.(3.1.2) can be neglected, leading to $\mathcal{P}(a, b) \xrightarrow{a \rightarrow \pm\infty} 0$, thus the integral in $\langle \mathcal{P} \rangle$, Eq.(3.1.3), is well defined $\forall b$. The existence of b^* , Eq.(3.1.4), depends on the model. For a fixed value of a , $\mathcal{P}(a, b)$ has a minimum along the curve $b_0(a) = 1/a$ with $\mathcal{P}(a, b_0(a)) = 0$. The minimum corresponds to CD driving, compare Eq.(3.1.2) with Eq.(3.1.1). Therefore, at least for small σ we expect b^* to exist and also $b^* \xrightarrow{\sigma \rightarrow 0} b_0(\mu) = 1/\mu$.

Expanding $b^*(\mu, \sigma)$ in powers of σ

$$b^*(\mu, \sigma) = \sum_{k=0}^{\infty} b_k(\mu) \sigma^k \quad (3.1.5)$$

$b^*(\sigma)$ is the minimum $F(b, \sigma) \equiv \int_{\mathbb{R}} \mathcal{P}(a, b) e^{-(a-\mu)^2/2\sigma^2} da$, dropping the irrelevant to the minimization prefactor $1/\sqrt{2\pi\sigma^2}$, which satisfies $F(b, -\sigma) = F(b, \sigma)$. From the uniqueness of the minimum $b^*(\sigma) = b^*(-\sigma)$.

For large σ , the global structure of b^* and $\mathcal{P}^*$ is dominated by the Normal PDF and is quite generic. Differentiating Eq.(3.1.3) w.r.t σ

$$\partial_{\sigma} \langle \mathcal{P} \rangle = -\frac{1}{\sigma} \langle \mathcal{P} \rangle + \frac{1}{\sigma^3} \langle (a - \mu)^2 \mathcal{P} \rangle$$

$\mathcal{P} \in [0, 1]$ implies $\langle \mathcal{P} \rangle, \langle (a - \mu)^2 \mathcal{P} \rangle > 0$. For small σ , the second term dominates and $\partial_{\sigma} \langle \mathcal{P} \rangle > 0$. For large σ , the first term dominates and $\partial_{\sigma} \langle \mathcal{P} \rangle < 0$. Thus we expect that $\mathcal{P}^*$ is increasing for small sigma until it reaches its peak and then decreases to

zero. Assuming the limit $b_\infty(\mu) \equiv \lim_{\sigma \rightarrow \infty} b^*(\mu, \sigma)$ exists, the asymptotic behavior is

$$\mathcal{P}^* \sim \frac{1}{\sqrt{2\pi\sigma^2}} \int_{\mathbb{R}} da (1 + \dots) \mathcal{P}(a, b_\infty(\mu) + \dots) \propto C/\sigma \rightarrow 0$$

Consequence of $b^*(-\sigma) = b^*(\sigma)$ is that in the asymptotic expansion of b^* the $1/\sigma$ term is missing, implying faster converges for b^* than $\mathcal{P}^*$ Fig.(3.2).

3.1.3 Toy model

The following example doesn't serve as an approximation or parameter fitting model for the actual problem Eq.(3.1.2). It's mere purpose is to make the definition of $b^*, \mathcal{P}^*$ more concrete Eq.(3.1.4) and further illustrate the generic behavior of Fig.(3.2). It has the advantage that all the calculations can be done analytically.

Let

$$\mathcal{P}(a, b) = e^{-\pi a^2} (ab - 1)^2 \quad (3.1.6)$$

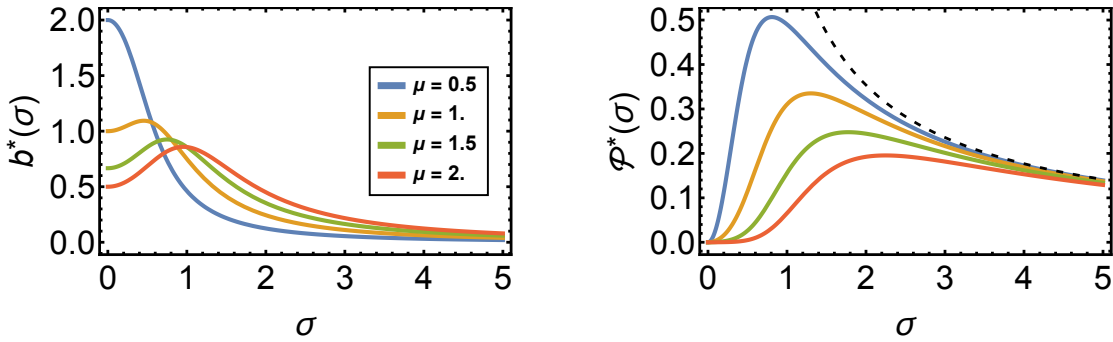


Figure 3.3. Graph of $b^*, \mathcal{P}^*$ for Eq.(3.1.7,3.1.8). Compare with the actual model Fig.(3.2). From the limit $b^*(\mu, 0) = 1/\mu$ we can read the values of μ .

In Eq.(3.1.3), $\langle \mathcal{P} \rangle(b; \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{\mathbb{R}} da (ab - 1)^2 e^{-a^2} e^{-\frac{(a-\mu)^2}{2\sigma^2}}$, the exponential e^{-a^2} can be absorbed in the measure by completing the square

$$a^2 + \frac{(a - \mu)^2}{2\sigma^2} = \frac{1}{2\left(\frac{\sigma}{\sqrt{1+2\sigma^2}}\right)^2} \left(a - \frac{\mu}{1+2\sigma^2}\right)^2 + \frac{\mu^2}{1+2\sigma^2}$$

with the new mean and variance being $\mu' = \frac{\mu}{1+2\sigma^2}$, $\sigma'^2 = \frac{\sigma^2}{1+2\sigma^2}$. The expectation $\langle \cdot \rangle$ can be expressed in terms of $\langle \cdot \rangle'$

$$\langle \mathcal{P} \rangle(b; \mu, \sigma) = \frac{e^{-\frac{\mu^2}{1+2\sigma^2}}}{\sqrt{1+2\sigma^2}} (b^2 I_2 - 2b I_1 + I_0)$$

with $I_0 = \langle 1 \rangle' = 1$, $I_1 = \langle a \rangle' = \mu'$, $I_2 = \langle a^2 \rangle' = \mu'^2 + \sigma'^2$. $\langle \mathcal{P} \rangle$ is quadratic in b and the critical quantities are easily found to be

$$b^* = \frac{\mu'}{\mu'^2 + \sigma'^2}, \quad \mathcal{P}^* = \frac{e^{-\frac{\mu^2}{1+2\sigma^2}}}{\sqrt{1+2\sigma^2}} \frac{\sigma'^2}{\mu'^2 + \sigma'^2}$$

Finally, converting back to μ, σ

$$b^*(\mu, \sigma) = \mu \frac{1 + 2\sigma^2}{\mu^2 + \sigma^2(1 + 2\sigma^2)} \quad (3.1.7)$$

$$\mathcal{P}^*(\mu, \sigma) = e^{-\frac{\mu^2}{1+2\sigma^2}} \frac{\sigma^2 \sqrt{1+2\sigma^2}}{\mu^2 + \sigma^2(1 + 2\sigma^2)} \quad (3.1.8)$$

Asymptotic behavior $\sigma \rightarrow \infty$

$$b^*(\mu, \sigma) \sim \frac{\mu}{\sigma^2} + \mathcal{O}(1/\sigma^4), \quad \mathcal{P}^*(\mu, \sigma) \sim \frac{1}{\sigma\sqrt{2}} + \mathcal{O}(1/\sigma^2) \quad (3.1.9)$$

3.2 Generalized System

As stated originally, the problem is too broad. We will restrict our attention to a special type of H_1 correction term, based on H_{CD} and Eq.(3.1.2). This brings us to the definition of the generalized system. The range of the parameter distribution is refined. In subsequent section we note the similarities and differences to Eq.(3.1.2). Finally, we consider the possibility of casting the probability minimization and the optimization of H_1 , as the area minimization of certain boundary curves.

3.2.1 Definition

Given the distribution $a \sim f_{\text{PDF}}$, the problem of finding the optimal correction term without extra constraints, is hard. Even for a TLS, the space of time-dependent Hamiltonians is spanned by $\text{span}_{\mathbb{R}}\{\mathbb{1}, \sigma_i\}$ and we are required to specify four real functions of time. Thus we will restrict our searching span and make an general ansatz based on H_{CD} and Eq.(3.1.1). For H_1 we will assume the form $H_1 = f_{\text{D}}\sigma_{\varphi}$ with $\sigma_{\varphi} \equiv \cos \varphi \sigma_1 + \sin \varphi \sigma_2$, relaxing the orthogonality condition $H_{\text{CD}} \perp H_0$ Eq.(2.3.9)². The profile function f_{D} will be modeled after f_{CD} in Eq.(2.3.10), being is a single peak function of time, vanishing at $|t| \rightarrow \infty$ and parametrized by a single parameter b which is now unrelated to a , as in Eq.(3.1.2).

We define the generalized Hamiltonian

$$H(t; a, b) \equiv -t\sigma_3 + a\sigma_1 + f_{\text{D}}(t; b)\sigma_{\varphi}, \quad \sigma_{\varphi} \equiv \sigma_1 \cos \varphi + \sigma_2 \sin \varphi \quad (3.2.1)$$

²A component parallel to σ_3 can be factored out, see prior to Eq.(2.1.1)

and the corresponding differential equations

$$i\partial_t |\psi\rangle = \left[-t\sigma_3 + a\sigma_1 + f_D(t;b)\sigma_\varphi \right] |\psi\rangle \quad (3.2.2)$$

There are two free parameters, the angle $\varphi \in [0, \frac{\pi}{2}]$ and the function $f_D(t;b)$ satisfying the properties listed in Tab.(3.1). These properties are satisfied by $f_{CD}(t;1/b)$ in Eq.(2.3.10). We present them as sufficient requirements for the construction. The choice of $1/b$ instead of b in f_D is conventional³.

Properties	
Dirac Seq.	$f_D(t;b) \xrightarrow{b \rightarrow \infty} \frac{\pi}{2} \delta(t)$
Peak	$f_D(0;b) = \frac{b}{2}$
Area	$\int_{\mathbb{R}} dt f_D(t;b) = \frac{\pi}{2}$
Even in time	$f_D(-t;b) = f_D(t;b)$
Odd in parameter	$f_D(t;-b) = -f_D(t;b)$
Asymptotic behavior	$f(t;b) \xrightarrow{t \rightarrow \pm\infty} 0$

Table 3.1. Defining properties of $f_D(t;b)$ in Eq.(3.2.1) and Eq.(3.2.2). $\delta(t)$ is the Dirac-delta function, centered at $t = 0$.

	$f_D(t;b)$
L	$\frac{b/2}{b^2 t^2 + 1}$
g	$\frac{b}{2} e^{-b^2 t^2 / \pi}$
s	$\frac{1}{2} \frac{\sin bt}{t}$
r	$\frac{b}{2} \mathbb{1}(t < \frac{\pi}{2b})$
t	$\frac{1}{2} \mathbb{1}(t < \frac{\pi}{b}) (b - \frac{ t }{\pi} b^2)$

Table 3.2. $b > 0$. $\mathbf{1}(A) \equiv \mathbf{1}_A$ denotes the indicator function. Example of functions satisfying the required properties in Tab.(3.1). For $b < 0$, $f_D(t;-b) = -f_D(t;b)$ and for $b = 0$, $f_D(t;0) = 0$, $\forall t$.

In Tab.(3.2) we have listed some elementary examples and in Fig.(3.4) their graphs. We do not aim to a systematic study of the whole class $\{f_D\}$. Two elements the list are special. The Lorentzian L, originating from H_{CD} Eq.(3.1.2), being the one after which the others are modeled and the rectangular r, for which many

³We could potentially relax some of them, e.g fixing the area to some other value, or add additional constraints, e.g $f_D(t;b) > 0$.

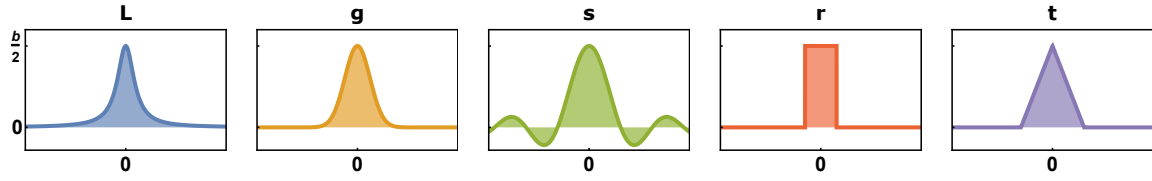


Figure 3.4. Graphs of $f_D(t; b)$, Tab.(3.2) as a function of time. At $t = 0$, $f_D(t; b) = b/2$ and the area under the graph, shaded region, is equal to $\pi/2$.

calculation can be done analytically and can also serve as a first order approximation to the other cases. The other choices are arbitrary. They are simple and provide enough variety for our study.

Due to the first property Tab.(3.1), $f_D(t; b)$ is a Dirac-sequence, in the parameter b . For a particular choice of f_D , the area and peak conditions Tab.(3.1) fix the exact functional form, e.g for the rectangular, the peak-area conditions fix the width and height of the pulse as function of b .

3.2.2 Refining the problem

As in Eq.(3.1.2), for a specific choice of φ and f_D the Hamiltonian in Eq.(3.2.1) generates transition probability $\mathcal{P}(a, b)$ which is then averaged over $a \sim \mathcal{N}(\mu, \sigma)$. As a function of the remaining parameter, $\langle \mathcal{P} \rangle(b; \mu, \sigma)$, has a minimum at b^* with minimum value $\mathcal{P}^*$, analogously to Eq.(3.1.4).

Although the large σ limit is theoretically viable, is it unphysical. Moreover, as discussed in previous section, the global behavior of $\mathcal{P}^*$ is dominated by the Normal distribution, having the generic behavior of Fig.(3.2), Fig.(3.3).

In the following sections we will primarily consider $a \sim \mathcal{N}(\mu, \sigma)$ with positive support, $a > 0$. This restricts $s \in [0, \sigma_{\max}]$ with $\sigma_{\max} \approx \mu/5$. Moreover, for μ the interesting limit is $\mu \rightarrow 0$ which numerically translates to $0 < \mu \lesssim 2$, since for large a , $\mathcal{P}(a, b) \rightarrow 0$ regardless of b . This can be traced back the LZ formula $\mathcal{P}(a) = e^{-\pi a^2}$. In combination with $\sigma \leq \mu/5$ and the symmetry $b^*(-\sigma) = b^*(\sigma)$, which means the first correction in the expansion Eq.(3.1.5) vanishes, we will (usually) make the identification $b^* = b_0$.

Additional justification is the following. For any choice of f_D, φ , $H_1 = f_D \sigma_\varphi$ should be compared against the default option $H_{CD} = f_D^L \sigma_2$ which is known to be robust under errors in the parameters. Thus higher order terms in the expansion Eq.(3.1.5) should not be in favor of H_{CD} .

3.2.3 Characteristic Curve

Given $H_1 = f_D \sigma_\varphi$, essential to our problem is the existence of $b_0(a)$, satisfying $\mathcal{P}(a, b_0(a)) = 0$ ⁴. We will call $b_0(a)$ the characteristic curve (CC). CC depends both on f_D and φ .

For $H_{CD} = f_D^L \sigma_2$, the CC, Fig.(3.5) (left), $b_0(a) = 1/a$, has a very precise origin: it corresponds to CD driving for the LZS, Eq.(3.1.2). Either by modifying $f_D \neq f_D^L$ of $\varphi \neq \frac{\pi}{2}$ in Eq.(3.2.1) destroys this property. Nevertheless, numerically we observe that for the general construction in Eq.(3.2.1), CC always exists. Typically, in the limit $a \rightarrow 0$, behaves similarly to $b_0 = 1/a$ and has more complicated structure in $a \rightarrow \infty$, which numerically translates to $a \gtrsim 2$. For certain choices of f_D like the rectangular Tab.(3.2), $b_0(a)$ can even become multivalued. This irregular behavior indicates there is no simple transformation between the general H_1 and $H_{CD} = f_D^L \sigma_2$ and the origin of $b_0(a)$ is different.

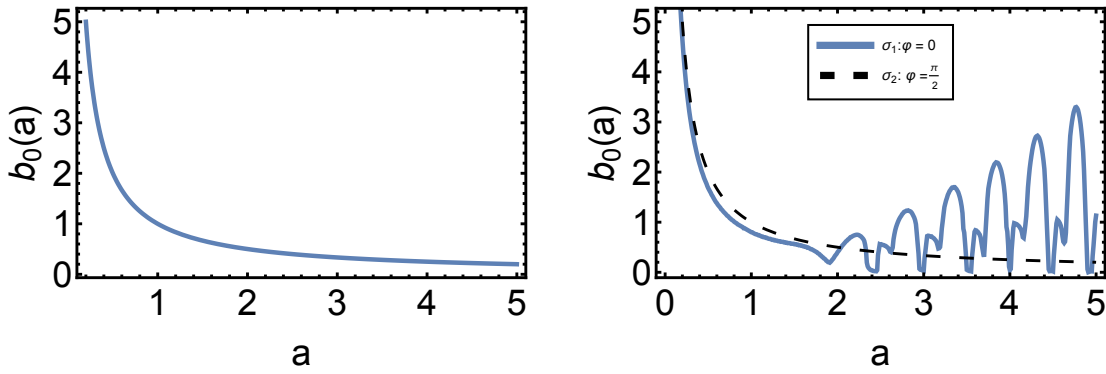


Figure 3.5. Characteristic curves with Lorentzian prefactor L. (Left) $\varphi = \frac{\pi}{2}$, $b_0(a) = 1/a$ corresponds to CD driving, Eq.(3.1.2),3.1.1. (Right) $\varphi = 0$. The curve is obtained numerically. For small a , the behavior is analogous to the graph on the left. For large a , $b_0(a)$ exhibits more complicated oscillatory behavior.

Another major difference is the behavior at finite times. $b_0(a)$ is defined as the root of the final probability $\mathcal{P}(a, b)$, without any reference to intermediate times. Only for H_{CD} , the probability is identically zero $\forall t$. For the other cases, typically there is a peak around $t = 0$, or multiple peaks, after which the probability decays to zero without oscillations. Interestingly, for $b = b_0(a)$, $\mathcal{P}(a, b_0(a); t)$ is symmetric in time, Fig.(3.6).

Other variation of the f_{CD} pulse, like $f'(t; b) = \lambda \frac{b/2}{b^2 t^2 + 1}$, $\lambda \in \mathbb{R}^*$ and $f''(t; \eta) = \eta \frac{a/2}{a^2 + t^2}$ can reliably produce roots for $\mathcal{P}(a, b)$ with the latter having an infinite number and even more complicated peak structure, Fig.(3.7). f' satisfies the same prop-

⁴Technically, a minimum with a value very close to zero could also work.

erties with f_D but violates the area condition, Tab.(3.1), and f'' is related to f_D in the following manner. Let $b = \frac{1}{\eta a}$, then $f_D = \eta \frac{a/2}{\eta^2 a^2 + t^2} \approx \eta \frac{a/2}{a^2 + t^2}$, for $\eta \approx 1$. For $\eta = 1$, we recover the pulse shape of H_{CD} and thus $\mathcal{P} = 0, \forall t$. Unexpectedly, for $\eta > 1$ there is an infinite number of extra roots. In [88], in the adiabatic limit via DDP formalism, they have obtained $\mathcal{P} \sim \cos^2 \frac{\eta\pi}{2} e^{-2\eta/3} e^{-\pi a^2}$, which validates the existence of the roots $\forall a, \eta$.

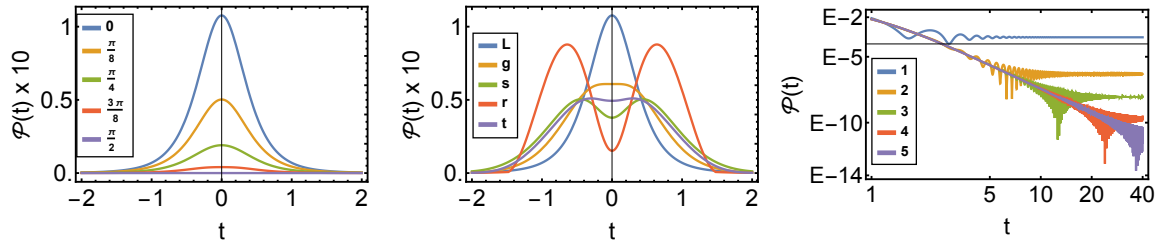


Figure 3.6. Time dependence of $\mathcal{P}(t; a, b_0(a))$. (Left) $a = 0.5$, L for different values of φ . (Middle) $a = 0.5$, $\varphi = 0$ and different prefactors Tab.(3.2). (Right) $a = 0.5$, L , $\varphi = 0$ and decimal increasing accuracy of $b_0(a)$ in Log-Log plot. By increasing the accuracy, the oscillations subside.

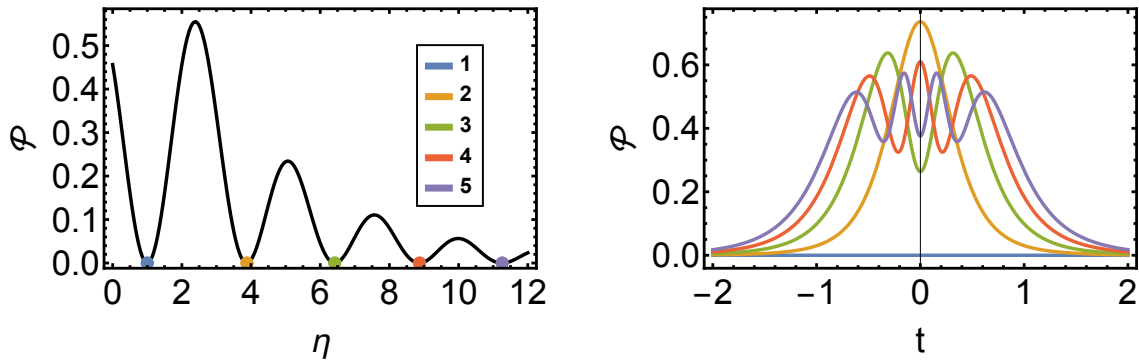


Figure 3.7. $\mathcal{P}$ as a function of η for $a = 0.5$, generated by $H_1 = \eta \frac{a/2}{a^2 t^2 + 1} \sigma_2$. The first root corresponds to CD driving, $\eta = 1$ and $\mathcal{P}$ is zero for all intermediate times. For the secondary, roots, we get a weird peak structure. The number of peak in the time domain increases by one for each subsequent root.

3.2.4 Boundary curves

The function $\mathcal{P}(a, b)$ in general is not know, except from the rectangular case r , Tab.(3.2). For the general problem, we only have information about the boundary cases $a = 0$, $b = 0$ and $b \rightarrow \pm\infty$. For $b = 0$, $\mathcal{P}(a, 0) = e^{-\pi a^2}$, $\forall f_D, \varphi$. For $b = 0$, the angle can be factored out and thus $\mathcal{P}(0, b)$ only depends on the choice of φ . Again,

the problem can only be solved exactly only for r , but partial information are available for the other cases via perturbation theory and other approximate methods. Interesting is the limit $b \rightarrow \pm\infty$. By definition all f_D 's satisfies $f_D \xrightarrow{b \rightarrow \infty} \frac{\pi}{2}\delta(t)$ and thus $\mathcal{P}(a, \infty)$ only depends on φ . The solution to this problem reduces to the solution of LZS, and the analytic expression for $\mathcal{P}(a, \pm\infty; \varphi)$ can be found. For more details see Sec.(?) and App.(B).

The two free parameters f_D, φ of the generalized system Eq.(3.2.2), control the two boundary curves $a = 0$ and $b \rightarrow \infty$ respectively, independently of one another, Fig.(3.8). Since we have control over the boundary curves, it is interesting to examine their effect on the function $\mathcal{P}(a, b)$ globally, and particularly around the minimum, Fig.(3.8).

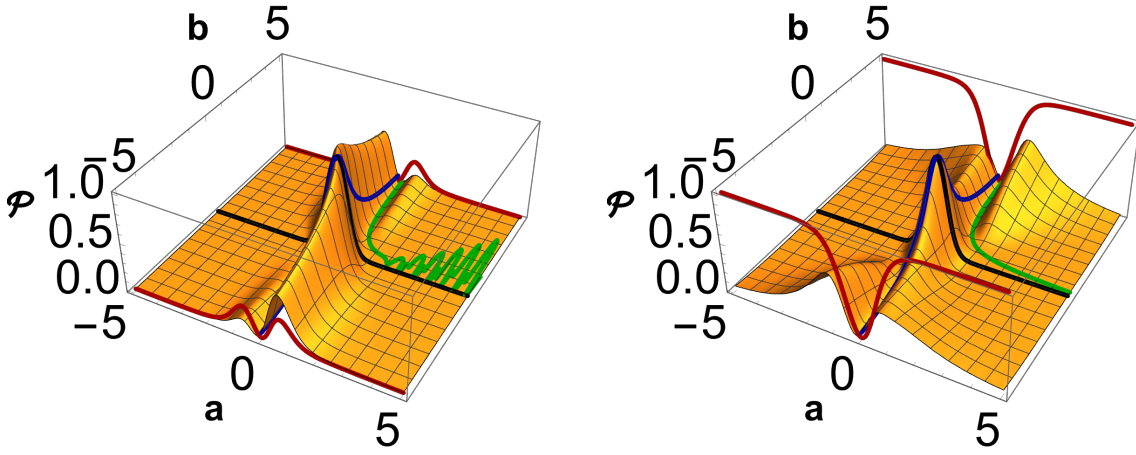


Figure 3.8. Plot of $\mathcal{P}(a, b)$ for Eq.(3.1.2) (right) and σ_2 replaced by σ_1 (left). The graphs have the symmetry $\mathcal{P}(a, -b) = \mathcal{P}(-a, b)$. For $b = 0$, $\mathcal{P}(a, 0) = e^{-\pi a^2}$, black curve. Green curve corresponds to the minimum $b_0(a)$ satisfying $\mathcal{P}(a, b_0(a)) = 0$. For σ_2 , $b_0(a) = 1/a$ corresponds to CD driving Eq.(3.1.2). For σ_1 , the curve exhibits more complicated structure. The blue curve corresponds to $a = 0$ which is the same in the two cases. The red curves correspond to $b \rightarrow \pm\infty$. Notice the the shape of the boundary curve affects to the area around the minimum, green curve. Blue, green and red curves intersect at infinity.

Chapter 4

Analytic Results

We collect all the analytic results related to the two boundary curves, the blue curve for vanishing gap $a \rightarrow 0$ and red curve for infinite control $b \rightarrow \infty$, Fig.(3.8). The two problems were initially motivated by the random gap problem and the minimization of the transition probability. The analytic findings are complementary to the numerical results, giving a possible interpretation for the latter. On the other hand, the two problems stand on their own as theoretical questions. We enumerate the main steps and key results while laborious calculations are reserved for the App.(B).

For $a = 0$, the angle parameter can be factored out, leaving only $f_D(t; b)$. The main figure is Fig.(4.1). In the limit $b \rightarrow 0$ the behavior is similar to LZS whereas in the other limit $b \rightarrow \infty$. The change in behavior from small to large couplings can be qualitatively understood via the gap structure. The rectangular case r , reduces to the LZS. Via Eq.(A.1.2,A.1.3), the analytic solution is found, including the relevant exponent. Lastly, we discuss the generalization to $a \neq 0$ and the connection to arbitrary prefactor f_D .

For $b \rightarrow \infty$, $f_D \rightarrow \frac{\pi}{2}\delta(t)$, Eq.(3.2.2) reduces to the LZS with Dirac delta function centered at $t = 0$. As is typically the case, the treatment of the Hamiltonian $H_0 + \lambda\delta(t)\sigma$ comes down to the unperturbed problem of H_0 . Again, via Eq.(A.1.2,A.1.3) we have found an analytic expression of the transition probability as a function of the coupling a and the angle parameter φ .

4.1 Vanishing gap ($a \rightarrow 0$)

For $a = 0$, the angle parameter in Eq.(3.2.1) can be eliminated by the rotation $U_\varphi \equiv \exp(i\frac{\varphi}{2}\sigma_3) = \cos\frac{\varphi}{2} + i\sin\frac{\varphi}{2}\sigma_3$. Using the commutation relations of the Pauli Matrices we get $U_\varphi^\dagger\sigma_1U_\varphi = \sigma_\varphi$, with $\sigma_\varphi \equiv \sigma_1\cos\varphi + \sigma_2\sin\varphi$. Effectively we can set $\varphi = 0$ and Eq.(3.2.1) leads to, App.(B.1.1)

$$i\partial_t |\psi\rangle = \left[-t\sigma_3 + f_D(t;b)\sigma_1 \right] |\psi\rangle \quad (4.1.1)$$

Of special interest are the two limits $b \rightarrow 0$ and $b \rightarrow \infty$ which we analyze in more detail in the following sections. In the next section, we have general results that apply to all cases in Tab.(3.2). Following that, the gap structure of L is analyzed in more detail. L is special for many reasons. First of all, is it the shape of the original H_{CD} . From the examples in Tab.(4.1), it is the only case with slope $n = 2$, Fig.(4.1) (right), and lastly, it has poles on the complex plane, in the time domain. After that, we treat the rectangular case and its generalizations.

4.1.1 Limits

For small $b \rightarrow 0$, Eq.(4.1.1) behaves as the LZS Eq.(2.1.1). Making the crude approximation $f_D(t;b) \approx f_D(0;b) = \frac{b}{2}$, $\forall t$, we get the LZS equation with a replaced by $b/2$, thus $\mathcal{P}(0,b) \stackrel{b \rightarrow 0}{\approx} e^{-\pi b^2/4}$. The validity of this approximation is further justified from perturbation theory. Treating $H_1 = f_D\sigma_1$ as a perturbation, $\|H_1\| \stackrel{b \rightarrow 0}{\rightarrow} 0$, to the trivially integrable $H_0 = -t\sigma_3$, up to second order we get, Eq.(C.1.8)

$$\mathcal{P}_{\text{pert}}(0,b) \approx \left(1 - \frac{1}{2}|V(b)|^2 \right)^2 \quad (4.1.2)$$

with $V(b) := \int_{\mathbb{R}} dt f_D(t;b)e^{-it^2}$. Because $f_D(t;b)$ depends non linearly b , Eq.(4.1.2) gives a better estimate than $\mathcal{P} = 1 - \frac{\pi b^2}{4} \approx e^{-\pi b^2/4}$, Tab.(4.1) (left) and Fig.(4.1) (left). The calculations can be found in App.(B.1.5).

On the other limit $b \rightarrow \infty$, the behavior is fundamentally different than the LZS. In contrast to the $a \rightarrow \infty$ in Eq.(2.1.1), in Eq.(4.1.1) the solution is well defined in the limit $b \rightarrow \infty$, $f_D \rightarrow \frac{\pi}{2}\delta(t)$. It is reasonable to expect a $1/b$ series expansion for $|\psi\rangle$, leading to an asymptotic behavior $\mathcal{P}(0,b) \stackrel{b \rightarrow \infty}{\sim} C + D/b^n$, instead of exponential decay. D, n depend on the f_D and due to the symmetry $\mathcal{P}(0,b) = \mathcal{P}(0,-b)$, Eq.(A.2.2), the exponent is even. For the examples in Tab.(3.2), for all but L, s we get $n = 8$.

$C = 0$ regardless of f_D . This can be seen by first taking the limit $b \rightarrow \infty$ and then solving the Eq.(4.1.1) with $f_D(t;b) \stackrel{b \rightarrow \infty}{\rightarrow} \frac{\pi}{2}\delta(t)$ (see next section for the general case

f_D	$V(b)$	$t_*^{\text{asym}}(b)$
L	$\frac{\pi}{2} e^{i/b^2} \text{Erfc}(\frac{i^{1/2}}{b})$	$(b\sqrt{2})^{-1/3}$
g	$\frac{b\sqrt{\pi}}{2} (b^2/\pi + i)^{-1/2}$	$\sqrt{2\pi} \frac{(\ln b)^{1/2}}{b}$
s	$\frac{\pi i^{1/2}}{2} \text{erf}(\frac{b}{2i^{1/2}})$	$\dots$
r	$\frac{b\sqrt{\pi}}{2i^{1/2}} \text{erf}(\frac{i^{1/2}\pi}{2b})$	$\pi/(2b)$
t	$2V^r(\frac{b}{2}) - i\frac{b^2}{2\pi} (e^{-i\pi^2/b^2} - 1)$	π/b

Table 4.1. (Left) Eq.(4.1.2) for the different functions in Tab.(3.2). In the limit $b \rightarrow 0 \Rightarrow \mathcal{P}(0, b) \rightarrow 1 - \frac{\pi b^2}{4} + \dots$ independently of f_D . (Right) Asymptotic expression for the minima of Eq.(4.1.4), for the function in Tab.(3.2). For L, $t_{*,L}^{\text{asym}}$ converges to zero slower than the other cases.

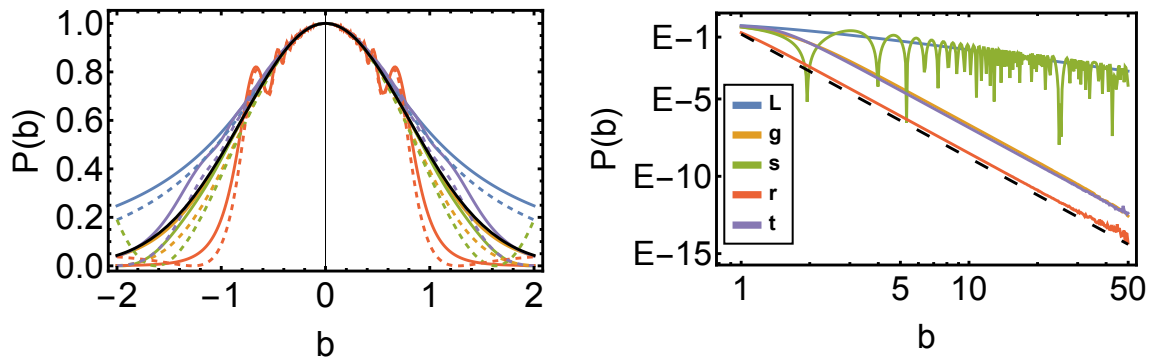


Figure 4.1. (Left) Numerical (solid lines) vs Eq.(4.1.2) (dashed) which is a good approximation for $|b| \lesssim 2$. Black curve corresponds to the $\mathcal{P} = e^{-\pi a^2/4}$. (Right) Log-Log scale, $\mathcal{P}(0, b)$ as a functions of b . Apart from L, s, all the curves are parallel to the rectangular with slope $n = 8$. It is already evident from the left graph that r and L are the two edge cases. Different cases correspond to Tab.(3.2).

with $a \neq 0$). Eq.(4.1.1) takes the form

$$i\partial_t |\psi\rangle = \left[-t\sigma_3 + \frac{\pi}{2}\delta(t)\sigma_1 \right] |\psi\rangle \quad (4.1.3)$$

Due to the presence of $\delta(t)$ in Eq.(4.1.3), the solution must necessarily have jump discontinuity at $t = 0$ which is given by $|\psi(0^+)\rangle = (-i\sigma_1) |\psi(0^-)\rangle$. For $t_f > 0$, integrating Eq.(4.1.3) in the symmetric interval $[t_f, -t_f]$ we get $|\psi(t_f)\rangle = -i\sigma_1 |\psi(-t_f)\rangle$ leading to $\mathcal{P}(0, \infty) = 0$.

4.1.2 Energy gap

The switch in behavior for large b can be qualitatively understood from instantaneous gap $\text{gap}(t; b) \equiv 2\sqrt{t^2 + f_D^2(t; b)}$. For the Lorentzian L, Tab.(3.2), $f_D^L(t; b) = \frac{b/2}{b^2 t^2 + 1}$ we have

$$\text{gap}(t; b) = 2\sqrt{t^2 + \frac{b^2/4}{(b^2 t^2 + 1)^2}} \quad (4.1.4)$$

Taking the time derivative

$$\partial_t \text{gap}(t; b) = \frac{t}{2\text{gap}(t; b)} \left(1 - \frac{b^4/2}{(b^2 t^2 + 1)^3} \right)$$

The second term in the parenthesis is upper bounded by its value at $t = 0$, $b^4/2$. For small $b < 2^{1/4}$

$$1 - \frac{b^2/4}{(b^2 t^2 + 1)^3} > 1 - \frac{b^4}{4} > 0$$

the sign is solely determined by the linear factor t . Thus at $t = 0$ we have a global minimum with the typical A.C. structure and as anticipated an exponential type behavior, Fig.(4.1) (left). For $b_* = 2^{1/4}$ a pitchfork bifurcation takes place [89]. The minimum becomes a (local) maximum and two other minima at positions $t = \pm t_*(b)$ appear. Their asymptotic behavior can be seen in Tab.(4.1) (right).

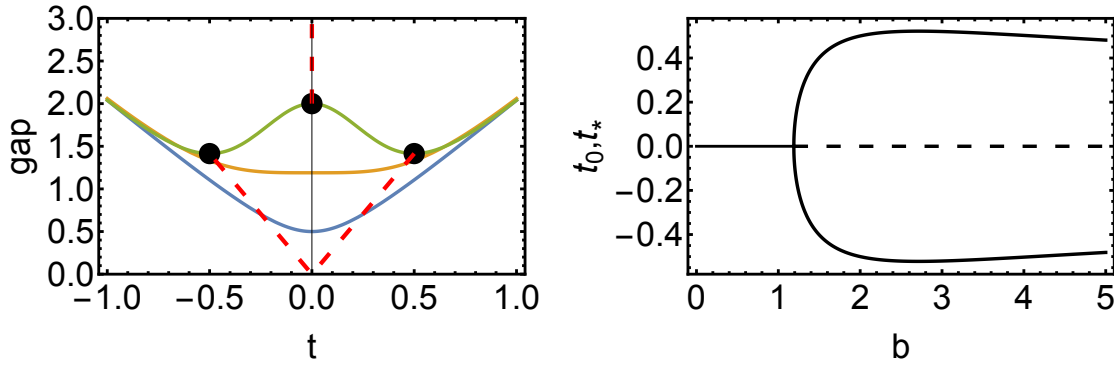


Figure 4.2. (Left) Eq.(4.1.4) as a function of time for $b = 0.5, 2^{1/4}, 2$. For $b > 2^{1/4}$, the minimum becomes maximum and two other roots are generated at values $t_*(b) = \pm \frac{1}{b} \sqrt{\frac{b^{4/3}}{2^{1/3}} - 1}$. The three roots (black points) move along the red dashed lines as b increases. For $b \rightarrow \infty$, $\text{gap}(t_*(b)) \approx t_*(b)$. (Right) Bifurcation diagram for the roots of the gap Eq.(4.1.4). Dashed corresponds to minimum and solid lines to maximum.

By construction in all cases, $f_D \xrightarrow{b \rightarrow \infty} \frac{\pi}{2} \delta(t)$ and therefore at $t = 0$ the gap becomes singular, approaching a delta function. The maximum itself is independent of f_D , with $\text{gap}(0; b) = b$ but the two minima carry additional information about f_D . From

their asymptotic behavior, Tab.(4.1) (right column), it is evident that the singularity is approached with different speeds, with L being the slowest. Although our sample is too small to draw a safe conclusion, the ratio with the other cases is approximately a power of four, as is the case for $\mathcal{P}$ in Fig.(4.1) (right). The slow decay of L is ultimately related to the heavy tails of the Lorentzian as a function of time, but it is not clear whether this is the only deciding factor ¹

Interesting is the behavior of Eq.(4.1.4) in the complex plane. The gap vanishes at 6 points $t_c(b)$, that we will collectively call crossing points, and has simple poles at $t_p(b) = \pm i/b$. The crossing points are given by the roots of the polynomial

$$t^2(t^2b^2 + 1)^2 + \frac{b^2}{4} = 0 \Rightarrow t(t^2b^2 + 1) \pm i\frac{b}{2} = 0 \Rightarrow t^3b^2 - t \mp \frac{b}{2} = 0, t \rightarrow it \quad (4.1.5)$$

The last equation is a depressed cubic, with the quadratic term missing. The real roots can be expressed via radicals and their behavior can be examined in detail.

As mentioned in previous chapter, the relevance of the crossing points in the transition probability was first noted by Landau and later developed to the DDP method [44–46]. According to that

$$\mathcal{P} \sim e^{-2\text{Im} \int_0^{t_c} \text{gap}(t) dt} \quad (2.1.11)$$

with t_c being the nearest to the $t = 0$ crossing point, in the upper complex plain $\text{Im}(t_c) > 0$. Eq.(2.1.11) gives the leading order behavior of $\mathcal{P}$ is the adiabatic limit but it is known to work surprisingly good beyond that. Specifically for the LZS reproduces the exact formula $\forall a$, Eq.(2.1.12). In order to apply the formula, the basic requirements are the existence of complex crossing and the gap analyticity in a strip contain the real line and the crossing point.

In Eq.(4.1.4), we have a polynomial of degree 6 with real coefficients, meaning 3 pairs of complex conjugate roots, 3 of them in the upper half plane. For small $b \rightarrow 0$, the main contribution comes from the imaginary root, closer to $t = 0$. From Eq.(4.1.5), $t_c = i\frac{b}{2}$ and Eq.(2.1.11) gives $\mathcal{P} \sim e^{-\pi b^2/4}$ analogously to Eq.(2.1.12), Fig.(4.3) (left). In the upper half plane (the situation is symmetric for $\text{Im}(t_c) < 0$), the two crossing points closed to each other collide at $b = b_*$, meaning the multiplicity of the purely imaginary root increases. For this special value, from Eq.(4.1.5) we have the system of equations

$$\left. \begin{array}{l} t^3b^2 - t \pm \frac{b}{2} = 0 \\ 3t^2b^2 - 1 = 0 \end{array} \right\} \Rightarrow \left. \begin{array}{l} t_* = \pm \frac{3b}{4} \\ b_* = \frac{2}{3^{3/4}} \end{array} \right\}$$

¹We can interpolate between the L and r with $f_{D,k}(t; b) \equiv \frac{b/2}{(g_k b t)^{2k+1}}$, $g_k \equiv (k \sin \frac{\pi}{2k})^{-1}$. For $k = 1$, $f_{D,1} = f_D^L$ and for $k \rightarrow \infty$, $f_{D,\infty} = f_D^r$. For $k = 2$ we get $n = 6$, skipping $n = 4$, and for $k = 3$, $n = 8$.

For $b \rightarrow \infty$, from Eq.(4.1.5), $t^6 b^4 + \frac{b^2}{4} = 0$, all the roots are uniformly distributed along the circle with radius $\rho = 1/(2b)^{1/3}$, Fig.(4.1.5). For multiple crossings, there is a generalized version of DDP in which all the roots contribute in a coherent sum. See [47, 90] and references therein. It is reasonable to assume that since all of them have the same distance from $t = 0$, the main contribution comes from the purely imaginary point.

The additional complication is that for $b \rightarrow \infty$, the singular point t_p lies between $t = 0$ and the target point t_c , as $t_c(b) \sim i/(2b)^{1/3}$ and $t_p(b) \sim i/b$. This technically forbids the application of DDP and the integral in Eq.(2.1.11) diverges. As in Fig.(4.2), we observe the qualitative change in behavior around $b \approx 1$, $b_* = 2^{1/4}, 2/3^{3/4}$ respectively.

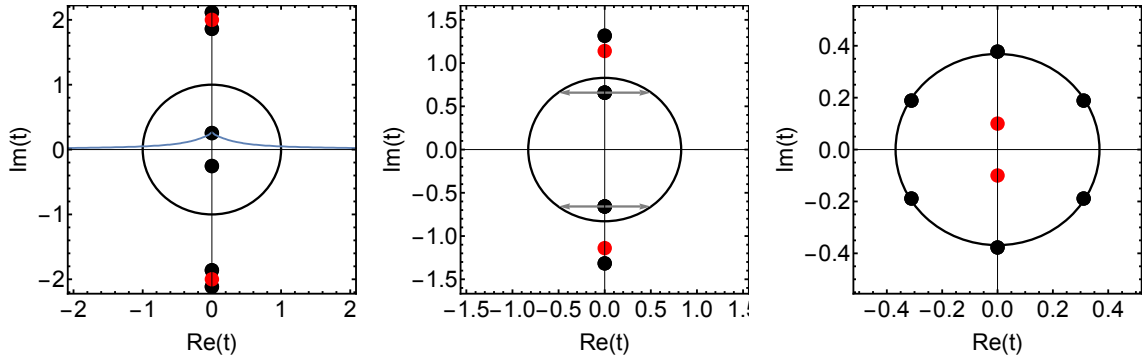


Figure 4.3. Black points correspond to the crossing points $\text{gap}(t_c; b) = 0$ and red points to the singularity $t_b(b) = \pm i/b$ of Eq.(4.1.4), in the complex plane. We are only interested in the upper half plane. (Left) $b = 0.5$, (Middle) $b = b_*$ and (Right) $b = 10$. For small b , the singularity doesn't affect the probability. The two black points closer to $t = 0$, more towards each other and at the critical value $b_* = \frac{2}{3^{3/4}}$ they collide (middle). Afterwards, they move horizontally. For large b (Right), all the roots approach the the cycle of radius $\rho = \frac{1}{(2b)^{1/3}}$. At large b , the singularity contributes to the probability.

The diverge of the integral in Eq.(2.1.11) for large b , can potentially account for the exponent $n = 2$, Fig.(4.1) (right). A hand wavy calculations is the following. We are interested only in the singular part. The term t^2 in Eq.(4.1.4) is not important.

$$\begin{aligned} \int_0^{i/(2b)^{1/3}} \sqrt{t^2 + \frac{b^2/4}{(b^2 t^2 + 1)^2}} dt &\approx i \int_0^{1/(2b)^{1/3}} dt \frac{b/2}{|1 - b^2 t^2|} \\ &= \frac{b}{2} \left[\int_0^{1/b-\varepsilon} dt \frac{1}{1 - b^2 t^2} + \int_{1/b+\varepsilon}^{1/(2b)^{1/3}} dt \frac{1}{b^2 t^2 - 1} \right] \end{aligned}$$

avoiding the singular point by making a Cauchy Principal Value regularization. For

the first integral, keeping only the singular term

$$\int_0^{1/b-\epsilon} dt \frac{1}{1-b^2 t^2} = \frac{1}{2} \int_0^{1/b-\epsilon} dt \frac{1}{1+bt} + \frac{1}{1-bt} = -\frac{1}{2b} \log(b\epsilon)$$

The second integrals gives the same contribution. Putting everything together we get $\mathcal{P} \sim e^{\pm 2 \log(b\epsilon)}$, with the minus sign corresponding to the same calculation going through the lower half plane.

4.1.3 Rectangular

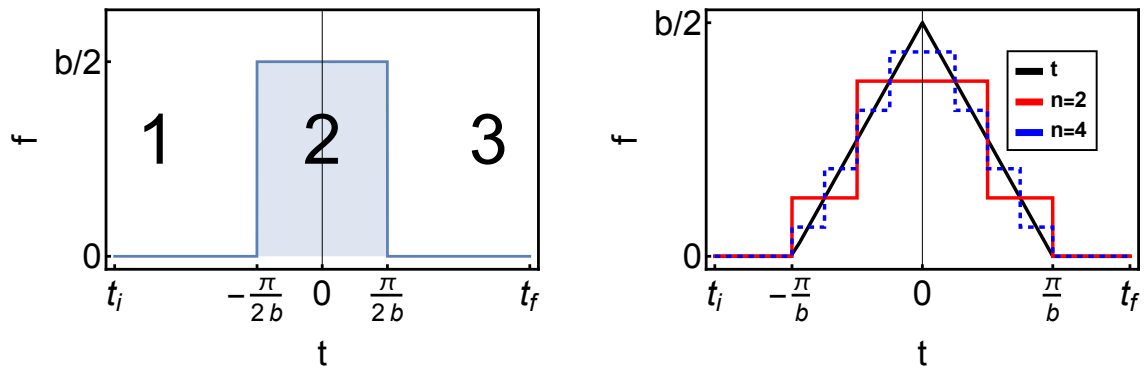


Figure 4.4. (Left) Spitting of the time interval $[t_i, t_f]$ in Eq.(4.1.6). (Right) Approximating a triangular pulse with rectangles, referring to Eq.(4.1.10). In the limit $n \rightarrow \infty$, we recover the exact shape of the pulse.

For the rectangular pulse with $\varphi = 0$, Eq.(4.1.1) becomes

$$i\partial_t |\psi\rangle = \left[-t\sigma_3 + \frac{b}{2} \mathbf{1}(|t| < \frac{\pi}{2b}) \right] |\psi\rangle, \quad b > 0 \quad (4.1.6)$$

The time-dependent coupling is piecewise constant. For $|t| > \frac{\pi}{2b}$ Eq.(4.1.6) is trivially integrable and for $|t| < \frac{\pi}{2b}$ reduces to the LZS with a replaced by $b/2$. The full solution is found by splitting the time evolution in appropriate time intervals, Fig.(4.4) (left)

$$[t_i, t_f] = [t_i, -\frac{\pi}{2b}] \cup [-\frac{\pi}{2b}, \frac{\pi}{2b}] \cup [\frac{\pi}{2b}, t_f]$$

and multiplying the corresponding time evolution matrices. Given $b > 0$, the endpoints t_i, t_f must be sufficiently large. In the end we make the identification $t_i = -t_f$ and take the limit $t_f \rightarrow +\infty$. After algebraic manipulations we get, App.(B.1.2)

$$\mathcal{P}^x(0, b) = \left(2 \left| \mathcal{M}\left(-\frac{ib^2}{16}, \frac{1}{2}, -i\frac{\pi^2}{4b^2}\right) \right|^2 - 1 \right)^2 \quad (4.1.7)$$

with $\mathcal{M}(\alpha, \beta; z)$ the Confluent Hypergeometric Function (Kummer's function) with

$$\alpha_b = -i\frac{b^2}{16}, \quad \beta = \frac{1}{2}, \quad z_b = -i\frac{\pi^2}{4b^2} \quad (4.1.8)$$

The two limits $b \rightarrow 0$ and $b \rightarrow \infty$ are examined in more detail. For $b \rightarrow 0 \Rightarrow z_b \rightarrow \infty$, from the asymptotic expansion of $\mathcal{M}(a, b; z)$ [27], Eq.(D.3.2), expanding in power of b , the leading terms are

$$\left| \mathcal{M}\left(-\frac{ib^2}{16}, \frac{1}{2}; -i\frac{\pi^2}{4b^2}\right) \right|^2 \stackrel{z \rightarrow \infty}{\sim} e^{-\frac{\pi b^2}{16}} (\cosh \frac{\pi b^2}{16} + \dots) = \frac{1}{2}(1 - e^{-\frac{\pi b^2}{8}}) = \frac{\pi b^2}{16} + \dots$$

and from Eq.(4.1.6) $\mathcal{P}^r(0, b) \stackrel{b \rightarrow 0}{\sim} 1 - \frac{\pi b^2}{4} \approx e^{-\pi b^2/4}$. This is consistent with previous results, see Tab.(4.1) and text previous to that, and further solidifies that for $b \rightarrow 0$, Eq.(4.1.6) and the more general Eq.(4.1.1) behave as the LZS.

More important is the limit $b \rightarrow \infty$ in which $a_b \rightarrow \infty$, $z_b \rightarrow 0$ with the product $a_b z_b = -\frac{\pi^2}{64}$ kept constant, Eq.(4.1.8). The key property that makes the calculation viable is Eq.(D.3.3). From that and utilizing the series representation of $\mathcal{M}$, Eq.(D.3.1) we find

$$\mathcal{P}^r(0, b) \stackrel{b \rightarrow \infty}{\sim} C + D/b^n + \dots \quad (4.1.9)$$

with $C = 0$, $D = (\pi/12)^2(\pi^2 - 12)^2 \approx 0.311$ and $n = 8$. The result is in complete agreement with numerics, Fig.(4.1) (right).

Using the same time splitting, Fig.(4.4) (left), we can also treat the case $a \neq 0$, for the rectangular pulse. Notice that we cannot set $\varphi = 0$ anymore. In regions (1),(3), $|t| > \frac{\pi}{2b}$ the solution reduces to the LZS. For region (2), $|t| < \frac{\pi}{2b}$, the full Hamiltonian Eq.(3.2.1) becomes

$$H = -t\sigma_3 + a\sigma_1 + \frac{b}{2}\sigma_\varphi$$

The trick is to merge the two couplings as follows

$$H = \begin{pmatrix} -t & a + \frac{b}{2}e^{-i\varphi} \\ a + \frac{b}{2}e^{i\varphi} & t \end{pmatrix}$$

leading to LZS with complex coupling $\mathbb{C} \ni a'(a, b, \varphi) \equiv a + \frac{b}{2}e^{-i\varphi}$. $\mathcal{P}^r$ as a function of the parameters a, b, φ can be found in closed form, App.(B.1.4).

Given any $f(t)$, we may partition the time interval $[t_i, t_f]$ as

$$t_i = t_1 < \dots < t_n = t_f$$

In each sub-interval $I_k \equiv [t_k, t_{k+1}]$, let $f_k \equiv f(t_\xi)$, $\xi \in I_k$

$$H_k = \begin{pmatrix} -t & a + f_k e^{-i\varphi} \\ a + f_k e^{i\varphi} & t \end{pmatrix}$$

Let $a_k \equiv a + f_k e^{-i\varphi}$, the total time evolution matrix is given by the product

$$\mathcal{U}(t_f, t_i) = \prod_{k=1}^{n-1} \mathcal{U}_0(t_{k+1}, t_k; a_k) \quad (4.1.10)$$

For a function f with compact support as the one in Fig.(4.4), Eq.(4.1.10) can give a good approximation even for small n . Let $t_{k+1} = t_k + \varepsilon$. $\mathcal{U}_0(t_k + \varepsilon, t_k; a) = \mathcal{U}_0(t_k, t_k) + \varepsilon \mathcal{U}_0^{(1)}(t_k, t_k) + \mathcal{O}(\varepsilon^2)$, with $\mathcal{U}_0(t_k, t_k) = \mathbb{1}$ and $\mathcal{U}_0^{(1)}(t_k, t_k) = -iH_k$ the derivative w.r.t the first argument

$$\mathcal{U}(t_f, t_i) \approx \prod_{k=1}^{n-1} (\mathbb{1} - i\varepsilon H_k) \approx \prod_{k=1}^{n-1} e^{-i\varepsilon H_k} \quad (4.1.11)$$

In the limit $n \rightarrow \infty$, the product in Eq.(4.1.10) becomes continuous. The expression is equivalent to the time ordered exponential [91, Theorem 4.2] which in practice is not possible to compute.

4.2 Infinite Control ($b \rightarrow \infty$)

For $b \rightarrow \infty$, $f_D \rightarrow \frac{\pi}{2}\delta(t)$, Eq.(3.2.1) takes the form

$$i\partial_t |\psi\rangle = \left[-t\sigma_3 + a\sigma_1 + \frac{\pi}{2}\delta(t)\sigma_\varphi \right] |\psi\rangle, \quad \sigma_\varphi \equiv \cos \varphi \sigma_1 + \sin \varphi \sigma_2 \quad (4.2.1)$$

with $a \neq 0$ ($a = 0$ was discussed previously). The main obstacle is determining the discontinuity conditions which is discussed in details in the first section and in App.(B.2.2). The solution to Eq.(4.2.1) reduces to the LZS and Eq.(A.1.2,A.1.3). The detailed derivation can be found in App.(B.2.3).

4.2.1 Discontinuity

Eq.(4.2.1) is first order in time. To match the $\delta(t)$ in the r.h.s, the solution must have jump discontinuity at $t = 0$. Let $\mathcal{N}$ be the matrix that connects the solution at $t = 0$, i.e $|\psi_+\rangle = \mathcal{N} |\psi_-\rangle$. In terms of the time evolution matrix, $\mathcal{N}$ is defined as $\mathcal{N} \equiv \mathcal{U}(0^+, 0^-)$. $\mathcal{N}$ is fixed from the differential equation itself but due to the discontinuity, extra care must be taken. The naive integration around $t = 0$ leads to the wrong condition. The correct expression arises by taking the matrix exponential of the prefactor of $\delta(t)$ in Eq.(4.2.1)

$$\mathcal{N} = e^{-i\frac{\pi}{2}\sigma_\varphi} = -i\sigma_\varphi \quad (4.2.2)$$

For the problem at hand, we can establish this rigorously. A quick argument is that around $t = 0$, Eq.(4.2.1) approximately becomes $i\partial_t |\psi\rangle \approx \frac{\pi}{2}\delta(t)\sigma_\varphi |\psi\rangle$ from which we get Eq.(4.2.2) after integration, treating $\delta(t)$ as a regular function. This is not surprising since $\delta(t)$ is well behaved under the integral.

The treatment of the discontinuity in Eq.(4.2.1) is the generalization of the one dimensional case discussed in [92, 93]. A similar problem about the one dimensional Dirac Equation can be found in [94]. Although is not stated explicitly in text, their approach is exactly the same, taking the matrix exponential of the prefactor of $\delta(t)$.

To treat the problem rigorously, we replace Eq.(4.2.1) with

$$i\partial_t |\psi_n\rangle = \left[-t\sigma_3 + a\sigma_1 + \frac{\pi}{2}\Delta_n(t)\sigma_\varphi \right] |\psi_n\rangle \quad (4.2.3)$$

with $\Delta_n(t) \xrightarrow{n \rightarrow \infty} \delta(t)$ and the needed solution defined as the pointwise limit $|\psi; t\rangle := \lim_{n \rightarrow \infty} |\psi_n; t\rangle$. $\forall n \in \mathbb{N}$ $|\psi_n\rangle$ can be glued at $t = 0$ such that the solution is continuous. The convergence to the limit is not uniform since $|\psi\rangle$ is discontinuous at $t = 0$ and the limiting function $|\psi\rangle$ "breaks" at $t = 0$.

The limit $n \rightarrow \infty$ is independent of the choice of Δ_n . The simplest choice is the sequence of rectangular pulses $\Delta_n(t) = \frac{n}{2}\mathbf{1}(|t| < \frac{1}{2n})$. For $|t| < \frac{1}{2n}$, in matrix notation Eq.(4.2.3) becomes

$$i\partial_t |\psi_n\rangle = \begin{pmatrix} -t & a_n \\ a_n^* & t \end{pmatrix} |\psi_n\rangle \quad (4.2.4)$$

with $a_n \equiv a + \frac{n}{2}e^{-i\varphi}$. Eq.(4.2.3) is the generalization of Eq.(2.1.1) with complex coupling $a \rightarrow a_n \in \mathbb{C}$. Let $\mathcal{U}_n := \mathcal{U}_0(\frac{\pi}{2n}, -\frac{\pi}{2n}; a_n)$. Then $|\psi(\frac{\pi}{2n})\rangle = \mathcal{U}_n |\psi(-\frac{\pi}{2n})\rangle$ and $\mathcal{U}_n \xrightarrow{n \rightarrow \infty} \mathcal{N}$.

The limit in question reduces to limits of product of PCF which have been studies in [95]. A direct calculation is also possible with the help of the series expansion of $D_\nu(z)$, Eq.(D.2.1) and careful rearrangement of the terms. Therefore, we can independently verify that $\mathcal{U}_n \xrightarrow{n \rightarrow \infty} \mathcal{N} = -i\sigma_\varphi$ in agreement with Eq.(4.2.2). For the technical details, see App.(B.2.2).

4.2.2 Solution

From Eq.(4.2.1,4.2.2)

$$\mathcal{U}_\infty(t_f, t_i; a) = \mathcal{U}_0(t_f, 0; a) \mathcal{N} \mathcal{U}_0(0, t_i; a) \quad (4.2.5)$$

Expanding the matrices in Eq.(4.2.5)

$$\mathcal{A}_\infty(t_f, t_i) = \mathcal{A}_0(0, t_i) \mathcal{B}_0(t_f, 0) e^{i\varphi} + \mathcal{A}_0(t_f, 0) \mathcal{B}_0^*(0, t_i) e^{-i\varphi} \quad (4.2.6)$$

We will consider symmetric integration with $t_f = -t_i$ in order to exploit the time symmetry Eq.(A.2.1)

$$\begin{aligned}\mathcal{A}_\infty(t_f, t_i) &= \mathcal{A}_0(0, t_i)\mathcal{B}_0(0, -t_f)e^{i\varphi} + \mathcal{A}_0^*(0, -t_f)\mathcal{B}_0^*(0, t_i)e^{-i\varphi} \\ &= \mathcal{A}_0(0, t_i)\mathcal{B}_0(0, t_i)e^{i\varphi} + \mathcal{A}_0^*(0, t_i)\mathcal{B}_0^*(0, t_i)e^{-i\varphi} \\ &= 2\text{Re}(\underbrace{\mathcal{A}_0(0, t_i)\mathcal{B}_0(0, t_i)}_{\mathcal{C}_0}e^{i\varphi})\end{aligned}\quad (4.2.7)$$

Taking the asymptotic expansions of PCF for $t_i \rightarrow -\infty$ and only keeping leading order terms

$$\mathcal{C}_0 = \frac{\Gamma(1-\nu)}{a\sqrt{\pi}}D_\nu^2(0)(e^{-\pi a^2/2} - 1)e^{i(\frac{\pi}{4}+\varphi)}, \quad \nu(a) = ia^2/2 \quad (4.2.8)$$

Further simplification can be made using the value of PCF at $z = 0$, $D_\nu(0) = 2^{\frac{\nu}{2}}\sqrt{\pi}\Gamma\left(\frac{1-\nu}{2}\right)$ Eq.(D.2.2) and properties of the Gamma function. The final form for $\mathcal{P}_\infty = |\mathcal{A}_\infty|^2$ is

$$\mathcal{P}_{\text{LZD}}(a) = (1 - e^{-\pi a^2})\cos^2(\chi(a) - \varphi) \quad (4.2.9)$$

with

$$\chi(a) = \frac{\pi}{4} - \arg \Gamma\left(\frac{2-\nu(a)}{2}\right) + \arg \Gamma\left(\frac{1-\nu(a)}{2}\right), \quad \nu(a) = i\frac{a^2}{2} \quad (4.2.10)$$

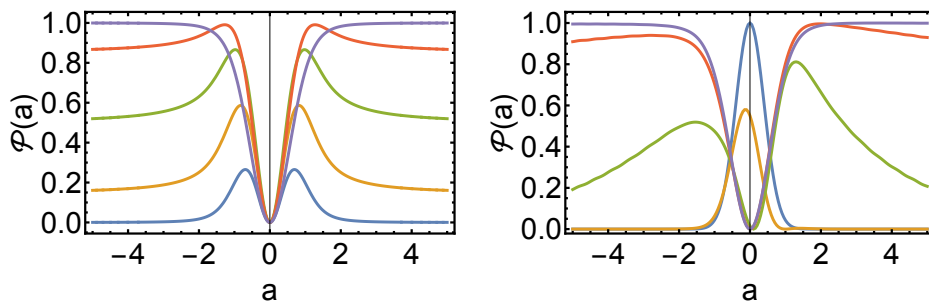


Figure 4.5. (Left) $\mathcal{P}(a, \infty)$ as a function of a , for different values of $\varphi \in \{0, \frac{\pi}{8}, \frac{\pi}{4}, \frac{3\pi}{8}, \frac{\pi}{2}\}$. (Right) $\mathcal{P}(a, b)$ as a function of a , for $\varphi = \frac{\pi}{2}$ and increasing values of $b \in \{0, 1, 10, 100, 1000\}$.

A slightly more general to Eq.(4.2.1) is

$$i\partial_t |\psi\rangle = \left[-t\sigma_3 + a\sigma_1 + \delta(t)\mathbf{n} \cdot \boldsymbol{\sigma} \right] |\psi\rangle \quad (4.2.11)$$

which leads to Eq.(B.2.20). In Eq.(4.2.10), for $a > 0$, $\chi(a)$ is an increasing function from $\pi/4$ to $\pi/2$. Its asymptotic expansion for large a is [33] $\chi(a) \stackrel{a \rightarrow \infty}{\sim} \frac{\pi}{2} - \frac{1}{2a^2} +$

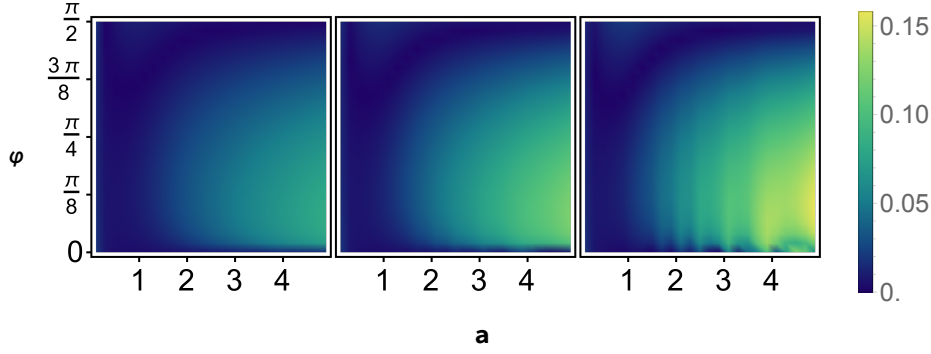


Figure 4.6. Relative error $\text{error}(x, y) \equiv \frac{|x-y|}{\max(x, y)}$ between numerical and analytical solution given by Eq.(4.2.9). $b = 10^3$ (left), $b = 10^4$ (middle) and $b = 10^5$ (right). For the middle graph, the values are multiplied by 10, while for the right graph by 100, in order to have a common legend. The average error, roughly satisfies $\langle \text{error} \rangle \propto 1/b$.

$\mathcal{O}(1/a^6)$. Dropping the exponential in Eq.(4.2.9), since it goes to zero faster than any power of $1/a$

$$\mathcal{P}_\infty(a) - \sin^2 \varphi \sim \frac{1}{2a^2} \sin 2\varphi + \frac{1}{8a^4} (2 \cos^2 \varphi - \sin^2 \varphi) + \mathcal{O}(1/a^6) \quad (4.2.12)$$

Typically, $\mathcal{P}_\infty$ approaches the limit $\sin^2 \varphi$ as $1/a^2$. For $\varphi = 0, \pi/2 \Rightarrow \sin 2\varphi = 0$, $\mathcal{P}_\infty(a) - \sin^2 \varphi \sim \frac{1}{4a^2}$. Only for $\varphi = 0$, the area $\int_{\mathbb{R}} da \mathcal{P}_\infty(a)$ is finite. Putting a cutoff at some value $a_{\max}$, $\varphi = 0$ minimizes the area of the red curve.

Chapter 5

Numerics

5.1 Roots

As discussed in detail in Section 3, important is the existence of the CC which are collectively the roots of the transition probability $\mathcal{P}(a, b)$. For the case $H_1 = H_{\text{CD}}$, $\mathcal{P}(a, 1/a) = 0$ due to the CD driving. For the other cases, the existence of CC is postulated, which is supported by the numerics. In the current section, we will mainly discuss the dependence of b_0 in the two parameters of the GLZS, φ and f_D , Eq.(3.2.1). In the final part, we will briefly examine the dependence on the protocol time T , for the finite time problem Eq.(2.1.13).

5.1.1 Existence

The existence (and uniqueness) of $b_0(a)$ is understood only in the case $H_1 = H_{\text{CD}}$. For the other cases, we don't have an analytic argument, but the numerics clearly indicate that the following is true: *Given f_D satisfying the properties in Tab.(3.1) and $\varphi \in [0, \frac{\pi}{2}]$, $\forall a, \exists b(a) : \mathcal{P}(a, b_0(a)) = 0$, with $\mathcal{P}(a, b)$ being the transition probability general by the full Hamiltonian in Eq.(3.2.1).*

In Fig.(5.3), we illustrate the existence of b_0 for the different function in Tab.(3.2) for gap parameter $a = 0.5$ and similarly in Fig.(5.2), existence of b_0 for different φ 's. One important observation for the numerics is that for $H_1 \neq H_{\text{CD}}$, the roots are systematically move to the left, meaning $b_0(a) < b_{0,\text{CD}} = 1/a$.

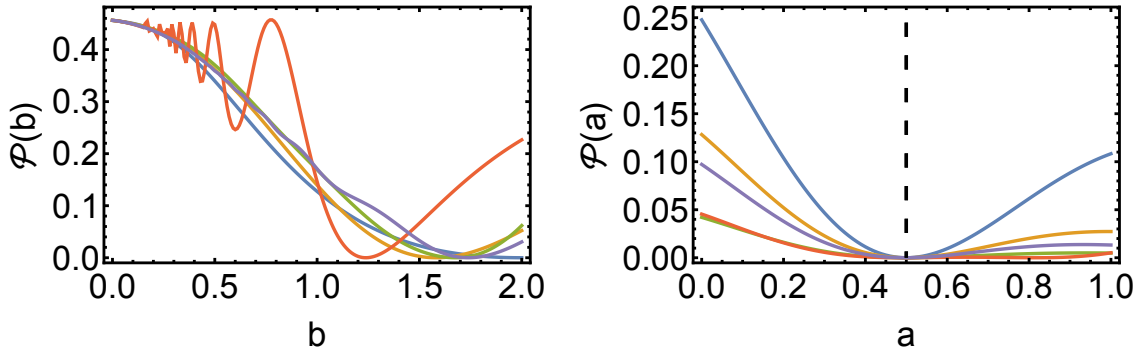


Figure 5.1. The colors and the functions f_D correspond to Fig.(3.6). (Left) $\mathcal{P}(0.5, b)$ as a function of b for different f_D . For the L, $b_0(0.5) = 2$. For the other cases, we can verify numerically the existence of b_0 . The roots systematically move to the left, i.e $b_0(a) < 1/a$ for $\# \neq L$. (Right) $\mathcal{P}(a, b_0(0.5))$ as a function of a , for control coupling $b_0(a)$. All the curves have a minimum (zero), at $a = 0.5$ by the definition of b_0 . It is already evident that L is worse than the other cases, regarding the average transition probability, see Fig.(3.1).

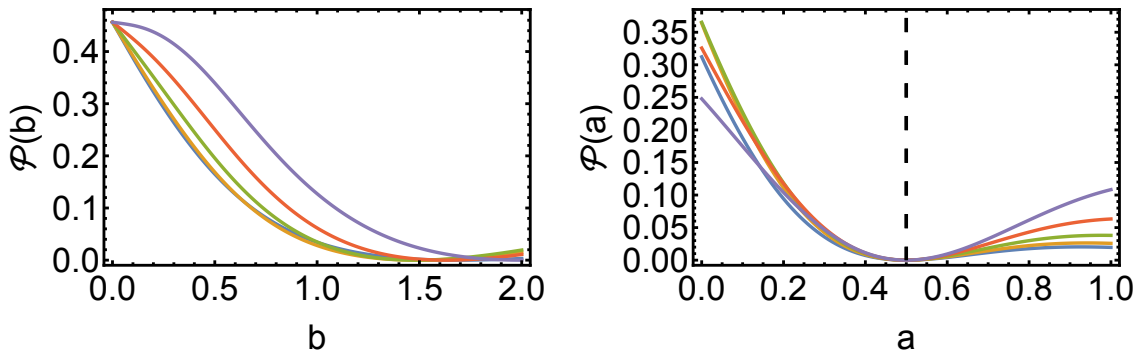


Figure 5.2. The colors and values of φ correspond to the middle graph in Fig.(3.6). (Left) $\mathcal{P}(0.5, b)$ as a function of b for different φ . For $\varphi = \frac{\pi}{2}$, $\sigma_\varphi = \sigma_2$, $b_0(0.5) = 2$. As in Fig.(5.1), we can verify the existence of b_0 numerically and also observe the systematic translation to the left of $b_0(a) = 1/a$. (Right) Analogously to Fig.(5.1). Referring to Fig.(3.1), the area under the corresponding curves amplified by the probability distribution, gives the average transition probability.

5.1.2 Time Peaks

Having established the existence of b_0 , one of the compromises in contrast to $H_1 = H_{\text{CD}}$ is that although $\mathcal{P}(a, b_0(a)) = 0$, the probability is not zero at intermediate times. This is not necessarily problematic in our case, since we are only interested in the minimization of the final transition probability, but can potentially be important to the stability of the system, especially in the case of Eq.(2.1.13), with finite time evolution.

In Fig.(3.6) (left and middle) we have briefly discussed the structure of the time peaks. In Fig.(5.3), we extend these two graphs, examining the behavior for the different prefactor functions in Tab.(3.2) and different angles φ . In the first column, we see the effect of different angles, for the five values $\varphi = \{0 : \frac{\pi}{8} : \frac{\pi}{2}\}$, as in Fig.(3.6) (left). In the second column, we see the dependence of b_0 in the angle parameter. Typically the dependence is not monotonous, but what is systematically present, is the location of the maximum at $\varphi = \frac{\pi}{2}$. This was also observed in Fig.(5.2). Lastly, on the third column we graph the φ dependence of the central value at $t = 0$ (solid line) and area (dashed line), for the function $\mathcal{P}(t, \cdot)$. For the Lorentzian prefactor L, the two quantities are in complete alignment but for the other cases, we have deviations, as it is evident from the first column. Both quantities measure the deviation from adiabaticity, with the area being a more reliable measure, Fig.(5.3).

The particular peak structure in each case is not quite understood and as discussed previously, in similar systems we can get even weirder behavior, with arbitrary many peaks, Fig.(3.7). What is true without exceptions in all cases, is the even symmetry of $\mathcal{P}(t; a, b_0(a))$ as a function of time. For $H_1 = H_{\text{CD}}$, $\mathcal{P}(t; a, 1/a) = 0, \forall t$, which is trivially an even function. There is clearly a relation between the time inversion symmetry of $\mathcal{P}$ and the existence of the root. Obviously, the presence of the symmetry implies the vanishing of the probability, since we start with $\mathcal{P} = 0$. The other direction is not clear whether it is true. Exploring further the relation between the two, could potentially lead to a formal proof for the existence of the CC, $b_0(a)$.

A Further consequence of the symmetry, is that $\mathcal{P}(t; a, b_0(a)) \xrightarrow{t \rightarrow \infty} 0$ goes to zero without oscillations, Fig.(3.6) (right). This is because for $t < 0$, $\mathcal{P}$ increases monotonically, see Fig.(3.1) (left) and Fig.(2.1) (middle).

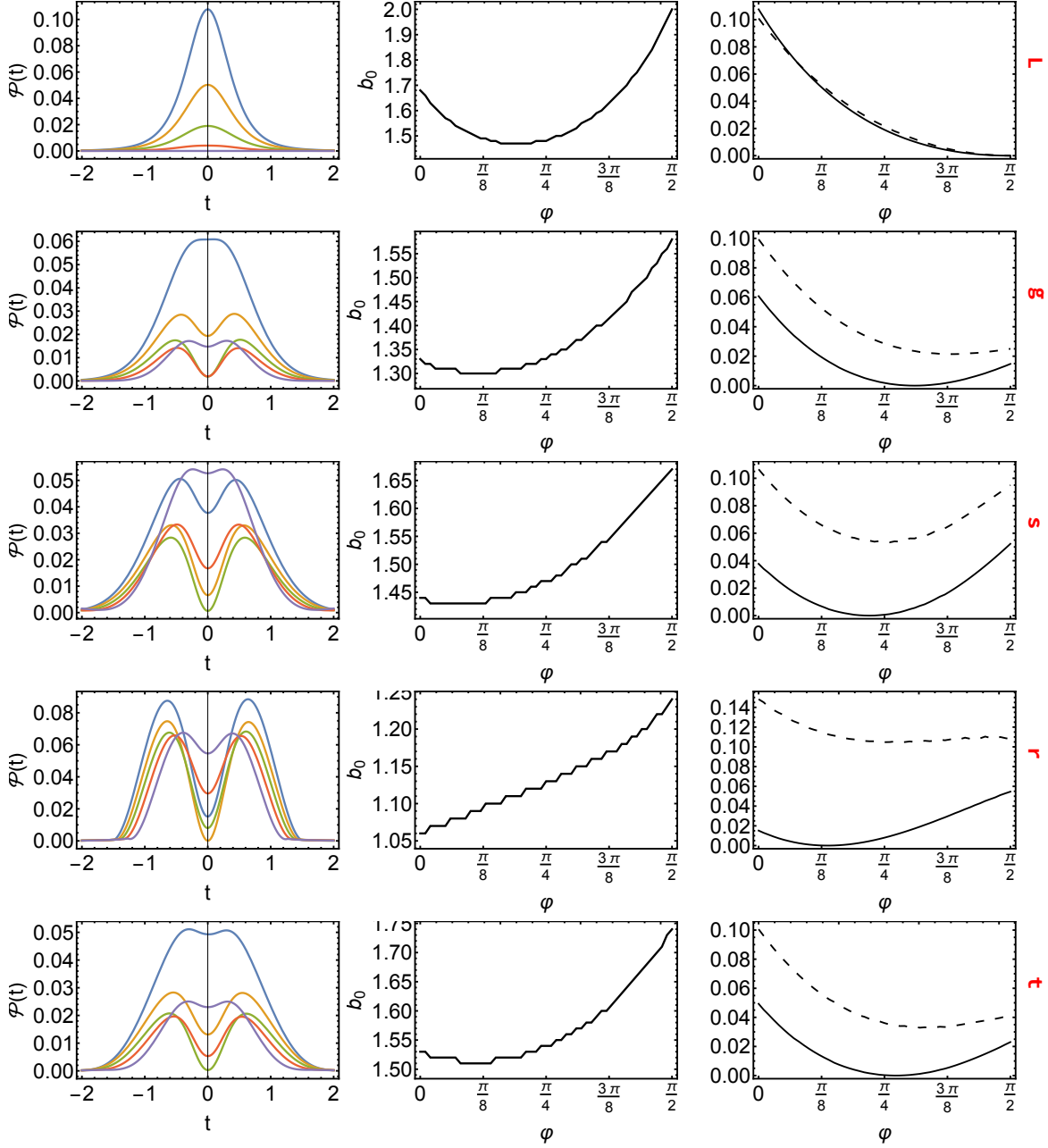


Figure 5.3. Peaks of the transition probability $\mathcal{P}(t; a, b_0(a))$, in the time domain, for various angles φ and the prefactors function in Tab.(3.2). For all the simulations, $a = 0.5$. In the first column, colors and φ values are the same with Fig.(3.6) (left). (Left) Although the final transition probability vanishes, the evolution is not adiabatic, typically having a peak or multiple peak around the point $t = 0$. (Middle) φ dependence of b_0 . Common feature is the $b_0(a) < 1/a$. (Left) $\mathcal{P}(0; a, b_0(a))$ and area under the curves of left column, as a function of φ . In the general case, the value at $t = 0$ is not a good measure of adiabaticity, as it demonstrated from the figures.

5.1.3 Finite Time

For the finite time version of Eq.(2.1.1), b_0 is defined analogously. There is the extra complication of the protocol time- T dependence the choice of the NLS, Tab.(2.1). We won't make a systematic analysis. This part serves as an illustration of the extra complications that arise for the finite system Eq.(2.1.13) and would be the basis for further examination in the future.

In Fig.(5.4), we have plotted the protocol time- T dependence for different values of the gap parameter a . The only modification to Eq.(2.3.10), is the replacement $\sigma_2 \rightarrow \sigma_1$. The time dependence of the control field f_{CD} is kept the same and also linear time dependence in Eq.(2.1.13). Regardless of the magnitude of a , for large enough T , we observe oscillatory behavior.

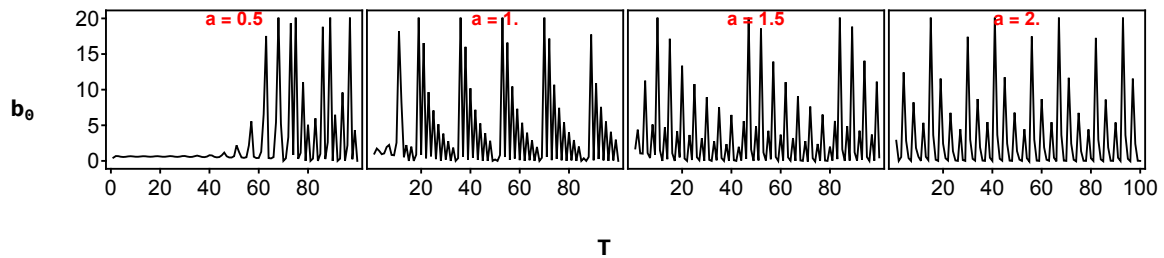


Figure 5.4. Linear sweep Lin with $\lambda_0 = 4$, Eq.(2.1.13), Tab.(2.1). In Eq.(2.3.10), we have replaced σ_2 with σ_1 . The profile function, is the original, Lorentzian pulse L , $f_D(t; b) = \frac{b/2}{\lambda^2(t) + b^2}$ with $1/b$, opposite to the typical convention that was used throughout the text.

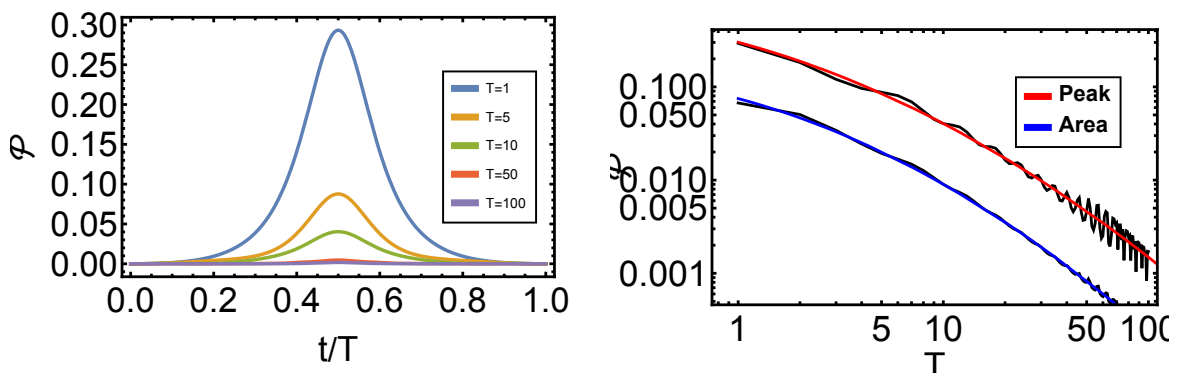


Figure 5.5. $a = 0.5$ The other parameter values are the same with Fig.(5.4). For $T \rightarrow \infty$, adiabatic limit, both peak and area go to zero, as expected from the AT.

It is not clear whether those oscillation Fig.(5.4) are detrimental to our problem since in the large T limit (adiabatic limit), $\mathcal{P}(t; \cdot) \rightarrow 0, \forall t$, for all the other parameter

values, Fig.(5.5). It is important to note that for $H_1 = H_{CD}$, there is no T dependence on CC, nor any dependence on the choice of NLS, Tab.(2.1) since $b_{0,CD} = 1/a$.

Ultimately, the oscillation are related to the oscillations in Fig.(3.5). Recalling the relation between Eq.(2.1.1) and Eq.(2.1.13), $a' \sim a\sqrt{T}$ with a' being the unit free gap parameter in Eq.(2.1.1). Summing up, for small gaps a and protocol times T , the T dependence is negligible. On the other hand, for large a and T , there is strong time dependence in $b_0(a)$ and the full consequences of that are not entirely clear.

5.1.4 Characteristic Curves

The notion of the Characteristic Curve was defined in Chapter (3) and it referees to the function $b_0(a)$ which satisfies, $\mathcal{P}(a, b_0(a)) = 0$. It depends both on the choice of φ and f_D in GLZS, Eq.(3.2.1). As discussed in previous section, apart from the case $b_{0,CD}(a) = 1/a$, we don't know for sure that such curve exists, but due to vast numerical evidence, we operate under the assumption that it does.

In the small gap limit $a \rightarrow 0$, the typical behavior is qualitatively the same as $b_{0,CD} = 1/a$: For $b_0(a) \xrightarrow{a \rightarrow 0} \infty$, see Chapter 4, first section, and for small $a > 0$, $b_0(a)$ monotonically decreases. Around the value $a \approx 2$, their behavior becomes more complicated. Either irregular oscillations are present and/or multiple branches are created whose origin is not understood at the moment, Fig.(3.5), Fig.(5.6).

Theoretically, even with those irregularities present, our construction can still work since only the existence of b_0 is required. Nevertheless, the oscillation, are a potential threat to the stability and should be examined in more detail. On the other hand, the multivaluedness can cause technical issues. The main branch, which is the one that extends to $a \rightarrow 0$, is the deformation of $b_{0,CD}(a) = 1/a$ and should be our first candidate, but there is always the potential that the secondary roots, might be a better option regarding $\langle \mathcal{P} \rangle$.

In Fig.(5.6), we have plotted the (approximate) CC for the different prefactors f_D in Tab.(3.2) and the angle parameters $\varphi = 0$ (left) and $\varphi = \frac{\pi}{2}$ (right). For $\varphi = \pi/2$ and prefactor L (top right sub-figure), $b_{0,CD} = 1/a$. Without any knowledge of the CD formalism and Eq.(2.3.10), the regularity of $b_{0,CD}$ in comparison to the other cases, should be a strong indication that $H_{CD} = f_D^L \sigma_2$.

Apart from the oscillation, the other typical pattern is the branching of roots. Detailed analysis shows that indeed branching is present. For example, for the r case, we have analytic evidence from Eq.(B.1.4), that possibly an infinite number of roots exists in the limit $a \rightarrow \infty$.

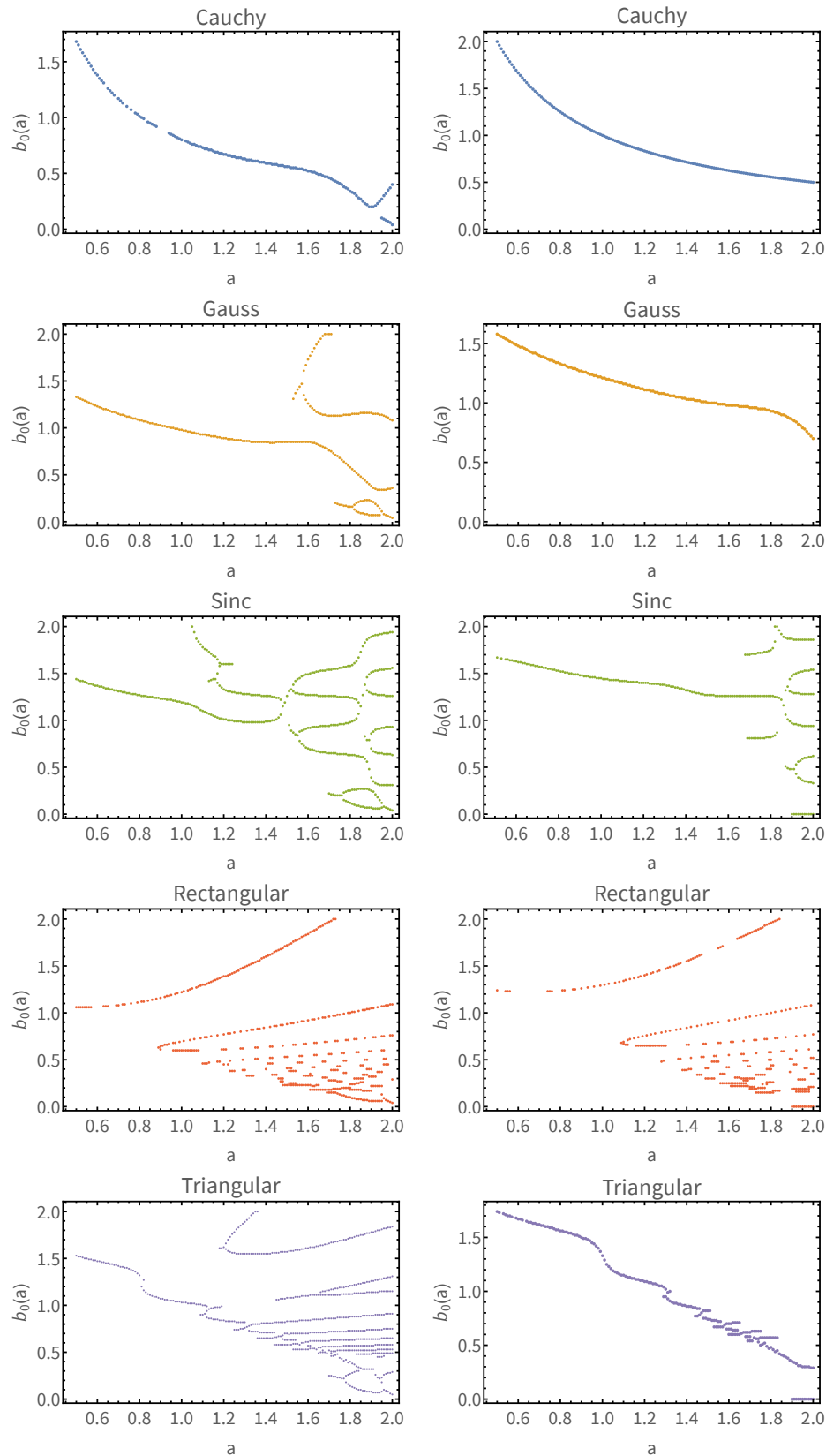


Figure 5.6. CC for f_D in Tab.(3.2) with $\varphi = 0$ (left) and $\varphi = \frac{\pi}{2}$ (right). In the top right graph, $b_{0,CD}(a) = 1/a$. We can clearly see the multivaluedness for $\varphi = 0$ and large a . See also Fig.(3.5), for the oscillatory part. Here CC is calculated approximately by setting a threshold below which the point is classified as a root (there should be no branching in the top left graph).

5.2 Random Gap

This section is concerned with the numerical calculation of b^* and most importantly $\mathcal{P}^*$, which is the minimum, average transition probability. For the gap distribution we assume $a \sim \mathcal{N}(\mu, \sigma)$. The important parameter range for μ and σ is small μ and $\sigma < \sigma_{\max} \equiv \mu/5$. This was discussed in Chapter 3. To summarize, the restriction $\sigma < \sigma_{\max}$ comes from $a > 0$. For large μ , $\mathcal{P} \rightarrow 0$, regardless of b, σ , Eq.(3.1.3). Moreover, following the discussion on the previous section, the definition of b_0 and consequently of $b^* = b_0 + \mathcal{O}(\sigma^2)$ is ambiguous for the GLZS, Eq.(3.2.1). Thus we will restrict to $0 < \mu \lesssim 2$.

The main purpose of this section is to establish two results. For the GLZS, $\varphi = 0$ is the optimal angle parameter, for the given parameter range of the distribution and moreover, the prefactor L is the worse among the one in the Tab.(3.2). As previously mentioned in Chapter 3, we will conflate b_0 with b^* and make the distinction when needed.

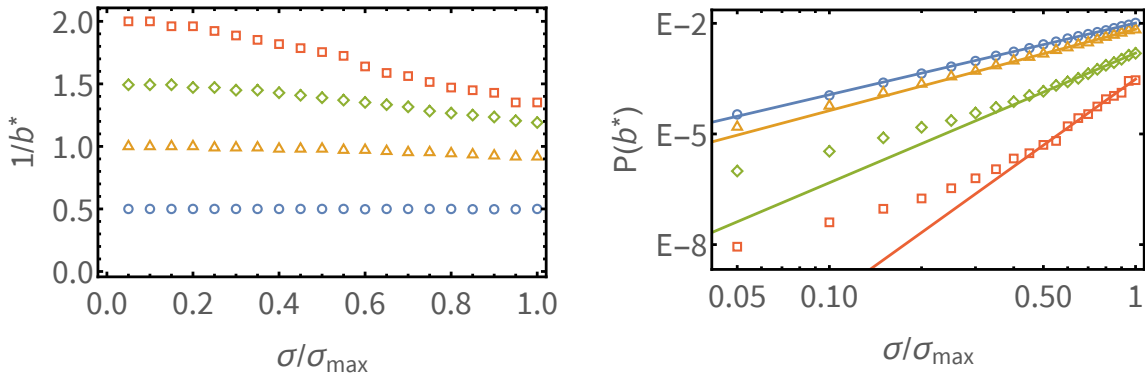


Figure 5.7. $H_1 = H_{\text{CD}}$ Eq.(3.1.2). b^* and $\mathcal{P}^*$ as a function of σ for $\mu = 0.5, 1.0, 1.5, 2.0$. The values of μ can be read by the limit $\sigma \rightarrow 0$ in the left graph. $\mathcal{P}^*$ decreasing with μ can be traced back to the LZ formula $\mathcal{P} = e^{-\pi\mu^2}$, although $\mathcal{P}^*$ is not monotonic in $\mu, \forall \mu$, see Fig.(5.8).

In Fig.(5.7) we see the typical behavior of b^* and $\mathcal{P}^*$, as a function of σ for different values of μ . It is evident that the σ dependence of b^* is weak and thus further justifies the identification $b^* = b_0$. For $H_1 \neq H_{\text{CD}}$ the dependence is slightly stronger and our numerical simulations indicate that the use of b^* instead of b_0 will be in favor of $H_1 \neq H_{\text{CD}}$. If possible, the numerical evaluation of b^* should be avoided since it is not cost efficient. For the result we want to establish, the first order term in the expansion of b^* Eq.(3.1.5) should be sufficient.

In the following two sections, we make the comparison between σ_1 and σ_2 , for the Lorentzian pulse function L , Tab.(3.2), followed by the f_D dependence. We briefly

discuss the implications of the finite time evolution Eq.(2.1.13) and the dependence on the protocol time. As it was previously elucidated, the problem can be transferred to the finite case as is, as long as we restrict our parameters in appropriately and as for the general case, the extension is not straightforward.

After that, we analyse the effect of different parameter imperfections in the pulse function f_D , to the stability of b^* and $\mathcal{P}^*$. This is an important question for the possibility of any experiment realization. Our qualitative analysis shows analogous behavior between σ_1 and σ_2 and at least from a first glance, the system is stable under the errors taking into consideration.

5.3 σ_1 vs σ_2

For all the simulations in this section, we used $b^* = b_0$. In Fig.(5.8) we see the typical behavior $\mathcal{P}^*$ for the two cases. As the variance of the gap increases, σ_1 outperforms σ_2 approximately by an order of magnitude. This is a conservative estimate since we only using b_0 .

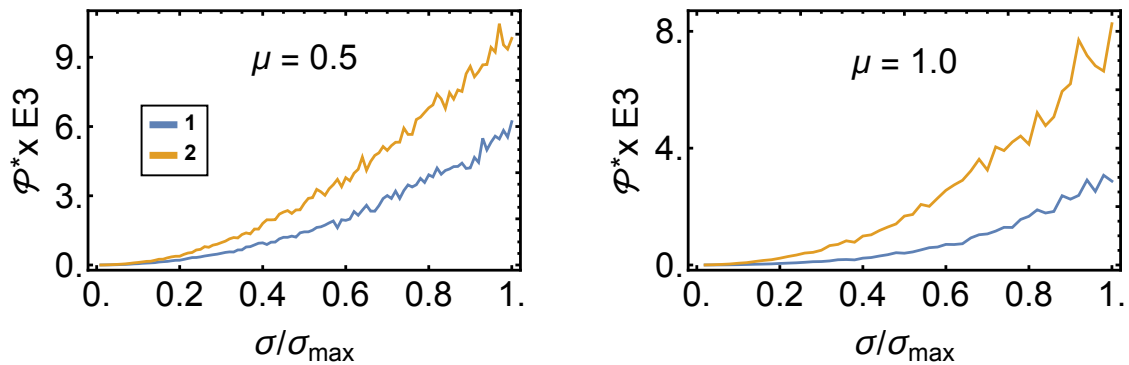


Figure 5.8. $b^* = b_0$. Lorentzian prefactor L Tab.(3.2). $\mathcal{P}^*$ as a function of σ for $\mu = 0.5$ (left) and $\mu = 1.0$ (right).

In Fig.(5.9), the μ dependence is analyzed in more detail. For each value of μ , we take $\sigma = \sigma_{\max} = \mu/5$. On the right panel of Fig.(5.9), the relative error between the two curves of the left is depicted. The advantage of σ_1 over σ_2 is not dramatic, but is systematic.

Finally, in the last figure of this section, Fig.(5.10), we have calculated the average area (in the time domain), of the transition probability, Fig.(3.1). As discussed in great detail previously, the main compromise of using the control σ_1 in place of σ_2 is the appearance of the peaks in the time domain. Although, even for σ_2 , the single control field H_{CD} cannot drive the full ensemble of system transitionlessly,

the average deviation from the adiabatic path is small.

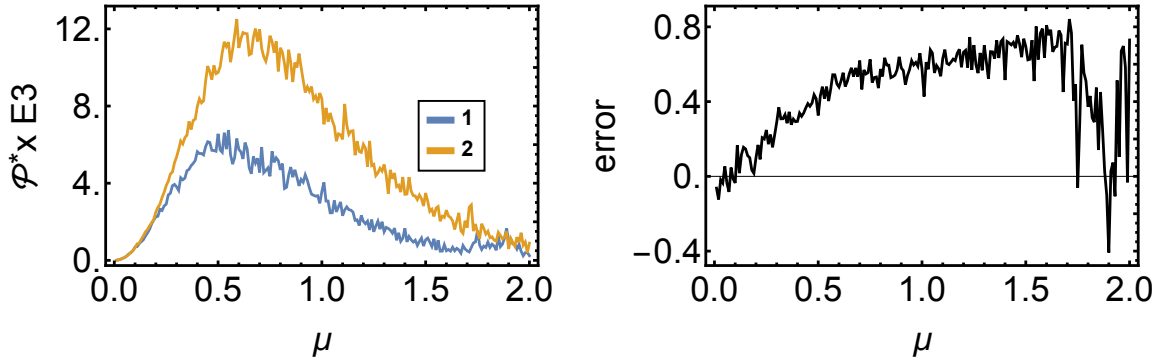


Figure 5.9. $\sigma = \sigma_{\max} = \mu/5, b = b_0$. runs = 1000., error = $\frac{x-y}{\max(x,y)}$. Lorentzian prefactor L Tab.(3.2).

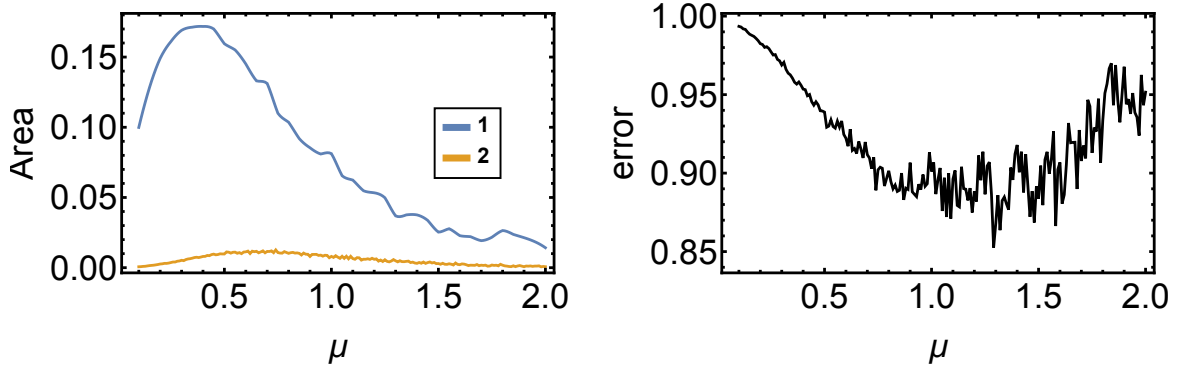


Figure 5.10. $\sigma = \sigma_{\max} = \mu/5, b = b_0$. runs = 1000., error = $\frac{x-y}{\max(x,y)}$. Average area as in Fig.(3.1) (left).

The previous analysis was done specifically for the Lorentzian case L. In Fig.(5.11) we extend this analysis for the other function of Tab.(3.2). The investigation is less thorough but the numerics clearly point to the same direction as before. σ_1 is always better than σ_2 across all functions f_D Tab.(3.2) and across all parameter values μ, σ of the Normal distribution.

Moreover, the comparison of the first row with the rest Fig.(5.11), clearly shows that L is worse among the the examples in Tab.(3.2). Again, although the improvement is not dramatic, it is systematic. This can be traced back to Fig.(4.1) (right). For $a = 0$, for the Lorentzian L, $\mathcal{P}(0, b) \stackrel{b \rightarrow \infty}{\sim} C/b^2$, the probability decays to zero as a inverse power of 2, wheres for the other cases (excluding s which is more complicated cases due to the oscillations), we typically have $n = 8$ as the leading exponent, Fig.(4.1) (right). The origin of $n = 2$ is mainly due to the heavy tails of L.

We finish this section with a brief reference to the finite time LZS, Eq.(2.1.13)

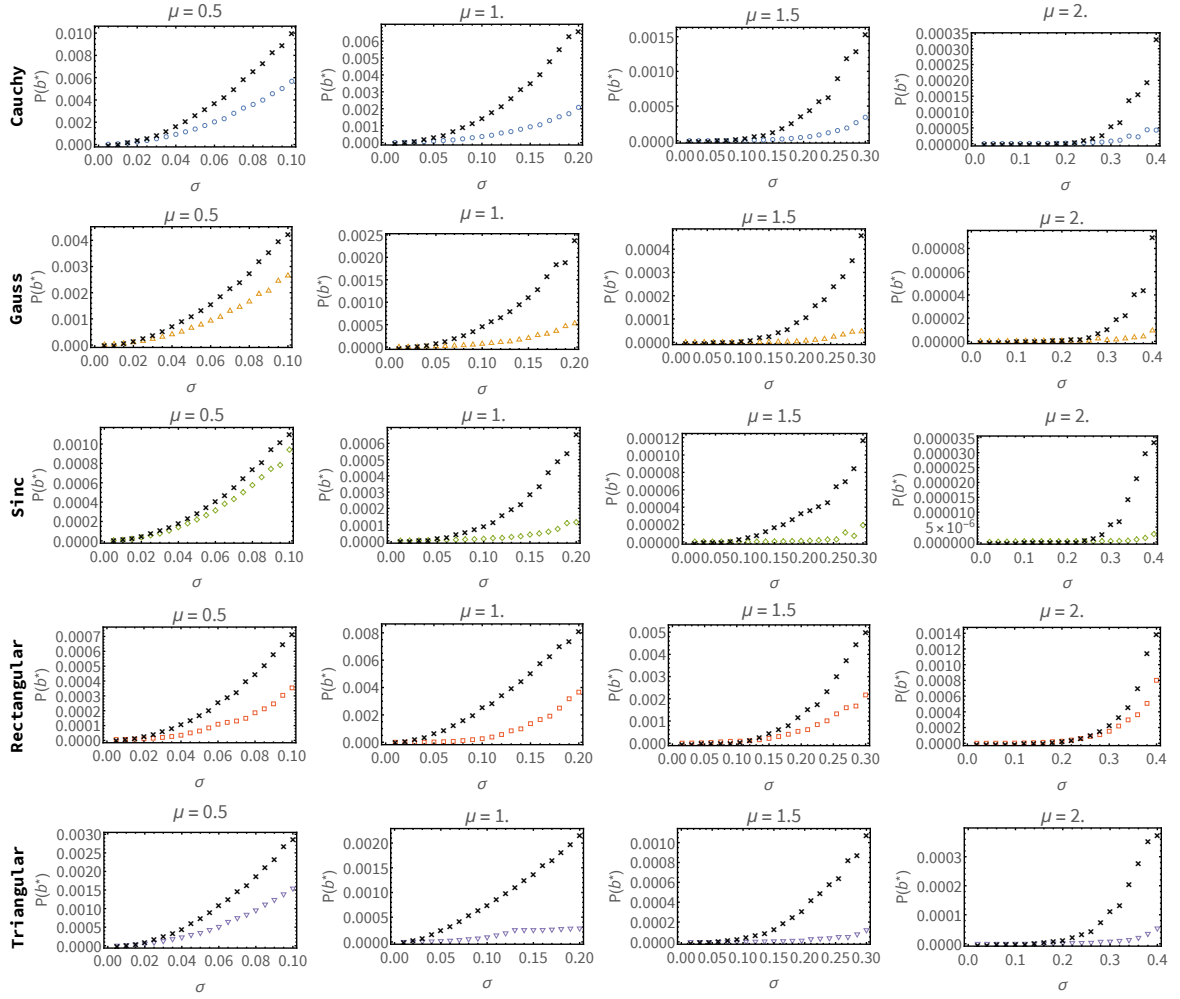


Figure 5.11. σ_1 vs σ_2 for different f_D , Tab.(3.2). Black marking correspond to σ_2 . We observe systematic advantage of σ_1 .

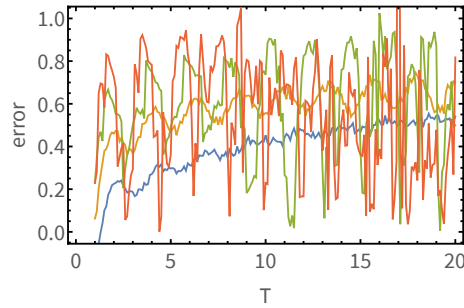


Figure 5.12. Relative error between σ_1 and σ_2 as in Fig.(5.9) for different values of $\mu = 0.5, 1, 1.5, 2.0$, $\sigma = \mu/5$, as a function of protocol time T . The figure feature the same problem that we mentioned before.

5.4 Stability

In the previous section, the advantage of σ_1 over σ_2 was established across all parameter values μ, σ of the probability distribution and for all the functions of Tab.(3.2). The reasonable next step is to study the stability of the two cases. We don't have a precise definition of stability in mind. The purpose of this section is to demonstrate the two cases are qualitatively equivalent, regarding the stability.

We have analyzed the effect of different types of errors in the prefactor function, Tab.(5.1). The first type of error, is the one that is usually taken into consideration in an experimental setup. The parameter ε affects both the peak and the area of the pulse function f_D . In the two other cases, we have made the appropriate modifications such that either the area or the pulse is kept constant, up to order ε^2 . This would require extra control of the experiment setup and it principle is more complicated to implement in practice.

	Function	Area	Peak
(1)	$(1 + \varepsilon) \frac{b/2}{t^2 + b^2}$	$\frac{\pi}{2}(1 + \varepsilon)$	$(1 + \varepsilon) \frac{b}{2}$
(2)	$\frac{b/2}{t^2(1 - \varepsilon)^2 + b^2}$	$\frac{\pi}{2} \frac{1}{1 - \varepsilon} = \frac{\pi}{2}(1 + \varepsilon + \dots)$	$\frac{b}{2}$
(3)	$(1 + \varepsilon) \frac{b/2}{t^2(1 - \varepsilon)^2 + b^2}$	$\frac{\pi}{2} \frac{1 + \varepsilon}{1 - \varepsilon} = \frac{\pi}{2}(1 - \varepsilon^2 + \dots)$	$(1 + \varepsilon) \frac{b}{2}$

Table 5.1. (1) The error affects both area and peak. (2) Fixing the peak (3) fixing the area up to second order in ε .

In Fig.(5.13), the relative error $\text{error}(x, y) \equiv \frac{|x - y|}{\max(x, y)}$, for $\mathcal{P}^*$, between the unperturbed ($\varepsilon = 0$) and the perturbed pulse is plotted. In the horizontal axis, we vary the standard deviation of the distribution of gaps $a \sim \mathcal{N}(\mu, \sigma)$ and in the horizontal axis, we vary the imperfection parameter ε . For the optimal control parameter, we have used $b^* = b_0$.

For the comparison between σ_1 and σ_2 , for the three cases Tab.(5.1), we notice typical variation patterns, with the same order of magnitude relative error. The case (2) Tab.(5.1) with the fixed peak height outperforms the other two cases by an order of magnitude.

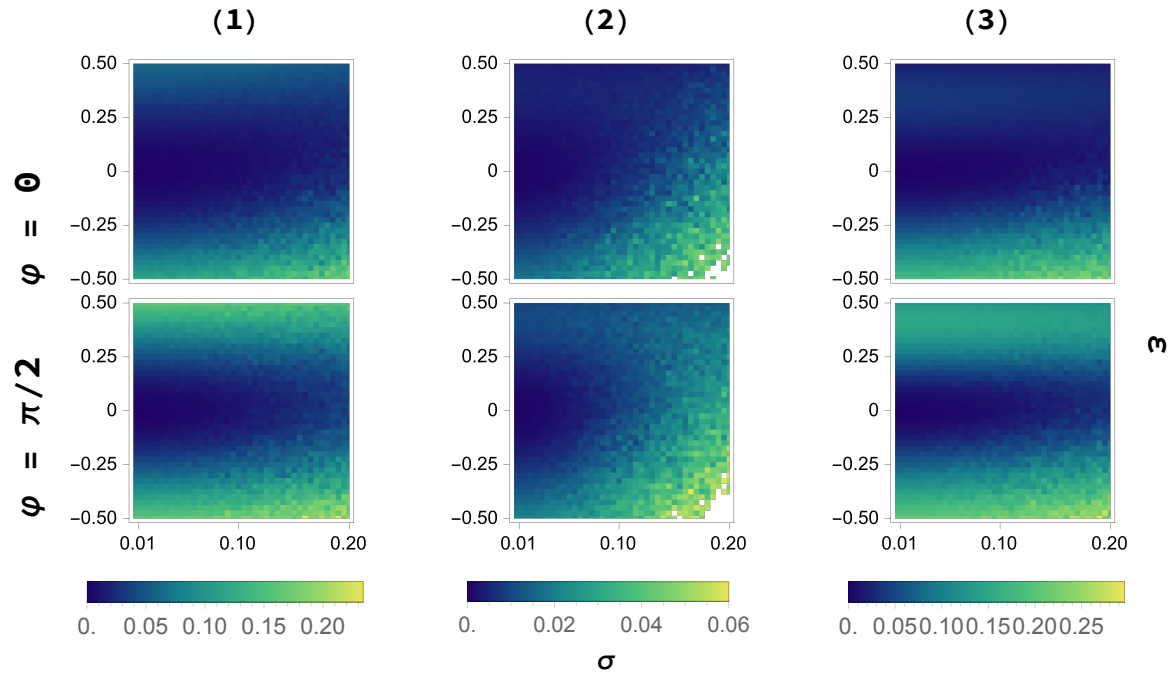


Figure 5.13. Effect of errors in parameter, Tab.(5.1). Fixing the peak improves the accuracy by one order of magnitude. $\mu = 0.5$. In the horizontal axis σ is $a \sim \mathcal{N}(\mu, \sigma)$ and in the vertical axis, the parameter ε , Tab.(5.1).

Lastly, we are considering the stability of the of the higher order terms in Eq.(3.1.5). If Fig.(5.14), we examine the stability of b^* , using the type (1) errors Tab.(5.1), with $\varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon)$ being a Gaussian random variable with small σ_ε . Again our surface level numerical analysis in this case, shows that at least qualitatively, the two cases σ_1 and σ_2 behave the same.

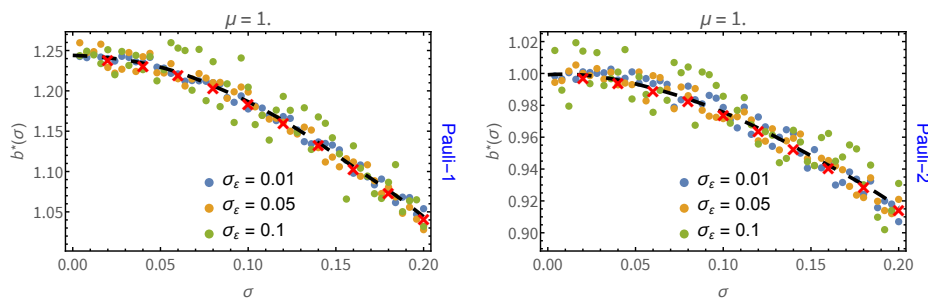


Figure 5.14. The unperturbed curve (black dashed) is extrapolated from the red crosses. The effect of small gaussian noise is qualitatively similar in the two cases.

Chapter 6

Summary

6.1 Conclusions

Although the random gap problem was motivated by experiments such as [17, 18], we have found some interesting analytic results that complement the numerical analysis of the optimization problem.

Based on H_{CD} we have defined the GLZS in Chapter 3. Limiting cases of the general system Eq.(3.2.1) are the vanishing gap, $a \rightarrow 0$ and the infinite control, $b \rightarrow \infty$. These two can be treated analytically and are the main topics of Chapter 4. Both reduce to the general solution of the original LZS and although our approach is not sophisticated, the results are original and we have discussed all the details.

The analytic are valuable addition to the numerical part. The main result there is that if the only concern is the minimization of the final transition probability, then H_{CD} can be replaced with a better correction term $H_1 = f_{\text{D}}\sigma_{\varphi}$. From a theoretical point of view, the angle parameter is related to the Dirac delta problem, infinite control, in which the parameter f_{D} is eliminated. The numerics show that the optimal angle parameter is $\varphi = 0$. At the same time $\varphi = 0$, minimizes the area of the $\mathcal{P}_{\text{LZD}}$ curve, Eq.(4.2.9). Similarly, f_{D} is related to the vanishing gap problem in which φ is factored out of the equation. The numerical analysis clearly indicates that the Lorentzian prefactor is the worst regarding the random gap problem. On the other hand, L has the worst asymptotic behavior with $n = 2$, Tab.(4.1.1) (right).

Our study was mostly based on the original LZS system, with linear time dependence and infinite integration time, since this is most suitable for theoretical analysis, with the hope that it could be generalized to the finite time version. Numerics suggest that the construction works for the finite version, in the limit $a \rightarrow 0, T \rightarrow 0$ whereas for large a, T , more systematic analysis is required, with the main issues already pointed out.

6.2 Outlook

The obvious continuation of this work would be the systematic study of the finite time LZS. Apart from the brute force numerical analysis, there are a number of open problems that also transfer to the finite version and their clarification could lead to overall better understanding.

Specifically, the basic requirement is the existence of the CC which we haven't managed to prove in the general case. Moreover, the defining conditions in Tab.(3.1) are assumed to sufficient but not necessary and further investigation of this is important. Secondly, one of the two main **limit**, infinite control was solved exactly, while the other one, vanishing gap still remain open. We are not interested in the full solution but merely in the calculation of the relevant exponent in Tab.(4.1). A better understanding of the underlying mechanics could potentially lead to a better choice of prefactor functions.

One of our main results, the formula $\mathcal{P}_{\text{LZD}}$ is related to other parts of the literature, specifically the transition time in the LZS [1]. It is not clear whether there is a deeper connection between the two and/or an experimental verification is viable.

Appendix A

Landau Zener

In the first section, we connect the LZS system to the Weber equation and arrive at the expression for the matrix evolution matrix via PCF Eq.(A.1.2), (A.1.3). Since these two equations are referenced many times throughout the text, we provide all the steps for their derivation. In the second section, we derive three properties that are relevant to our work. In the last section, we review one of the alternative derivations of the LZ formula which has some interest as a standalone calculation.

A.1 Landau Zener System

The LZS Eq.(2.1.1) with complex coupling takes the form

$$i\partial_t |\psi\rangle = \begin{pmatrix} -t & a \\ a^* & t \end{pmatrix} |\psi\rangle, \quad a \in \mathbb{C} \quad (\text{A.1.1})$$

The general solution, for $a \in \mathbb{R}$ can be found in [1, 19, 23]. The extension to $a \in \mathbb{C}$ is trivial.

A.1.1 General Solution

Let $|\psi\rangle = (\psi_1, \psi_2)$. Eq.(A.1.1) is written as

$$\begin{aligned} i\dot{\psi}_1 &= -t\psi_1 + a\psi_2 \\ i\dot{\psi}_2 &= a^*\psi_1 + t\psi_2 \end{aligned}$$

By differentiation, the system decouples

$$\ddot{\psi}_1 + (t^2 + |a|^2 - i)\psi_1 = 0$$

and similarly for ψ_2 . Making the substitutions

$$z = t\sqrt{2}e^{-i\pi/4}, \quad \varphi(z) := \psi(t(z)), \quad \frac{d}{dt} = \sqrt{2}e^{-i\pi/4} \frac{d}{dz}, \quad \nu = i|a|^2/2$$

$$\varphi_1''(z) + \left(\frac{1}{2} + \nu - \frac{z^2}{4}\right)\varphi_1(z) = 0 \quad (2.1.2)$$

and similarly for φ_2 . Eq. (2.1.2) is the Weber equation and its solutions are the Parabolic Cylinder Functions $D_\nu(z)$ [24]. Given a solution $\varphi_\nu(z)$ then $\varphi_\nu(-z)$ and $\varphi_{-1-\nu}(\pm iz)$ are also independent solutions [24]. Any two of the four span the general solution of Eq.(2.1.2)

$$\begin{aligned} \varphi_1(z) &= c_1 D_\nu(z) + c_2 D_\nu(-z) \\ \varphi_2(z) &= \frac{a^*}{\sqrt{2}} e^{-i\pi/4} (-c_1 D_{\nu-1}(z) + c_2 D_{\nu-1}(-z)) \end{aligned}$$

$\varphi_2(z)$ follows from $\varphi_1(z)$ in combination with Eq.(D.2.7). The constants $c_1, c_2 \in \mathbb{C}$ are determined by the initial conditions. Let $\lambda = a^* e^{-i\pi/4} / \sqrt{2}$ and

$$M(z) \equiv \begin{pmatrix} D_\nu(z) & D_\nu(-z) \\ -\lambda D_{\nu-1}(z) & \lambda D_{\nu-1}(-z) \end{pmatrix}$$

$M(z)$ can be inverted with the help of Eq.(D.2.8)

$$M^{-1}(z) = \frac{\Gamma(1-\nu)}{\lambda\sqrt{2\pi}} \begin{pmatrix} \lambda D_{\nu-1}(-z) & -D_\nu(-z) \\ \lambda D_{\nu-1}(z) & D_\nu(z) \end{pmatrix}$$

Let $\boldsymbol{\varphi}_i = M(z_i)\mathbf{c}$ and $\boldsymbol{\varphi}_f = M(z_f)\mathbf{c}$. Combining the previous equations

$$\boldsymbol{\varphi}_f = M(z_f)\mathbf{c} = M(z_f)M^{-1}(z_i)\boldsymbol{\varphi}_i = \mathcal{U}_0(t_f, t_i)\boldsymbol{\varphi}_i$$

with $\mathcal{U}_0(t_f, t_i) = M(z_f)M^{-1}(z_i)$

$$\mathcal{U}_0 \equiv \begin{pmatrix} \mathcal{A}_0 & \mathcal{B}_0 \\ -\mathcal{B}_0^* & \mathcal{A}_0^* \end{pmatrix} \quad (2.1.4)$$

and $\mathcal{A}_0, \mathcal{B}_0$

$$\mathcal{A}_0(t_f, t_i; a) = \frac{\Gamma(1-\nu)}{\sqrt{2\pi}} \left[D_\nu(z_f) D_{\nu-1}(-z_i) + D_\nu(-z_f) D_{\nu-1}(z_i) \right] \quad (A.1.2)$$

$$\mathcal{B}_0(t_f, t_i; a) = \frac{\Gamma(1-\nu)}{a^* \sqrt{\pi}} e^{i\frac{\pi}{4}} \left[-D_\nu(z_f) D_\nu(-z_i) + D_\nu(-z_f) D_\nu(z_i) \right] \quad (A.1.3)$$

$$\nu := i \frac{|a|^2}{2}, \quad z_i = \sqrt{2} e^{-i\frac{\pi}{4}} t_i, \quad z_f = \sqrt{2} e^{-i\frac{\pi}{4}} t_f \quad (A.1.4)$$

In Eq.(A.1.2),(A.1.3), there 6 different terms. Using the asymptotic expansion of PCF in $t_f > 0, t_i < 0$ and keeping leading order terms in $1/t_i, 1/t_f$ [23, 24, 96] we

get

$$\begin{aligned}
D_\nu(z_f) &\sim \exp\left(\frac{1}{8}\pi|a|^2 + i\varphi_f\right) \\
D_\nu(-z_i) &\sim \exp\left(\frac{1}{8}\pi|a|^2 + i\varphi_i\right) \\
D_{\nu-1}(-z_i) &\sim \frac{\exp\left(\frac{1}{8}\pi|a|^2 + i\varphi_i + i\frac{\pi}{4}\right)}{\sqrt{2}|t_i|} \\
D_\nu(-z_f) &\sim \exp\left(-\frac{3}{8}\pi|a|^2 + i\varphi_f\right) + \frac{\sqrt{\pi}}{\Gamma(-\nu)|t_f|} \exp\left(-\frac{1}{8}\pi|a|^2 - i\varphi_f + i\frac{\pi}{4}\right) \\
D_\nu(z_i) &\sim \exp\left(-\frac{3}{8}\pi|a|^2 + i\varphi_i\right) + \frac{\sqrt{\pi}}{\Gamma(-\nu)|t_i|} \exp\left(-\frac{1}{8}\pi|a|^2 - i\varphi_i + i\frac{\pi}{4}\right) \\
D_{\nu-1}(z_i) &\sim \frac{\sqrt{2\pi}}{\Gamma(1-\nu)} \exp\left(-\frac{1}{8}\pi|a|^2 - i\varphi_i\right) \\
&\quad - \frac{1}{\sqrt{2}|t_i|} \exp\left(-\frac{3}{8}\pi|a|^2 + i\varphi_i + i\frac{\pi}{4}\right)
\end{aligned}$$

The leading order term in Eq.(A.1.2),(A.1.3) are

$$\mathcal{A}_0(t_f, t_i) \sim e^{-\pi|a|^2/2 + i(\varphi_f - \varphi_i)}, \quad \mathcal{B}_0(t_f, t_i) \sim -(1 - e^{-\pi|a|^2})^{1/2} e^{i\vartheta} \quad (\text{A.1.5})$$

$$\vartheta = \varphi_i + \varphi_f + \frac{\pi}{4} + \arg \Gamma(1 - \nu) + \arg a \quad (\text{A.1.6})$$

$$\varphi_i := \frac{1}{2}(t_i^2 + \frac{1}{2}|a|^2 \ln 2t_i^2), \quad \varphi_f := \frac{1}{2}(t_f^2 + \frac{1}{2}|a|^2 \ln 2t_f^2) \quad (\text{A.1.7})$$

The transition probability is defined as in Eq.(2.1.9). From Eq. (A.1.5), directly follows

$$\mathcal{P}_0(a) = e^{-\pi|a|^2} \quad (\text{A.1.8})$$

A.1.2 Half evolution

$$z_f = \sqrt{2}e^{-i\pi/4}t, t_f > 0$$

$$\begin{aligned}
\mathcal{A}_{0,+} &= \frac{\Gamma(1-\nu)}{\sqrt{2\pi}} D_{\nu-1}(0) \left(D_\nu(-z_f) + D_\nu(z_f) \right) \\
\mathcal{B}_{0,+} &= \frac{\Gamma(1-\nu)}{a^* \sqrt{\pi}} e^{i\frac{\pi}{4}} D_\nu(0) \left(-D_\nu(z_f) + D_\nu(-z_f) \right) \\
\mathcal{A}_{0,-} &= \frac{\Gamma(1-\nu)}{\sqrt{2\pi}} D_\nu(0) \left(D_{\nu-1}(z_f) + D_{\nu-1}(-z_f) \right) \\
\mathcal{B}_{0,-} &= \frac{\Gamma(1-\nu)}{a^* \sqrt{\pi}} e^{i\frac{\pi}{4}} D_\nu(0) \left(-D_\nu(z_f) + D_\nu(-z_f) \right)
\end{aligned}$$

$$\begin{aligned}
\mathcal{A}_{0,+} &\sim \frac{\Gamma(1-\nu)}{\sqrt{2\pi}} D_{\nu-1}(0) (e^{-3\pi a^2/8} + e^{\pi a^2/8}) e^{i\varphi_f} \\
\mathcal{B}_{0,+} &\sim \frac{\Gamma(1-\nu)}{a^* \sqrt{\pi}} D_{\nu}(0) (e^{-3\pi a^2/8} - e^{\pi a^2/8}) e^{i(\varphi_f + \frac{\pi}{4})} \\
\mathcal{A}_{0,-} &\sim D_{\nu}(0) e^{-\pi a^2/8 - i\varphi_f} \\
\mathcal{B}_{0,-} &\sim \frac{\Gamma(1-\nu)}{a \sqrt{\pi}} D_{\nu}(0) (e^{-3\pi a^2/8} - e^{\pi a^2/8}) e^{i(\varphi_f + \frac{\pi}{4})} \\
|\mathcal{A}_{0,+}|^2 &\sim \frac{1}{2} (1 + e^{-\pi a^2/2})
\end{aligned}$$

A.2 Symmetries

Eq.(A.1.1) ($a \in \mathbb{R}$) exhibits the following properties that also generalize to $b \neq 0$

$$i\partial_t |\psi\rangle = \left[-t\sigma_3 + a\sigma_1 + f_D(t;b)\sigma_\varphi \right] |\psi\rangle \quad (3.2.2)$$

with $\sigma_\varphi \equiv \cos \varphi \sigma_1 + \sin \varphi \sigma_2$.

1. "Time reversal symmetry": Formalizing the "trick" used in [97], we can relate $\mathcal{U}_0(t, 0)$ and $\mathcal{U}_0(0, -t)$, $t > 0$. Let $\tau := -t$ and $|\varphi(\tau)\rangle \equiv \sigma_3 |\psi(-\tau)\rangle$. From Eq.(3.2.2)

$$\begin{aligned} -i\partial_\tau |\psi(-\tau)\rangle &= \left(\tau\sigma_3 + a\sigma_1 + f_D(\tau;b)\sigma_\varphi \right) |\psi(-\tau)\rangle, \quad f_D(\tau;b) = f_D(-\tau;b) \\ i\partial_\tau |\psi(-\tau)\rangle &= \left(-\tau\sigma_3 - a\sigma_1 - f_D(\tau;b)\sigma_\varphi \right) |\psi(-\tau)\rangle \\ i\partial_\tau (\sigma_3 |\psi(-\tau)\rangle) &= \sigma_3 \left(-\tau\sigma_3 + a\sigma_1 - f_D(\tau;b)\sigma_\varphi \right) \sigma_3^2 |\psi(-\tau)\rangle, \quad \sigma_3^3 = \mathbb{1} \\ i\partial_\tau |\varphi(\tau)\rangle &= \sigma_3 \left(-\tau\sigma_3 + a\sigma_1 + f_D(\tau;b)\sigma_\varphi \right) \sigma_3 |\varphi(\tau)\rangle, \quad \sigma_3 \sigma_{1,2} \sigma_3 = -\sigma_{1,2} \\ i\partial_\tau |\varphi(\tau)\rangle &= H(t; a, b) |\varphi(\tau)\rangle \end{aligned}$$

Relabel τ with t . From the uniqueness of solutions (up to irrelevant complex phases)

$$|\varphi(t)\rangle = \mathcal{U}(t, 0) |\varphi(0)\rangle \Rightarrow |\psi(0)\rangle = \sigma_3 \mathcal{U}^\dagger(t, 0) \sigma_3 |\psi(-t)\rangle$$

and therefore

$$\sigma_3 \mathcal{U}^\dagger(t, 0) \sigma_3 = \mathcal{U}(0, -t)$$

Expanding the matrices

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \mathcal{A}_+ & \mathcal{B}_+ \\ -\mathcal{B}_+^* & \mathcal{A}_+^* \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \stackrel{!}{=} \begin{pmatrix} \mathcal{A}_+^* & \mathcal{B}_+ \\ -\mathcal{B}_+^* & \mathcal{A}_+ \end{pmatrix}$$

we get

$$\mathcal{A}_- = \mathcal{A}_+^*, \quad \mathcal{B}_- = \mathcal{B}_+ \quad (\text{A.2.1})$$

with $\mathcal{A}_\pm, \mathcal{B}_\pm$ being the elements of $\mathcal{U}(t, 0)$ and $\mathcal{U}(0, -t)$ respectively.

2. The generalization of $\mathcal{P}_0(a) = \mathcal{P}_0(-a)$ Eq.(2.1.10)

$$\mathcal{P}(a, b) = \mathcal{P}(-a, -b) \quad (\text{A.2.2})$$

Using the properties $\sigma_3 \sigma_j \sigma_3 = -\sigma_j$, $j = 1, 2$ and $f(t; b) = -f(t; -b)$ Tab.(3.1)

$$H(t; a, b) = -t\sigma_3 + a\sigma_1 + f(t; b)\sigma_\varphi = \sigma_3 H(t; -a, -b) \sigma_3$$

from which follows

$$\mathcal{U}(t_f, t_i; a, b) = \sigma_3 \mathcal{U}(t_f, t_i; -a, -b) \sigma_3$$

and subsequently

$$\mathcal{A}(t_f, t_i; a, b) = \mathcal{A}(t_f, t_i; -a, -b)$$

which proves Eq.(A.2.2) by taking the limits $t_f \rightarrow +\infty, t_i \rightarrow -\infty$.

3. In Eq.(A.1.5), letting $t_f = -t_i$ leads to $\mathcal{A}_0 \in \mathbb{R}$. This is a consequence of Eq.(A.2.1) and the property $\mathcal{U}(t_f, t_i) = \mathcal{U}(t_f, t_0) \mathcal{U}(t_0, t_i)$. For $t_f = -t_i = t > 0$ and $t_0 = 0$

$$\mathcal{U}(t) = \mathcal{U}_+(t) \mathcal{U}_-(t)$$

Expanding the matrices

$$\begin{aligned} \mathcal{A} &= \mathcal{A}_+ \mathcal{A}_- - \mathcal{B}_+ \mathcal{B}_-^* \\ \mathcal{B} &= \mathcal{A}_+ \mathcal{B}_- + \mathcal{A}_-^* \mathcal{B}_+ \end{aligned}$$

and in combination with Eq.(A.2.1)

$$\mathcal{A} = |\mathcal{A}_+|^2 - |\mathcal{B}_+|^2 = 2|\mathcal{A}_+|^2 - 1 = 2|\mathcal{A}_-|^2 - 1 \in \mathbb{R} \quad (\text{A.2.3})$$

$$\mathcal{B} = 2\mathcal{A}_+ \mathcal{B}_+ = 2\mathcal{A}_-^* \mathcal{B}_- \quad (\text{A.2.4})$$

A.3 LZ via Dyson Series

The first account of this calculation can be found in the Appendix of [39]. The result is obtained by summing the Dyson series, treating the term $H_1 = a\sigma_1$ as a perturbation to the trivially integrable $H_0 = -t\sigma_3$. The proof is very brief and no technical details are provided.

Essential is the change of variables that disentangle the multi dimensional integrals. Quoting from [39]

$$\begin{aligned} x_1 &= t_1 \\ x_p &= t_1 + \sum_{j=1}^{p-1} t_{2j+1} - t_{2j}, \quad 2 \leq p \leq n \\ y_p &= t_{2p} - t_{2p-1} \end{aligned} \quad (\star\star)$$

An extended version of the proof can be found in [98] and other places but $(\star\star)$ is cited from [39] without any further justification. The transformation works for all orders and allows us to calculate the general term in closed form, from which the LZ formula emerges as the exponential series. $(\star\star)$ is arguably unmotivated and more importantly, the range of the new variables is not apparent. In contrast to the compact form of $(\star\star)$, we will break down the coordinate transformation into multiple steps, making the geometric meaning evident.

In the same spirit, an alternative approach can be found in [40]. The Dyson series are summed without relying on sophisticated change of variables. A similar calculation arises in a classical problem, related to the quantum mechanical Landau Zener [99, 100].

The starting point is Eq.(C.1.7) for $f(t) \equiv a \in \mathbb{R}^*$.

$$\mathcal{A}_1 = 1 + \sum_{n=1}^{\infty} (-i)^{2n} a^{2n} \int_{I_{2n}} \prod_{j=1}^{2n} dt_j \exp(i\Lambda_{2n}) \quad (\text{A.3.1})$$

$$\Lambda_{2n} = \sum_{k=1}^n (-1)^k t_{2k}^2 \quad (\text{C.1.6})$$

with $I_n = \{t_1 > t_2, \dots > t_n\} \subset \mathbb{R}^n$.

The first step is the change of variables, which works $\forall n \in \mathbb{N}$ (in our case replace $n \rightarrow 2n$). Let $(t_1, \dots, t_n) \in I_n \subset \mathbb{R}^n$

$$\left\{ \begin{array}{l} t_1 - t_2 = y_1 \\ t_2 - t_3 = y_2 \\ \vdots \\ t_{n-1} - t_n = y_{n-1} \\ t_n = x \end{array} \right\} \Rightarrow \left\{ \begin{array}{l} t_1 = y_1 + y_2 + \dots + y_{n-1} + x \\ t_2 = y_2 + \dots + y_{n-1} + x \\ \vdots \\ t_n = y_{n-1} + x \\ t_n = x \end{array} \right. \quad (\text{A.3.2})$$

The Jacobian of the transformation is upper triangular with $\det J = 1$

$$J = \begin{pmatrix} 1 & 1 & \dots & 1 \\ 0 & 1 & \dots & 1 \\ \vdots & \ddots & & \\ 0 & 0 & \dots & 1 \end{pmatrix}$$

and the new coordinates take values in

$$x \in (-\infty, +\infty), \quad y_i \in (0, +\infty), \quad i = 1, \dots, n-1$$

In order to understand the geometric meaning behind Eq.(A.3.2), consider the case $n = 3$

$$\begin{aligned} t_1 - t_2 &= y_1 \\ t_2 - t_3 &= y_2 \\ y_3 &= x \end{aligned}$$

with $(t_1, t_2, t_3) \in I_3 = \{t_1 > t_2 > t_3\} \subset \mathbb{R}^3$. The first equation describes a family of planes, parametrized by y_1

$$\Pi(y_1) := \{(t_1, t_2, t_3) \in \mathbb{R}^3 : t_1 - t_2 = y_1\}$$

and the system of the first two equations describes lines (rank = 2, $3 - 2 = 1$) parametrized by y_1, y_2

$$E(y_1, y_2) := \{t_1 - t_2 = y_1, t_2 - t_3 = y_2\}$$

Since $\Pi(y_1)$ are orthogonal to (t_1, t_2) plane and parallel to each other, $\{\Pi(y_1)\}_{y_1>0}$ is a partition of the half space $t_1 > t_2$, blue planes in Fig.A.1 (left). Similarly, for constant $y_1 > 0$, the lines $\{E(y_1, y_2)\}_{y_2>0}$ are parallel to each other and partition the half plane $\Pi(y_1)|_{t_2>t_3}$, red lines in Fig.A.1 (left). I_3 decomposes into parallel lines

$$I_3 = \bigcup_{y_1>0} \Pi(y_1) = \bigcup_{y_1>0} \bigcup_{y_2>0} E(y_1, y_2)$$

The parameter $x \in (-\infty, +\infty)$, parametrizes each such line.

Back to Eq.(A.3.2), for $n \rightarrow 2n$, the integrals in Eq.(C.1.5) transforms to

$$\int_{I_{2n}} dt_1 \dots dt_{2n} = \int_{-\infty}^{\infty} dx \times \prod_{k=1}^{2n-1} \int_0^{\infty} dy_k$$

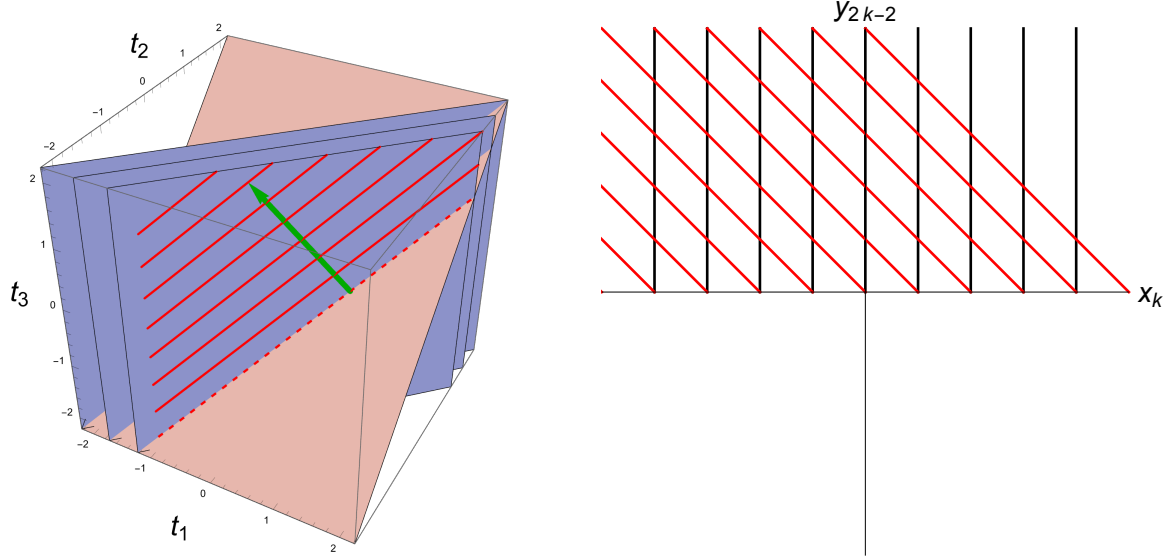


Figure A.1. Left: $n = 3$. Blue planes correspond to $t_1 - t_2 = y_1$, parametrized by $y_1 > 0$. For constant y_1 , red lines correspond to $t_2 - t_3 = y_2 < 0$ ($y_2 < 0$ for better visualization). y_2 takes values across the green axes and x along the red lines. **Right:** (x_k, y_{2k-2}) plane. Red lines correspond to fixed x_{k-1} and black lines to fixed $y_{2k-2} > 0$.

From Eq.(C.1.6), grouping together consecutive terms and substituting Eq.(A.3.2)

$$\begin{aligned}
 -\Lambda_{2n} &= (t_1^2 - t_2^2) + \cdots + (t_{2n-1}^2 - t_{2n}^2) \\
 &= (t_1 - t_2)(t_1 + t_2) + \cdots + (t_{2n-1} - t_{2n})(t_{2n-1} + t_{2n}) \\
 &= y_1(2t_2 + y_1) + \cdots + y_{2n-1}(2t_n + y_{2n-1}) \\
 &= (y_1^2 + y_3^2 + \cdots + y_{2n-1}^2) + \\
 &\quad + 2y_1(y_2 + y_3 + \cdots + y_{2n-1} + x) \\
 &\quad + 2y_3(y_4 + y_5 + \cdots + y_{2n-1} + x) \\
 &\quad + \cdots \\
 &\quad + 2y_{2n-1}x
 \end{aligned}$$

The odd-odd products, eg. $y_1y_3, y_1y_5 \dots$ complete the square $(y_1 + y_3 + \cdots + y_{2n-1})^2$

$$\begin{aligned}
 -\Lambda_{2n} &= (y_1 + y_3 + \cdots + y_{2n-1})^2 + \\
 &\quad + 2y_1(y_2 + y_4 + \cdots + y_{2n-2} + x) \\
 &\quad + 2y_3(y_4 + y_6 + \cdots + y_{2n-2} + x) \\
 &\quad + \cdots \\
 &\quad + y_{2n-3}(y_{2n-2} + x) \\
 &\quad + y_{2n-1}x
 \end{aligned}$$

The next step is to make a sequence of change of variables that simplify the last expression

$$x_n = x, \quad x_{k-1} = x_k + y_{2k-2}, \quad k = 1, \dots, n-1 \quad (\text{A.3.3})$$

$x_{k-1} \in \mathbb{R}$ labels the red lines and x_k runs takes values along $x_{k-1} = \text{const}$ line, $x_{k-1} > x_k$, A.1 (right). Iteratively, $x_1 > x_2 > \dots > x_n$.

Continuing from where we left

$$-\Lambda_{2n} = (y_1 + y_3 + \dots + y_{2n-1})^2 + 2(x_1 y_1 + x_2 y_3 + \dots + x_n y_{2n-1})$$

and after relabeling $y_{2k-1} \rightarrow y_k$

$$-\Lambda_{2n} = \left(\sum_{k=1}^n y_k\right)^2 + 2 \sum_{k=1}^n x_k y_k \quad (\text{A.3.4})$$

Combining all the above with Eq.(C.1.5)

$$\mathcal{A}_1^{(2n)} = \int_{-\infty}^{\infty} dx_1 \int_{x_1}^{\infty} dx_2 \dots \int_{x_{n-1}}^{\infty} dx_n \times \prod_{k=1}^n \int_0^{\infty} dy_k e^{i\Lambda_{2k}(x,y)} \quad (\text{A.3.5})$$

Under the integral $\prod_{k=1}^n \int_0^{\infty} dy_k$, $e^{i\Lambda_{2n}(x,y)}$ has permutation invariance in x 's. It is sufficient to prove the statement for transpositions $x_i \leftrightarrow x_j$ since every permutation decomposes to a finite product of transpositions [101]. Let

$$-\Lambda_{2n}(x_i \leftrightarrow x_j) = \exp\left(\left(\sum_{k=1}^n y_k\right)^2 + 2(\dots + x_i y_j + x_j y_i + \dots)\right)$$

Under the integral $\prod_{k=1}^n \int_0^{\infty} dy_k$, y_i, y_j are dummy variables and thus we can relabel $y_i \leftrightarrow y_j$ which effectively negates the transposition of x_i, x_j . The term $\sum_{k=1}^n y_k$ is obviously unaffected.

Let $I_\pi = \{x_{\pi(1)} > \dots > x_{\pi(n)}\}$ with $\pi \in S_n$, S_n being the symmetric group, or group of permutations of length n . Up to measure zero set, $\{I_\pi\}_{\pi \in S_n}$ form a partition of $\mathbb{R}^n$.

$$\int_{\mathbb{R}^n} dx_1 \dots dx_n f(x_1, \dots, x_n) = \int_{\cup_{\pi \in S_n} I_\pi} dx_1 \dots dx_n f(x_1, \dots, x_n)$$

After relabeling $x_{\pi(k)} \rightarrow x_k \Rightarrow x_k = x_{\pi(\pi^{-1}(k))} \rightarrow x_{\pi^{-1}(k)}$, using the permutation invariance of f and $|S_n| = n!$ we get

$$\begin{aligned} \sum_{\pi \in S_n} \int_{I_\pi} dx_1 \dots dx_n f(x_1, \dots, x_n) &= \sum_{\pi \in S_n} \int_{I_{\text{id}}} dx_1 \dots dx_n f(x_{\pi^{-1}(1)}, \dots, x_{\pi^{-1}(n)}) \\ &= \sum_{\pi \in S_n} \int_{I_{\text{id}}} dx_1 \dots dx_n f(x_1, \dots, x_n) \\ &= n! \int_{I_{\text{id}}} dx_1 \dots dx_n f(x_1, \dots, x_n) \end{aligned}$$

From Eq.(A.3.5), using the previous result

$$\mathcal{A}_1^{(2n)} = \frac{1}{n!} \int_{-\infty}^{\infty} dx_n \cdots \int_{-\infty}^{\infty} dx_1 \times \int_0^{\infty} dy_n \cdots \int_0^{\infty} dy_1 e^{i\Lambda_{2n}(x,y)} \quad (\text{A.3.6})$$

The final expression is obtained with the help of the Dirac delta properties

$$\int_{\mathbb{R}} dx_k e^{ix_k y_k} = \frac{\pi}{2} \delta(y_k) \quad (\text{A.3.7})$$

$$\int_0^{\infty} dy \delta(y) f(y) = \frac{1}{2} f(0) \quad (\text{A.3.8})$$

$$\begin{aligned} \mathcal{A}_1^{(2n)} &= \frac{1}{n!} \prod_{k=1}^n \int_{\mathbb{R}} dx_k e^{-2ix_k y_k} \left(\prod_{j=1}^n \int_0^{\infty} dy_j \right) e^{-i(\sum_{l=1}^n y_l)^2} \\ &= \frac{\pi^n}{n!} \left(\prod_{j=1}^n \int_0^{\infty} dy_j \delta(y_j) \right) e^{-i(\sum_{l=1}^n y_l)^2} \\ &= \frac{\pi^n}{2^n n!} \end{aligned}$$

with the last equality obtained by repeated application of Eq.(A.3.8). Finally from Eq.(A.3.6)

$$\mathcal{A}_1 = 1 + \sum_{k=1}^{\infty} \frac{(-i)^{2k}}{k!} \frac{\pi^k a^{2k}}{2^k} = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{-\pi a^2}{2} \right)^k = e^{-\pi a^2/2}$$

The use of Eq.(A.3.8) is ambiguous since $\delta(t)$ is centered at the boundary of the integration. [40] suffers from similar problem regarding the step function. Although Eq.(A.3.8) can be regarded as part of the definition of the Dirac delta, [93, 102], an additional justification in our case is the following. The second order term in the series can be also calculated via Eq.(C.1.8), which reduces to the known Gaussian integral

$$\int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{t_1} dt_2 e^{i(t_2^2 - t_1^2)} = \frac{1}{2} \left| \int_{-\infty}^{+\infty} dt_1 e^{-it_1^2} \right|^2 = \frac{1}{2} \left| \sqrt{\frac{\pi}{-i}} \right|^2 = \frac{\pi}{2}$$

On the other hand, applying the coordinate transformation Eq.(A.3.2) for $n = 2$

$$\begin{aligned} \int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{t_1} dt_2 e^{i(t_2^2 - t_1^2)} &= \int_{-\infty}^{\infty} dx \int_0^{\infty} dy e^{-iy(y+2x)} \\ &= \int_0^{\infty} dy e^{-iy^2} \int_{-\infty}^{\infty} dx e^{-2ixy} \\ &= \pi \int_0^{\infty} dy e^{-iy^2} \delta(y) \stackrel{!}{=} \frac{\pi}{2} \end{aligned}$$

thus $\int_0^{\infty} dy e^{-iy^2} \delta(y) \stackrel{!}{=} \frac{1}{2}$.

Appendix B

Complementary to Section 4

B.1 Vanishing gap ($a \rightarrow 0$)

B.1.1 φ independence

For $a = 0$, Eq.(3.2.2) takes the form

$$i\partial_t |\psi\rangle = (-t\sigma_3 + f_D(t;b)\sigma_\varphi) |\psi\rangle \quad (4.1.1)$$

The angle φ can be set to $\varphi = 0$. Let $U_\varphi := \exp(i\frac{\varphi}{2}\sigma_3)$. Expanding the matrix exponential, $U_\varphi = \cos \frac{\varphi}{2} \mathbf{1} + i \sin \frac{\varphi}{2} \sigma_3$. U_φ rotates σ_1 to σ_φ

$$\begin{aligned} U_\varphi^\dagger \sigma_1 U_\varphi &= (\cos \frac{\varphi}{2} - i \sin \frac{\varphi}{2} \sigma_3) \sigma_1 (\cos \frac{\varphi}{2} + i \sin \frac{\varphi}{2} \sigma_3) \\ &= (\cos \frac{\varphi}{2} \sigma_1 - i \sin \frac{\varphi}{2} \sigma_3 \sigma_1) (\cos \frac{\varphi}{2} + i \sin \frac{\varphi}{2} \sigma_3) \\ &= \cos^2 \frac{\varphi}{2} \sigma_1 + i \sin \frac{\varphi}{2} \cos \frac{\varphi}{2} [\sigma_1, \sigma_3] + \sin \frac{\varphi}{2} \sigma_3 \sigma_1 \sigma_3 \\ &= (\cos^2 \frac{\varphi}{2} - \sin^2 \frac{\varphi}{2}) \sigma_1 + 2 \sin \frac{\varphi}{2} \cos \frac{\varphi}{2} \sigma_2 \\ &= \sigma_1 \cos \varphi + \sigma_2 \sin \varphi \\ &= \sigma_\varphi \end{aligned}$$

Substituting $\sigma_\varphi = U_\varphi^\dagger \sigma_1 U_\varphi$ in Eq.(4.1.1)

$$\begin{aligned} i\partial_t |\psi\rangle &= \left[-t\sigma_3 + f_D(t;b) U_\varphi^\dagger \sigma_1 U_\varphi \right] |\psi\rangle, \quad [U_\varphi, \sigma_3] = 0 \\ &= U_\varphi^\dagger \left[-t\sigma_3 + f_D(t;b) \sigma_1 \right] U_\varphi |\psi\rangle \\ &= U_\varphi^\dagger H(t;0,b) U_\varphi |\psi\rangle \end{aligned}$$

we get $\mathcal{U}^\varphi = U_\varphi^\dagger \mathcal{U}^{\varphi=0} U_\varphi$ and

$$\begin{aligned} \mathcal{P}^\varphi &= |\langle + | \mathcal{U}^\varphi | + \rangle|^2 \\ &= \left| \langle + | U_\varphi^\dagger \mathcal{U}^{\varphi=0} U_\varphi | + \rangle \right|^2, \quad U_\varphi | + \rangle = e^{i\frac{\varphi}{2}} | + \rangle \\ &= \left| \langle + | + \rangle \mathcal{U}^{\varphi=0} | + \rangle \right|^2 \\ &= \mathcal{P}^{\varphi=0} \end{aligned}$$

B.1.2 Derivation of Eq.(4.1.7)

Setting $\varphi = 0$ in Eq.(3.2.2) and $f_D = f_D^r$

$$i\partial_t |\psi\rangle = \left[-t\sigma_3 + \frac{b}{2} \mathbf{1} \left(|t| < \frac{\pi}{2b} \right) \sigma_1 \right] |\psi\rangle, \quad b > 0 \quad (4.1.6)$$

For $b = 0$, $i\partial_t |\psi\rangle = -t\sigma_3 |\psi\rangle \Rightarrow |\psi_f\rangle = e^{i\tilde{\zeta}\sigma_3} |\psi_i\rangle$, $\tilde{\zeta} := \frac{t_f^2 - t_i^2}{2}$. For $|\psi_i\rangle = |+\rangle$, $|\psi_f\rangle = e^{i\tilde{\zeta}\sigma_3} |+\rangle = e^{i\tilde{\zeta}} |+\rangle \Rightarrow \mathcal{P}(0,0) = 1$. For $b > 0$, Eq.(4.1.1) splits into three parts, see Fig.(4.4)

$$\begin{aligned} t < -\frac{\pi}{2b}, \quad i\partial |\psi\rangle &= -t\sigma_3 |\psi\rangle \\ t \in [-\frac{\pi}{2b}, \frac{\pi}{2b}], \quad i\partial |\psi\rangle &= (-t\sigma_3 + \frac{b}{2}\sigma_1) |\psi\rangle \\ t > \frac{\pi}{2b}, \quad i\partial |\psi\rangle &= -t\sigma_3 |\psi\rangle \end{aligned}$$

Let $t_b \equiv \frac{\pi}{2b}$. For $|t| > t_b$, the time evolution is trivial. For $|t| < t_b$, Eq.(4.1.6) reduces to Eq.(A.1.1) with $a \rightarrow \frac{b}{2}$.

Let $t_i = -t_f$ and $t_f > t_b$. From Eq.(??)

$$\mathcal{A}(t_f - t_f; 0, b) = 2|\mathcal{A}(t_f, 0; 0, b)|^2 - 1 \quad (B.1.1)$$

Splitting the time evolution $[0, t_f]$ to $[0, t_b] \cup [t_b, t_f]$

$$\mathcal{A}(t_f, 0; 0, b) = e^{i(t_f^2 - t_b^2)/2} \mathcal{A}_0(t_b, 0; \frac{b}{2}) \quad (B.1.2)$$

with $\mathcal{A}_0$ given by Eq.(A.1.2)

$$\mathcal{A}_0(t_b, 0; b/2) = \frac{\Gamma(1 - \nu_b)}{\sqrt{2\pi}} D_{\nu_b-1}(0) (D_{\nu_b}(z_b) + D_{\nu_b}(-z_b)) \quad (B.1.3)$$

$$\nu_b = ib^2/8, \quad z_b = \sqrt{2}t_b e^{-i\pi/4}$$

The last equations simplifies further using the value of PCF at $z = 0$, Eq.(D.2.2), the relation between the even part of PCF to the Confluent Hypergeometric Function, Eq.(D.2.9), and the Legendre Duplication formula for the Gamma function, Eq.(D.1.3) Combining the above

$$\mathcal{A}(t_f, 0; b, 0) = e^{-it_f^2/2} \mathcal{M}\left(-\frac{ib^2}{16}, \frac{1}{2}, -i\frac{\pi^2}{4b^2}\right) \quad (B.1.4)$$

$$\mathcal{A}(t_f, -t_f; b, 0) = 2 \left| \mathcal{M}\left(-\frac{ib^2}{16}, \frac{1}{2}, -i\frac{\pi^2}{4b^2}\right) \right|^2 - 1 \quad (\text{B.1.5})$$

The limit $t_f \rightarrow \infty$ in the last equation is trivial since t_f drops out. Combining the above we get

$$\mathcal{P}^r(0, b) = \left(2 \left| \mathcal{M}\left(-\frac{ib^2}{16}, \frac{1}{2}, -i\frac{\pi^2}{4b^2}\right) \right|^2 - 1 \right)^2 \quad (\text{4.1.7})$$

with $\mathcal{M}(\alpha, \beta; z) = {}_1F_1(\alpha, \beta; z)$ the Confluent Hypergeometric Function, see Eq.(D.3.1).

$${}_1F_1(\alpha, \beta; z) := \sum_{k=0}^{\infty} \frac{(\alpha)^k}{(\beta)^k} \frac{z^k}{k!}, \quad (\text{D.3.1})$$

with $(a)^k = a(a+1)\dots(a+k-1)$ the rising factorial. Eq.(4.1.7) was derived for $b > 0$ but is true $\forall b \in \mathbb{R}$ since $\mathcal{P}(0, b)$ is even in b , Eq.(A.2.2), and the value at $b = 0$ understood as the limit $\lim_{b \rightarrow 0} \mathcal{P}^r(0, b) = 1$, see Eq.(D.3.2).

B.1.3 Derivation of Eq.(4.1.9)

In Eq.(4.1.7), in the limit $b \rightarrow \infty$, $\alpha_b = -i\frac{b^2}{16} \rightarrow \infty$ and $z_b = -i\frac{\pi^2}{4b^2} \rightarrow 0$ but the product $x \equiv \alpha z$ is kept constant. $\mathcal{M}(\alpha, \beta, -|x|/\alpha)$ is related to the Bessel function of the 1st kind, Eq.(D.3.3)

$$\lim_{\alpha \rightarrow \infty} \mathcal{M}(\alpha, \beta, -|x|/\alpha) = \Gamma(\beta) |x|^{\frac{1}{2}(1-\beta)} J_{1-\beta}(2\sqrt{|x|}) \quad (\text{D.3.3})$$

Let $y = 2\sqrt{|x|}$. For $\beta = 1/2$, $J_{-1/2}(y) = \sqrt{\frac{2}{\pi y}} \cos y$, $\Gamma(\frac{1}{2}) = \sqrt{\pi}$, Eq.(D.3.3) becomes

$$\lim_{\alpha \rightarrow \infty} \mathcal{M}(\alpha, \frac{1}{2}, -\frac{y^2}{4\alpha}) = \cos(y) \quad (\text{B.1.6})$$

For $x = \frac{\pi^2}{64}$, $y = \frac{\pi}{4}$, combining Eq.(B.1.6) with Eq.(4.1.7) $\lim_{b \rightarrow \infty} \mathcal{P}^r(0, b) = 0$.

Let $\epsilon \equiv \frac{1}{\alpha} = i\frac{16}{b^2} \rightarrow 0$. We want to expand Eq.(4.1.7) in powers of ϵ and find the leading order behavior. To do so, we have to keep up to ϵ^2 terms in Eq.(D.3.1).

$$\begin{aligned} (\alpha)^k z^k &= \alpha(\alpha+1)\dots(\alpha+k-1)z^k = (\alpha z)^k (1 + \frac{1}{\alpha}) \dots (1 + \frac{k-1}{\alpha}) \\ &= x^k (1 + \epsilon)(1 + 2\epsilon) \dots (1 + (k-1)\epsilon) \\ &= x^k p_k(\epsilon) \end{aligned}$$

with

$$p_k(\epsilon) \equiv (1 + \epsilon)(1 + 2\epsilon) \dots (1 + (k-1)\epsilon) \quad (\text{B.1.7})$$

$p_k(\epsilon)$ is a polynomial in ϵ of order $k-1$. The coefficients $p_k^{(i)}$ with $p_k(\epsilon) = \sum_{i=0}^{k-1} p_k^{(i)} \epsilon^i$ can be found recursively using the relation $p_{k+1} = p_k(1 + k\epsilon)$. We will only need $p_k^{(0)} = 1$, $p_k^{(1)}$ and $p_k^{(2)}$. $p_k^{(1)}$ is given by the known sum

$$p_k^{(1)} = 1 + 2 + \dots + k-1 = \frac{k(k-1)}{2}, \quad k \geq 2 \quad (\text{B.1.8})$$

For $p_k^{(2)}, p_{k+1} = p_k(1+k) = (1+p_k^{(1)}\epsilon + p_k^{(2)}\epsilon^2 + \dots)(1+k\epsilon) \Rightarrow p_{k+1}^{(2)} = p_k^{(2)} + kp_k^{(1)}$ from which $p_k^{(2)}$ reduces to known sums of powers $p_k^{(2)} = \sum_{i=2}^{k-1} ip_i^{(1)} = \sum_{i=2}^{k-1} i \frac{i(i-1)}{2}$

$$p_k^{(2)} = \frac{1}{24}k(k-1)(k-2)(3k-1), \quad k \geq 3 \quad (\text{B.1.9})$$

Rearranging the series in Eq.(D.3.3) in power of ϵ

$$\begin{aligned} \mathcal{M}(\alpha, \beta; z) &= \sum_{k=0}^{\infty} \frac{(\alpha)^k z^k}{(\beta)^k k!} = \sum_{k=0}^{\infty} \frac{x^k p_k(\epsilon)}{(\beta)^k k!} \\ &= 1 + \frac{x}{(\beta)^{11!}} + \frac{x^2}{(\beta)^{22!}}(1+\epsilon) + \frac{x^3}{(\beta)^{33!}}(1+\epsilon)(1+2\epsilon) + \dots \\ &= (1 + \frac{x}{(\beta)^{11!}} + \frac{x^2}{(\beta)^{22!}} + \dots) + \epsilon(\frac{x^2}{(\beta)^{22!}} + 3\frac{x^3}{(\beta)^{33!}} + \dots) + \epsilon^2(2\frac{x^3}{(\beta)^{33!}} + 11\frac{x^4}{(\beta)^{44!}} + \dots) + \dots \\ &= \sum_{k=0}^{\infty} \frac{1}{(\beta)^k} \frac{x^k}{k!} + \epsilon \sum_{k=2}^{\infty} \frac{p_k^{(1)}}{(\beta)^k} \frac{x^k}{k!} + \epsilon^2 \sum_{k=3}^{\infty} \frac{p_k^{(2)}}{(\beta)^k} \frac{x^k}{k!} + \dots \\ &= \sum_{k=0}^{\infty} \frac{1}{(\beta)^k} \frac{x^k}{k!} + \epsilon \sum_{k=0}^{\infty} \frac{p_k^{(1)}}{(\beta)^k} \frac{x^k}{k!} + \epsilon^2 \sum_{k=0}^{\infty} \frac{p_k^{(2)}}{(\beta)^k} \frac{x^k}{k!} + \dots \end{aligned}$$

shifting the sums to zero in second to last line for free since $p_k^{(i)} = 0, k < i$. Let

$$\mathcal{M}(\alpha, \beta; z) \equiv c_0 + \epsilon c_1 + \epsilon^2 c_2 + \dots \quad (\text{B.1.10})$$

$$c_0 \equiv \sum_{k=0}^{\infty} \frac{1}{(\beta)^k} \frac{x^k}{k!} \quad (\text{B.1.11})$$

$$c_1 \equiv \sum_{k=0}^{\infty} \frac{p_k^{(1)}}{(\beta)^k} \frac{x^k}{k!} \quad (\text{B.1.12})$$

$$c_2 \equiv \sum_{k=0}^{\infty} \frac{p_k^{(2)}}{(\beta)^k} \frac{x^k}{k!} \quad (\text{B.1.13})$$

By definition, $\epsilon = 16i/b^2$, even powers of ϵ are real and odd terms are imaginary. From Eq.(B.1.10)

$$\begin{aligned} |\mathcal{M}(\alpha, \beta, z)|^2 &= \left| (c_0 - |\epsilon|^2 c_2) + \epsilon c_1 \right|^2 = (c_0 - |\epsilon|^2 c_2)^2 + |\epsilon|^2 c_1^2 \\ &= c_0^2 + (c_1^2 - 2c_0 c_2) |\epsilon|^2 + \cancel{c_2^2 |\epsilon|^4} \end{aligned}$$

and from Eq.(4.1.7)

$$\begin{aligned} \mathcal{P}(0, b) &= (2|\mathcal{M}(\alpha, \beta, z)|^2 - 1)^2 \\ &= ((2c_0^2 - 1) + 2(c_1^2 - 2c_0 c_2) |\epsilon|^2 + \dots)^2 \end{aligned} \quad (\text{B.1.14})$$

The constants $c_i, i = 0, 1, 2$ can be calculated in closed form with the help of Eq.(D.3.3).

From Eq.(B.1.6), $c_0 = \lim_{b \rightarrow \infty} \mathcal{M}(\alpha_b, \beta; z_b) = \cos(\pi/4) = 1/\sqrt{2}$. c_1 can be calculated as follows:

$$2p_k^{(1)} = k^2 - k = 2 - 4(k+1) + (k+1)(k+2)$$

$$\begin{aligned}
 c_1 &= \sum_{k=0}^{\infty} \frac{p_k^{(1)}}{(\beta)^k k!} \frac{x^k}{k!} = \frac{1}{2} \sum_{k=0}^{\infty} \frac{k^2 - k}{(\beta)^k k!} x^k \\
 &= \frac{1}{2} \sum_{k=0}^{\infty} \frac{x^k}{(\beta)^k k!} \left(2 - 4(k+1) + (k+1)(k+2) \right) \\
 &= \sum_{k=0}^{\infty} \frac{x^k}{(\beta)^k k!} - 2 \sum_{k=0}^{\infty} \frac{(k+1)x^k}{(\beta)^k k!} + \frac{1}{2} \sum_{k=0}^{\infty} \frac{(k+1)(k+2)x^k}{(\beta)^k k!} \\
 &= \left[\sum_{k=0}^{\infty} \frac{x^k}{(\beta)^k k!} - 2 \frac{d}{dx} \sum_{k=0}^{\infty} \frac{x^{k+1}}{(\beta)^k k!} + \frac{1}{2} \frac{d^2}{dx^2} \sum_{k=0}^{\infty} \frac{x^{k+2}}{(\beta)^k k!} \right] \Big|_{x \rightarrow -\pi^2/64} \\
 &= \left[\sum_{k=0}^{\infty} \frac{x^k}{(\beta)^k k!} - 2 \frac{d}{dx} \left(x \sum_{k=0}^{\infty} \frac{x^k}{(\beta)^k k!} \right) + \frac{1}{2} \frac{d^2}{dx^2} \left(x^2 \sum_{k=0}^{\infty} \frac{x^k}{(\beta)^k k!} \right) \right] \Big|_{x \rightarrow -\pi^2/64} \\
 &= \left[\cos(y) + \frac{4}{y} \frac{d}{dy} \left(-\frac{y^2}{4} \cos(y) \right) + \frac{2}{y^2} \left(\frac{d^2}{dy^2} - \frac{1}{y} \frac{d}{dy} y \right) \left(\frac{y^4}{16} \cos(y) \right) \right] \Big|_{y \rightarrow \pi/4} \\
 &= \frac{1}{8} y \left(\sin(y) - y \cos(y) \right) \Big|_{y \rightarrow \pi/4} \\
 &= \frac{\pi(4 - \pi)}{128\sqrt{2}}
 \end{aligned}$$

For c_2 the calculation is similar.

$$c_1 = \frac{\pi(4 - \pi)}{128\sqrt{2}} \approx 0.015, \quad c_2 = \frac{\pi(3\pi^3 - 8\pi^2 + 48\pi - 192)}{98304\sqrt{2}} \approx -0.0006 \quad (\text{B.1.15})$$

Substituting back to Eq.(B.1.14)

$$\begin{aligned}
 \mathcal{P}(0, b) &\stackrel{b \rightarrow \infty}{\sim} \left[(2c_0^2 - 1) + 2(c_1^2 - 2c_0c_2)|\epsilon|^2 \right]^2, \quad \epsilon = 1/a_b, \quad \alpha_b = -ib^2/16 \\
 &= 4 \cdot 16^4 \cdot (c_1^2 - 2c_0c_2)^2 \frac{1}{b^8} \\
 &= D/b^8, \quad D \equiv (\pi/12)^2(\pi^2 - 12)^2 \approx 0.311
 \end{aligned}$$

B.1.4 Rectangular with non zero gap

$$H(t; a, b) = H_0(t; a) + H_{\text{CD}}(t; b)$$

$$H_0(t; a) = -t\sigma_3 + a\sigma_1 = \begin{pmatrix} -t & a \\ a & t \end{pmatrix}$$

$$H_{\text{CD}}^\varphi(t; b) = V(t; b) \left(\sigma_1 \cos \varphi + \sigma_2 \sin \varphi \right)$$

For $b = 0$, $V(t; b) = 0$

$$U_0(t_f, t_i; a) = \begin{pmatrix} U_{0,11} & U_{0,12} \\ -U_{0,12}^* & U_{0,11}^* \end{pmatrix}$$

$$\begin{aligned}
U_{0,11} &= \frac{\Gamma(1-\nu(a))}{\sqrt{2\pi}} \left(D_{\nu(a)}(z_f) D_{\nu(a)-1}(-z_i) + D_{\nu(a)}(-z_f) D_{\nu(a)-1}(z_i) \right) \\
U_{0,12} &= \frac{\Gamma(1-\nu(a))}{a^* \sqrt{\pi}} e^{i\frac{\pi}{4}} \left(-D_{\nu(a)}(z_f) D_{\nu(a)}(-z_i) + D_{\nu(a)}(-z_f) D_{\nu(a)}(z_i) \right) \\
\nu(a) &= i \frac{|a|^2}{2}, \quad z_f = t_f \sqrt{2} e^{-i\frac{\pi}{4}}, \quad z_i = t_i \sqrt{2} e^{-i\frac{\pi}{4}}
\end{aligned}$$

For the rectangular pulse $V(t; b) = \frac{b}{2} 1\left(|t| < \frac{\pi}{2b}\right)$, the full Hamiltonian H reduces to H_0 . For $|t| < \frac{\pi}{2b}$

$$\begin{aligned}
H^\varphi(t; a, b) &= \begin{pmatrix} -t & a \\ a & t \end{pmatrix} + \frac{b}{2} \cos \varphi \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{b}{2} \sin \varphi \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\
&= \begin{pmatrix} -t & a + \frac{b}{2} e^{-i\varphi} \\ a + \frac{b}{2} e^{i\varphi} & t \end{pmatrix} \\
&= H_0(t; a')
\end{aligned}$$

$$a'(a, b, \varphi) := a + \frac{b}{2} e^{-i\varphi}$$

extending the definition of $H_0(t; a)$ to complex argument a . For the time evolution matrix, with $|t_f|, |t_i| \gg 1, t_f > 0, t_i < 0$

$$\mathcal{U}(t_f, t_i; a, b) = \mathcal{U}_0(t_f, \frac{\pi}{2b}; a) \mathcal{U}_0(\frac{\pi}{2b}, -\frac{\pi}{2b}; a') \mathcal{U}_0(-\frac{\pi}{2b}, t_i; a)$$

We will use the shorthand notation $\mathcal{U} = \mathcal{U}_+ \mathcal{U}_0 \mathcal{U}_-$ and similarly for the matrix elements $\mathcal{A}, \mathcal{B}$. The transition probability is given by $\mathcal{P} = |\mathcal{A}|^2$. Expanding the matrices we get

$$\mathcal{P} = \mathcal{A}_+ \mathcal{A}_0 \mathcal{A}_- - \mathcal{B}_+ \mathcal{B}_0^* \mathcal{A}_- - \mathcal{A}_+ \mathcal{B}_0 \mathcal{B}_-^* - \mathcal{B}_+ \mathcal{A}_0^* \mathcal{B}_- \quad (\text{B.1.16})$$

Using the time symmetry Eq.(A.2.1)

$$\begin{aligned}
\mathcal{P} &= \mathcal{A}_-^* \mathcal{A}_0 \mathcal{A}_- - \mathcal{B}_- \mathcal{B}_0^* \mathcal{A}_- - \mathcal{A}_-^* \mathcal{B}_0 \mathcal{B}_-^* - \mathcal{B}_- \mathcal{A}_0^* \mathcal{B}_-^* \\
&= |\mathcal{A}_-|^2 \mathcal{A}_0 - |\mathcal{B}_-|^2 \mathcal{A}_0^* - 2 \operatorname{Re}(\mathcal{A}_- \mathcal{B}_- \mathcal{B}_0^*)
\end{aligned}$$

Due to the symmetric integration, $\mathcal{A}_0 \in \mathbb{R}$ Eq.(A.2.3) and from the unitarity of $\mathcal{U}_-$, $|\mathcal{B}_-|^2 = 1 - |\mathcal{A}_-|^2$

$$\mathcal{P} = (2|\mathcal{A}_-|^2 - 1) \mathcal{A}_0 - 2 \operatorname{Re}(\mathcal{A}_- \mathcal{B}_- \mathcal{B}_0^*) \quad (\text{B.1.17})$$

with

$$\begin{aligned}
\mathcal{A}_- &\sim e^{-\pi a^2/8} D_\nu\left(\frac{\pi}{2b}\right) e^{-i\varphi_f} \\
\mathcal{B}_- &\sim \frac{\Gamma(1-\nu)}{a\sqrt{\pi}} e^{i\pi/4+i\varphi_f} e^{\pi a^2/8} \left[D_\nu\left(\frac{\pi}{2b}\right) e^{-\pi a^2/2} - D_\nu\left(-\frac{\pi}{2b}\right) \right] \\
\mathcal{A}_- \mathcal{B}_- &\sim \frac{\Gamma(1-\nu)}{a\sqrt{\pi}} e^{i\pi/4} \left[D_\nu\left(\frac{\pi}{2b}\right) e^{-\pi a^2/2} - D_\nu\left(-\frac{\pi}{2b}\right) \right]
\end{aligned}$$

After further algebraic manipulations using the formulas in App.(D), $\mathcal{P}^x(a, b)$ takes the form

$$\mathcal{P}(a, b) = \left(F(a, b) \mathcal{A}_0(a', b) + 2\pi \operatorname{Re}\{G(a, b) \mathcal{B}_0^*(a', b)\} \right)^2 \quad (\text{B.1.18})$$

$$F(a, b) := 2e^{-\pi a^2/4} |D^+(a, b)|^2 - 1$$

$$G(a, b) := \frac{\Gamma(1 - \nu(a))}{a\sqrt{\pi}} D^+(a, b) (-D^-(a, b) + e^{-\pi a^2/2} D^+(a, b))$$

$$\mathcal{A}_0(a, b) := \left| {}_1F_1\left(-\frac{\nu(a)}{2}, 1/2, -i\frac{\pi^2}{4b^2}\right) \right|^2 - \frac{\pi^2 |a|^2}{4b^2} \left| {}_1F_1\left(\frac{1-\nu(a)}{2}, 3/2, -i\frac{\pi^2}{4b^2}\right) \right|^2$$

$$\mathcal{B}_0(a, b) := \frac{a}{b} e^{i\pi/4} {}_1F_1\left(\frac{1+\nu(a)}{2}, 1/2, i\frac{\pi^2}{4b^2}\right) {}_1F_1\left(\frac{1-\nu(a)}{2}, 3/2, -i\frac{\pi^2}{4b^2}\right)$$

$$D^\pm(a, b) := D_{\nu(a)}\left(\pm z\left(\frac{\pi}{2b}\right)\right), \quad z(t) := t\sqrt{2}e^{-i\pi/4}$$

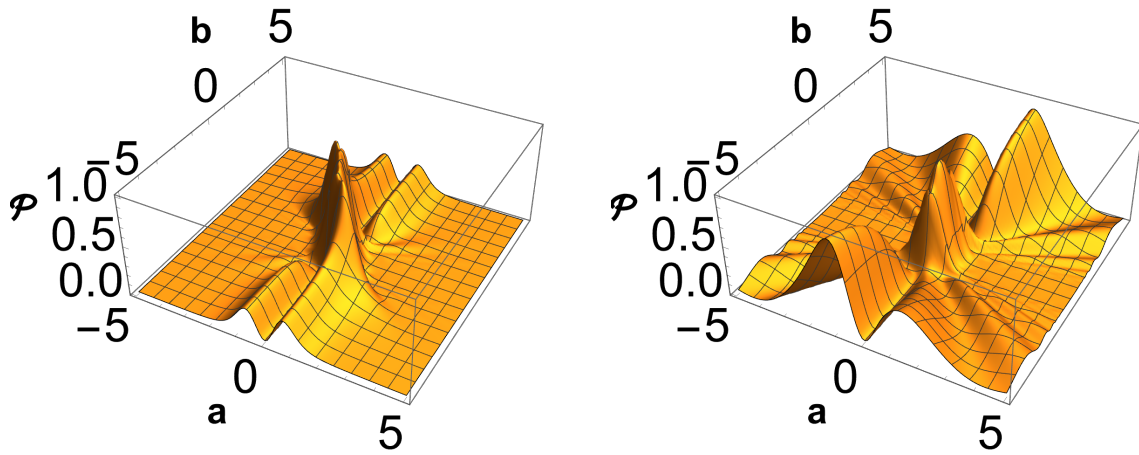


Figure B.1. 3D plot of Eq.(B.1.18), $\varphi = 0$ (left) and $\varphi = \frac{\pi}{2}$ (right). Compare with Fig.(3.8).

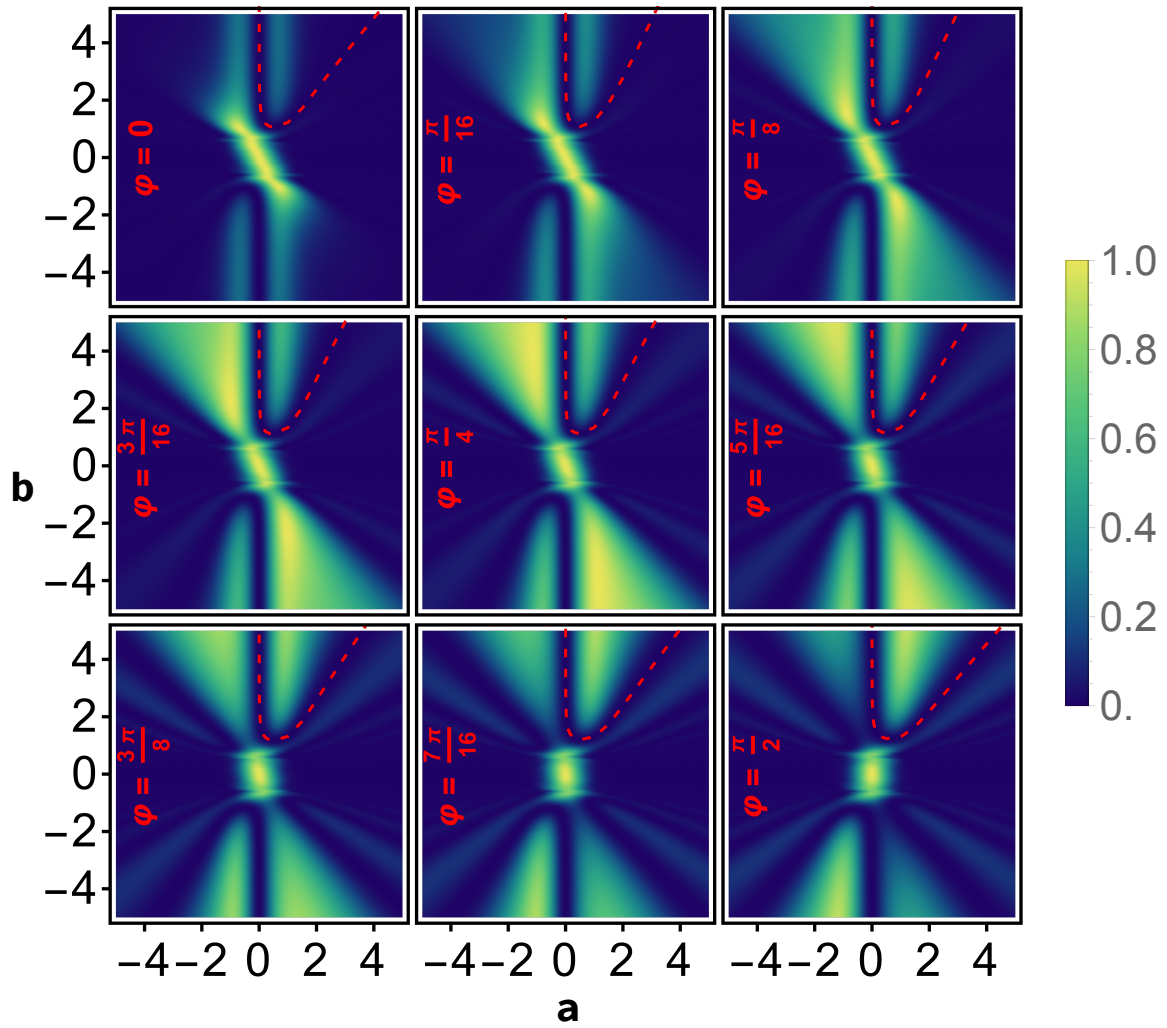


Figure B.2. Heatmap plot of Eq.(B.1.18) for different values of φ . The red dashed line corresponds to the the main branch of the CC. The secondary branched as partially visible.

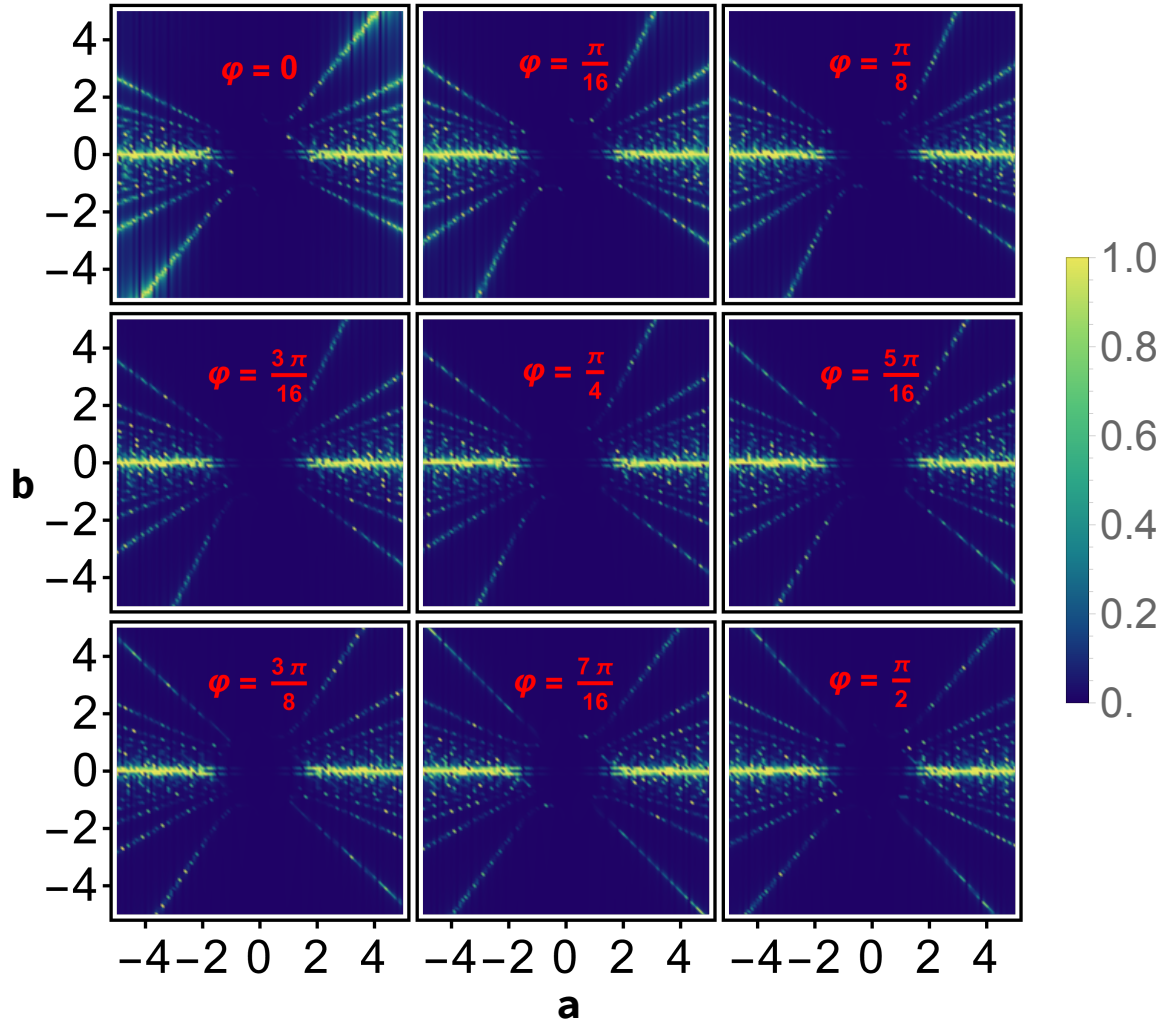


Figure B.3. Relative error between analytic and numerical evaluation of Eq.(B.1.18).

B.1.5 Calculations for Tab.(4.1)

Calculation for the Tab.(4.1).

$$V(b) \equiv \int_{\mathbb{R}} dt e^{-it^2} f_D(t; b)$$

We will make use of the Gaussian integral $\int_{\mathbb{R}} dt e^{-at^2} = (\frac{\pi}{a})^{1/2}$ and the definitions of the error and complementary error functions, $\text{erf}(\cdot)$, $\text{Erfc}(\cdot)$ [27]

$$\text{erf}(z) \equiv \frac{2}{\sqrt{\pi}} \int_0^z dz e^{-z^2}, \quad \text{Erfc}(z) \equiv 1 - \text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty dz e^{-z^2},$$

In all the calculations we assume $b > 0$. For $b = 0$, $f_D(t, 0) = 0$ due to $f_D(t; -b) = -f_D(t; b)$ and $\mathcal{P}(0) = 1$. Similarly for $b < 0$, $V(-b) = -V(b)$, $\mathcal{P}(-b) = \mathcal{P}(b)$, with $\mathcal{P} \equiv \mathcal{P}_{\text{pert}}$, Eq.(4.1.2).

- L : Using the identity $\int_0^\infty d\zeta e^{-\zeta x} = \frac{1}{x}$, $x > 0$

$$\begin{aligned}
 V^L(b) &= \frac{b}{2} \int_{\mathbb{R}} dt \frac{e^{-it^2}}{b^2 t^2 + 1} \\
 &= \frac{b}{2} \int_{\mathbb{R}} dt e^{-it^2} \int_0^\infty d\zeta e^{-\zeta(b^2 t^2 + 1)} \\
 &= \frac{b}{2} \int_0^\infty d\zeta e^{-\zeta} \int_{\mathbb{R}} dt e^{-t^2(b^2 \zeta + i)} \\
 &= \frac{b\sqrt{\pi}}{2} \int_0^\infty d\zeta \frac{e^{-\zeta}}{(b^2 \zeta + i)^{1/2}}, \quad u \equiv (b^2 \zeta + i)^{1/2} \\
 &= \frac{\sqrt{\pi}}{b} e^{i/b^2} \int_{i^{1/2}}^\infty du e^{-u^2/b^2} = \sqrt{\pi} e^{i/b^2} \int_{i^{1/2}/b}^\infty du e^{-u^2} \\
 &= \frac{\pi}{2} e^{i/b^2} \text{Erfc}\left(\frac{i^{1/2}}{b}\right)
 \end{aligned}$$

- g: Standard Gaussian integral

$$\begin{aligned}
 V^g(b) &= \frac{b}{2} \int_{\mathbb{R}} dt e^{-it^2} e^{-b^2 t^2 / \pi} \\
 &= \frac{b}{2} \int_{\mathbb{R}} dt e^{-t^2(b^2 / \pi + i)} \\
 &= \frac{b\sqrt{\pi}}{2} \left(\frac{b^2}{\pi} + i \right)^{-1/2}
 \end{aligned}$$

- s: Use the identity $\int_0^b d\zeta \cos(t\zeta) = \frac{\sin(bt)}{t}$

$$\begin{aligned}
 V^s(b) &= \frac{1}{2} \int_{\mathbb{R}} dt e^{-it^2} \frac{\sin(bt)}{t} \\
 &= \frac{1}{2} \int_{\mathbb{R}} dt e^{-it^2} \int_0^b d\zeta \cos(\zeta t) \\
 &= \frac{1}{2} \int_0^b d\zeta \int_{\mathbb{R}} dt e^{-it^2} \cos(\zeta t) \\
 &= \frac{1}{4} \int_0^b d\zeta \left[\int_{\mathbb{R}} dt e^{-i(t^2 - \zeta t)} + e^{-i(t^2 + \zeta t)} \right] \\
 &= \frac{1}{4} \int_0^b d\zeta e^{i\zeta^2/4} \left[\int_{\mathbb{R}} dt e^{-i(t - \zeta/2)^2} + e^{-i(t + \zeta/2)^2} \right], \quad t \pm \zeta \rightarrow t \\
 &= \frac{\sqrt{\pi}}{2} \int_0^b d\zeta e^{i\zeta^2/4}, \quad u \equiv \frac{\zeta}{2i^{1/2}} \\
 &= \sqrt{\pi} i^{1/2} \int_0^{\frac{b}{2i^{1/2}}} du e^{-u^2} \\
 &= \frac{\pi i^{1/2}}{2} \text{erf}\left(\frac{b}{2i^{1/2}}\right)
 \end{aligned}$$

- r: Use the definition of $\text{erf}(\cdot)$

$$\begin{aligned}
 V^r(b) &= \frac{b}{2} \int_{\mathbb{R}} dt e^{-it^2} \mathbb{1}(|t| < \frac{\pi}{2b}) \\
 &= \frac{b}{2} \int_{-\frac{\pi}{2b}}^{\frac{\pi}{2b}} dt e^{-it^2} \\
 &= b \int_0^{\frac{\pi}{2b}} dt e^{-it^2} \\
 &= \frac{b}{i^{1/2}} \int_0^{\frac{i^{1/2}\pi}{2b}} dt e^{-t^2} \\
 &= \frac{b\sqrt{\pi}}{2i^{1/2}} \text{erf}\left(\frac{i^{1/2}\pi}{2b}\right)
 \end{aligned}$$

- t: Reduces to the r case

$$\begin{aligned}
 V^t(b) &= \frac{1}{2} \int_{\mathbb{R}} dt e^{-it^2} \mathbb{1}(|t| < \frac{\pi}{b}) (b - \frac{|t|}{\pi} b^2) \\
 &= \frac{1}{2} \int_{-\frac{\pi}{b}}^{\frac{\pi}{b}} dt e^{-it^2} (b - \frac{|t|}{\pi} b^2) \\
 &= 2V^r\left(\frac{b}{2}\right) - \frac{b^2}{\pi} \int_0^{\frac{\pi}{b}} dt t e^{-it^2} \\
 &= 2V^r\left(\frac{b}{2}\right) - i \frac{b^2}{2\pi} (e^{-i\pi^2/b^2} - 1)
 \end{aligned}$$

B.2 Infinite control ($b \rightarrow \infty$)

B.2.1 Dirac Delta

[103, 104]....**some general stuff** For functions with discontinuity there is an ambiguity in the action of Dirac delta. Assuming the left and right limits exists, it is reasonable to define

$$\int_{\varepsilon}^{\varepsilon} dt \delta(t) f(t) = \frac{f(0^+) + f(0^-)}{2} \quad (\text{B.2.1})$$

This is also known as the weak/strong definition of Dirac Delta [102]. In [92, 93] it was noted that this property can potentially lead to inconsistencies when applied to differential equations. We will argue that in case the Dirac delta arises as the limit of a Dirac sequence Eq.(B.2.1) is correct and the inconsistencies in [92, 93] can be understood by careful analysis. This is relevant to the discontinuity in Eq.(4.2.1).

As the prototypical example of Dirac sequence we will consider $\Delta_n(t) \equiv n\mathbb{1}(|t| < \frac{1}{2n})$, the sequence of rectangular pulses. Assume f is continuous apart from possibly $t = 0$ and the two limits $f(0^{\pm}) := \lim_{x \rightarrow 0^{\pm}} f(x)$ exists. The following property is true

$$\forall \varepsilon > 0, \lim_{n \rightarrow \infty} \int_{-\varepsilon}^{\varepsilon} dt \Delta_n(t) f(t) = \frac{f(0^+) + f(0^-)}{2} \quad (\text{B.2.2})$$

It is sufficient to show $\int_0^{\varepsilon} dt \Delta_n(t) f(t) = \frac{f(0^+)}{2}$. For n large enough s.t. $\frac{1}{2n} < \varepsilon$, equivalently $\int_0^{\frac{1}{2n}} dt n f(t) = \frac{f(0^+)}{2}$. Let

$$I_n \equiv \left| n \int_0^{\frac{1}{2n}} f(t) dt - \frac{f(0^+)}{2} \right|$$

We will show that $I_n \rightarrow 0$.

$$I_n = n \left| \int_0^{\frac{1}{2n}} dt (f(t) - f(0^+)) \right| \leq n \int_0^{\frac{1}{2n}} dt |f(t) - f(0^+)|$$

$$\lim_{n \rightarrow \infty} \int_0^{\frac{1}{2n}} dt f(t) = \frac{f(0^+)}{2}$$

From the definition of $\lim_{t \rightarrow 0^+} f(t) = f(0^+)$, $\forall \varepsilon > 0$, $\exists \delta > 0$:

$$0 < t < \delta \Rightarrow |f(t) - f(0^+)| < \varepsilon/2$$

$\exists n_0 : \frac{1}{2n_0} < \delta$. For $n > n_0$, $\forall t \in (0, \frac{1}{2n})$

$$0 < t < \frac{1}{2n} < \frac{1}{2n_0} < \delta \Rightarrow |f(t) - f(0^+)| < \varepsilon/2$$

$$I_n \leq n \int_0^{\frac{1}{2n}} dt \varepsilon/2 = \varepsilon$$

By definition $\lim_{n \rightarrow \infty} I_n = 0$ which proves the property Eq.(B.2.1).

For $f(t)$ continuous at $t = 0$, $\lim_{x \rightarrow 0^\pm} f(x) = f(0)$

$$\lim_{n \rightarrow \infty} \int_{-\frac{1}{2n}}^{\frac{1}{2n}} dt \Delta_n(t) f(t) = f(0)$$

Consider now the differential equations, as in [92, 93]

$$\dot{x}_n = \lambda \Delta_n(t) x_n$$

For $t \in (-\frac{1}{2n}, \frac{1}{2n})$

$$\begin{aligned} x_n(t) &= \exp\left(n\lambda \int_{-1/2n}^t dt'\right) x_n(-\frac{1}{2n}) = \exp\left(n\lambda(t + \frac{1}{2n})\right) x_n(-\frac{1}{2n}) \\ x_n(\frac{1}{2n}) &= e^\lambda x_n(-\frac{1}{2n}) \xrightarrow{n \rightarrow \infty} x(0^+) = e^\lambda x(0^-) \\ x_n(\varepsilon) - x_n(-\varepsilon) &= n\lambda \int_{-\varepsilon}^{\varepsilon} dt x_n(t) \end{aligned} \quad (\text{B.2.3})$$

First taking the limit $\varepsilon \rightarrow 0$, both sides of Eq.(B.2.3) vanish from the continuity of $x_n(t)$. On the other hand, for large enough n s.t $\frac{1}{2n} < \varepsilon$

$$x_n(\varepsilon) - x_n(-\varepsilon) = n\lambda e^{\lambda/2} \int_{-1/2n}^{1/2n} dt e^{n\lambda t} = e^{\lambda/2} e^{n\lambda t} \Big|_{t=-1/2n}^{t=1/2n} = e^\lambda - 1$$

therefore in the limit $\lim_{\varepsilon \rightarrow 0} \lim_{n \rightarrow \infty} x(0^+) - x(0^-) = e^\lambda - 1 \Rightarrow x(0^+) - x(0^-) = e^\lambda - 1$ which is consistent with Eq.(B.2.3).

The inconsistency arises from the following interpretation

$$\lim_{n \rightarrow \infty} \int_{-\varepsilon}^{\varepsilon} dt \Delta_n(t) x_n(t) \stackrel{\times}{=} \lim_{n \rightarrow \infty} \int_{-\varepsilon}^{\varepsilon} dt \Delta_n(t) x(t) \stackrel{\checkmark}{=} \frac{x(0^+) + x(0^-)}{2}$$

It's the first equality that fails and not the second one.

B.2.2 Discontinuity Limit

Calculation of the limit $\mathcal{U}_n := \mathcal{U}_0(\frac{\pi}{2n}, -\frac{\pi}{2n}; a + \frac{n}{2}e^{-i\varphi})$, $\mathcal{U}_n \xrightarrow{n \rightarrow \infty} \mathcal{N} = -i\sigma_\varphi$

$$\mathcal{U}_n = \begin{pmatrix} \mathcal{A}_n & \mathcal{B}_n \\ -\mathcal{B}_n^* & \mathcal{A}_n^* \end{pmatrix} \quad (\text{B.2.4})$$

with $\mathcal{A}_n, \mathcal{B}_n$ given by Eq.(A.1.2, A.1.3) $t_i \rightarrow -\frac{\pi}{2n}, t_f \rightarrow \frac{\pi}{2n}, a \rightarrow a_n \equiv a + \frac{n}{2}e^{-i\varphi}$

$$\mathcal{A}_n \equiv \frac{\Gamma(1 - \nu_n)}{\sqrt{2\pi}} \left[D_{\nu_n}(z_n) D_{\nu_n-1}(z_n) + D_{\nu_n}(-z_n) D_{\nu_n-1}(-z_n) \right] \quad (\text{B.2.5})$$

$$\mathcal{B}_n \equiv \frac{\Gamma(1 - \nu_n)}{a_n^* \sqrt{\pi}} e^{i\pi/4} \left[D_{\nu_n}^2(-z_n) - D_{\nu_n}^2(z_n) \right] \quad (\text{B.2.6})$$

$$z_n = \sqrt{2} e^{-i\pi/4} \frac{\pi}{2n} = \frac{\pi e^{-i\pi/4}}{n\sqrt{2}}, \quad \nu_n = \frac{i}{2} |a_n|^2 = \frac{i}{2} (a^2 + na \cos \varphi + \frac{n^2}{4}) \quad (\text{B.2.7})$$

$$z_n^2 \nu_n = \frac{\pi^2}{16} (1 + \mathcal{O}(1/n)) \Rightarrow z_n = \frac{\pi}{4\sqrt{\nu_n}} (1 + \mathcal{O}(1/n)) \quad (\text{B.2.8})$$

Direct Calculation

Substituting Eq.(D.2.1) in Eq.(B.2.5,B.2.6) and rearranging in powers of $1/n$, we find that there are infinite terms of order 1 that contribute in the limit $n \rightarrow \infty$. From Eq.(D.2.1)

$$D_\nu(z) = C \sum_{k=0}^{\infty} c_k z^k, \quad C = 2^{\nu/2} \pi^{1/2} e^{z^2/4}, \quad c_k = \frac{(-\sqrt{2})^k}{k! \Gamma(\frac{1-k-\nu}{2})}, \quad (\text{D.2.1})$$

Substituting Eq.(D.2.1) in Eq.(B.2.6) and after algebraic manipulations

$$\begin{aligned} \mathcal{B}_n &= \frac{\Gamma(1-\nu_n)}{a_n^* \sqrt{\pi}} e^{i\pi/4} (D_\nu(-z) + D_\nu(z)) (D_\nu(-z) - D_\nu(z)) \\ &= -\frac{4C^2 e^{i\pi/4}}{\sqrt{\pi}} \frac{z_n^2 \nu_n}{z_n a_n^*} \frac{c_0 c_1 \Gamma(1-\nu_n)}{\nu_n} \sum_{k=0}^{\infty} \frac{c_{2k}}{c_0} z^{2k} \sum_{l=0}^{\infty} \frac{c_{2l+1}}{c_1} z^{2l} \end{aligned} \quad (\text{B.2.9})$$

In the last equation, each contributes to the limit $n \rightarrow \infty$.

- For the two sums, the leading terms are the known series of $\cos(\pi/4)$ and $\sin(\pi/4)$

$$\begin{aligned} \frac{c_{2k}}{c_0} &= \frac{(-\sqrt{2})^{2k}}{(2k)!} \frac{\Gamma(\frac{1-\nu_n}{2})}{\Gamma(\frac{1-\nu_n-2k}{2})} = \frac{2^k}{(2k)!} \left(\frac{1-\nu_n}{2} - 1\right) \dots \left(\frac{1-\nu_n}{2} - k\right) \sim \frac{(-1)^k}{(2k)!} \nu_n^k \\ \sum_{k=0}^{\infty} \frac{c_{2k}}{c_0} z^{2k} &= \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} (z_n^2 \nu_n)^k \sim \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} (\pi/4)^{2k} = \cos(\pi/4) = \frac{1}{\sqrt{2}} \end{aligned}$$

Similarly

$$\sum_{l=0}^{\infty} \frac{c_{2l+1}}{c_1} z^{2l} \sim \sum_{l=0}^{\infty} \frac{(-1)^l}{(2l+1)!} (\pi/4)^{2l} = \frac{4}{\pi} \sin(\pi/4) = \frac{4}{\pi\sqrt{2}}$$

•

$$\begin{aligned} c_0 c_1 \Gamma(1-\nu_n) &= (-\sqrt{2}) \frac{\Gamma(1-\nu_n)}{\Gamma(\frac{1-\nu_n}{2}) \Gamma(-\frac{\nu_n}{2})} = -\frac{\sqrt{2}}{\sqrt{\pi}} 2^{-\nu_n} \frac{\Gamma(1-\frac{\nu_n}{2})}{\Gamma(-\frac{\nu_n}{2})} \\ &= -\frac{\sqrt{2}}{\sqrt{\pi}} 2^{-\nu_n} \left(-\frac{\nu_n}{2}\right) = \frac{2^{-\nu_n} \nu_n}{\sqrt{2\pi}} \\ \frac{c_0 c_1 \Gamma(1-\nu_n)}{\nu_n} &= \frac{2^{-\nu_n}}{\sqrt{2\pi}} \end{aligned}$$

•

$$z_n^2 \nu_n \sim \frac{\pi^2}{16}, \quad z_n a_n^* = \frac{\pi}{n\sqrt{2}} e^{-i\pi/4} \left(a_+ \frac{n}{2} e^{i\varphi}\right) \sim \frac{\pi}{2\sqrt{2}} e^{i(-\pi/4+\varphi)}$$

Combining the above results

$$\begin{aligned} \mathcal{B}_n &= -4 \frac{(2^{\nu_n} \pi e^{z_n^2/2}) e^{i\pi/4}}{\sqrt{\pi}} \frac{2^{-\nu_n}}{\sqrt{2\pi}} \frac{2\sqrt{2}}{\pi e^{i(-\pi/4+\varphi)}} \frac{\pi^2}{16} \frac{4}{2\pi} \\ &= -e^{i(\pi/2-\varphi)} = -ie^{-i\varphi} \end{aligned} \quad (\text{B.2.10})$$

$\lim_{n \rightarrow \infty} \mathcal{A}_n$ can be calculated by

$$|\mathcal{A}_n| = \sqrt{1 - |\mathcal{B}_n|^2} \xrightarrow{n \rightarrow \infty} \sqrt{1 - |-ie^{-i\varphi}|^2} = 0, \Rightarrow \mathcal{A}_n \xrightarrow{n \rightarrow \infty} 0 \quad (\text{B.2.11})$$

From Eq.(B.2.4,B.2.5,B.2.6)

$$\begin{aligned} \mathcal{U}_n &= \begin{pmatrix} \mathcal{A}_n & \mathcal{B}_n \\ -\mathcal{B}_n^* & \mathcal{A}_n^* \end{pmatrix} \xrightarrow{n \rightarrow \infty} \begin{pmatrix} 0 & -ie^{-i\varphi} \\ -ie^{i\varphi} & 0 \end{pmatrix} \\ &= -i \begin{pmatrix} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{pmatrix} = -i \begin{pmatrix} 0 & \cos \varphi - i \sin \varphi \\ \cos \varphi + i \sin \varphi & 0 \end{pmatrix} \\ &= -i(\cos \varphi \sigma_1 + \sin \varphi \sigma_2) \\ &= -i\sigma_\varphi \end{aligned}$$

Indirect calculation

Limits of PCF similar to Eq.(B.2.5,B.2.6) can be found in [95]

$$\begin{aligned} \lim_{\beta \rightarrow 0} \left[\frac{\Gamma(s/\beta)}{\sqrt{\beta}} D_{-s/\beta}(x\sqrt{\beta} - \frac{\alpha}{\sqrt{\beta}}) D_{-s/\beta}(y\sqrt{\beta} + \frac{\alpha}{\sqrt{\beta}}) \right] \\ = \frac{\sqrt{2\pi}}{\sqrt{\alpha^2 + 4s}} \exp \left(-\frac{\sqrt{\alpha^2 + 4s}}{2}(x+y) \right), \quad \text{Re}(s) > 0, \quad x, y \in \mathbb{R} \quad (\text{B.2.12}) \end{aligned}$$

From Eq.(B.2.6) and the recurrence relation of PCF, Eq.(D.2.5), similar formulas for limits of products of PCF with different orders can be derived. As in the previous section, we only need to calculate $\lim_{n \rightarrow \infty} \mathcal{B}_n$. Let

$$\mathcal{B}_n^\pm := \frac{\Gamma(1 - \nu_n)}{a_n^* \sqrt{\pi}} D_{\nu}^2(\pm z_n) e^{i\pi/4} \quad (\text{B.2.13})$$

with $\mathcal{B}_n = \mathcal{B}_n^- - \mathcal{B}_n^+$, see Eq.(B.2.6).

$$\begin{aligned} \mathcal{B}_n^+ &= \frac{\Gamma(1 - \nu_n)}{a_n^* \sqrt{\pi}} D_{\nu}^2(z_n) e^{i\pi/4}, \quad \Gamma(1+z) = z\Gamma(z) \\ &= \frac{-\nu_n \Gamma(-\nu_n)}{a_n^* \sqrt{\pi}} D_{\nu_n}^2(z_n) e^{i\pi/4}, \quad \nu_n = i \frac{|a_n|^2}{2} \\ &= -\frac{i}{2\sqrt{\pi}} a_n \Gamma(-\nu_n) D_{\nu_n}^2(z_n) e^{i\pi/4} \\ &= -\frac{i}{2\sqrt{\pi}} \left(\not{a} + \frac{n}{2} e^{-i\varphi} \right) \Gamma(-\nu_n) D_{\nu_n}^2(z_n) e^{i\pi/4} \\ &= -\frac{i}{4\sqrt{\pi}} n e^{i(\pi/4 - \varphi)} \Gamma(-\nu_n) D_{\nu_n}^2(z_n) \end{aligned}$$

dropping irrelevant terms. Let $\beta := -1/\nu_n \sim 8i/n^2 \Rightarrow n \sim 2\sqrt{2}e^{i\pi/4}/\sqrt{\beta}$

$$\begin{aligned}\mathcal{B}_n^+ &= \frac{-i}{\sqrt{2\pi}} e^{i(\pi/2-\varphi)} \frac{\Gamma(1/\beta)}{\sqrt{\beta}} D_{-1/\beta}^2 \left(-i\frac{\pi}{4}\sqrt{\beta} + \dots \right) \\ &= \frac{e^{-i\varphi}}{\sqrt{2\pi}} \frac{\Gamma(1/\beta)}{\sqrt{\beta}} D_{-1/\beta}^2 \left(-i\frac{\pi}{4}\sqrt{\beta} + \dots \right)\end{aligned}$$

From Eq.(B.2.12), for $x = y = -i\pi/4$, $a = 0$, $\mathcal{B}_n^+ \xrightarrow{n \rightarrow \infty} ie^{-i\varphi}/2$. Similarly $\mathcal{B}_n^- \xrightarrow{n \rightarrow \infty} -ie^{-i\varphi}/2$ (for $x = y = i\pi/4, a = 0$) and $\mathcal{B}_n \xrightarrow{n \rightarrow \infty} -ie^{-i\varphi}$. In [95], Eq.(B.2.12) was initially derived for $x, y \in \mathbb{R}$ but it is valid for $x, y \in \mathbb{C}$ since left and right sides are analytic functions of x, y .

B.2.3 Landau Zener with Dirac Delta

Let $\mathbf{n} = (n_1, n_2, n_3) \in \mathbb{R}^3$ and

$$i\partial_t |\psi\rangle = \left[-t\sigma_3 + a\sigma_1 + \delta(t)(\mathbf{n} \cdot \boldsymbol{\sigma}) \right] |\psi\rangle, \quad a \neq 0 \quad (4.2.11)$$

Let $t_f > 0$. Using the shorthand notation

$$\mathcal{U}_\infty(t_f) = \mathcal{U}_{0,+}(t_f) \mathcal{N} \mathcal{U}_{0,-}(t_f) \quad (4.2.5)$$

with

$$\mathcal{N} = e^{-i|\mathbf{n}|(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})} = \cos |\mathbf{n}| - i \sin |\mathbf{n}|(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \quad (B.2.14)$$

Expanding the matrices in Eq.(4.2.5)

$$\mathcal{A}_\infty = C_0 \cos |\mathbf{n}| - i \frac{n_3}{|\mathbf{n}|} \sin |\mathbf{n}| C_3 + \sin |\mathbf{n}| \left(\frac{n_1}{|\mathbf{n}|} C_1 + \frac{n_2}{|\mathbf{n}|} C_2 \right) \quad (B.2.15)$$

with $C_i(a), i = 0, 1, 2, 3$

$$C_0 = (\mathcal{U}_{0,+} \mathcal{U}_{0,-})_{11} = (\mathcal{U}_0)_{11} \quad (B.2.16)$$

$$C_1 = -i(\mathcal{A}_{0,-} \mathcal{B}_{0,-} - \mathcal{A}_{0,+} \mathcal{B}_{0,-}^*) = 2\text{Im}(\mathcal{A}_{0,-} \mathcal{B}_{0,-}) \quad (B.2.17)$$

$$C_2 = \mathcal{A}_{0,-} \mathcal{B}_{0,-} + \mathcal{A}_{0,+} \mathcal{B}_{0,-}^* = 2\text{Re}(\mathcal{A}_{0,-} \mathcal{B}_{0,-}) \quad (B.2.18)$$

$$C_3 = \mathcal{A}_{0,+} \mathcal{A}_{0,-} + \mathcal{B}_{0,+} \mathcal{B}_{0,-}^* = |\mathcal{A}_{0,+}|^2 + |\mathcal{B}_{0,+}|^2 = 1 \quad (B.2.19)$$

applying the properties of the time evolution matrix and Eq.(??,??). $\mathcal{A}_0, \mathcal{B}_0$ are given by Eq.(A.1.2,A.1.3) with $t_f \rightarrow 0$ and $t_i \rightarrow -t_f, z_f = \sqrt{2}e^{-i\pi/4}t_f$

$$\begin{aligned}\mathcal{A}_{0,-} &= \frac{\Gamma(1-\nu)}{\sqrt{2\pi}} D_\nu(0) \left(D_{\nu-1}(z_f) + D_{\nu-1}(-z_f) \right) \\ \mathcal{B}_{0,-} &= \frac{\Gamma(1-\nu)}{a\sqrt{\pi}} e^{i\frac{\pi}{4}} D_\nu(0) \left(-D_\nu(z_f) + D_\nu(-z_f) \right)\end{aligned}$$

Keeping leading order terms in t_f , Eq.(D.2.3), C_0 becomes $C_0 = e^{-\pi a^2/2}$, Eq.(A.1.5) and

$$\begin{aligned} \mathcal{A}_{0,-} &\sim D_\nu(0)e^{-\pi a^2/8 - i\varphi_f} \\ \mathcal{B}_{0,-} &\sim \frac{\Gamma(1-\nu)}{a\sqrt{\pi}} D_\nu(0)(e^{-3\pi a^2/8} - e^{\pi a^2/8})e^{i(\varphi_f + \frac{\pi}{4})} \\ \mathcal{A}_{0,-}\mathcal{B}_{0,-} &= \frac{\Gamma(1-\nu)}{a\sqrt{\pi}} D_\nu^2(0)(e^{-\pi a^2/2} - 1)e^{i\frac{\pi}{4}} \end{aligned} \quad (4.2.8)$$

In the last equation, t_f drops out. Substituting Eq.(D.2.2) and after further algebraic manipulations we get

$$\begin{aligned} \mathcal{A}_{0,-}\mathcal{B}_{0,-} &= \frac{2^\nu \sqrt{\pi}}{a} \frac{\Gamma(1-\nu)}{\Gamma^2\left(\frac{1-\nu}{2}\right)} (e^{-\pi a^2/2} - 1)e^{i\frac{\pi}{4}} \\ &= \frac{\sqrt{\pi}}{a} (e^{-\pi a^2/2} - 1) \frac{|\Gamma(1-\nu)|}{|\Gamma(\frac{1-\nu}{2})|^2} e^{i\omega(a)} \end{aligned}$$

with

$$\omega(a) \equiv \frac{\pi}{4} + \frac{a^2}{2} \ln 2 + \arg \Gamma(1-\nu) - 2 \arg \Gamma\left(\frac{1-\nu}{2}\right)$$

Let $x \equiv \pi \frac{a^2}{2}$. Using the formula $\sinh(x) = 2 \sinh(\frac{x}{2}) \cosh(\frac{x}{2})$ and properties Eq.(D.1.5, D.1.6), the ratio of Γ functions becomes

$$\frac{|\Gamma(1-\nu)|}{|\Gamma(\frac{1-\nu}{2})|^2} = \frac{|a|}{\sqrt{2\pi}} \frac{\cosh \frac{x}{2}}{\sqrt{\sinh x}} = \frac{|a|}{2\sqrt{\pi}} \frac{1}{\sqrt{\tanh \frac{x}{2}}}$$

from which

$$\mathcal{A}_{0,-}\mathcal{B}_{0,-} = \frac{|a|}{2a} \frac{e^{-x} - 1}{\sqrt{\tanh \frac{x}{2}}} e^{i\omega(a)} = -\text{sgn}(a) \frac{1}{2} \sqrt{1 - e^{-\pi a^2}} e^{i\omega(a)}$$

with $\text{sgn}(a) := \frac{|a|}{a}$. $\omega(a)$ can be written in an equivalent more familiar form. From the Legendre duplication formula, Eq.(D.1.3) with $z = \frac{1-\nu}{2}$

$$\frac{\Gamma(1-\nu)}{\Gamma(\frac{1-\nu}{2})} = \frac{1}{\sqrt{\pi}} 2^{-\nu} \Gamma\left(\frac{2-\nu}{2}\right)$$

from which follows

$$\begin{aligned} \arg \frac{\Gamma(1-\nu)}{\Gamma(\frac{1-\nu}{2})} &= \arg(2^{-\nu} \Gamma(\frac{2-\nu}{2}) / \sqrt{\pi}) = \arg(2^{-\nu} \Gamma(\frac{2-\nu}{2})) \\ &= \arg 2^{-i a^2/2} + \arg \Gamma(\frac{2-\nu}{2}) \\ &= -\frac{a^2}{2} \ln 2 + \arg \Gamma(\frac{2-\nu}{2}) \end{aligned}$$

and

$$\arg \Gamma(1 - \nu) - \arg \Gamma\left(\frac{1-\nu}{2}\right) = -\frac{a^2}{2} \ln 2 + \arg \Gamma\left(\frac{2-\nu}{2}\right)$$

From the last equation we get $\omega(a) = \frac{\pi}{2} - \chi(a)$ with $\chi(a)$

$$\begin{aligned} \chi(a) &= \frac{\pi}{4} + \arg \Gamma\left(\frac{1 - \nu(a)}{2}\right) - \arg \Gamma\left(\frac{2 - \nu(a)}{2}\right) \\ &= \frac{\pi}{4} + \arg \frac{\Gamma\left(\frac{1-\nu(a)}{2}\right)}{\Gamma\left(\frac{2-\nu(a)}{2}\right)} \end{aligned} \quad (4.2.10)$$

Combinite all the above

$$\begin{aligned} \mathcal{A}(a) &= e^{-\pi a^2/2} \cos |\mathbf{n}| - i \frac{n_3}{|\mathbf{n}|} \sin |\mathbf{n}| \\ &\quad - \operatorname{sgn}(a) \sqrt{1 - e^{-\pi a^2}} \sin |\mathbf{n}| \left[\frac{n_1}{|\mathbf{n}|} \cos \chi(a) + \frac{n_2}{|\mathbf{n}|} \sin \chi(a) \right] \end{aligned} \quad (B.2.20)$$

For $n_3 = 0$, let $\mathbf{n} = |\mathbf{n}|(\cos \varphi, \sin \varphi, 0)$, Eq.(B.2.20) reduces to

$$\mathcal{A}_\infty(a) = e^{-\pi a^2/2} \cos |\mathbf{n}| - \operatorname{sgn}(a) \sqrt{1 - e^{-\pi a^2}} \sin |\mathbf{n}| \cos(\chi(a) - \varphi) \quad (B.2.21)$$

and for $|\mathbf{n}| = \frac{\pi}{2}$

$$\mathcal{A}_\infty(a) = -\operatorname{sgn}(a) \sqrt{1 - e^{-\pi a^2}} \cos(\chi(a) - \varphi) \quad (B.2.22)$$

$$\mathcal{P}_\infty(a) = (1 - \mathcal{P}_0) \cos^2(\chi(a) - \varphi) \quad (4.2.9)$$

with $\mathcal{P}_0 = e^{-\pi a^2}$ and $\chi(a)$ given by Eq.(4.2.10).

B.2.4 $\chi(a)$

$\chi(a) = \pi/4 + \chi_0(a)$ with $\chi_0(a) \equiv \arg f(a)$ and

$$f(a) \equiv \frac{\Gamma\left(\frac{1-\nu(a)}{2}\right)}{\Gamma\left(1 - \frac{\nu(a)}{2}\right)}, \quad \nu(a) = ia^2/2 \quad (B.2.23)$$

Attempt to prove the monotonicity of $\chi_0(a)$. Polar representation $f(a) = |f(a)|e^{if(a)}$

$$\log f(a) = \log |f(a)| + i \arg f(a) \Rightarrow \arg f(a) = \operatorname{Im} \log f$$

$$\begin{aligned} \partial_a \arg f(a) &= \partial_a \operatorname{Im} \log f(a) = \operatorname{Im} \partial_a \log f(a) \\ &= \operatorname{Im} \left[ia \partial_\nu \left(\log \Gamma\left(\frac{1-\nu}{2}\right) - \log \Gamma\left(1 - \frac{\nu}{2}\right) \right) \right] \\ &= \frac{a}{2} \operatorname{Re} \left(\psi\left(1 - \frac{\nu}{2}\right) - \psi\left(\frac{1-\nu}{2}\right) \right) \end{aligned}$$

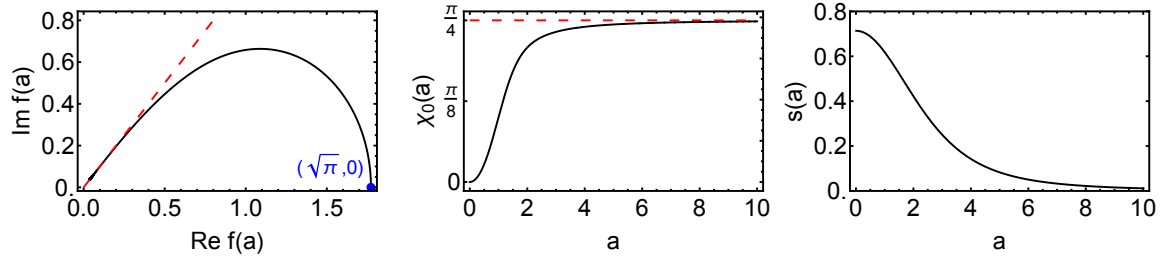


Figure B.4. (Left) The image of $[0, \infty)$ under $\chi_0 : \mathbb{R} \mapsto \mathbb{C}$. For $a = 0$, $f(0) = \frac{\Gamma(1/2)}{\Gamma(1)} = \sqrt{\pi}$, blue point. For increasing a , $f(a)$ remains in the first quadrant and asymptotically approaches the diagonal. (Middle) $\chi_0(a) = \arg f(a)$. For $a = 0$ the argument is zero. $\chi_0(a)$ is an increasing function of a and asymptotically approaches the value $\pi/4$. (Right) The positive sign of $s(a)$ shows that $\chi_0(a)$ is increasing.

with $\psi(z) \equiv \Gamma'(z)/\Gamma(z)$ the Digamma function [27]. From the series representation of $\psi(z)$ [27]

$$\begin{aligned}
 \psi(1 - \frac{\nu}{2}) - \psi(\frac{1-\nu}{2}) &= \sum_{k=0}^{\infty} \frac{1}{k + \frac{1-\nu}{2}} - \frac{1}{k + 1 - \frac{\nu}{2}} \\
 &= \frac{1}{2} \sum_{k=0}^{\infty} \frac{1}{(k + \frac{1}{2} - \frac{\nu}{2})(k + 1 - \frac{\nu}{2})} \\
 \operatorname{Re}(\psi(1 - \frac{\nu}{2}) - \psi(\frac{1-\nu}{2})) &= \frac{1}{2} \sum_{k=0}^{\infty} \frac{(k + \frac{1}{2})(k + 1) - \frac{a^2}{16}}{((k + \frac{1}{2})^2 + \frac{a^2}{16})((k + 1)^2 + \frac{a^2}{16})} \\
 &> \frac{1}{2} \sum_{k=0}^{\infty} \frac{(k + \frac{1}{2})^2 - \frac{a^2}{16}}{((k + 1)^2 + \frac{a^2}{16})^2} \\
 &= \frac{1}{2} \sum_{l=1}^{\infty} \frac{(l - \frac{1}{2})^2 - \frac{a^2}{16}}{(l^2 + \frac{a^2}{16})^2} \\
 s(a) &\equiv \sum_{l=1}^{\infty} \frac{(l - \frac{1}{2})^2 - \frac{a^2}{16}}{(l^2 + \frac{a^2}{16})^2}
 \end{aligned}$$

For $a/4 < 1$, all the terms in $s(a)$ are positive and thus $s(a)$ positive. We haven't managed to prove this $\forall a > 0$ which is evidently true by the numerics.

For the asymptotic expansion of $\mathcal{P}_{\infty}(a) \sim \cos^2(\chi(a) - \varphi)$: The asymptotic expansion for the ratio of Γ functions in Eq.(B.2.23) can be obtained by Stirling formula $\Gamma(z) \sim e^z z^{z-\frac{1}{2}}(1 + \frac{1}{12z} + \dots)$, or the more efficient expansion described in [105], from which [27]

$$z^{b-a} \frac{\Gamma(z+a)}{\Gamma(z+b)} \sim 1 + \frac{(a-b)(a+b-1)}{2z} + \frac{1}{12} \binom{a-b}{2} (3(a+b-1)^2 - a+b-1) \frac{1}{z^2} + \dots$$

Then the expansion for $\arg(\cdot)$ and $\mathcal{P}_{\infty}$ in Eq.(4.2.9) follows.

$$\chi(a) \sim \frac{\pi}{2} - \frac{1}{2a^2} - \frac{1}{3a^6} - \frac{8}{5a^{10}} + \mathcal{O}(1/a^{14})$$

From Eq.(4.2.9) up to second order

$$\begin{aligned}
 \mathcal{P}_\infty(a) &\sim \cos^2\left(\frac{\pi}{2} - \frac{1}{2a^2} - \varphi\right) \\
 &= \sin^2\left(\frac{1}{2a^2} + \varphi\right) \\
 &= \left(\sin \frac{1}{2a^2} \cos \varphi + \cos \frac{1}{2a^2} \sin \varphi\right)^2 \\
 &= \sin^2 \frac{1}{2a^2} \cos^2 \varphi + \frac{1}{2} \sin \frac{1}{a^2} \sin 2\varphi + \cos^2 \frac{1}{2a^2} \sin^2 \varphi \\
 &\sim \frac{1}{4a^4} \cos^2 \varphi + \frac{1}{2a^2} \sin 2\varphi + \left(1 - \frac{1}{8a^4}\right) \sin^2 \varphi \\
 &= \sin^2 \varphi + \frac{1}{2a^2} \sin 2\varphi + \frac{1}{8a^4} (2 \cos^2 \varphi - \sin^2 \varphi)
 \end{aligned}$$

Appendix C

Other calculations

C.1 Dyson Series

Eq.(C.1.8) is relevant to the calculations in Tab.(4.1) and Eq.(C.1.7) is relevant to App.(A.3)

C.1.1 Generalities

Let

$$i\partial_t |\psi\rangle = (H_0 + H_1) |\psi\rangle \quad (\text{C.1.1})$$

Assuming $\mathcal{U}_0$ is the time evolution matrix for the unperturbed Hamiltonian H_0 , i.e $(i\partial_t \mathcal{U}_0 - H_0) |\psi\rangle = 0$, we make the change of basis (interaction picture) [25].

$$|\psi; t\rangle = \mathcal{U}_0(t, t_0) |\varphi; t\rangle, \quad \partial_t |\psi\rangle = \partial_t \mathcal{U}_0 |\varphi\rangle + \mathcal{U}_0 \partial_t |\varphi\rangle$$

with $t_0 \in \mathbb{R}$. Eq.(C.1.1) transform to $\underbrace{i(\partial_t \mathcal{U}_0 - H_0) \mathcal{U}_0}_{=0} |\varphi\rangle + i\mathcal{U}_0 \partial_t |\varphi\rangle - H_1 \mathcal{U}_0 |\varphi\rangle = 0$

$$i\partial_t |\varphi\rangle = H_1^{\text{I}}(t) |\varphi\rangle, \quad H_1^{\text{I}}(t) \equiv \mathcal{U}_0^\dagger H_1 \mathcal{U}_0 \quad (\text{C.1.2})$$

The solution to Eq.(C.1.2), $|\varphi; t_f\rangle = \mathcal{U}_1(t_f, t_i) |\varphi; t_i\rangle$, is formally written as

$$\begin{aligned} \mathcal{U}_1(t_f, t_i) = \mathbb{1} + (-i) \int_{t_i}^{t_f} dt_1 H_1^{\text{I}}(t_1) + (-i)^2 \int_{t_i}^{t_f} dt_1 \int_{t_i}^{t_1} dt_2 H_1^{\text{I}}(t_1) H_1^{\text{I}}(t_2) + \dots \\ + (-i)^n \int_{t_i}^{t_f} dt_1 \dots \int_{t_i}^{t_{n-1}} dt_n H_1^{\text{I}}(t_1) \dots H_1^{\text{I}}(t_n) \end{aligned} \quad (\text{C.1.3})$$

which is known as the Dyson series. The n -th term, is a n -th dimensional integral over the simplex $I_n := \{t_1 > t_2 > \dots > t_n\}$. The series rarely converge in the usual sense and in case they do, finding the general term in closed form and summing

the series is a difficult task. If $\|H_1\| \ll 1$, truncating $\mathcal{U}_1$ at a finite order gives a good approximation.

Let $\mathcal{U}$ denote the full time evolution of Eq.(C.1.1), i.e $(i\partial_t \mathcal{U} - H) |\psi\rangle = 0$. Using the above definitions, the following relation holds

$$\mathcal{U}(t_f, t_i) = \mathcal{U}_0(t_f, t_0) \mathcal{U}_1(t_f, t_i) \mathcal{U}_0^{-1}(t_i, t_0) \quad (\text{C.1.4})$$

For symmetric integration, $t_f = -t_i$, $t_0 = 0$, $\mathcal{U}_0^{-1}(t_1, t_2) = \mathcal{U}_0(t_2, t_1)$ and assuming $\mathcal{U}_0$ has the symmetries Eq.(A.2.1), (??)

$$\mathcal{U}(t_f, -t_f) = \mathcal{U}_0(t_f, 0) \mathcal{U}_1(t_f, -t_f) \mathcal{U}_0(0, -t_f)$$

$$\begin{aligned} \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & \mathcal{A}^* \end{pmatrix} &= \begin{pmatrix} \mathcal{A}_{0,+} & \mathcal{B}_{0,+} \\ -\mathcal{B}_{0,+}^* & \mathcal{A}_{0,+}^* \end{pmatrix} \begin{pmatrix} \mathcal{A}_1 & \mathcal{B}_1 \\ -\mathcal{B}_1^* & \mathcal{A}_1^* \end{pmatrix} \begin{pmatrix} \mathcal{A}_{0,-} & \mathcal{B}_{0,-} \\ -\mathcal{B}_{0,-}^* & \mathcal{A}_{0,-}^* \end{pmatrix} \\ &= \begin{pmatrix} \mathcal{A}_{0,+} & \mathcal{B}_{0,+} \\ -\mathcal{B}_{0,+}^* & \mathcal{A}_{0,+}^* \end{pmatrix} \begin{pmatrix} \mathcal{A}_1 & \mathcal{B}_1 \\ -\mathcal{B}_1^* & \mathcal{A}_1^* \end{pmatrix} \begin{pmatrix} \mathcal{A}_{0,+}^* & \mathcal{B}_{0,+} \\ -\mathcal{B}_{0,+}^* & \mathcal{A}_{0,+} \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \mathcal{A} &= 2 \operatorname{Re} \left(\mathcal{A}_1 |\mathcal{A}_{0,+}|^2 - \mathcal{A}_{0,+} \mathcal{B}_1 \mathcal{B}_{0,+}^* \right) - \mathcal{A}_1^* \\ &= \mathcal{A}_1 (2|\mathcal{A}_{0,+}|^2 - 1) - 2 \operatorname{Re}(\mathcal{A}_{0,+} \mathcal{B}_{0,+}^* \mathcal{B}_1) \end{aligned} \quad (\text{C.1.5})$$

C.1.2 Application to LZS

Let $H_0 = -t\sigma_3$, $H_1 = f(t)\sigma_1$ with $f(t) = f(-t)$, $f(t) \in \mathbb{R}$. The unperturbed system, $(i\partial_t - H_0) |\psi\rangle = 0$, is trivially integrable with $\mathcal{U}_0(t_f, 0) = e^{it^2/2\sigma_3} \Rightarrow \mathcal{A}_{0,+}(t_f) = e^{it_f^2/2}$, $\mathcal{B}_{0,+}(t_f) = 0$. From Eq.(C.1.5)

$$\mathcal{A}(t_f, -t_f) = \mathcal{A}_1(t_f, -t_f)$$

$$H_1^{\text{I}}(t) := \mathcal{U}_0^\dagger(t, 0) H_1(t) \mathcal{U}_0(t, 0) = f(t) e^{-it^2/2\sigma_3} \sigma_1 e^{it^2/2\sigma_3} = f(t) \begin{pmatrix} 0 & e^{-it^2} \\ e^{it^2} & 0 \end{pmatrix}$$

Similarly

$$H_1^{\text{I}}(t_1) H_1^{\text{I}}(t_2) = f(t_1) f(t_2) \begin{pmatrix} e^{-i(t_1^2 - t_2^2)} & 0 \\ 0 & e^{i(t_1^2 - t_2^2)} \end{pmatrix}$$

Notice that only even terms contribute to the diagonal part $\mathcal{A}_1$

$$\prod_{k=1}^{2n} H_1^{\text{I}}(t_k) = \prod_{k=1}^{2n} f(t_k) \begin{pmatrix} \exp(i\Lambda_{2n}(t_1, \dots, t_{2n})) & 0 \\ 0 & * \end{pmatrix}$$

with $*$ the complex conjugate of the diagonal element and

$$\Lambda_{2n}(t_1, \dots, t_{2n}) \equiv \sum_{k=1}^{2n} (-1)^k t_k^2 \quad (\text{C.1.6})$$

From Eq.(C.1.3)

$$\mathcal{A}_1 = 1 + \sum_{n=1}^{\infty} (-i)^{2n} \int_{I_{2n}} \prod_{j=1}^{2n} dt_j \prod_{k=1}^{2n} f(t_k) \exp(i\Lambda_{2n}) \quad (\text{C.1.7})$$

with $I_n = \{t_1 > t_2 > \dots > t_n\}$. Assuming $f(t) = f(-t)$ and $f(t) \in \mathbb{R}$, the second term in the series Eq.(C.1.7) has the following simplification

$$\begin{aligned} \mathcal{A}_1^{(2)} &= \int_{-\infty}^{\infty} dt_1 \underbrace{f(t_1) e^{-it_1^2/2}}_{\text{even in } t_1} \int_{-\infty}^{t_1} dt_2 f(t_2) e^{it_2^2/2} \\ &= \frac{1}{2} \int_{-\infty}^{\infty} dt_1 f(t_1) e^{-it_1^2/2} \left(\int_{-\infty}^{t_1} dt_2 f(t_2) e^{it_2^2/2} + \underbrace{\int_{-\infty}^{-t_1} dt_2 f(t_2) e^{it_2^2/2}}_{t_2 \rightarrow -t_2} \right) \\ &= \frac{1}{2} \int_{-\infty}^{\infty} dt_1 f(t_1) e^{-it_1^2/2} \int_{-\infty}^{+\infty} dt_2 f(t_2) e^{it_2^2/2} \\ &= \frac{1}{2} \left| \int_{-\infty}^{\infty} dt_1 f(t_1) e^{-it_1^2/2} \right|^2 \\ \mathcal{A}_1^{(2)} &= \frac{1}{2} \left| \int_{-\infty}^{\infty} dt_1 f(t_1) e^{-it_1^2/2} \right|^2 \end{aligned} \quad (\text{C.1.8})$$

The trick doesn't generalize to higher order terms.

C.2 AGP

Complementary calculation to Section 2.3.

C.2.1 Main equations

$$\begin{aligned}
 \partial_t H_0 &= D + \sum_n E_n Q_n + \sum_n E_n Q_n^\dagger \\
 &= D + \left(\sum_n Q_n\right) H_0 + H_0 \left(\sum_n Q_n^\dagger\right) \\
 &= D + \left(\sum_n Q_n\right) H_0 - H_0 \left(\sum_n Q_n\right) \\
 &= D + \frac{1}{i} [H_{\text{CD}}, H_0]
 \end{aligned}$$

$$\begin{aligned}
 H &= \sum_n E_n P_n - i \sum_n \langle n | \partial_t n \rangle P_n + i \sum_n Q_n \\
 &= H_0 - i \sum_n \langle n | \partial_t n \rangle P_n + i \sum_{n,m} P_m Q_n \\
 &= H_0 + i \sum_{n \neq m} P_m Q_n
 \end{aligned}$$

$P_m Q_n = |m\rangle \langle m | \partial_t n \rangle \langle n|$. Differentiate $H_0 |n\rangle = E_n |n\rangle$ and project to $\langle m|$

$$\langle m | \partial_t n \rangle = \frac{\langle m | \partial_t H_0 | n \rangle}{E_n - E_m}, \quad P_m Q_n = \frac{P_m \partial_t H_0 P_n}{E_n - E_m}$$

C.2.2 Orthogonality conditions

We make repeated use of the cyclic property of trace, the linearity and the basis independence [86]. Referring to Eq.(2.3.3), $H_{\text{CD}} = i \sum_n Q_n$

1. H_{CD}

$$\text{tr}(H_{\text{CD}}) = \text{tr} \sum_n Q_n = \text{tr} \sum_n |\partial_t n\rangle \langle n| = \sum_n \langle n | \partial_t n \rangle$$

2. $H_0 H_{\text{CD}}$

$$\begin{aligned}
 \text{tr}(H_0 H_{\text{CD}}) &= \text{tr} \left(H_0 \sum_n Q_n \right) = \text{tr} \sum_n H_0 Q_n = \text{tr} \sum_n H_0 |\partial_t n\rangle \langle n| \\
 &= \sum_n \langle n | H_0 | \partial_t n \rangle = \sum_n E_n \langle n | \partial_t n \rangle
 \end{aligned}$$

3. $\partial_t H_0 H_{\text{CD}}$

$$\begin{aligned}
\text{tr}(\partial_t H_0 H_{\text{CD}}) &= \text{tr} \sum_n \partial_t H_0 Q_n = \text{tr} \sum_n \partial_t H_0 |\partial_t n\rangle \langle n| \\
&= \text{tr} \sum_n D |\partial_t n\rangle \langle n| + \frac{1}{i} \text{tr} \sum_n [H_{\text{CD}}, H_0] |\partial_t n\rangle \langle n| \\
&= \text{tr} \sum_{n,m} \partial_t E_m P_m |\partial_t n\rangle \langle n| + \frac{1}{i} \text{tr} \sum_n [H_{\text{CD}}, H_0] |\partial_t n\rangle \langle n| \\
&= \sum_n \partial_t E_n \langle n | \partial_t n \rangle
\end{aligned}$$

The last equality follows from

$$\begin{aligned}
\text{tr} \sum_{n,m} \partial_t E_m P_m |\partial_t n\rangle \langle n| &= \sum_{n,m} \partial_t E_m \langle n | P_m | \partial_t n \rangle \\
&= \sum_{n,m} \partial_t E_m \langle m | \partial_t n \rangle \delta_{nm} \\
&= \sum_n \partial_t E_n \langle n | \partial_t n \rangle
\end{aligned}$$

$$\begin{aligned}
\text{tr} \sum_n [H_{\text{CD}}, H_0] |\partial_t n\rangle \langle n| &= \frac{1}{i} \text{tr} \left([H_{\text{CD}}, H_0] \sum_n |\partial_t n\rangle \langle n| \right) \\
&= -\text{tr}([H_{\text{CD}}, H_0] H_{\text{CD}}) \\
&= -\text{tr}(H_{\text{CD}} H_0 H_{\text{CD}} - H_0 H_{\text{CD}} H_{\text{CD}}) \\
&= \text{tr}(H_0 H_{\text{CD}} H_{\text{CD}}) - \text{tr}(H_{\text{CD}} H_0 H_{\text{CD}}) \\
&= 0
\end{aligned}$$

By redefining the phases, $|n'\rangle = e^{-\int^t \langle n | \partial_t n \rangle} |n\rangle$

$$\begin{aligned}
\langle n' | n' \rangle &= \langle n | n \rangle = 1 \\
\partial_t |n'\rangle &= -\langle n | \partial_t n \rangle |n'\rangle + |\partial_t n\rangle e^{-\int^t \langle n | \partial_t n \rangle} \\
\langle n' | \partial_t n' \rangle &= -\langle n | \partial_t n \rangle \langle n' | n' \rangle + \langle n | \partial_t n \rangle = 0
\end{aligned}$$

we can impose the condition $\langle n | \partial_t n \rangle = 0$ (parallel gauge), thus

$$\text{tr}(H_{\text{CD}}) = \text{tr}(H_0 H_{\text{CD}}) = \text{tr}(\partial_t H_0 H_{\text{CD}}) = 0$$

Referring to Eq.(2.3.8)

1. $\text{tr } H_{\text{CD}} = 0$

$$\begin{aligned} \text{tr} \sum_{n \neq m} \frac{P_m \partial_n H_0 P_n}{E_n - E_m} &= \sum_{n \neq m} \frac{\text{tr}(P_m \partial_t H_0 P_n)}{E_n - E_m} \\ &= \sum_{n \neq m} \frac{\text{tr}(P_n P_m \partial_t H_0)}{E_n - E_m} \\ &= \sum_{n \neq m} \frac{\text{tr}(\delta_{nm} \partial_t H_0)}{E_n - E_m} \\ &= 0 \end{aligned}$$

2. $\text{tr}(H_0 H_{\text{CD}}) = 0$

$$\begin{aligned} \text{tr} \left(H_0 \sum_{n \neq m} \frac{P_m \partial_n H_0 P_n}{E_n - E_m} \right) &= \sum_{n \neq m} \frac{E_m}{E_n - E_m} \text{tr}(P_m \partial_t H_0 P_n) \\ &= \sum_{n \neq m} \frac{E_m}{E_n - E_m} \text{tr}(P_n P_m \partial_t H_0) \\ &= \text{tr}(\partial_t H_0) \sum_{n \neq m} \frac{E_m}{E_n - E_m} \delta_{nm} \\ &= 0 \end{aligned}$$

3. $\text{tr}(\partial_t H_0 H_{\text{CD}}) = 0$

$$\text{tr} \left(\partial_t H_0 \sum_{n \neq m} \frac{P_m \partial_t H_0 P_n}{E_n - E_m} \right) = \sum_{n \neq m} \frac{\text{tr}(\partial_t H_0 P_m \partial_t H_0 P_n)}{E_n - E_m} = 0$$

because $a_{nm} \equiv \text{tr}(\partial_t H_0 P_m \partial_t H_0 P_n)$ is symmetric, $a_{nm} = a_{mn}$ applying the cyclic property of trace twice, therefore $b_{nm} \equiv a_{nm} / (E_n - E_m)$ is antisymmetric and $\sum_{n \neq m} b_{nm} = 0$.

C.2.3 Derivation of f_{CD}

From Eq.(2.3.7), $[H_0, \partial_t H_0 + i[H_{\text{CD}}, H_0]] = 0$ with $H_{\text{CD}} = f_{\text{CD}} \sigma_2$ and $H_0 = -t\sigma_3 + a\sigma_1$, using the properties of Pauli Matrices $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$ [25]

$$i[H_{\text{CD}}, H_0] = if_{\text{CD}}[\sigma_2, -t\sigma_3 + a\sigma_1] = 2f_{\text{CD}}(t\sigma_1 + a\sigma_3)$$

$$\left[-t\sigma_3 + a\sigma_1, -\sigma_3 + 2f_{\text{CD}}(t\sigma_1 + a\sigma_3) \right] = 0$$

$$2(a^2 + t^2)f_{\text{CD}}[\sigma_1, \sigma_3] - a[\sigma_1, \sigma_3] = 0 \Rightarrow f_{\text{CD}} = \frac{a}{2a^2 + t^2}$$

Alternative derivation, using the series expansion

$$A^{(1)} = ic_1[H_0, \partial_t H_0]$$

$$D = \partial_t H_0 + i[A^{(1)}, H_0] = \partial_t H_0 - c_1 [[H_0, \partial_t H_0], H_0]$$

$$D^2 = (\partial_t H_0)^2 - c_1 \left(\partial_t H_0 [[H_0, \partial_t H_0], H_0] + [[H_0, \partial_t H_0], H_0] \partial_t H_0 \right) + c^2 [[H_0, \partial_t H_0], H_0]^2$$

Using the cyclic property of trace

$$\text{tr } D^2 = \text{tr}(\partial_t H_0)^2 - 2c_1 \text{tr}(\partial_t H_0 [[H_0, \partial_t H_0], H_0]) + c^2 \text{tr} [[H_0, \partial_t H_0], H_0]^2$$

The minimum is found by $\partial_{c_1} \text{tr } D^2 \stackrel{!}{=} 0$

$$c_1^* = \frac{\text{tr}(\partial_t H_0 [[H_0, \partial_t H_0], H_0])}{\text{tr} [[H_0, \partial_t H_0], H_0]^2}$$

$$[H_0, \partial_t H_0] = [-t\sigma_3 + a\sigma_1, -\sigma_3] = 2ia\sigma_2$$

$$[[H_0, \partial_t H_0], H_0] = 2ia[\sigma_2, -t\sigma_3 + a\sigma_1] = 4a(t\sigma_1 + a\sigma_3)$$

$$\partial_t H_0 [[H_0, \partial_t H_0], H_0] = -4a\sigma_3(t\sigma_1 + a\sigma_3) = -4at\sigma_3\sigma_1 - 4a^2\sigma_3^2$$

$$[[H_0, \partial_t H_0], H_0]^2 = 16a^2(t\sigma_1 + a\sigma_3)^2 = 16a^2(t^2\sigma_1^2 + a^2\sigma_3^2)$$

Using the properties $\text{tr}(\sigma_1\sigma_3) = 0$ and $\sigma_i^2 = \mathbb{1}$, $\text{tr } \sigma_i^2 = 2$, $c_1^* = -\frac{1}{t^2+a^2}$ and $A^* = \frac{a/2}{a^2+t^2}\sigma_2$.

Appendix D

Special Functions

Our main references for the following collection of formulas are [24, 27, 106]

D.1 Gamma Function

$$\Gamma(z+1) = z\Gamma(z) \quad (\text{D.1.1})$$

$$\Gamma(1-z)\Gamma(z) = \frac{\pi}{\sin \pi z} \quad (\text{D.1.2})$$

$$\Gamma(z)\Gamma\left(\frac{1}{2}+z\right) = 2^{1-2z}\sqrt{\pi}\Gamma(2z) \quad (\text{D.1.3})$$

$$|\Gamma(bi)|^2 = \frac{\pi}{b \sinh \pi b} \quad (\text{D.1.4})$$

$$\left|\Gamma\left(\frac{1}{2}+bi\right)\right|^2 = \frac{\pi}{\cosh \pi b} \quad (\text{D.1.5})$$

$$|\Gamma(1+bi)|^2 = \frac{\pi b}{\sinh \pi b} \quad (\text{D.1.6})$$

D.2 Parabolic Cylinder Functions

$$D_\nu(z) = 2^{\nu/2}\pi^{1/2}e^{z^2/4}\sum_{k=0}^{\infty}\frac{(-z\sqrt{2})^k}{k!\Gamma(\frac{1-k-\nu}{2})} \quad (\text{D.2.1})$$

$$D_\nu(0) = \frac{2^\nu\sqrt{\pi}}{\Gamma(\frac{1-\nu}{2})} \quad (\text{D.2.2})$$

$$D_\nu(z) \sim z^\nu e^{-z^2/4}(1 + \mathcal{O}(1/z)), \quad |\arg z| < \frac{3\pi}{4} \quad (\text{D.2.3})$$

$$D_\nu(z) = e^{i\pi\nu}D_\nu(-z) + \frac{\sqrt{2\pi}}{\Gamma(-\nu)}e^{i(\nu+1)\pi/2}D_{-\nu-1}(-iz) \quad (\text{D.2.4})$$

$$D_{\nu+1}(z) - zD_\nu(z) + \nu D_{\nu-1}(z) = 0 \quad (\text{D.2.5})$$

$$\frac{d}{dz}(e^{z^2/4}D_\nu(z)) = \nu e^{z^2/4}D_{\nu-1}(z) \quad (D.2.6)$$

$$\frac{d}{dz}D_\nu(z) = \nu D_{\nu-1}(z) - \frac{z}{2}D_\nu(z) \quad (D.2.7)$$

$$D_\nu(z)D_{\nu-1}(z) + D_\nu(-z)D_{\nu-1}(z) = \frac{\sqrt{2\pi}}{\Gamma(1-\nu)} \quad (D.2.8)$$

$$D_\nu(z) + D_\nu(-z) = \frac{\sqrt{\pi}2^{(\nu+2)/2}}{\Gamma(\frac{1-\nu}{2})}e^{-z^2/4}\mathcal{M}(-\frac{\nu}{2}, \frac{1}{2}, \frac{z^2}{2}) \quad (D.2.9)$$

$$D_\nu(z) - D_\nu(-z) = \frac{z2^{(\nu+3)/2}\sqrt{\pi}}{\Gamma(-\nu/2)}e^{-z^2/4}\mathcal{M}(\frac{1-\nu}{2}, \frac{3}{2}, \frac{z^2}{2}) \quad (D.2.10)$$

D.3 Confluent Hypergeometric Functions

$$\mathcal{M}(\alpha, \beta; z) := \sum_{k=0}^{\infty} \frac{(\alpha)_k}{(\beta)_k} \frac{z^k}{k!} \quad (D.3.1)$$

$$\mathcal{M}(\alpha, \beta; z) \stackrel{z \rightarrow \infty}{\sim} \Gamma(\beta) \left(\frac{e^z z^{\alpha-\beta}}{\Gamma(\alpha)} + \frac{(-z)^{-\alpha}}{\Gamma(\beta-\alpha)} \right), \quad |\arg z| < \frac{3\pi}{2} \quad (D.3.2)$$

$$\lim_{\alpha \rightarrow \infty} \mathcal{M}(\alpha, \beta, -|x|/\alpha) = \Gamma(\beta)|x|^{\frac{1}{2}(1-\beta)} J_{1-\beta}(2\sqrt{|x|}) \quad (D.3.3)$$

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