Beyond the Rotating Wave Approximation Dynamics of High-Fidelity Quantum Gates

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by
Evangelos Varvelis

First examiner: Prof. David P. DiVincenzo
Second examiner: Prof. Fabian Hassler

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Abstract

An important aspect for practical quantum computation is the ability to precisely manipulate the fundamental unit of quantum information, the qubit, through coupling the qubit to a drive signal. Closely connected to this is our capability to predict the dynamic behavior of the system qubit-gate accurately. In this thesis, we give an extended review from a different perspective of a framework, presented in [1], for the description of the time evolution of such systems. The methodology applied in [1] relies on a perturbative calculation of an effective Hamiltonian based on the Magnus expansion. We will use this effective Hamiltonian formalism to predict the time evolution of a high fidelity quantum gate for singlet-triplet qubits developed in [2] using a phenomenological model. Finally, we will present a new approach of calculating the effective Hamiltonian. This new approach is aimed at finding a non-recursive formula for the effective Hamiltonian, thereby reducing the computational cost of determining such effective Hamiltonians. In the process of doing so, we obtain some simplifications as well as motivate new directions for further development of the formalism.
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Introduction

I am a quantum engineer, but on Sundays I have principles

John S. Bell

In order to describe the state of a quantum system of $N$ subsystems with two degrees of freedom each, like a system of $N$ spin $\frac{1}{2}$ particles, the number of real parameters one would have to keep track of grows exponentially with $N$ even if we require that the state is normalized and also use the invariance of states under multiplication with global phases. Of course this is a system that cannot be efficiently simulated by a classical computer for large $N$. In 1982, Feynman suggested for the first time that one should use a "quantum" computer instead to simulate such a system, in his famous keynote talk [3].

Since then, there have been great advancements in the field of quantum information which have drawn the attention of many scientists from various disciplines as well as the industry. The developments in this field have been both theoretical, like Peter Shor’s algorithm for prime factorization [4] in 1994, and experimental, like the first demonstration of a logical controlled-NOT operation by C. Monroe and D. Wineland [5] using ion trap qubits in 1995. However, that is not to say that everything has been figured out. There are still many challenges ahead of us.

One of these challenges that is of relevance for this thesis is the issue of improving our control over the information unit of the quantum computer, the qubit. One approach to deal with this problem is to improve the accuracy of our description for the dynamics of systems that involve qubits and some control unit or drive.

The standard procedure for solving such a dynamics problem, is to bring the system to a rotating frame that cancels the terms of the orginal Hamiltonian of the system that rotate the same way and amplify the frequency of the counter-rotating terms. The latter terms are then effectively averaged out to zero since they are rapidly oscillating. This is the Rotating Wave Approximation (RWA). In this thesis, we will try to describe the dynamics of such systems with an effective Hamiltonian formalism derived in [1]. The effective Hamiltonian is calculated perturbatively as a power series of the inverse of the frequency of the drive and in this framework the RWA is simply the zeroth order of the expansion. At the core of this formalism lies the Magnus expansion, a perturbative solution of the time-dependent Schrödinger equation that preserves unitarity at all orders of expansion. The Magnus expansion has gained a lot of attention in the last decade, with applications of it appearing in the field of quantum information and beyond [6, 7]. We will introduce these concepts more thoroughly in Chapter 1.
In the second chapter, we will apply this effective Hamiltonian formalism to describe the dynamics of a high fidelity quantum gate for singlet-triplet qubits, developed in [2]. This is a system of a relatively strong drive compared to its frequency which means that low orders of the effective Hamiltonian expansion will fail to describe the dynamics to desirable precision. However, this is an interesting calculation that accentuates the weaknesses and the strengths of the formalism.

In the final chapter a different approach to the effective Hamiltonian is being investigated. Namely we will try to derive an explicit formula for the effective Hamiltonian which will lead into some new insights about the formalism.
Chapter 1

Magnus-Taylor Expansion and Effective Hamiltonians

In this chapter we present our main tools for the calculation of time evolution operators using time-dependent perturbation theory developed in [1]. In section 1 we give a brief review of the derivation of the Magnus expansion and motivate its use a tool for solving the time-dependent Schrödinger equation, while in sections 2 and 3 we present two different methods for calculating it. Next, in section 3 we present a modification of the Magnus expansion, namely the Magnus-Taylor expansion which is required in order to calculate effective Hamiltonian which is presented in detail in section 5.

1.1 Magnus Expansion

A frequently occurring differential equation in physics is

$$\frac{dX(t)}{dt} = A(t)X(t),$$

(1.1)

where $X(t)$ and $A(t)$ can be any kind of operators acting on some space. A differential equation that falls into this category and is also of greatest significance for us is of course the Schrödinger equation:

$$i\frac{d|\psi(t)\rangle}{dt} = \mathcal{H}(t)|\psi(t)\rangle,$$

(1.2)

written in natural units, where one can identify $X(t)$ as the state of the system under consideration and $A(t)$ as $-i\mathcal{H}(t)$, the Hamiltonian of the system up to a factor of $-i$. The standard methodology of dealing with this problem in the case of a time dependent Hamiltonian is to switch to a Heisenberg picture by introducing the time evolution operator $U(t, t_0)$ for the state:

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle \Rightarrow U(t_0, t_0) = I,$$

(1.3)

where we denote the identity operator with $I$. In this Heisenberg picture the dynamics are described by the differential equation

$$i\frac{dU(t, t_0)}{dt} = \mathcal{H}(t)U(t, t_0).$$

(1.4)
Chapter 1. Magnus-Taylor Expansion and Effective Hamiltonians

Its solution using the Dyson series is

\[
U(t, t_0) = T \exp \left( -i \int_{t_0}^{t} \mathcal{H}(\tau) d\tau \right),
\]  

where \( T \) is the time ordering operator.

An alternative approach of finding the solution of Eq. (1.1) is to make use of the Magnus Expansion (ME) [8]. The idea here is to assume that there is a solution of the form

\[
X(t) = e^{\Omega(t)} \quad \text{with} \quad X(t_0) = I \quad \text{and} \quad \Omega(t) = \sum_{n=0}^{\infty} \Omega_n(t).
\]  

Here the expansion happens in the exponent rather than the entire exponential. By substituting the ansatz into the differential equation one can show by exploiting some algebraic properties and as long as convergence criteria are met (see Appendix A) that

\[
\Omega(t) = \sum_{n=0}^{\infty} \frac{B_n}{n!} \int_{t_0}^{t} \text{ad}_{\Omega(t)} A(t) dt,
\]  

with \( B_n \) the \( n \)th Bernoulli number and \( \text{ad}_{\Omega(t)} A(t) = [\Omega(t), A(t)] \) and so on. Then by introducing an auxiliary parameter \( \varepsilon \) in the \( \Omega(t) \) expansion:

\[
\Omega(t) = \sum_{n=0}^{\infty} \varepsilon^n \Omega_n(t)
\]  

and substituting this into Eq. (1.7) one can derive the terms of the ME as they are also presented in [9]

\[
\Omega_0(t) = \int_{t_0}^{t} d\tau A(\tau)
\]  

\[
\Omega_1(t) = \frac{1}{2} \int_{t_0}^{t} d\tau \int_{t_0}^{\tau} d\tau_1 [A(\tau), A(\tau_1)]
\]  

\[
\Omega_2(t) = \frac{1}{6} \int_{t_0}^{t} d\tau \int_{t_0}^{\tau} d\tau_1 \int_{t_0}^{\tau_1} d\tau_2 ([A(\tau), [A(\tau_1), A(\tau_2)]] + [A(\tau_2), [A(\tau_1), A(\tau)]])
\]  

\[
\vdots
\]  

by comparing orders of \( \varepsilon \) and in the end send \( \varepsilon \rightarrow 1 \).

All of these terms are anti-Hermitian if \( A(t) \) is anti-Hermitian. This can be easily seen by considering two operators \( A = -A^\dagger \) and \( B = -B^\dagger \), then

\[
[A, B] = B^\dagger A^\dagger - A^\dagger B^\dagger = (-1)^2 BA - (-1)^2 AB = -[A, B].
\]  

adding a third operator of the same kind \( C = -C^\dagger \) leads to

\[
\]  

(1.12)
1.1. Magnus Expansion

and so it can be easily proved by induction that the \( n \) right nested commutator of anti-Hermitian operators \( A_1, \ldots, A_{n+1} \) is also anti-Hermitian

\[
\left[ A_1, \left[ A_2, \ldots, \left[ A_n, A_{n+1} \right] \ldots \right] \right] = -\left[ A_1, \left[ A_2, \ldots, \left[ A_n, A_{n+1} \right] \ldots \right] \right], \tag{1.14}
\]

therefore the ME is anti-Hermitian at all orders for anti-Hermitian \( A(t) \).

A final remark about the ME, is that in case \( A(t) \) is constant in time, all commutators vanish and therefore we obtain the exact solution of the system at zeroth order in the ME

\[
U(t, t_0) = e^{\Omega(t)} = e^{\Omega_0(t)} = \exp \left( \int_{t_0}^{t} d\tau A \right) = e^{A(t-t_0)}. \tag{1.15}
\]

In the general case we will have

\[
U(t, t_0) = \exp \sum_{n=0}^{\infty} \Omega_n(t), \tag{1.16}
\]

where \( \Omega_n(t) \) are calculated as stated above with \( A(t) = -i\mathcal{H}(t) \) for the Schrödinger equation. A detailed derivation of the above can be found in [9].

The ME comes with some very significant advantages. First of all, unitarity of the time evolution operator is preserved at all orders of the expansion, as can be easily seen from Eq. (1.6) combined with the fact that the ME is anti-Hermitian at any order. This preservation of unitarity is not a feature of the Dyson series. Furthermore, due to the nested commutator form of the ME terms, there are cases where one can obtain the exact result by going only up to a finite order in the expansion. Usually, this will occur when some higher order commutator vanishes at all times.

As an example case where the exact solution is obtained at finite order, consider the forced harmonic oscillator

\[
\mathcal{H}(t) = \omega_0 \left( a^\dagger a + \frac{1}{2} \right) + f(t) (a^\dagger + a) \tag{1.17}
\]

with \( a \) \((a^\dagger)\) the annihilation (creation) operator of the harmonic oscillator and \( f(t) \) some real function. In the interaction picture, this Hamiltonian transforms into

\[
\mathcal{H}_{\text{int}}(t) = f(t) (e^{i\omega_0 t} a^\dagger + e^{-i\omega_0 t} a). \tag{1.18}
\]

From this it is simple to see that

\[
[[\mathcal{H}_{\text{int}}(t_1), \mathcal{H}_{\text{int}}(t_2)], \mathcal{H}_{\text{int}}(t_3)] = 0 \tag{1.19}
\]

and therefore the ME terminates at first order. On the contrary probing the same problem with the Dyson series would require to go up to infinite order to obtain the full result. More examples are given in [9].

Unfortunately, there are some drawbacks too. The most obvious one is the exponential increase in complexity of calculations as we move on to higher orders. Even looking at the first three orders of the ME one can easily spot this by comparing
Eqs. (1.9) and (1.11). A more subtle drawback is the fact that after calculating the ME we merely obtain the generator of the time evolution. For practical, though non-numerical applications one would still have to expand the exponential of the already truncated ME, which of course will also be truncated at some point, therefore slowing down the convergence and adding more computational complexity. However, this last disadvantage is somewhat mediated by the fact that for many applications the generator of the time evolution operator is sufficient to work with.

1.2 Algorithmic Calculation of the Magnus Expansion

In the last section we presented the first three orders of the ME. At first glance these terms do not seem to follow any particular pattern, which would of course make the calculation up to arbitrary orders extremely complicated. Fortunately, a variety of algorithmic ways to calculate higher order terms have been developed, which rely on recursive relations. In the present section, we briefly present the method of our choice for the work presented in this thesis.

The algorithm requires to be seeded with the zeroth order Magnus term as stated in Eq. (1.9). Starting from this, a series of $S_j^n(t)$ components needs to be calculated depending on the desired order. The lower index of the $S_j^n(t)$ components counts the order in the ME with $n > 0$ and the upper index takes integer values in the range $[1, n]$. So for instance

1st order terms: $S_1^1(t)$
2nd order terms: $S_2^1(t), S_2^2(t)$
3rd order terms: $S_3^1(t), S_3^2(t), S_3^3(t)$

\[ S_1^1(t) = [\Omega_{n-1}(t), A(t)], \]
\[ S_2^j(t) = \sum_{m=0}^{n-j} [\Omega_m(t), S_{n-m-1}^{j-1}(t)]. \]

Once all necessary $S_j^n(t)$ components have been obtained we can calculate the $n$th order Magnus term by

\[ \Omega_n(t) = \sum_{j=1}^{n} \frac{B_j}{j!} \int_{t_0}^{t} d\tau S_j^n(\tau), \]

where again $B_j$ is the $j$th Bernoulli number. An alternative algorithm can be found in [10] and further details about the algorithm presented here are given in [9].
1.3   Diagramatic Calculation of the Magnus Expansion

The algorithmic calculation of the ME has also a diagrammatic counterpart, developed in [11], which we present in this section. Essentially, the diagrammatic calculation of the ME boils down to finding all the possible binary rooted trees we can create for a specific order. Our main building tools are:

(i) Endpoints of each branch of the tree: $\bullet = -i\mathcal{H}(\tau)$

(ii) Vertical lines that denote integration of whatever lies on top of them

(iii) Bifurcations that indicate commutation of whatever lies on top of them

The last two elements combine to form left skewed bifurcations

\[
\begin{align*}
\bullet_1 & \quad \bullet_2 = \left[ \int_{t_0}^{t} d\tau (\bullet_1), \bullet_2 \right],
\end{align*}
\]

where the squares can be either endpoints or sub-trees and the upper bound of the integral is the variable of integration below the bifurcation. Notice that the left skewed bifurcation is antisymmetric with respect to its branches, meaning that if we interchange them we end up with the same term but opposite sign. Furthermore, each tree has an $\alpha$-factor. For an endpoint it is simply

\[
\alpha(\bullet) = 1. \quad (1.23)
\]

For a generic tree, in order to calculate the $\alpha$-factor we locate all the second layer independent integrations (graphically that means a vertical line that has only one other vertical line underneath it) and cut those branches to end up with a tree of the form

\[
\begin{align*}
\eta_1 & \quad \eta_2 \quad \eta_3 \quad \vdots \\
& \quad \eta_s
\end{align*}
\]

which we call the truncated tree. Then the $\alpha$-factor is given by

\[
\alpha(\eta) = \frac{B_s}{s!} \prod_{n=1}^{s} \alpha(\eta_n). \quad (1.24)
\]

If we define a vertex as a point where exactly three lines meet then: $s$ is the number of vertices in the truncated tree, $B_s$ is the $s$th Bernoulli number, $\eta$ denotes our original tree and $\eta_n$ are the sub-trees emerging from the truncation of the main tree.

Now that we know the building blocks of our diagrammatic procedure we only need the rules by which we construct our trees:
(i) Start with the tree trunk, a vertical line.
(ii) In order to build the $m$th order term of the ME, keep adding left skewed bifurcations adjacently and upwards until the number of vertices is $m$.
(iii) Add an endpoint to the end of each branch of the resulting tree.
(iv) Write down all possible trees for $m$ vertices.
(v) Calculate the corresponding $\alpha$-factors.
(vi) Sum all the diagrams obtained multiplied with their corresponding $\alpha$-factor.

As an example we calculate the first three orders of the ME. For the zeroth order we need to add the tree trunk and then we need zero vertices, therefore the only possible diagram is

$$\eta_0 = \int_{t_0}^{t_0 + t_c} d\tau \mathcal{H}(\tau)$$

and $\alpha(\eta_0) = 1$. For the first order of the ME we start with the tree trunk. Now we need one vertex and therefore we only need to add one left skewed bifurcation, so the only possible diagram is

$$\eta_1 = \int_{t_0}^{t_0 + t_c} d\tau \left[ \int_{t_0}^{\tau} d\tau_1 \mathcal{H}(\tau_1), \mathcal{H}(\tau) \right].$$

The truncated tree will look exactly like the original and therefore

$$\alpha(\eta_1) = B_1 \frac{1}{1!} \alpha(\bullet) = -\frac{1}{2}.$$  \hspace{1cm} (1.25)

For the second order of the ME we get two trees,

$$\eta_{21} = \int_{t_0}^{t_0 + t_c} d\tau \left[ \int_{t_0}^{\tau} d\tau_1 \mathcal{H}(\tau_1), \left[ \int_{t_0}^{\tau_1} d\tau_2 \mathcal{H}(\tau_2), \mathcal{H}(\tau) \right] \right],$$

$$\eta_{22} = \int_{t_0}^{t_0 + t_c} d\tau \left[ \int_{t_0}^{\tau} d\tau_1 \left[ \int_{t_0}^{\tau_1} d\tau_2 \mathcal{H}(\tau_2), \mathcal{H}(\tau_1) \right], \mathcal{H}(\tau) \right],$$

with corresponding $\alpha$ factors

$$\alpha(\eta_{21}) = B_2 \frac{1}{2!} \alpha(\bullet)^2 = \frac{1}{12} \text{ and } \alpha(\eta_{22}) = B_1 \frac{1}{1!} \alpha(\eta_1) = \frac{1}{4}.$$  \hspace{1cm} (1.26)
1.4. Magnus-Taylor Expansion

Note here that the second order looks quite different from what we obtained in Eq. (1.11). However using Fubini’s theorem

\[
\int_a^b dx \int_a^x dy f(x, y) = \int_a^b dy \int_y^b dx f(x, y),
\]

(1.27)

the Jacobi identity

\[
[A, [B, C]] + [C, [A, B]] + [B, [C, A]] = 0
\]

(1.28)

and appropriate relabeling of the integration variables we can bring the second order term that we derived here in the form of Eq. (1.11).

1.4 Magnus-Taylor Expansion

In the previous sections we have seen that we can obtain useful information about the time evolution operator of a given system using the ME as long as we are given the explicit form of the Hamiltonian. But what happens if we have a Hamiltonian that has some explicit time dependence as well as some implicit time dependence through \(N\) unspecified functions \(H_j(t)\) for \(1 \leq j \leq N\)? The answer is that we can still obtain some useful information using the Magnus-Taylor Expansion (MTE).

The idea here, as introduced in [1], is to use the Magnus formalism presented in the previous sections with the addition that the unspecified functions \(H_j(t)\) are substituted with their corresponding Taylor expansions around a time \(\tau_0 \in [t_0, t]\) up to some order \(n\). We write for the lowest order in the ME

\[
\Omega_0(t) = -i \int_{t_0}^t d\tau \mathcal{H}[\tau, H_j(\tau)] \rightarrow \mathcal{M}_0^n \left[ \mathcal{H}(\tau); t, t_0, \tau_0 \right] = -i \int_{t_0}^t d\tau \mathcal{H} \left[ \tau, T^n_j(\tau; \tau_0) \right],
\]

(1.29)

where we denoted

\[
T^n_j(\tau; \tau_0) = \sum_{k=0}^n \frac{1}{k!} \frac{\partial^k H_j(\tau_0)}{\partial \tau^k}(\tau - \tau_0)^k
\]

(1.30)

and we also introduced the notation

\[
\mathcal{M}^n_m \left[ \mathcal{H}(\tau); t, t_0, \tau_0 \right]
\]

(1.31)

for the MTE term of order \(m\) in the ME and order \(n\) in the Taylor expansion, which is thus distinguished from the simple Magnus counterpart \(\Omega_m\). To abbreviate this we will refer to \(\mathcal{M}^n_m(t)\) as the \((m, n)\)-MTE term. For consistency, two conditions have to be met:

- The length of the integration interval should not exceed the radius of convergence of the ME
- The Taylor expansion must converge, which means that the unspecified functions \(H_j(t)\) must be analytic.
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As we will see at the end of this chapter, there is a way around the second restriction using the formalism of the so-called kick operators, but before we get into that let us try to apply the MTE on a specific problem.

Consider the harmonically driven qubit with a transverse drive

\[ H(t) = \frac{\omega_0}{2} \sigma_z + \frac{H_1(t)}{2} \cos(\omega t + \phi) \sigma_x, \]  
(1.32)

with \( \omega_0 \) the frequency of the qubit, \( H_1(t) \) some time dependent amplitude function, \( \omega \) the frequency of the drive, \( \phi \) some phase and the Pauli matrices \( \sigma_x, \sigma_y, \sigma_z \). To simplify the problem we assume resonance \( \omega = \omega_0 \) and \( \phi = 0 \),

\[ H(t) = \frac{\omega}{2} \sigma_z + \frac{H_1(t)}{2} \cos(\omega t) \sigma_z. \]  
(1.33)

From now on we will refer to this system as our toy model. The standard methodology for dealing with such a Hamiltonian is to shift the discussion to a rotating frame using the transformation

\[ H' = U^\dagger H U - i U^\dagger \frac{\partial U}{\partial t}, \]  
(1.34)

and then apply a Rotating Wave Approximation (RWA). So for our case, we would rotate the frame using \( U = \exp(-i \omega t \sigma_z/2) \), to get

\[ H_{\text{rot}}(t) = \frac{H_1(t)}{4} (\sigma_x + \cos 2\omega t \sigma_x - \sin 2\omega t \sigma_y) \]  
(1.35)

and the RWA Hamiltonian for this frame

\[ \mathcal{H}_{\text{RWA}}(t) = \frac{H_1(t)}{4} \sigma_x. \]  
(1.36)

Assuming \( t_0 = 0 \), the corresponding Dyson time evolution operator according to Eq. (1.5) is

\[ U_{\text{RWA}}(t, 0) = T \exp \left( -i \int_0^t \mathcal{H}_{\text{RWA}}(\tau) d\tau \right) = \exp \left( -i \frac{t}{4} \int_0^t H_1(\tau) d\tau \sigma_x \right). \]  
(1.37)

However, by using the MTE, instead of the RWA we can still get some useful insight about the evolution of the system and as a matter of fact we may be able to obtain information about more subtle effects that would be completely missed out by the RWA. Now let us try to approach this problem with a MTE including up to (1,1)-MTE terms. To simplify the calculation a bit further we choose the evolution time \( t = \pi/\omega \). Applying the formulas for zeroth and first order we obtain

\[ \mathcal{M}_0 \left[ \mathcal{H}_{\text{rot}}(\tau); \frac{\pi}{\omega}, 0, \tau_0 \right] = -i \int_0^{\frac{\pi}{\omega}} d\tau \mathcal{H}_{\text{rot}}[\tau, T_1(\tau; \tau_0)], \]  
(1.38)

\[ \mathcal{M}_1 \left[ \mathcal{H}_{\text{rot}}(\tau); \frac{\pi}{\omega}, 0, \tau_0 \right] = -\frac{1}{2} \int_0^{\frac{\pi}{\omega}} d\tau \int_0^{\tau} d\tau_1 \left[ \mathcal{H}_{\text{rot}}[\tau, T_1(\tau; \tau_0)], \mathcal{H}_{\text{rot}}[\tau_1, T_1(\tau_1; \tau_0)] \right]. \]  
(1.39)
1.4. Magnus-Taylor Expansion

with

\[ T_1^1(\tau; \tau_0) = H_1(\tau_0) + \dot{H}_1(\tau_0)(\tau - \tau_0) \]  

(1.40)

and therefore

\[ \mathcal{H}_{\text{rot}}[\tau, T_1^1(\tau; \tau_0)] = \frac{1}{4} \left( H_1(\tau_0) + \dot{H}_1(\tau_0)(\tau - \tau_0) \right) (\sigma_x + \cos 2 \omega \tau \sigma_x - \sin 2 \omega \tau \sigma_y). \]  

(1.41)

By putting everything together and introducing a dimensionless variable \( \beta_0 = 2 \omega \tau_0 \) we get

\[ M_0^1 \left[ \mathcal{H}_{\text{rot}}(\tau); \frac{\pi}{\omega}, 0, \tau_0 \right] = -\frac{i \pi H_1(\tau_0)}{4 \omega} \sigma_x + \frac{i \pi \dot{H}_1(\tau_0)}{8 \omega^2} (\beta_0 - \pi) \sigma_x - \frac{i \pi \ddot{H}_1(\tau_0)}{8 \omega^2} \sigma_y, \]  

(1.42)

\[ M_1^1 \left[ \mathcal{H}_{\text{rot}}(\tau); \frac{\pi}{\omega}, 0, \tau_0 \right] = \frac{i \pi H_1(\tau_0)^2}{32 \omega^2} \sigma_z + O \left( \frac{1}{\omega^3} \right), \]  

(1.43)

where we will ignore terms \( O(1/\omega^3) \) because even only with terms of order \( 1/\omega^2 \) we are already beyond the RWA which is valid for \( H_1(t)/\omega \ll 1 \).

Note that in \( O(1/\omega^3) \) there are also terms proportional to \( \tau_0/\omega^2 \) which at first glance do not seem to be of order \( 1/\omega^3 \). However, we are working in natural units and so we may choose to express everything in terms of energy. Time variables or parameters have dimensions of inverse energy and our standard unit for energy throughout this thesis will be the frequency \( \omega \). In other words we always express time variables and parameters as a dimensionless quantities divided by the frequency. For instance

\[ \tau_0 = \frac{\beta_0}{2 \omega}, \]  

(1.44)

where the factor of 2 is inserted for reasons that will become clear later. Therefore \( \tau_0/\omega^2 = \beta_0/2 \omega^3 \) is indeed of order \( 1/\omega^3 \) in natural units.

The time evolution operator in this case is

\[ U_{\text{MTE}} \left( \frac{\pi}{\omega}, 0 \right) = \exp \left[ -\frac{i \pi}{4} \left( \frac{H_1(\tau_0)}{\omega} \sigma_x - \frac{\dot{H}_1(\tau_0)}{2 \omega^2} ((\beta_0 - \pi) \sigma_x - \sigma_y) - \frac{H_1(\tau_0)^2}{8 \omega^2} \sigma_z \right) \right]. \]  

(1.45)

In comparison, the corresponding time evolution operator for the RWA if we also Taylor expand the amplitude function up to order one is

\[ U_{\text{RWA}} \left( \frac{\pi}{\omega}, 0 \right) = \exp \left[ -\frac{i \pi}{4} \left( \frac{H_1(\tau_0)}{\omega} \sigma_x - \frac{\dot{H}_1(\tau_0)}{2 \omega^2} (\beta_0 - \pi) \sigma_x \right) \right]. \]  

(1.46)

Even from this equation it is evident that the MTE includes the RWA as well as further corrections in the time evolution operator of the system. Such a relation will indeed be established explicitly in the following section.
1.5 Effective Hamiltonian

1.5.1 What Is the Effective Hamiltonian

In the previous section we have seen that we can approximate the evolution of a quantum system using the MTE to a sufficient degree. However, even though the time evolution of a system may be useful in its own right, we would like to be able to extract information about our system in a more generalized and systematic way.

A tool for doing this for periodically driven systems is the effective Hamiltonian. The effective Hamiltonian is axiomatically defined as:

**Definition 1.5.1** Assume a Hamiltonian \( H(t) \) acting on a two-dimensional Hilbert space \( \mathbb{H}_2 \). The effective Hamiltonian \( H_{\text{eff}}(t) \) is a Hamiltonian acting on the same space, that generates a time evolution which stroboscopically coincides with the time evolution generated by the original Hamiltonian \( H(t) \):

\[
\exists t_c : T \exp \left( -i \int_{t_0}^{t_0 + nt_c} H(\tau) d\tau \right) = T \exp \left( -i \int_{t_0}^{t_0 + nt_c} H_{\text{eff}}(\tau, t_0) d\tau \right), \forall n \in \mathbb{Z}^+.
\]

In the following sections we will see that this is the only relation required to derive all the properties of the effective Hamiltonian. For the moment the effective Hamiltonian of a particular system may be considered as a Hamiltonian that exhibits the same behavior as the actual Hamiltonian periodically. The goal, in order for...
1.5. Effective Hamiltonian

this formalism to be meaningful, is to end up with an effective Hamiltonian that is generally easier to deal with than the actual Hamiltonian. Although we will also introduce some new terminology, most of the theory presented in section 1.5 can be found in more detail in [1].

1.5.2 Relation Between the Hamiltonian and the Corresponding Effective Hamiltonian

In order to derive the effective Hamiltonian we must first relate it to the actual Hamiltonian of a given system. At first, we notice that Eq. (1.47) can be rewritten as

\[ T \exp \left( -i \int_{t_0}^{t_0 + n t_c} \mathcal{H}(\tau) d\tau \right) = T \exp \left( -i \int_{t_0}^{t_0 + n t_c} \mathcal{H}_{\text{eff}}(\tau, t_0) d\tau \right), \forall n \in \mathbb{Z}^+. \]  

(1.48)

To see why this is true let us rewrite Eq. (1.47) using the \( U \) notation

\[ U(t_0 + nt_c, t_0) = U_{\text{eff}}(t_0 + nt_c, t_0), \forall n \in \mathbb{Z}^+. \]  

(1.49)

By exploiting the group multiplication property of the time evolution operator we can also write Eq. (1.49) as

\[ U(t_0 + nt_c, t_0 + (n-1)t_c) U(t_0 + (n-1)t_c, t_0) = U_{\text{eff}}(t_0 + nt_c, t_0 + (n-1)t_c) U_{\text{eff}}(t_0 + (n-1)t_c, t_0). \]  

(1.50)

According to Eq. (1.49) we should also have

\[ U(t_0 + (n-1)t_c, t_0) = U_{\text{eff}}(t_0 + (n-1)t_c, t_0) \]  

(1.51)

and therefore Eq. (1.48) is proved.

Using Eq. (1.48) as a starting point is still not particularly helpful since the time ordering operator prohibits us from making any kind of connection between \( \mathcal{H}(t) \) and \( \mathcal{H}_{\text{eff}}(t) \). This is where ME comes in handy, we write again Eq. (1.48) using the ME

\[ e^{\Omega[H(\tau);n,t_c,t_0]} = e^{\Omega[H_{\text{eff}}(\tau);n,t_c,t_0]}, \forall n \in \mathbb{Z}^+. \]  

(1.52)

This statement is equally valid for the MTE as well

\[ e^{M[H(\tau);n,t_c,t_0,\tau_0]} = e^{M[H_{\text{eff}}(\tau);n,t_c,t_0,\tau_0]}, \forall n \in \mathbb{Z}^+ \]  

(1.53)

and in order to make the MTE exponents dimensionally meaningful and compact we define

\[ \overline{\mathcal{H}} = \frac{i}{t_c} \mathcal{M} [\mathcal{H}(\tau); n, t_c, t_0, \tau_0] \Rightarrow \overline{\mathcal{H}}^{(ij)} = \frac{i}{t_c} \mathcal{M}^{(ij)} [\mathcal{H}(\tau); n, t_c, t_0, \tau_0]. \]  

(1.54)

Substitution of Eq. (1.54) into Eq. (1.53) yields

\[ e^{-i\overline{\mathcal{H}} t_c} = e^{-i\mathcal{H}_{\text{eff}} t_c}, \forall n \in \mathbb{Z}^+, \]  

(1.55)
where now the "bar" quantities are still the MTE, only up to a factor of $i/t_c$, which is why from now on when we refer to "MTE" we will refer to the one with dimensions of energy. The MTE terms in this new notation are

\[
\tilde{H}^{(0,i)} = \frac{1}{t_c} \int_{t_0+(n-1)t_c}^{t_0+nt_c} d\tau \frac{d}{d\tau} \left[ \mathcal{H} \left[ \tau, T_j^i(\tau; \tau_0) \right] \right]
\]

\[
\tilde{H}^{(1,i)} = -\frac{i}{2t_c} \int_{t_0+(n-1)t_c}^{t_0+nt_c} d\tau \int_{t_0+(n-1)t_c}^{\tau} d\tau_1 \mathcal{H} \left[ \tau, T_j^i(\tau; \tau_0) \right] \mathcal{H} \left[ \tau_1, T_j^i(\tau_1; \tau_0) \right]
\] (1.56)

\[
\vdots
\]

If the reader got confused about the factors involved here recall that besides multiplying Eqs. (1.9) to (1.11) with the $i/t_c$ factor we also need to substitute $A(\tau) = -i \mathcal{H}(t)$. The advantage that Eq. (1.55) offers towards deriving $H_{\text{eff}}(t)$ is that we can now see directly the relation between the effective Hamiltonian and the actual Hamiltonian of the system

\[
\tilde{H} = \tilde{H}_{\text{eff}}.
\] (1.58)

meaning that the Hamiltonians $\mathcal{H}$ and $H_{\text{eff}}$ must have the same MTE.

Before this section is concluded we introduce the generic form of the effective Hamiltonian. Since we are mostly going to deal with harmonically driven systems, we would like our effective Hamiltonian to have some explicit dependence on the parameter of importance which is of course the frequency of the drive $\omega$. Therefore we expand the effective Hamiltonian in terms of $1/\omega$

\[
H_{\text{eff}}(t; t_0) = \sum_{k=0}^{\infty} \frac{h_k(t; t_0)}{\omega^k},
\] (1.59)

and by setting $\mu = 1/\omega$ we obtain

\[
h_k(t; t_0) = \frac{D^k H_{\text{eff}}}{D\mu^k}.
\] (1.60)

At this point we define for notational convenience the Polynomial Coefficient Operator (PCO):

- For a Polynomial function $P(\mu)$

\[
\frac{D^k P(\mu)}{D\mu^k} = \frac{D^k}{D\mu^k} \left( \sum_{n=0}^{N} a_n \mu^n \right) = \sum_{n=0}^{N} a_n \frac{D^k}{D\mu^k} \mu^n = \sum_{n=0}^{N} a_n \delta_{kn} = a_k
\] (1.61)

- For any non-Polynomial function $f(\mu)$

\[
\frac{D^k f(\mu)}{D\mu^k} = \delta_{k0} f(\mu).
\] (1.62)

- Linearity

\[
\frac{D^k}{D\mu^k} (\alpha A(\mu) + \beta B(\mu)) = \alpha \frac{D^k A(\mu)}{D\mu^k} + \beta \frac{D^k B(\mu)}{D\mu^k}
\] (1.63)
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- Product rules

\[ A, B \text{ non polynomial functions} \Rightarrow \frac{D^k(A(\mu)B(\mu))}{D\mu^k} = \delta_{k0}A(\mu)B(\mu) \quad (1.64) \]

\[ A(\mu) = \sum_{n=0}^{N} a_n \mu^n, B \text{ non polynomial function} \Rightarrow \frac{D^k(A(\mu)B(\mu))}{D\mu^k} = a_k B(\mu) \quad (1.65) \]

\[ A(\mu) = \sum_{n=0}^{N_a} a_n \mu^n, B(\mu) = \sum_{m=0}^{N_b} b_m \mu^m \Rightarrow \frac{D^k(A(\mu)B(\mu))}{D\mu^k} = \sum_{n=0}^{k} a_n b_{k-n}. \quad (1.66) \]

1.5.3 Dimensional Analysis Filter for the Magnus-Taylor Expansion

As we have seen in the toy model application, the MTE terms are generally of the form

\[ \lambda \prod_{k=1}^{m} \partial_{t}^{d_k} H_{j_k}(\tau_0) \quad (1.67) \]

with \( \lambda \) some dimensionless constant, \( j_k \) the function index of the \( k \)th factor of the product and \( d_k \) the derivative order of the \( k \)th factor of the product. In the final chapter of this thesis we will prove that this is in fact the most general form of the dimension full factors of the MTE. Dimensional considerations however cannot allow any combination of these parameters. Specifically, the MTE should have dimensions of energy and by extension terms like the one in (1.67) should also have dimensions of energy. Since we are working in natural units, dimensions of time \([t]\) are equal to inverse dimensions of energy \([E]^{-1}\) and so \( \omega \sim [E] \) and \( \partial_{t}^{d_k} H_{j_k} \sim [E]^{d_k+1} \). The dimensional restriction in this case is

\[ m + \sum_{k=1}^{m} d_k = n + 1. \quad (1.68) \]

So far, each time we used the MTE the choice of order for the ME and Taylor expansion was arbitrary. In the following section it will be vital to have a methodical way of selecting these orders so that our MTE will include terms of some specified order in \( \frac{1}{\omega} \). The need for such order fixing arises from our choice of expansion in Eq. (1.59) and the fact that we will construct our effective Hamiltonian from Eq. (1.58)

Let us see how Eq. (1.68) restricts our choice of ME and Taylor orders, by considering the toy model. For this application we had only one amplitude function and therefore the only possible value for \( j_k \) is one, so (1.67) becomes

\[ \lambda \prod_{k=1}^{m} \partial_{t}^{d_k} H_{1}(\tau_0) \quad (1.69) \]

Assume we wished to find all the possible \( 1/\omega^n \) terms in the MTE. The zeroth order of the MTE depends on the Hamiltonian and by extension on \( T^p_1(\tau;\tau_0) \) (see Eq. (1.30)) as well, which of course includes no products of any derivatives, so the
only possible value for \( m \) would be 1. In this order of the expansion, the dimensional restriction (1.68) gives \( d_1 = n \), thus in order to go up to order \( 1/\omega^n \) in the zeroth order of the MTE we need to go up to order \( n \) in the Taylor expansion. The first order of the MTE depends on the commutator of the Hamiltonian with itself at different times and by extension on \( T^p_1(\tau; \tau_0) T^p_1(\tau_1; \tau_0) \) as well, which includes only products of two Taylor terms, so the only possible value for \( m \) would be two. In this order of the expansion, the dimensional restriction (1.68) gives \( d_1 + d_2 = n - 1 \) which of course does not have a unique solution. However, we are trying to track the order of the Taylor expansion needed and therefore the highest order of derivative that can be involved, so the solution we are interested in is \((d_1, d_2) = (n - 1, 0)\) or \((0, n - 1)\). Therefore in order to go up to order \( 1/\omega^n \) in the first order we need to go up to order \( n - 1 \) in the Taylor expansion. Notice however that by going up to order \( n - 1 \) we guarantee only that any terms of order \( 1/\omega^n \) that the ME first order can contribute, will be included. That said, there will still be some higher order terms that we will have to throw out by hand. For instance \((\partial_t^{n-1} H_1(\tau_0))^2\) is an example of a term that will be included following this line of reasoning, yet dimensional analysis tells us that it is an \( 1/\omega^{2n} \) term.

We can keep going up in the ME order following this process, but the question now is when should we stop. The general pattern that emerges here is that the \( \nu \)-th order of the ME will include terms of the form (1.67) for \( m = \nu + 1 \). If we solve Eq. (1.68) for the sum of \( d_k \)'s,

\[
\sum_{k=1}^{m} d_k = n - m + 1,
\]

it becomes clear that by keeping \( n \) constant and going up to higher orders in the MTE and in turn higher \( m \), will lead to a dilution of the \( d_k \)'s. Therefore the higher we go in the MTE the lower the orders of the derivatives relevant. From this it is easy to extrapolate that the highest order derivative that may appear in the MTE will be in the zeroth order. Furthermore, it is evident from Eq. (1.70) that there is a point of maximal dilution for the \( d_k \)'s which is reached when

\[
\sum_{k=1}^{m} d_k = 0 \Rightarrow m = n + 1 \text{ and } d_k = 0, \forall k.
\]

This value for \( m \) corresponds to the \( n \)th order of the ME. Beyond that order, all terms involved are of order \( O(1/\omega^{n+1}) \). Combining all of the above leads to the emergence of the following theorem:

**Theorem 1.5.1** The truncated Magnus-Taylor expansion \( \tilde{H} = \sum_{j=0}^{N} \tilde{H}^{(j,N-j)} \) includes all the possible terms of order up to \( N \) in \( 1/\omega \) of the full Magnus-Taylor expansion.
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1.5.4 Recursive Formula for the Effective Hamiltonian

The recursive formula that we will present here produces a truncated $H_{\text{eff}}(t; t_0)$ up to some order $N$ in $1/\omega$

$$H_N = H_{\text{eff}}(t; t_0, N) = \sum_{k=0}^{N} \frac{h_k(t; t_0)}{\omega^k}.$$  \hspace{1cm} (1.72)

To initiate the recursion we must first calculate the $N = 0$ term. Our starting point is Eq. (1.58) where we will compare the $\omega^0$ terms in the effective Hamiltonian $M_{\text{TE}}$ to the corresponding ones in the actual Hamiltonian $M_{\text{TE}}$

$$\frac{D^0 H_{\text{eff}}}{D \mu^0} = \frac{D^0 \tilde{H}}{D \mu^0}.$$  \hspace{1cm} (1.73)

By setting $N = 0$ in Eq. (1.72) it can be easily seen that

$$H_0 = h_0(t; t_0) \Rightarrow \tilde{H}_0 = \tilde{h}_0,$$  \hspace{1cm} (1.74)

thus

$$\frac{D^0 \tilde{h}_0}{D \mu^0} = \frac{D^0 \tilde{H}}{D \mu^0}.$$  \hspace{1cm} (1.75)

For the left hand side of this equation we would need to calculate the MTE of $h_0(t; t_0)$. Unfortunately, if we choose to Taylor expand around some specific time we will not be able to retrieve the time dependence of $h_0(t; t_0)$, so instead we will expand around the running time $t \in [t_0 + (n-1)t_c, t_0 + nt_c]$. For the rest of this thesis the MTE will always be expanded around the running time unless it is explicitly stated otherwise. To clarify what is meant by running time, consider that there are two time variables involved here. One of them is $\tau$, the integration variable for the MTE and the other is $t$, time as it would be measured in a laboratory. By expanding around this running time, the Taylor expansion becomes not only a function of $\tau$ but also a function of the point of expansion $t$. Thanks to Theorem (1.5.1) there is no longer any ambiguity in which order in the MTE or Taylor do we need to go up to. Here we need $\omega^{-0}$ terms therefore we only need

$$\tilde{h}_0 = \tilde{h}_0^{(0,0)} + O \left( \frac{1}{\omega} \right) \Rightarrow$$

$$\frac{D^0 \tilde{h}_0}{D \mu^0} = \frac{1}{t_c} \frac{D^0}{D \mu^0} \left( \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} T_0^0(\tau; t) d\tau \right) = \frac{1}{t_c} \frac{D^0}{D \mu^0} \left( \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} h_0(t; t_0) d\tau \right) = \frac{h_0(t; t_0)}{t_c} \frac{D^0}{D \mu^0} \left( \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} d\tau \right) = h_0(t; t_0)$$  \hspace{1cm} (1.76)

and now we have obtained the zero order term of the effective Hamiltonian

$$h_0(t; t_0) = \frac{D^0 \tilde{H}}{D \mu^0}.$$  \hspace{1cm} (1.77)
For our toy model Eq. (1.78) would imply that
\[
h_0(t; t_0) = \frac{D^0}{D\mu^0} \left( \mathcal{H}_{rot} \left( 1, \frac{\pi}{\omega}, 0, t \right) \right)
= \frac{i\pi}{\omega} \frac{D^0}{D\mu^0} \left( M_0^1 \left[ \mathcal{H}_{rot}(\tau); \frac{\pi}{\omega}, 0, t \right] \right) = \frac{H_1(t)}{4} \sigma_x = \mathcal{H}_{RWA}(t),
\]
(1.79)
thus the zeroth order of the effective Hamiltonian is identified with the RWA. This is why the effective Hamiltonian formalism has also been called the "exact" RWA in [1].

Now we proceed with calculating the next term of the effective Hamiltonian. We use the truncated effective Hamiltonian for
\[
N = 1 \quad \mathcal{H}_1 = \frac{h_1(t; t_0)}{\omega} + h_0(t; t_0),
\]
(1.80)
where \( h_0(t; t_0) \) is given in Eq. (1.78). Here we would like to compare the \( 1/\omega \) terms of the MTE of the effective Hamiltonian to the corresponding ones in the MTE of the actual Hamiltonian,
\[
\frac{D\mathcal{H}_1}{D\mu} = \frac{D\mathcal{H}}{D\mu},
\]
(1.81)
with
\[
\mathcal{H}_1 = \mathcal{H}_1^{(0,1)} + \mathcal{H}_1^{(1,0)} + O \left( \frac{1}{\omega^2} \right)
\]
(1.82)
and therefore
\[
\frac{D\mathcal{H}_1}{D\mu} = \frac{D\mathcal{H}_1^{(0,1)}}{D\mu} + \frac{D\mathcal{H}_1^{(1,0)}}{D\mu}.
\]
(1.83)
From Eq. (1.56) we can see that the zeroth order term of the MTE is linear in its argument
\[
\mathcal{H}_1^{(0,1)} = \frac{\tilde{h}_1^{(0,1)}}{\omega} + \tilde{h}_0^{(0,1)}
= \frac{h_1(t; t_0)}{\omega} + h_0(t; t_0) + \left( \frac{\hat{h}_1(t; t_0)}{\omega} + \hat{h}_0(t; t_0) \right) I_1 + O \left( \frac{1}{\omega^2} \right),
\]
(1.84)
where we denoted
\[
I_1 = \frac{1}{t_c} \int_{t_0+(n-1)t_c}^{t_0+nt_c} (\tau - t) d\tau = t_0 - t + \left( n - \frac{1}{2} \right) t_c.
\]
(1.85)
There are a lot of time parameters involved in this integral however and according to what we have seen in Eq. (1.44), this integral is bound to have some \( \omega \) dependence. Substituting the time parameters with their dimensionless counterparts as in Eq. (1.44) we get
\[
I_1 = \frac{1}{2\omega} \left( \beta_0 - \beta + \left( n - \frac{1}{2} \right) \beta_c \right) = \frac{\tilde{I}_1}{\omega},
\]
(1.86)
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with

\[ \tilde{I}_1 = \frac{D I_1}{D \mu} = \frac{1}{2} \left( \beta_0 - \beta + \left( n - \frac{1}{2} \right) \beta_c \right), \]  \hspace{1cm} (1.88)

therefore Eq. (1.84) can be written as

\[ \tilde{H}_1^{(0,1)} = \frac{h_1(t; t_0)}{\omega} + h_0(t; t_0) + \frac{\dot{h}_0(t; t_0)}{\omega} \tilde{I}_1 + O \left( \frac{1}{\omega^2} \right). \]  \hspace{1cm} (1.89)

Applying the PCO on each side of Eq. (1.89) gives

\[ \frac{D \tilde{H}_1^{(0,1)}}{D \mu} = h_1(t; t_0) + \dot{h}_0(t; t_0) \tilde{I}_1. \]  \hspace{1cm} (1.90)

Unfortunately no other order of the MTE exhibits linearity, thus complicating their calculation. For \( \tilde{H}_1^{(1,0)} \) however, calculations are trivial since we only need zero order in the Taylor expansion. Specifically, we will have

\[ \tilde{H}_1^{(1,0)} = -\frac{i}{2 \epsilon} \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} d\tau \int_{t_0 + (n-1)t_c}^{\tau} d\tau_1 \left[ \frac{h_1(t; t_0)}{\omega} + h_0(t; t_0), h_1(t; t_0) + h_0(t; t_0) \right], \]  \hspace{1cm} (1.91)

but of course

\[ \left[ \frac{h_1(t; t_0)}{\omega} + h_0(t; t_0), h_1(t; t_0) + h_0(t; t_0) \right] = 0 \Rightarrow \tilde{H}_1^{(1,0)} = 0 \]  \hspace{1cm} (1.92)

and therefore solving Eq. (1.81) with respect to \( h_1(t; t_0) \) yields

\[ h_1(t; t_0) = \frac{D \tilde{H}}{D \mu} - \dot{h}_0(t; t_0) \tilde{I}_1. \]  \hspace{1cm} (1.93)

However this equation is not particularly suggestive of the underlying pattern for the recursion in this form. Using Eqs. (1.88) and (1.86) and the fact that \( \dot{h}_0(t; t_0) \) commutes with the PCO we can bring Eq. (1.93) to the form

\[ h_1(t; t_0) = \frac{D \tilde{H}}{D \mu} - \dot{h}_0(t; t_0) \frac{D I_1}{D \mu} \]  \hspace{1cm} (1.94)

\[ = \frac{D \tilde{H}}{D \mu} - \dot{h}_0(t; t_0) \frac{D}{D \mu} \left( \frac{1}{t_c} \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} (\tau - t) d\tau \right) \]  \hspace{1cm} (1.95)

\[ = \frac{D \tilde{H}}{D \mu} - \frac{D}{D \mu} \left( \frac{1}{t_c} \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} \dot{h}_0(t; t_0) (\tau - t) d\tau \right). \]  \hspace{1cm} (1.96)

We note here that

\[ \frac{D}{D \mu} \left[ \frac{1}{t_c} \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} h_0(t; t_0) d\tau \right] = \frac{D h_0(t; t_0)}{D \mu} = 0 \]  \hspace{1cm} (1.97)

and now we subtract this complicated zero in Eq. (1.96)

\[ h_1(t; t_0) = \frac{D \tilde{H}}{D \mu} - \frac{D}{D \mu} \left[ \frac{1}{t_c} \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} \left( \dot{h}_0(t; t_0) (\tau - t) + h_0(t; t_0) \right) d\tau \right]. \]  \hspace{1cm} (1.98)
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in order to identify the integral in the derivative as the MTE of \( h_0(t; t_0) \) and therefore write

\[
h_1(t; t_0) = \frac{DH}{D\mu} - \frac{D\tilde{h}_0}{D\mu}.
\] (1.99)

To proceed with the derivation of the recursive formula, we make the ansatz for the \( i \)th recursion

\[
h_i(t; t_0) = \frac{D^iH}{D\mu^i} - \frac{D^i\tilde{h}_i}{D\mu^i}
\] (1.100)

and will now prove it inductively. Assume Eq. (1.100) to be valid, then it must also hold for

\[
h_{i+1}(t; t_0) = \frac{D^{i+1}H}{D\mu^{i+1}} - \frac{D^{i+1}\tilde{h}_{i+1}}{D\mu^{i+1}}.
\] (1.101)

Using Eq. (1.100) we can calculate

\[
\mathcal{H}_i = \sum_{k=0}^{i} \frac{h_k(t; t_0)}{\omega^k}
\] (1.102)

and the effective Hamiltonian for \( N = i + 1 \) will be

\[
\mathcal{H}_{i+1} = \sum_{k=0}^{i+1} \frac{h_k(t; t_0)}{\omega^k} = \sum_{k=0}^{i} \frac{h_k(t; t_0)}{\omega^k} + \frac{h_{i+1}(t; t_0)}{\omega^{i+1}} = \mathcal{H}_i + \frac{h_{i+1}(t; t_0)}{\omega^{i+1}}.
\] (1.103)

From Eq. (1.58) we require

\[
\frac{D^{i+1}\tilde{H}_{i+1}}{D\mu^{i+1}} = \frac{D^{i+1}\tilde{H}}{D\mu^{i+1}},
\] (1.104)

with

\[
\tilde{H}_{i+1} = \sum_{k=0}^{i+1} \mathcal{H}_{i+1} = \mathcal{H}_{i+1}^{(0, i+1)} + \sum_{k=1}^{i+1} \mathcal{H}_{i+1}^{(k, i+1 - k)} = \mathcal{H}_i^{(0, i+1)} + \frac{\tilde{h}_{i+1}^{(0, i+1)}}{\omega^{i+1}} + \sum_{k=1}^{i+1} \mathcal{H}_{i+1}^{(k, i+1 - k)}.
\] (1.105)

But

\[
\tilde{h}_{i+1}^{(0, i+1)} = h_{i+1}(t; t_0) + O\left(\frac{1}{\omega}\right) \Rightarrow \tilde{h}_{i+1} = \mathcal{H}_i + \frac{h_{i+1}(t; t_0)}{\omega^{i+1}} + \sum_{k=1}^{i+1} \frac{\tilde{h}_{i+1}^{(k, i+1 - k)}}{\omega^{i+1}} + O\left(\frac{1}{\omega^{i+2}}\right)
\] (1.106)

and so we now need to find the \( O\left(\frac{1}{\omega^{i+2}}\right) \) terms in the sum to simplify it. In general, \( \mathcal{H}_{i+1}^{(k, i+1 - k)} \) will be consisted of \( k \) nested commutators accompanied by \( k + 1 \) integrations

\[
\mathcal{H}_{i+1}^{(k, i+1 - k)} \sim \int \frac{\prod_{\nu=1}^{k+1} d\tau_\nu}{t_c} \left[ \mathcal{H}_{eff}(\tau_1; t_0, i + 1), ..., [\mathcal{H}_{eff}(\tau_k; t_0, i + 1), \mathcal{H}_{eff}(\tau_{k+1}; t_0, i + 1)]\right]
\] (1.107)

\[
\sim \int \frac{\prod_{\nu=1}^{k+1} d\beta_\nu}{\beta_c(2\omega)^k} \left[ \mathcal{H}_{eff}\left(\frac{\beta_1}{2\omega}; t_0, i + 1\right), ..., \left[ \mathcal{H}_{eff}\left(\frac{\beta_{k+1}}{2\omega}; t_0, i + 1\right), \mathcal{H}_{eff}\left(\frac{\beta_{k+1}}{2\omega}; t_0, i + 1\right)\right]\right].
\] (1.108)
1.5. Effective Hamiltonian

For instance
\[
\mathcal{H}_{i+1}^{(1,i)} = \frac{1}{2\omega_\beta_c} \int_{\beta_i}^{\beta_f} \! d\beta_1 \int_{\beta_i}^{\beta_1} \! d\beta_2 \left[ \mathcal{H}_{\text{eff}} \left( \frac{\beta_1}{2\omega}; t_0, i + 1 \right), \mathcal{H}_{\text{eff}} \left( \frac{\beta_2}{2\omega}; t_0, i + 1 \right) \right] (1.109)
\]
\[
= \frac{1}{2\omega_\beta_c} \int_{\beta_i}^{\beta_f} \! d\beta_1 \int_{\beta_i}^{\beta_1} \! d\beta_2 \left[ \mathcal{H}_{\text{eff}} \left( \frac{\beta_1}{2\omega}; t_0, i \right) + \frac{h_{i+1} \left( \frac{\beta_1}{2\omega}; t_0 \right)}{\omega_\beta_c} \right] (1.110)
\]
\[
= \mathcal{H}_i^{(0,i)} + O \left( \frac{1}{\omega_\beta_c^{i+2}} \right) , (1.111)
\]
where we denoted for concreteness \( \beta_i = \beta_0 + (n-1)\beta_c \) and \( \beta_{f} = \beta_0 + n\beta_c \). It can be similarly shown that
\[
\mathcal{H}_{i+1}^{(k,i+1-k)} = \mathcal{H}_i^{(k,i+1-k)} + O \left( \frac{1}{\omega_\beta_c^{i+k+1}} \right) , (1.113)
\]
so we can now write
\[
\mathcal{H}_{i+1} = \mathcal{H}_i^{(0,i+1)} + \frac{h_{i+1}(t; t_0)}{\omega_\beta_c^{i+1}} + \sum_{k=1}^{i+1} \mathcal{H}_i^{(k,i+1-k)} + O \left( \frac{1}{\omega_\beta_c^{i+2}} \right) = \mathcal{H}_i + \frac{h_{i+1}(t; t_0)}{\omega_\beta_c^{i+1}} + O \left( \frac{1}{\omega_\beta_c^{i+2}} \right) . (1.114)
\]
Application of the \( i + 1 \) order PCO with respect to \( \mu \) yields
\[
\frac{D_i^{i+1} \mathcal{H}_{i+1}}{D\mu^{i+1}} = \frac{D_i^{i+1} \mathcal{H}_i}{D\mu^{i+1}} + h_{i+1}(t; t_0) . (1.115)
\]
By substituting Eq. (1.115) into Eq. (1.104) and solving for \( h_{i+1}(t; t_0) \) we confirm Eq. (1.101), thus concluding our inductive proof.

1.5.5 Reduction to the Fundamental Magnus Interval

So far, all of our results hold only for the \( n \)th Magnus interval \([t_0 + (n-1)t_c, t_0 + nt_c]\). If we wished to calculate the effective Hamiltonian for a time interval \([t_i, t_f]\), we would have to divide this interval to \( n \) sub-intervals of equal range \( t_c \) and repeat the cumbersome calculation presented in the previous section for each one of them. There is a way, however, to reduce the entire calculation to what is called the Fundamental Magnus Interval (FMI),
\[
[t_0, t_0 + t_c] (1.116)
\]
which we shall now present.

Assume a Hamiltonian of the form
\[
\mathcal{H}(t) = \sum_i f_i(t) + \sum_j H_j(t)g_j(t) (1.117)
\]
where \( f_i(t), g_j(t) \) are some known periodic functions with the same period or constants and \( H_j(t) \) are some unspecified amplitude functions. The zero order MTE for this Hamiltonian would be

\[
\bar{H}(0,p) = \frac{1}{t_c} \sum_i \int_{t_0+(n-1)t_c}^{t_0+nt_c} d\tau f_i(\tau) + \frac{1}{t_c} \sum_j \int_{t_0+(n-1)t_c}^{t_0+nt_c} d\tau T_j^p(\tau; t) g_j(\tau),
\]

(1.118)

with

\[
T_j^p(\tau; t) = \sum_{k=0}^p \frac{1}{k!} \frac{d^k H_j(t)}{d\tau^k}(\tau - t)^k
\]

(1.119)

and we choose \( t_c \) to coincide with the period of the periodic functions involved. This is why we chose to define \( \beta_0 = 2\omega t_0 \), because for the toy model in the rotating frame \( t_c = \pi/\omega \) and with the same convention we will have \( \beta_c = 2\omega t_c = 2\pi \). We can choose to shift the integration variable in order to transform the integral in the FMI

\[
\tau \rightarrow \tilde{\tau} + (n-1)t_c \Rightarrow \int_{t_0+(n-1)t_c}^{t_0+nt_c} d\tau \rightarrow \int_{t_0}^{t_0+t_c} d\tilde{\tau},
\]

(1.120)

thus Eq. (1.118) is written as

\[
\bar{H}(0,p) = \frac{1}{t_c} \sum_i \int_{t_0}^{t_0+t_c} d\tilde{\tau} f_i(\tilde{\tau}+(n-1)t_c) + \frac{1}{t_c} \sum_j \int_{t_0}^{t_0+t_c} d\tilde{\tau} T_j^p(\tilde{\tau}+(n-1)t_c; t) g_j(\tilde{\tau}+(n-1)t_c).
\]

(1.121)

By exploiting the periodicity of the \( f_i(t) \) and \( g_j(t) \) functions however we can write

\[
\bar{H}(0,p) = \frac{1}{t_c} \sum_i \int_{t_0}^{t_0+t_c} d\tilde{\tau} f_i(\tilde{\tau}) + \frac{1}{t_c} \sum_j \int_{t_0}^{t_0+t_c} d\tilde{\tau} T_j^p(\tilde{\tau}+(n-1)t_c; t) g_j(\tilde{\tau}).
\]

(1.122)

For simplicity we insert the shifted amplitude functions

\[
\tilde{H}_j(\tilde{\tau}) = H_j(\tilde{\tau}+(n-1)t_c) = H_j(\tilde{\tau}),
\]

(1.123)

with corresponding Taylor expansions

\[
\tilde{T}_j^p(\tilde{\tau}; \tilde{\ell}) = \sum_{k=0}^p \frac{1}{k!} \frac{d^k \tilde{H}_j(\tilde{\ell})}{d\tilde{\tau}^k}(\tilde{\tau} - \tilde{\ell})^k
\]

(1.124)

and \( \tilde{\ell} \) has to be chosen inside the interval that \( \tilde{\tau} \) lives therefore

\[
\tilde{\ell} = t - (n-1)t_c.
\]

(1.125)

Eq. (1.122) can now be written as

\[
\bar{H}(0,p) = \frac{1}{t_c} \sum_i \int_{t_0}^{t_0+t_c} d\tilde{\tau} f_i(\tilde{\tau}) + \frac{1}{t_c} \sum_j \int_{t_0}^{t_0+t_c} d\tilde{\tau} \tilde{T}_j^p(\tilde{\tau}; \tilde{\ell}) g_j(\tilde{\tau}),
\]

(1.126)
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notice however that

\[
\tilde{T}_j(\tilde{\tau}; \tilde{t}) = \sum_{k=0}^{p} \frac{1}{k!} \frac{d^k \tilde{H}_j(\tilde{t})}{d\tilde{\tau}^k} (\tilde{\tau} - \tilde{t})^k
\]

(1.127)

\[
= \sum_{k=0}^{p} \frac{1}{k!} \frac{d^k H_j(t)}{d\tau^k} (\tau - t)^k
\]

(1.128)

\[
= \sum_{k=0}^{p} \frac{1}{k!} \frac{d^k H_j(t)}{d\tau^k} (\tau - (n-1)t_c - t + (n-1)t_c)^k = \tilde{T}_j(\tau; t),
\]

(1.129)

where we went from the first line to the second using Eq. (1.123) and the chain rule:

\[
\frac{d}{d\tilde{\tau}} = \frac{d\tau}{d\tilde{\tau}} \frac{d}{d\tau} = \frac{d}{d\tau},
\]

(1.130)

In the third line we substituted \(\tilde{\tau}\) and \(\tilde{t}\) from Eq. (1.120) and Eq. (1.125) respectively. Since Eqs.(1.118) and (1.126) are equivalent for arbitrary \(n\) we conclude that, at least in the zeroth order of the ME, the MTE obtained in the FMI is valid for arbitrary times. The question now is if we can do this for higher orders as well.

The integrand in the first order of the ME will be

\[
[\mathcal{H}(\tau_1), \mathcal{H}(\tau_2)] = \sum_{i_1,i_2} [f_{i_1}(\tau_1), f_{i_2}(\tau_2)] + \sum_{i_1,j_2} [f_{i_1}(\tau_1), g_{j_2}(\tau_2)] H_{j_2}(\tau_2) + \sum_{j_1,j_2} [g_{j_1}(\tau_1), f_{i_2}(\tau_2)] H_{j_1}(\tau_1) + \sum_{j_1,j_2} [g_{j_1}(\tau_1), g_{j_2}(\tau_2)] H_{j_1}(\tau_1) H_{j_2}(\tau_2),
\]

(1.131)

but since the functions involved in the commutators are periodic in the same period the commutator itself will also be a periodic function and so we can write this as

\[
[\mathcal{H}(\tau_1), \mathcal{H}(\tau_2)] = \sum_i F_i(\tau_1, \tau_2) + \sum_j G_j(\tau_1, \tau_2) \eta_j(\tau_1, \tau_2)
\]

(1.132)

where \(F_i(\tau_1, \tau_2)\) and \(G_j(\tau_1, \tau_2)\) are periodic in both of their arguments and

\[
\eta_j(\tau_1, \tau_2) = H_{j_1}(\tau_1) H_{j_2}(\tau_2).
\]

(1.133)

From these three equations in the last paragraph it is easy to generalise to

\[
[\mathcal{H}(\tau_1), [\mathcal{H}(\tau_2), [... [\mathcal{H}(\tau_{m-1}), \mathcal{H}(\tau_m)]...]]] = \sum_i F_i(\tau_1, ..., \tau_m) + \sum_j G_j(\tau_1, ..., \tau_m) \eta_j(\tau_1, ..., \tau_m)
\]

(1.134)

with

\[
\eta_j(\tau_1, ..., \tau_m) = \prod_{s=1}^{m} H_{js}(\tau_s)
\]

(1.135)

and corresponding term for the MTE will be

\[
\hat{H}^{(m,p)} \propto \frac{1}{t_c} \sum_i \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} \cdots \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} d\tau_1 \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} d\tau_2 \cdots \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} d\tau_n F_i(\tau_1, ..., \tau_m)
\]

\[+ \frac{1}{t_c} \sum_j \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} \cdots \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} d\tau_1 \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} d\tau_2 \cdots \int_{t_0 + (n-1)t_c}^{t_0 + nt_c} d\tau_n G_j(\tau_1, ..., \tau_m) \prod_{s=1}^{m} T_s^p(\tau_s; t).
\]

(1.136)
Figure 1.2: First three Magnus intervals of: (blue) the time evolution generated from the toy model Hamiltonian in the rotated frame, (orange) the time evolution generated by the effective Hamiltonian and (red) the time evolution generated by RWA, in the Bloch sphere for a Gaussian amplitude function $H_1(t)$ and initial state $|0\rangle$.

By shifting again every integration variable as $\tau_a \rightarrow \tilde{\tau}_a + (n-1)t_c$ we will have

$$
\int_{t_0+(n-1)t_c}^{t_0+nt_c} d\tau_1 \int_{t_0+(n-1)t_c}^{t_0+nt_c} d\tau_2 \cdots \int_{t_0+(n-1)t_c}^{t_0+nt_c} d\tau_n \rightarrow \int_{t_0}^{t_0+t_c} d\tilde{\tau}_1 \int_{t_0}^{t_0+t_c} d\tilde{\tau}_2 \cdots \int_{t_0}^{t_0+t_c} d\tilde{\tau}_n,
$$

exploiting the periodicities and using the shifted function Taylor expansions we write

$$
\bar{H}^{(m,p)} \propto \frac{1}{t_c} \sum_i \int_{t_0}^{t_0+t_c} d\tilde{\tau}_1 \int_{t_0}^{t_0+t_c} d\tilde{\tau}_2 \cdots \int_{t_0}^{t_0+t_c} d\tilde{\tau}_n F_i(\tilde{\tau}_1, \cdots, \tilde{\tau}_m) + \frac{1}{t_c} \sum_j \int_{t_0}^{t_0+t_c} d\tilde{\tau}_1 \int_{t_0}^{t_0+t_c} d\tilde{\tau}_2 \cdots \int_{t_0}^{t_0+t_c} d\tilde{\tau}_n G_j(\tilde{\tau}_1, \cdots, \tilde{\tau}_m) \prod_{s=1}^{m} \tilde{T}_j^p(\tilde{\tau}_s; \tilde{t}).
$$

and so according to Eq. (1.129) we have now proved that the MTE obtained in the FMI for arbitrary order in the expansion is valid for arbitrary times. From now on we will always calculate the MTE in the FMI and drop the $n$ dependence from any relevant quantities. If a Hamiltonian satisfies the criteria to have its corresponding effective Hamiltonian reduced in the FMI we will say that the effective Hamiltonian is $FMI$ reducible.

### 1.5.6 Application to the Toy Model

Now that our effective Hamiltonian toolkit is complete, let us calculate the first order effective Hamiltonian for our toy model. The period of the explicit periodic
1.5. Effective Hamiltonian

functions in $H_{\text{rot}}(\tau)$ is $\pi/\omega$, so we choose $t_c = \pi/\omega$ and we start by calculating the zero order term

$$h_0(t; t_0) = \frac{D^0H_{\text{rot}}}{D\mu^0} = \frac{D^0H_{\text{rot}}^{(0,0)}}{D\mu^0} = H_{\text{RWA}}(t) = \frac{H_1(t)}{4}\sigma_x. \quad (1.139)$$

For the first order term as we have seen in Eq. (1.93),

$$h_1(t; t_0) = \frac{DH_{\text{rot}}}{D\mu} - \dot{h}_0(t; t_0)\tilde{I}_1 = \frac{DH_{\text{rot}}}{D\mu} - \frac{H_1(t)\tilde{I}_1}{4}\sigma_x, \quad (1.140)$$

where $\tilde{I}_1$ is given in Eq. (1.88) and

$$\dot{H}_{\text{rot}} = \dot{H}_{\text{rot}}^{(0,1)} + \dot{H}_{\text{rot}}^{1,0}. \quad (1.141)$$

Now we compute each term separately:

$$\dot{H}_{\text{rot}}^{(0,1)} = \frac{\omega}{\pi} \int_{t_0}^{t_0 + \frac{\pi}{\omega}} d\tau H_{\text{rot}} [\tau, T_1^1(\tau; t)]$$

$$= \left( \frac{H_1(t)}{4} + \frac{H_1(t)}{8\omega} (\beta_0 - \beta + \pi + \sin \beta_0) \right)\sigma_x + \frac{H_1(t)}{8\omega} \cos \beta_0 \sigma_y, \quad (1.142)$$

$$\dot{H}_{\text{rot}}^{1,0} = -\frac{i\omega}{2\pi} \int_{t_0}^{t_0 + \frac{\pi}{\omega}} d\tau \int_{t_0}^{\tau} d\tau_1 \left[ H_{\text{rot}} [\tau, T_1^0(\tau; t)] , H_{\text{rot}} [\tau_1, T_1^0(\tau_1; t)] \right]$$

$$= \frac{H_1(t)^2}{32\omega} (1 - 2 \cos \beta_0)\sigma_z \quad (1.143)$$

therefore

$$\frac{DH_{\text{rot}}}{D\mu} = \frac{DH_{\text{rot}}^{(0,1)}}{D\mu} + \frac{DH_{\text{rot}}^{1,0}}{D\mu}$$

$$= \frac{H_1(t)}{8} (\beta_0 - \beta + \pi + \sin \beta_0)\sigma_x + \frac{H_1(t)}{8\omega} \cos \beta_0 \sigma_y + \frac{H_1(t)^2}{32} (1 - 2 \cos \beta_0)\sigma_z. \quad (1.144)$$

Substitution of this equation and Eq. (1.88) in Eq. (1.140) yields

$$h_1(t; t_0) = \frac{H_1(t)}{8} \sin \beta_0 \sigma_x + \frac{H_1(t)}{8\omega} \cos \beta_0 \sigma_y + \frac{H_1(t)^2}{32} (1 - 2 \cos \beta_0)\sigma_z, \quad (1.145)$$

So in conclusion the first order effective Hamiltonian will be

$$H_1(t) = \frac{h_1(t; t_0)}{\omega} + h_0(t; t_0)$$

$$= \frac{H_1(t)}{4}\sigma_x + \frac{H_1(t)}{8\omega} \sin \beta_0 \sigma_x + \frac{H_1(t)}{8\omega} \cos \beta_0 \sigma_y + \frac{H_1(t)^2}{32\omega} (1 - 2 \cos \beta_0)\sigma_z. \quad (1.146)$$
Chapter 1. Magnus-Taylor Expansion and Effective Hamiltonians

Figure 1.3: The envelope shown in (a) exhibits non-analyticities at $t_d = 0$, $t_{\text{gate}}/2$ and $t_{\text{gate}}$. The axes in (b) represent the spherical latitude $\theta$ and longitude $\phi$ on a rotated Bloch sphere whose $|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$ state defines the north pole. The qubit is initialized to the north pole ($\phi = 0, \theta = 0$). Shown are the exact (red) and effective (blue) trajectories ($\beta_0 = 0.45$), where the latter is supplemented by the use of kick operators (dotted lines) that connect the effective trajectories for times $t < t_d$ and $t > t_d$. For the second discontinuity at $t_d = t_{\text{gate}}/2$, the corresponding point on each trajectory is indicated (diamond), and the dotted line is labeled by the kick operator $K_j$. Around this discontinuity, generators of evolution operators along several sections of the exact and stroboscopic trajectories on the FMI are labeled $\Omega_A$ through $\Omega_D$.

1.5.7 Kick Operators

The effective Hamiltonian formalism we presented here works only as long as the MTE converges. Assuming that the ME converges, the only other requirement for convergence of the MTE is for the amplitude functions to be analytic. Merely for completeness, here we discuss a strategy to be followed when computing the time evolution of a system that contains a drive function $H_j(t)$ that exhibits a non-analyticity at time $t_d = t_{\text{gate}}/2$, using the kick operator.

In the intervals $t < t_d$ and $t > t_d$ the amplitude function is analytic and therefore we can calculate the effective Hamiltonian for each interval separately. Following the time evolution of the Hamiltonian up to some time $t_L < t_d$ we would like to find a way to transition to the time $t_R > t_d$. To do this we reverse the effective Hamiltonian evolution using its ME to get back to the last point of stroboscopic coincidence with the ME of the actual Hamiltonian for $t < t_d$. From there we use the evolution generated by the ME of the actual Hamiltonian to get at $t = t_d$, followed by an application of the evolution generated by the ME of the actual Hamiltonian to get to the first point of stroboscopic coincidence with the ME of the effective Hamiltonian for $t > t_d$. Finally we use the inverse time evolution generated by the effective Hamiltonian ME to get to $t = t_R$. Putting all of this together we define:

$$e^{K_j} = e^{-\Omega_D}e^{\Omega_A}e^{-\Omega_B}e^{\Omega_C},$$  \hspace{1cm} (1.150)$$

where $K_j$ is the kick operator corresponding to this discontinuity and it can be calculated by successively using the Baker-Campbell-Hausdorff formula. However we will deal with analytic amplitude functions and therefore the kick operators are irrelevant for us.
Chapter 2

High Fidelity Singlet-Triplet Qubit Gate

In this chapter, we use the effective Hamiltonian formalism presented in the previous chapter to describe the dynamics of a Singlet-Triplet qubit gate. A brief review of the Singlet-Triplet qubit and a description of the gate under consideration are presented in section 1. In section 2, we apply numerical methods to obtain an analytic expression for the Hamiltonian of the gate in order to proceed with the calculation of the corresponding effective Hamiltonian in section 3.

2.1 Numerical Pulse Optimization Scheme for Singlet-Triplet Qubit Gates

In this chapter we will focus on applying the effective Hamiltonian formalism we presented in the previous chapter to the Singlet-Triplet Qubit (STQ) gate introduced in [2].

The STQ we will consider here consists of two coupled GaAs quantum dots. An external magnetic field is applied to energetically separate the triplet states with $m_s \neq 0$ thus isolating the singlet state

$$|S\rangle = \frac{\left|01\right> - \left|10\right>}{\sqrt{2}} \quad (2.1)$$

and the $m_s = 0$ triplet state

$$|T_0\rangle = \frac{\left|01\right> + \left|10\right>}{\sqrt{2}}. \quad (2.2)$$

These states correspond to the logical $|0\rangle_L$ and $|1\rangle_L$. From now on we will drop the $L$ index and simply refer to the singlet, triplet states as $|0\rangle$ and $|1\rangle$ respectively.

Some advantages of choosing this system as a potential qubit include:

1) Long coherence times.

2) Realizable single and two qubit operations.
3) Universal single qubit control (although subject to large noise).

More information about the STQ can be found in [13], where it was originally introduced. The novel idea in [2] is to use an iterative procedure that rectifies systematic errors emerging from the application of numerical voltage pulses, by creating successive pulses using data from the experiment at each step. This way, a fidelity higher than $99.9\%$ is achieved for $\pi$ and $\frac{\pi}{2}$ gates. The strength of this numerical pulse optimization scheme is that it was tailored to account for the noise sources specific to the STQ system used in [2].

The Hamiltonian for this system is

$$H_{CG}(t) = \frac{\Delta B_z}{2} \sigma_z + J(\epsilon(t)) \sigma_x \quad (2.3)$$

where $\Delta B_z$ is an Overhauser magnetic field gradient (see [14]) originating from the different magnetic field that each dot is coupled to, $\epsilon(t)$ are pulses created by arbitrary waveform generators and $J(\epsilon(t))$ is a transfer function described by the phenomenological model

$$J(\epsilon(t)) = J_0 \exp \left( \frac{\epsilon(t)}{\epsilon_0} \right). \quad (2.4)$$

From now one we shall refer to this system as the Cerfontaine Gate (CG).

### 2.2 Numerical Analysis

#### 2.2.1 Fitting

We would like to thank the authors of [2], for a sharing the data of a pulse sequence $\{t, \epsilon(t)\}$ that corresponds to a $\frac{\pi}{2}$ gate around the $y$ axis in the Bloch sphere. In the first stage of analyzing the data we would like to find an analytic expression that approximates $J(t)$. In order to achieve this, we plugged the $\{t, \epsilon(t)\}$ data into Eq. (2.4) using $J_0 = \epsilon_0 = 1 \text{ ns}^{-1}$ to obtain a new data set $\{t, J(t)\}$. For this new data we used a linear combination of Gaussian functions as our fitting model

$$J(t) = \sum_{n=0}^{N} \alpha_n \exp \left( -\frac{(t - t_n)^2}{\sigma_n} \right), \quad (2.5)$$

where $\alpha_n$, $t_n$ and $\sigma_n$ are $3N$ parameters to be numerically determined. For $N = 11$ and using Mathematica’s FindFit command we end up with the fit presented in Figure 2.1.

Even though the fit we obtained for $J(t)$ describes the behavior of the system rather accurately, as it is evident from Figure 2.1, it is of no use to us in this form because it has no apparent periodic time dependent components. Without any periodic components we cannot reduce the calculation of the Magnus-Taylor Expansion (MTE) to the Fundamental Magnus Interval (FMI) and therefore we cannot obtain an effective Hamiltonian for arbitrary times. We solved this problem, by performing a frequency decomposition of this $J(t)$ signal, which is presented in the next section.
2.2. Numerical Analysis

Figure 2.1: (left) The \{t, J(t)\} data set (blue) and \(J(t)\) fit (red) for the gate pulse sequence \(\{t, \epsilon(t)\}\) with a time step \(\Delta t = 0.2\) ns starting from \(t_0 = 0\) ns and finishing at \(t_{\text{gate}} = 18\) ns. (right) The Bloch sphere trajectory generated by the Hamiltonian (2.3) for \(J(t)\) as an interpolating function of the data \(\{t, J(t)\}\) (blue) and for \(J(t)\) fitted according to our model given in Eq. (2.5) for \(N = 11\) (red). The initial state for both evolutions is the \(|0\rangle\) state and the final state of each trajectory is depicted by the vectors coloured with the same colour as the trajectory they correspond to.

2.2.2 Frequency Decomposition of the Drive

As it has already been mentioned in the previous section, we would like to extract the periodic time dependent components of \(J(t)\). To this end, we first calculate the Fourier transform from

\[
\tilde{J}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt J(t) e^{i\omega t}.
\]  

(2.6)

Ideally \(|\tilde{J}(\omega)|\) would give us a spectrum of the form presented in the left plot of Figure 2.2. From this spectrum we would isolate each frequency \(\omega\) corresponding to the peaks centered around \(\omega = 0, \omega_d\) and \(-\omega_d\), with \(\omega_d\) being the frequency of [Diagram of Fourier spectrum]

Figure 2.2: (left) Idealised absolute value of the Fourier transform of the CG drive \(J(t)\) and (right) corresponding frequency decomposition using the window functions Eqs. (2.16), (2.17).
the drive, using a window function \( W(\omega) \) and then invert the Fourier transform for each component separately. For the ideal spectrum we would have a zero frequency mode
\[
J_0(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega W_0(\omega) \tilde{J}(\omega) e^{-i\omega t} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \tilde{J}_0(\omega) e^{-i\omega t} \tag{2.7}
\]
and a non zero frequency mode
\[
J_1(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega W_1(\omega) \tilde{J}(\omega) e^{-i\omega t} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \tilde{J}_1(\omega) e^{-i\omega t} \tag{2.8}
\]
with
\[
J_1(t) = J_{1c}(t) \cos(\omega_dt + \phi_c) + J_{1s}(t) \sin(\omega_dt + \phi_s). \tag{2.9}
\]
Therefore, the frequency decomposition of \( J(t) \) would be
\[
J(t) = J_0(t) + J_1(t) = J_0(t) + J_{1c}(t) \cos(\omega_dt + \phi_c) + J_{1s}(t) \sin(\omega_dt + \phi_s). \tag{2.10}
\]
The reason we called the spectrum presented in Figure 2.2 ideal is because it leads to a \( J(t) \) given in Eq. (2.10) which in turn leads to a Hamiltonian
\[
\mathcal{H}_{\text{ideal}}(t) = \frac{\Delta B_z}{2} \sigma_z + J_0(t) \sigma_x + J_{1c}(t) \cos(\omega_dt + \phi_c) \sigma_x + J_{1s}(t) \sin(\omega_dt + \phi_s) \sigma_x \tag{2.11}
\]
that is quite similar to our toy model Hamiltonian Eq. (1.32).

The actual spectrum we obtain for \( J(t) \) however is more complicated than the ideal spectrum, and it is presented in Figure 2.3, so in this case we obtain many additional components
\[
J(t) = \sum_{n=0}^{\infty} J_n(t) = J_0(t) + \sum_{n=1}^{\infty} J_{n,c}(t) \cos(\omega_nt + \phi_{n,c}) + \sum_{n=1}^{\infty} J_{n,s}(t) \sin(\omega_nt + \phi_{n,s}). \tag{2.12}
\]
Of course it is not practical to use such an infinite sum representation for \( J(t) \), which means that we will truncate the series at some finite order \( N_J \), thus ending up with a residual drive component \( \delta J(t) \),
\[
J(t) = \sum_{n=0}^{N_J} J_n(t) + \delta J(t) \tag{2.13}
\]
Unfortunately, the \( J(t) \) decomposition in Eq. (2.12) results in a CG Hamiltonian that does not have a FMI-reducible effective Hamiltonian. If, however, the decomposition was of the form
\[
J(t) = \sum_{n=0}^{\infty} J_n(t) = J_0(t) + \sum_{n=1}^{\infty} J_{n,c}(t) \cos(n\omega_dt + \phi_{n,c}) + \sum_{n=1}^{\infty} J_{n,s}(t) \sin(n\omega_dt + \phi_{n,s}), \tag{2.14}
\]
then it would be guaranteed that all the trigonometric functions will be periodic in at least \( 2\pi/\omega_d \) allowing us thus to reduce the effective Hamiltonian in the FMI
\( [0, 2\pi/\omega_d] \).
2.2. Numerical Analysis

Figure 2.3: (left) Actual absolute value of the Fourier transform of the CG drive $J(t)$ and (right) corresponding frequency decomposition using the window functions Eqs. (2.16), (2.17), for a frequency decomposition scheme with a divergent effective Hamiltonian.

For our windowing scheme we used pairs of Fermi-functions

\[
W_{\text{Fermi}}(\omega) = \frac{1}{1 + e^{\beta(\omega - \omega_{\text{high}})}} - \frac{1}{1 + e^{\beta(\omega - \omega_{\text{low}})}}
\]  

(2.15)

which essentially simulates a square window: it is approximately 1 for $\omega \in [\omega_{\text{low}}, \omega_{\text{high}}]$ and approximately 0 otherwise. The important difference to the square window is the fact that the decay of the function at $\omega_{\text{low}}$ and $\omega_{\text{high}}$ is continuous. In order to isolate the the $n$th component of the spectrum $\tilde{J}(\omega)$ we use the window functions

\[
W_0(\omega) = \frac{1}{1 + e^{\beta(\omega - \omega_0)}} - \frac{1}{1 + e^{\beta(\omega + \omega_0)}},
\]

(2.16)

\[
W_n(\omega) = \frac{1}{1 + e^{\beta(\omega - \omega_n)}} - \frac{1}{1 + e^{\beta(\omega - \omega_{n-1})}} + \frac{1}{1 + e^{\beta(\omega + \omega_{n-1})}} - \frac{1}{1 + e^{\beta(\omega + \omega_n)}}, \quad n \in \mathbb{Z}^+,
\]

(2.17)

where $\omega_0$ is the frequency that corresponds to the first minimum of the positive part of the spectrum, $\omega_1$ is the second minimum and so on. This choice of windowing functions makes the analytic calculation of the inverse Fourier transform integrals very complicated and computationally impractical, but it guarantees that the decomposition we end up with will be of the form of Eq.(2.14).

In order to determine the inverse Fourier transform of each component we instead calculate the corresponding integrals numerically for a thousand equally spaced different times $t$ inside the time interval $[0, t_{\text{gate}}]$. This way we obtain new data sets which we then fit to find the corresponding components of $J(t)$. For the zero frequency mode we use the fitting model

\[
J_0(t) = \sum_{n=1}^{3} \alpha_{0n} \exp \left( -\frac{(t - t_{0n})^2}{s_{0n}} \right)
\]

(2.18)

and for the non-zero frequency modes we use

\[
J_n(t) = \alpha_{n,c} e^{-\frac{(t - t_{n,c})^2}{s_{n,c}}} \cos(n\omega_dt + \phi_{n,c}) + \alpha_{n,s} e^{-\frac{(t - t_{n,s})^2}{s_{n,s}}} \sin(n\omega_dt + \phi_{n,s}).
\]

(2.19)
Chapter 2. High Fidelity Singlet-Triplet Qubit Gate

Figure 2.4: First attempt fits for $J_0(t)$ (blue), $J_1(t)$ (green), $J_2(t)$ (orange) and the $\delta J_{\text{res}}(t)$ noise term (red)

Once we determine all terms up to $n = N_J$, the $\delta J(t)$ component is calculated as

$$\delta J(t) = J(t) - \sum_{n=0}^{N_J} J_n(t), \quad (2.20)$$

where we expect $\delta J(t) \ll J(t)$. Notice that as soon as we introduce a finite $N_J$, which is equivalent to saying $\delta J(t) \neq 0$, the FMI-reducibility of the effective Hamiltonian is lost.

Our first attempt to resolve the $\delta J(t)$ issue was to notice that if we use a $N_J = 1$ decomposition for $J(t)$, the dominant part of $\delta J(t)$ is the $2\omega_d$ peak. For this case we could potentially fit $\delta J(t)$ as a $2\omega_d$ mode by introducing more parameters for the amplitude functions, namely

$$\delta J(t) = \delta J_c(t) \cos(2\omega_dt + \phi_{2c}) + \delta J_s(t) \sin(2\omega_dt + \phi_{2s}) \quad (2.21)$$

$$= \left( \sum_{n=1}^{6} \alpha_n c e^{-\frac{(t-t_n,c)^2}{\tau_{n,c}^2}} \right) \cos(2\omega_dt + \phi_{2c}) + \left( \sum_{n=1}^{5} \alpha_n s e^{-\frac{(t-t_n,s)^2}{\tau_{n,s}^2}} \right) \sin(2\omega_dt + \phi_{2s}). \quad (2.22)$$

The hope with this approach was that we can end up with a residual $\delta J_{\text{res}}(t)$ component

$$\delta J_{\text{res}}(t) = J(t) - J_0(t) - J_1(t) - \delta J(t) \quad (2.23)$$

which could be safely ignored and this is exactly what we obtained. This decomposition of $J(t)$ is presented in Figure 2.4.

Unfortunately, while this is an incredibly accurate fitting which results in a truly insignificant $\delta J_{\text{res}}(t)$ component, the effective Hamiltonian for this decomposition is divergent. This is a result of the fact that the derivatives of the amplitudes $\delta J_c(t)$ and $\delta J_s(t)$ tend towards a delta-function-like behavior much faster than the powers
2.2. Numerical Analysis

Figure 2.5: In all of these graphs we plot the ratio of the maximum absolute value of the \( n \)th derivative of the amplitudes for the \( 2\omega_d \) trigonometric terms, over the \( n \)th power of the drive frequency \( \omega_d \) versus the value of \( n \) in the range \([0, 3]\). The red curves correspond to the \( \delta J(t) \) fitting as a \( 2\omega_d \) mode, which leads to a divergent effective Hamiltonian while the blue curves correspond \( J_2(t) \) fitting which leads to a convergent effective Hamiltonian. In the first row we have the ratio mentioned above for the amplitudes of the cosine terms and in the second row we have the same measure for the sine terms.

![Graphs showing the ratio of maximum absolute values of derivatives to powers of \( \omega_d \) for different values of \( n \).]({})

The drive frequency tend to infinity as we increase the order (see Eq. (1.59)). We could write this statement as

\[
\lim_{n \to \infty} \frac{1}{\omega^n} \max_t |\partial^n_t \delta J_c(t)| = \infty \quad \text{and} \quad \lim_{n \to \infty} \frac{1}{\omega^n} \max_t |\partial^n_t \delta J_s(t)| = \infty, \quad (2.24)
\]

where by \( \max_t |\partial^n_t \delta J_c(t)| \) and \( \max_t |\partial^n_t \delta J_s(t)| \) we denote the maximum value of the amplitude functions of the cosine and the sine respectively. Of course these limits should not be taken with a grain of salt, and rather be interpreted as a qualitative statement or perhaps a reasonable guess inspired by the trend presented by the red curves in Figure 2.5.

As noted above, despite the accuracy of this fitting, it is of no use to our formalism, therefore we resort to using the decomposition in Eq. (2.13) for \( N_J = 1, 2, 3 \) and deal with the \( \delta J(t) \) issue later on. In Figure 2.7 we present the \( N_J = 2 \) decomposition.
Figure 2.6: (left) Actual absolute value of the Fourier transform of the CG drive $J(t)$ and (right) corresponding frequency decomposition using the window functions Eqs. (2.16), (2.17), for a frequency decomposition scheme with a convergent effective Hamiltonian.

Figure 2.7: Final fits for $J_0(t)$ (blue), $J_1(t)$ (green), $J_2(t)$ (orange) and $\delta J(t)$ (red).
2.3. Effective Hamiltonian Description of the System

The Hamiltonian we end up with is

\[ H_{CG}(t) = \frac{\Delta B_z}{2} \sigma_z + \frac{J_0(t)}{2} \sigma_x + \frac{1}{2} \sum_{n=1}^{N_J} J_{n,c}(t) \cos(n\omega_d t + \phi_{n,c}) \sigma_x + \frac{1}{2} \sum_{n=1}^{N_J} J_{n,s}(t) \sin(n\omega_d t + \phi_{n,s}) \sigma_x + \delta J(t) \sigma_x \] (2.25)

and in order to simplify our future calculations we use the trigonometric identities

\[ \cos(\alpha + \beta) = \cos(\alpha) \cos(\beta) - \sin(\alpha) \sin(\beta) \] (2.26)
\[ \sin(\alpha + \beta) = \sin(\alpha) \cos(\beta) + \cos(\alpha) \sin(\beta) \] (2.27)

as well as the definitions

\[ \tilde{J}_{n,c}(t) = J_{n,c}(t) \cos(\phi_{n,c}) + J_{n,s}(t) \sin(\phi_{n,s}) \] (2.28)
\[ \tilde{J}_{n,s}(t) = J_{n,s}(t) \cos(\phi_{n,s}) - J_{n,c}(t) \sin(\phi_{n,c}) \] (2.29)

to write our Hamiltonian as

\[ H_{CG}(t) = \frac{\Delta B_z}{2} \sigma_z + \frac{1}{2} \left[ J_0(t) + \sum_{n=1}^{N_J} \tilde{J}_{n,c}(t) \cos(n\omega_d t) + \sum_{n=1}^{N_J} \tilde{J}_{n,s}(t) \sin(n\omega_d t) \right] \sigma_x \] (2.30)

From now on, we also drop the \( d \) index for the frequency of the drive since this is the only relevant frequency anymore.

2.3 Effective Hamiltonian Description of the System

2.3.1 Choice of Rotating Frame

The choice of frame that we will use for our analysis is one of the key aspects of simplifying the problem as much as possible. However, there is no real measure of how ”simplifying” a frame is and therefore the choice of any particular one entails some degree of arbitrariness.

Before getting into any more details and since we are going to discuss quite a few different frames it is useful to decide on a systematic way of labeling those frames. To this end, we name each frame by the the transformation that maps the lab frame of the system to this frame, so “going to the \( \mathcal{R}_n(\theta) \) frame” means that we use the transformation

\[ |\psi(t)\rangle_{new} = \mathcal{R}_n^\dagger(\theta) |\psi(t)\rangle_{old} \quad \text{and} \quad \mathcal{H}_{new}(t) = \mathcal{R}_n^\dagger(\theta) \mathcal{H}_{old}(t) \mathcal{R}_n(\theta) - i \mathcal{R}_n^\dagger(\theta) \partial_t \mathcal{R}_n(\theta) \] (2.31)

with

\[ \mathcal{R}_n(\theta) = e^{-i \frac{\theta}{2} (\hat{n} \cdot \vec{\sigma})} \] (2.32)
Figure 2.8: Bloch sphere time evolution of the toy model (blue) in the lab frame (left) and the $R_z(\omega_q t)$ frame (right) alongside the RWA trajectory (red). In both cases the initial state is $|0\rangle$ and the final state is depicted by a vector of the same colour as the trajectory it corresponds to.

In order to shape our ideal frame, we draw inspiration from our toy model. There, we chose a rotating frame around the qubit axis $z$ with frequency equal to the frequency of the qubit. According to our naming convention this will be the $R_z(\omega_q t)$ frame. The resulting transformation is visualized in Figure 2.8. In this rotating frame, the RWA generates a trajectory on the Bloch sphere which follows the actual trajectory of the full Hamiltonian rather closely. In Chapter 1, however, we have seen that the RWA is the zeroth order of our effective Hamiltonian. Finding a frame in which the RWA becomes an, as accurate as possible, description of the real time evolution would thus be a good indication that most of the information for the system is contained within the zeroth order effective Hamiltonian. Therefore higher order terms contribute only small corrections in this frame, thus allowing us to safely truncate it at some low order.

Due to the admittedly "engineered" similarity of our Hamiltonian for the Cerfontaine Gate

$$H_{CG}(t) = \frac{\Delta B_z}{2} \sigma_z + 1 \left[ J_0(t) + \sum_{n=1}^{N_J} \tilde{J}_{n,c}(t) \cos(n\omega t) + \delta J(t) \right] \sigma_x$$

with the corresponding one for the toy model

$$H_{TM}(t) = \frac{\omega_q}{2} \sigma_z + \frac{H_1(t)}{2} \cos(\omega_d t + \phi),$$

going to the $R_z(\omega_q t)$ frame might be an appropriate choice for this Hamiltonian as well. Ignoring the $\delta J(t)$ term for the moment, there is still one glaring difference between the two models and that is the zero frequency mode of the drive $J_0(t)$. 

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2.3. Effective Hamiltonian Description of the System

To deal with this issue we consider the Schrödinger equation on the Bloch sphere

$$\frac{d\vec{r}(t)}{dt} = 2\vec{H}(t) \times \vec{r}(t) \quad (2.35)$$

where $\vec{r}(t)$ is the Bloch vector of the state and $\vec{H}(t)$ is defined as

$$\mathcal{H}(t) = \vec{H}(t) \cdot \vec{\sigma} = H_x(t)\sigma_x + H_y(t)\sigma_y + H_z(t)\sigma_z \quad (2.36)$$

with $\mathcal{H}(t)$ some single qubit Hamiltonian. In order to absorb the zero frequency mode of the drive (part of the $H_x(t)$ component) into the qubit component of the Hamiltonian ($H_z(t)$ component) we clearly need to rotate of the system around the $y$ axis with an angle

$$\phi_0(t) = \arctan\left(\frac{J_0(t)}{\Delta B_z}\right). \quad (2.37)$$

The transformation for this frame is

$$\mathcal{R}_y(\phi_0(t)) = e^{-i\phi_0(t)\sigma_y} \quad (2.38)$$

and the Hamiltonian becomes

$$\mathcal{H}_y(t) = \frac{\Omega(t)}{2} \sigma_z + \frac{J(t) - J_0(t)}{2} \sigma'_x - \partial_t \phi_0(t) \sigma_y \quad (2.39)$$

where

$$J(t) - J_0(t) = \left[ \sum_{n=1}^{N_f} \tilde{J}_{n,c}(t) \cos(n\omega t) + \sum_{n=1}^{N_f} \tilde{J}_{n,s}(t) \sin(n\omega t) + \delta J(t) \right] \quad (2.40)$$

and $\Omega(t) = \sqrt{\Delta B_z^2 + J_0(t)^2}$. The fact that the Bloch sphere trajectory in this frame exhibits a similar spiraling behavior as the toy model in the lab frame, as can be seen in Figure 2.10, is encouraging.

Now that we have “hidden” the zero frequency mode of the drive in the qubit term we can proceed with moving to the $\mathcal{R}_z(t\Omega(t))\mathcal{R}_y(\phi_0(t))$ frame, with its corresponding trajectory depicted in Figure 2.10. Unfortunately, even the RWA trajectory appears to be a bad approximation, as a result of the Hamiltonian in this frame being pathogenic in various ways. The most prominent issue is the emergence of terms proportional to trigonometric functions that oscillate with the time dependent frequency of the qubit, such as $\sin(\omega t + \Omega(t)t), \cos(\omega t - \Omega(t)t)$ and others, which prevent us from reducing the system to the FMI. One way around this would be to expand these trigonometric terms using Eqs. (2.26) - (2.27), and then absorb the terms that oscillate with $\Omega(t)$ into some new definition of the amplitude functions.
Figure 2.10: Bloch sphere time evolutions of the Cerfontaine Gate in the lab frame (upper left), the $R_y(\phi_0(t))$ frame (upper right), the $R_z(t\Omega(t))R_y(\phi_0(t))$ frame (lower left) and the $R_z(\omega t)R_y(\phi_0(t))$ frame. In each graph, the blue vector is the final state predicted by the model, the purple vector indicates the initial state of the system in the corresponding frame, and the yellow one the experimental final state. The red trajectories represent the RWA in the corresponding frame.
2.3. Effective Hamiltonian Description of the System

Unfortunately, in that case we end up with a Hamiltonian whose effective Hamiltonian diverges. Particularly, the new drive amplitudes that are proportional to either \( \sin(\Omega(t)t) \) or \( \cos(\Omega(t)t) \) have derivatives that exhibit a similar behavior to the ones indicated by the red curves in Figure 2.5, and thus lead to divergent terms in the effective Hamiltonian.

Finally, we move the system to a variation of the \( \mathcal{R}_z(\Omega(t))\mathcal{R}_y(\phi_0(t)) \) frame, namely the \( \mathcal{R}_z(\omega t)\mathcal{R}_y(\phi_0(t)) \) frame, where we use the constant frequency of the drive instead of the time dependent frequency of the qubit, as the frequency of rotation for the frame. Although the RWA trajectory in this frame does not follow the actual trajectory as closely as we anticipated, the resulting Hamiltonian is much more well behaved. Therefore, we will use this one for our calculations. In Figure 2.10 we present the trajectory generated by the actual Hamiltonian in this frame alongside the RWA. The Hamiltonian in this frame is

\[
\begin{align*}
\mathcal{H}_{yz}(t) &= \mathcal{H}_{\text{FMI}}(t) + \delta \mathcal{H}(t), \\
\mathcal{H}_{\text{FMI}}(t) &= \mathcal{H}_{\text{qubit}}(t) + \mathcal{H}_0(t) + \sum_{j=1}^{3} \mathcal{H}_{j,c}(t) + \sum_{j=1}^{3} \mathcal{H}_{j,s}(t), \\
\mathcal{H}_{\text{qubit}}(t) &= \frac{\Delta(t)}{2} = \frac{\Omega(t) - \omega}{2}, \\
\mathcal{H}_0(t) &= -\partial_0 \phi_0(t) (\sin(\omega t)\sigma_x + \cos(\omega t)\sigma_y), \\
\mathcal{H}_{1,c}(t) &= \left( \sum_{n=1}^{N_j} \tilde{J}_{n,c}(t) \cos[(n-1)\omega t] + \tilde{J}_{n,c}(t) \cos[(n+1)\omega t] \right) \frac{\delta B_z}{4\Omega(t)} \sigma_x, \\
\mathcal{H}_{2,c}(t) &= \left( \sum_{n=1}^{N_j} \tilde{J}_{n,c}(t) \sin[(n-1)\omega t] - \tilde{J}_{n,c}(t) \sin[(n+1)\omega t] \right) \frac{\delta B_z}{4\Omega(t)} \sigma_y, \\
\mathcal{H}_{3,c}(t) &= \left( \sum_{n=1}^{N_j} \tilde{J}_{n,c}(t) \cos(n\omega t) \right) \frac{J_0(t)}{2\Omega(t)} \sigma_z, \\
\mathcal{H}_{1,s}(t) &= \left( \sum_{n=1}^{N_j} \tilde{J}_{n,s}(t) \sin[(n-1)\omega t] + \tilde{J}_{n,s}(t) \sin[(n+1)\omega t] \right) \frac{\delta B_z}{4\Omega(t)} \sigma_x, \\
\mathcal{H}_{2,s}(t) &= \left( \sum_{n=1}^{N_j} \tilde{J}_{n,s}(t) \cos[(n+1)\omega t] - \tilde{J}_{n,s}(t) \cos[(n-1)\omega t] \right) \frac{\delta B_z}{4\Omega(t)} \sigma_y, \\
\mathcal{H}_{3,s}(t) &= \left( \sum_{n=1}^{N_j} \tilde{J}_{n,s}(t) \sin(n\omega t) \right) \frac{J_0(t)}{2\Omega(t)} \sigma_z, \\
\delta \mathcal{H}(t) &= \frac{\delta J(t)}{2\Omega(t)} \left( J_0(t) \sigma_z + \delta B_z \cos(\omega t)\sigma_x - \delta B_z \sin(\omega t)\sigma_y \right).
\end{align*}
\]

2.3.2 The Effective Hamiltonian and Fidelity

Now that we have our Hamiltonian in the preferred frame of reference, we wish to calculate the effective Hamiltonian. However there is still the pending question of how to deal with the \( \delta \mathcal{H}(t) \) component of the Hamiltonian.
Figure 2.11: In this graph we have plotted the average absolute value of $J_{\text{res}}(t) = J(t) - \sum_{m=0}^{n} J_m(t)$ in the interval $[0, t_{\text{gate}}]$, as a percentage of the average absolute value of $J(t)$ in the same interval, for different values of the order $n$ of our spectral decomposition for $J(t)$.

To deal with this, we need to consider the relevance of the $\delta J(t)$ term in our calculations, compared to the rest of the components of the frequency decomposition. We notice that the $\delta J(t)$ we computed initially by doing a decomposition of $J(t)$, Eq. (2.14), up to order $J_1(t)$, was roughly of the same order as $J_1(t)$. However when we extended our decomposition up to order $J_2(t)$ the $\delta J(t)$ component decreased significantly in amplitude. This trend suggests that if one was to keep decomposing $J(t)$ using our frequency decomposition scheme, there would be some order $N_J$ for which

$$\delta J(t) = J(t) - \sum_{n=0}^{N_J} J_n(t) \ll J(t)$$

(2.53)

This trend is presented in Figure 2.11. Although, this might seem like an optimistic observation, there is a significant tradeoff with this approach, namely, our already cumbersome Hamiltonian will keep increasing in size, which in turn leads to an exponential increase in the complexity of the calculation of the effective Hamiltonian.

With these observations in mind we choose to describe the evolution of the system in two different ways. In both cases, we first calculate the first order effective Hamiltonian, $\mathcal{H}_1(t)$, of the FMI-reducible component of the Hamiltonian, Eq. (2.43). In the first approach, we completely ignore the $\delta \mathcal{H}(t)$ component of the full Hamiltonian but substitute $\mathcal{H}_{\text{FMI}}(t)$ with $\mathcal{H}_1(t)$ and calculate the time evolution of the system with the one generated by $\mathcal{H}_1(t)$

$$U_{CG}(t_{\text{gate}}, 0) = \mathcal{T} \exp \left( \int_0^{t_{\text{gate}}} (\mathcal{H}_{\text{FMI}}(\tau) + \delta \mathcal{H}(\tau)) d\tau \right)$$

$$\approx \mathcal{T} \exp \left( \int_0^{t_{\text{gate}}} \mathcal{H}_{\text{FMI}}(\tau) d\tau \right) \approx \mathcal{T} \exp \left( \int_0^{t_{\text{gate}}} \mathcal{H}_1(\tau) d\tau \right).$$

(2.54)

In the second approach, we account for the $\delta \mathcal{H}(t)$ component of the full Hamiltonian but substitute $\mathcal{H}_{\text{FMI}}(t)$ with $\mathcal{H}_1(t)$ and calculate the time evolution generated by
2.3. Effective Hamiltonian Description of the System

\[ \mathcal{H}_1(t) + \delta \mathcal{H}(t) \] numerically

\[ U_{\text{CG}}(t_{\text{gate}}, 0) = T \exp \left( \int_0^{t_{\text{gate}}} (\mathcal{H}_{\text{FMI}}(\tau) + \delta \mathcal{H}(\tau)) d\tau \right) \]

\[ \approx T \exp \left( \int_0^{t_{\text{gate}}} (\mathcal{H}_1(\tau) + \delta \mathcal{H}(\tau)) d\tau \right). \] (2.55)

Next, we repeat this procedure for the second order effective Hamiltonian \( \mathcal{H}_2(t) \) and finally we repeat all these calculations for three frequency decompositions of the drive with \( N_J = 1, 2, 3 \). The corresponding trajectories in the Bloch sphere for \( N_J = 2 \) are presented in Figure 2.12, using a two-dimensional representation of the Bloch sphere.

There is one final complication to resolve, but fortunately this is also the simplest one. As we have already stated in subsection 1.5.2, the effective Hamiltonian evolution is in agreement with the actual evolution of the system only stroboscopically. This means that we can only compare the actual evolution of the system \( U(t_{\text{gate}}, 0) \) with the one generated by the effective Hamiltonian \( U_{\text{eff}}(t_{\text{gate}}, 0) \) as long as

\[ t_{\text{gate}} = \lambda t_c = \frac{2\pi \lambda}{\omega} \text{ with } \lambda \in \mathbb{Z}, \] (2.56)

with \( t_c \) being the length of the FMI and \( \omega \) the frequency of the drive. However, it appears that for our case

\[ t_{\text{gate}} - \frac{2\pi \lambda}{\omega} = \delta t \neq 0 \] (2.57)

for any integer \( \lambda \). We fix the \( \lambda \) by requiring that the absolute value of \( \delta t \) becomes minimal, which leads to \( \lambda = 3 \) and \( \delta t > 0 \), meaning that the full time evolution of the system lasts slightly over three Magnus intervals. For this value of \( \lambda \), we have

\[ \frac{\delta t}{t_{\text{gate}}} = 4.8 \cdot 10^{-2} \quad \text{and} \quad \frac{\langle J(t) \rangle_{\delta t}}{\Delta B_z} = \frac{1}{\Delta B_z \delta t} \int_{\frac{6\pi}{\omega}}^{\frac{6\pi}{\omega} + \delta t} dt J(t) = 2.25 \cdot 10^{-10}. \] (2.58)

Here the first calculation is the ratio of the final step to the the total operation time of the gate and the second calculation is the ratio of the average value of the drive in the final step \( \delta t \) compared to the frequency of the free qubit \( \Delta B_z \). These values of course suggests that in the brief time interval \([6\pi/\omega, 6\pi/\omega + \delta t]\) the CG Hamiltonian in the lab frame is very well approximated as the free qubit Hamiltonian

\[ \mathcal{H}_{CG}(t) = \frac{\Delta B_z}{2} \sigma_z + \frac{J(t)}{2} \sigma_x \approx \frac{\Delta B_z}{2} \sigma_z \] (2.59)

and it will generate a time evolution

\[ U_{\text{free}} \left( \frac{6\pi}{\omega} + \delta t, \frac{6\pi}{\omega} \right) = e^{-i \frac{\Delta B_z}{2} \delta t \sigma_z}, \] (2.60)

which can be trivially calculated in this frame and then transferred into the rotating frame \( \mathcal{R}_z(\omega t) \mathcal{R}_y(\phi_0(t)) \). We will use this approximation for both approaches in
Figure 2.12: Bloch sphere trajectories in bloch angle coordinates $\phi/\pi \in [-1, 1]$ and $\theta/\pi \in [0, 1]$ in the $R_z(\omega t)R_y(\phi_0(t))$ frame. In both diagrams, the blue curve corresponds to the time evolution generated by the full CG Hamiltonian while the green one indicates the one generated by the RWA. The solid red trajectory on the top diagram corresponds to the time evolution operator of the first order effective Hamiltonian of the FMI Hamiltonian for three Magnus intervals $t_c$, while the same line in the bottom diagram corresponds to the second order effective Hamiltonian. The solid orange trajectory on the top is the time evolution generated by the first order effective Hamiltonian plus the $\delta H(t)$ component, again for three Magnus intervals $t_c$. In the bottom diagram we present the same evolution but for second order effective Hamiltonian. Finally the dashed lines are simply the $U_{\text{free}}$ continuation of each effective trajectory for the final $\delta t$ time step.
2.3. Effective Hamiltonian Description of the System

order to complete the evolution using the group multiplication property of the time evolution operator

\[ U_{\text{full}}(t_{\text{gate}}, 0) = U_{\text{free}} \left( \frac{6\pi}{\omega} + \delta t, \frac{6\pi}{\omega} \right) U_{\text{eff}} \left( \frac{6\pi}{\omega}, 0 \right). \]  

(2.61)

Although the trajectories presented in Figure 2.12 already suggest that the effective Hamiltonian does not accurately predict the evolution of this system, we present this miss-match even more explicitly with the following table of fidelities. Their definitions follow right after the table:

<table>
<thead>
<tr>
<th>( N )</th>
<th>( F(U_{\text{FMI}}) )</th>
<th>( F(U_{\text{RWA}}) )</th>
<th>( F(U_{1}) )</th>
<th>( F(U_{1+\delta}) )</th>
<th>( F(U_{2}) )</th>
<th>( F(U_{2+\delta}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>98.14</td>
<td>98.76</td>
<td>67.59</td>
<td>71.99</td>
<td>91.65</td>
<td>86.52</td>
</tr>
<tr>
<td>2</td>
<td>99.83</td>
<td>98.76</td>
<td>79.99</td>
<td>81.71</td>
<td>97.52</td>
<td>97.13</td>
</tr>
<tr>
<td>3</td>
<td>99.79</td>
<td>98.76</td>
<td>79.48</td>
<td>80.65</td>
<td>97.86</td>
<td>97.27</td>
</tr>
</tbody>
</table>

We calculate these average gate fidelities using the definition given in [15], which is an adjustment of the expression given in [16] and originally derived in [17],

\[ F(U) = \frac{100}{d+1} \left( \frac{1}{d} \left| \text{tr} \left( U_{\text{ideal}}^\dagger U \right) \right|^2 + 1 \right), \]  

(2.62)

where \( U \) is the time evolution operator of the gate whose fidelity to some ideal gate, with time evolution operator \( U_{\text{ideal}} \), we wish to calculate. For all of these fidelities we used

\[ U_{\text{ideal}}(t_{\text{gate}}, 0) = \mathcal{T} \exp \left( -i \int_{0}^{t_{\text{gate}}} \mathcal{H}_{\text{CG}}(\tau) d\tau \right), \]  

(2.63)

expressed in the same frame as the time evolution operator that we want to compare it to and calculated numerically.

The first fidelity in the above table, \( F(U_{\text{FMI}}) \), is that of the time evolution operator of the CG in the \( \mathcal{R}_z(\omega t)\mathcal{R}_y(\phi_0(t)) \) frame ignoring the \( \delta \mathcal{H}(t) \) term

\[ U_{\text{FMI}}(t_{\text{gate}}, 0) = \mathcal{T} \exp \left( -i \int_{0}^{t_{\text{gate}}} (\mathcal{H}_{\text{CG}}(\tau) - \delta \mathcal{H}(\tau)) d\tau \right) \]  

\[ = \mathcal{T} \exp \left( -i \int_{0}^{t_{\text{gate}}} \mathcal{H}_{\text{FMI}}(\tau) d\tau \right). \]  

(2.64)

The fidelity for this operator indicates the significance of the \( \delta J(t) \) in the description of the system. From the values listed in the \( F(U_{\text{FMI}}) \) column of the table we can see that the contribution of \( \delta J(t) \) is truly insignificant for all orders of frequency decomposition \( N \), perhaps excluding the first order, but in any case this fidelity does not seem to vary significantly with \( N \) either. This is in fact a very useful result, since it allows us to use a low order frequency decomposition, say up to \( J_2(t) \), and focus on increasing the accuracy by increasing only the order of the effective Hamiltonian.

The second fidelity we calculate in the above table, \( F(U_{\text{RWA}}) \), is that of the time evolution operator of the RWA Hamiltonian in the \( \mathcal{R}_z(\omega t)\mathcal{R}_y(\phi_0(t)) \) frame

\[ U_{\text{RWA}}(t_{\text{gate}}, 0) = \mathcal{T} \exp \left( -i \int_{0}^{t_{\text{gate}}} \mathcal{H}_{\text{RWA}}(\tau) d\tau \right). \]  

(2.65)
The most striking feature of this fidelity is that it is independent of the order of the frequency decomposition. This is reasonable since the RWA Hamiltonian only accounts for the slowly oscillating terms which include $J_0(t)$ and $J_1(t)$

\[
H_{\text{RWA}}(t) = \frac{\Delta(t)}{2} \sigma_z + \frac{\Delta B_z \tilde{J}_{1,c}(t)}{4\Omega(t)} \sigma_x - \frac{\Delta B_z \tilde{J}_{1,s}(t)}{4\Omega(t)} \sigma_y.
\] (2.66)

All other terms of the spectrum are excluded from the RWA and therefore including them in the full system Hamiltonian does not make any difference.

The third fidelity we calculate in the above table, $F(U_1)$, is that of the time evolution operator generated by the first order effective Hamiltonian $H_1(t)$ up to time $6\pi/\omega$ and assisted by $U_{\text{free}}$ in the last $\delta t$ time step as discussed in Eq. (2.61)

\[
U_1(t_{\text{gate}}, 0) = U_{\text{free}} \left( t_{\text{gate}}, \frac{6\pi}{\omega} \right) \cdot \mathcal{T} \exp \left( -i \int_0^{\frac{6\pi}{\omega}} H_1(\tau) d\tau \right).
\] (2.67)

The values listed in this column show that the first order effective Hamiltonian fails to describe the evolution of the system and it even performs worse than the RWA. Including the $\delta H(t)$ term into the effective evolution to calculate the fidelities presented in the fourth fidelity column, $F(U_{1+\delta})$, where

\[
U_{1+\delta}(t_{\text{gate}}, 0) = U_{\text{free}} \left( t_{\text{gate}}, \frac{6\pi}{\omega} \right) \cdot \mathcal{T} \exp \left( -i \int_0^{\frac{6\pi}{\omega}} (H_1(\tau) + \delta H(\tau)) d\tau \right)
\] (2.68)

does not seem to improve the situation either.

Finally, to ensure the reader about the accuracy of our model for the CG we calculate the fidelity of our model to the experimental data

\[
F(U_{\text{exp}}) = 99.59\%
\] (2.69)

In the last two columns of the table we present the same fidelities as in the previous two but for the second order effective Hamiltonian, $F(U_2)$ and $F(U_{2+\delta})$. In these columns we see a dramatic increase in fidelity compared to the first order effective Hamiltonian results, but still lower performance than the RWA. This behavior suggests that even with a second order effective Hamiltonian we have not included the most significant terms of the expansion yet and therefore need to go to higher orders in order to achieve higher fidelity than the RWA. Unfortunately, it is very hard to calculate higher order effective Hamiltonians with the method presented in Chapter 1 and this is the problem that inspired our search for an alternative way of calculating the effective Hamiltonian, which we will present in the following chapter.
Chapter 3

Analytic Expression for the Effective Hamiltonian

In this chapter we develop an alternative formulation for the calculation of the effective Hamiltonian. Our search for such an alternative formulation was inspired by the fact that we were unable to obtain higher orders of the effective Hamiltonian using the methods presented in chapter 1. In section 1 we present a formula for the calculation of the Magnus-Taylor expansion which we will use in section 2 to calculate the first three orders of the effective Hamiltonian of a generic Hamiltonian. Even though, we do not succeed to obtain a formula for any order of the effective Hamiltonian we do obtain some simplifications for the methods that we have already presented in chapter 1. Finally in section 4, we demonstrate the equivalence of Magnus, Magnus-Taylor and effective Hamiltonian expansions for the case of constant drive amplitudes.

3.1 An Explicit Formula for the Magnus-Taylor Expansion

We assume a Hamiltonian of the form

\[ H(t) = \sum_{n} A_n(t) g_n(\omega t) \sigma_n, \ n \in \mathbb{Z}, \]  

(3.1)

where \( A_n(t) \) are unspecified amplitude functions, \( g_n(\omega t) \) are functions that satisfy the condition

\[ g_n(\omega t) = g_n(\omega t + k\omega t_c), \ \forall n, k \in \mathbb{Z} \]  

(3.2)

and \( \sigma_n \) are operators.

While most formulas used for the Magnus expansion are defined recursively, according to [18] we can compute the nth order Magnus-expansion (ME) via the non-recursive formula

\[ \Omega_N = t_c \int_{\mathcal{T}_N} \sum_{p \in \mathcal{P}^{N-1}} (-1)^d_p \frac{d_p!(N - d_p - 1)!}{N!} [A(\tau_{p(1)}), A(\tau_{p(2)}), \ldots, A(\tau_{p(N-1)}), A(\tau_N)] \ldots]. \]  

(3.3)
Let us decode this expression term by term. First of all, \( t_c \) is the length of the FMI, Eq. (1.116), as before and we have also denoted the \( N \)-fold nested integration as

\[
\int_{T_N} = \frac{1}{t_c} \int_{t_0}^{t_0 + t_c} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{N-1}} dt_N. \tag{3.4}
\]

The sum \( \sum_{p \in \mathcal{P}^{N-1}} \) runs over all permutations \( p \) in the group of all \( N-1 \) permutations \( \mathcal{P}^{N-1} \), \( d_p \) is the number of index descents \( (p(i) > p(i + 1)) \) in \( p \) and \( A(t) = -i\mathcal{H}(t) \).

To convey a sense of what the permutation descents are we will consider a specific example. Before that, we use the simplified notation used in [18], namely

\[
[A(\tau_{p(1)}), [A(\tau_{p(2)}), \ldots, A(\tau_{p(N-1)}), A(\tau_N)] \ldots] = A[p(1), p(2), \ldots, p(N-1), N] = A[p, N]. \tag{3.5}
\]

Assume we are interested in the \( N = 4 \) case and therefore we sum over \( \mathcal{P}^3 \), then the possible permutations and their corresponding descents are

\[
\]

\[
d_{123} = 0 \quad d_{132} = 1 \quad d_{213} = 1 \quad d_{231} = 1 \quad d_{312} = 1 \quad d_{321} = 2.
\]

Note that the last index always takes the maximum value and therefore never contributes to the calculation of the descents.

Now we wish to re-express Eq. (3.3) using our conventions and notation from Chapter 1. Again, here the order \( N \) starts from 1 so we leave the left hand side \( N \) as it is and shift \( N \to N + 1 \) in the right hand side

\[
\Omega_N = t_c \int_{T_{N+1}} \sum_{p \in \mathcal{P}^N} (-1)^{d_p} \frac{d_p! (N - d_p)!}{(N + 1)!} A[p, N + 1], \tag{3.6}
\]

thus \( N \) now starts from 0 in this version of the formula. Next, we multiply each side with the factor \( i/t_c \) to obtain the ME formula with dimensions of energy

\[
\tilde{\mathcal{H}}^{(N)} = i \int_{T_{N+1}} \sum_{p \in \mathcal{P}^N} (-1)^{d_p} \frac{d_p! (N - d_p)!}{(N + 1)!} A[p, N + 1] \tag{3.7}
\]

Furthermore, as we have already stated \( A(t) = -i\mathcal{H}(t) \) and so

\[
\tilde{\mathcal{H}}^{(N)} = (-i)^N \int_{T_{N+1}} \sum_{p \in \mathcal{P}^N} (-1)^{d_p} \frac{d_p! (N - d_p)!}{(N + 1)!} \mathcal{H}[p, N + 1]. \tag{3.8}
\]

This is the \( N \)th term of the ME expressed faithfully to our conventions.

For the Magnus-Taylor Expansion (MTE) up to \( 1/\omega^m \) we will have

\[
\mathcal{H}[p, N + 1] = \left[ \mathcal{H} \left[ T_{n_1}^{m-N}(\tau_{p(1)}, t), \tau_{p(1)} \right], \mathcal{H} \left[ T_{n_2}^{m-N}(\tau_{p(2)}, t), \tau_{p(2)} \right], \cdots \right.
\]

\[
\cdots \left[ \mathcal{H} \left[ T_{n_N}^{m-N}(\tau_{p(N)}, t), \tau_{p(N)} \right], \mathcal{H} \left[ T_{n_{N+1}}^{m-N}(\tau_{N+1}, t), \tau_{N+1} \right] \right] \right]. \tag{3.9}
\]
3.1. An Explicit Formula for the Magnus-Taylor Expansion

where we used the notation in Eq. (1.30) for the Taylor expansion. Using our ansatz for the Hamiltonian in Eq. (3.1) we can write this as

$$
\mathcal{H}[p, N + 1] = \sum_{n_1, \ldots, n_{N+1}} T_{n_{N+1}}^{m-N} (\tau_{N+1}, t) g_{n_{N+1}} (\tau_{N+1}) \prod_{j=1}^{N} T_{n_{p(j)}}^{m-N} (\tau_{p(j)}, t) g_{n_{p(j)}} (\tau_{p(j)}) \cdot [\sigma_{n_1}, [\sigma_{n_2}, \cdots, [\sigma_{n_N}, [\sigma_{n_{N+1}}]]]] .
$$

(3.10)

However, the components that are now outside the commutator actually commute and the \(n_j\)'s are independent summation indices that run over the same range of values. As a result, if we take each permutation in \(P^N\) separately and choose for each one to do the relabeling \(n_j \rightarrow n_{p(j)}, \forall j \in [1, N] \cap \mathbb{Z}\), due to the commutativity of the terms outside the commutator, we effectively cancel out the permutational dependence for these terms. To visualize this consider the following example

\[
\sum_{p \in P^2} \sum_{n_1, n_2, n_3} F_{n_1}(t_{p(1)}) F_{n_2}(t_{p(2)}) F_{n_3}(t_3) [\sigma_{n_1}, [\sigma_{n_2}, [\sigma_{n_3}, \sigma_{n_4}]]] =
\]

\[
\sum_{n_1, n_2, n_3} (F_{n_1}(t_1) F_{n_2}(t_2) F_{n_3}(t_3) [\sigma_{n_1}, [\sigma_{n_2}, [\sigma_{n_3}, \sigma_{n_4}]]] + F_{n_1}(t_1) F_{n_2}(t_2) F_{n_3}(t_3) [\sigma_{n_1}, [\sigma_{n_2}, [\sigma_{n_3}, \sigma_{n_4}]]]) =
\]

\[
\sum_{n_1, n_2, n_3} (F_{n_1}(t_1) F_{n_2}(t_2) F_{n_3}(t_3) [\sigma_{n_1}, [\sigma_{n_2}, [\sigma_{n_3}, \sigma_{n_4}]]] + F_{n_1}(t_1) F_{n_2}(t_2) F_{n_3}(t_3) [\sigma_{n_1}, [\sigma_{n_2}, [\sigma_{n_3}, \sigma_{n_4}]]]) =
\]

\[
\sum_{p \in P^2} \sum_{n_1, n_2, n_3} F_{n_1}(t_1) F_{n_2}(t_2) F_{n_3}(t_3) [\sigma_{n_{p(1)}}, [\sigma_{n_{p(2)}}, [\sigma_{n_{p(3)}}, \sigma_{n_4}]]] .
\]

(3.11)

Using this notational trick we end up with

$$
\mathcal{H}[p, N + 1] = \sum_{n_1, \ldots, n_{N+1}} \prod_{j=1}^{N+1} T_{n_j}^{m-N} (\tau_j, t) g_{n_j} (\tau_j) \sigma[p, N + 1],
$$

(3.12)

where we defined similar to Eq. (3.5)

$$
\sigma[p, N + 1] = \left( \prod_{j=1}^{N} \text{ad}_{\sigma_{n_{p(j)}}} \right) \sigma_{N+1} = \left[ \sigma_{n_{p(1)}}, [\sigma_{n_{p(2)}}, [...], [\sigma_{n_{p(N)}}, [\sigma_{N+1}, [...]]] \right] .
$$

(3.13)

Writing down the Taylor expansions explicitly and using the definition in Eq. (3.5) we can get

$$
\mathcal{H}[p, N + 1] = \sum_{n_1, \ldots, n_{N+1}} \sum_{k_1, \ldots, k_{N+1} = 0}^{m-N} \prod_{j=1}^{N+1} \frac{1}{k_j !} \frac{\partial^{k_j} A_{n_j}(t)}{\partial \tau_j^{k_j}} (\tau_j - t)^{k_j} g_{n_j}(\tau_j) \sigma[p, N + 1].
$$

(3.14)

Substitution of this into Eq. (3.8) yields

$$
\mathcal{H}^{(N, m-N)} = \frac{(-i)^N}{(N+1)!} \sum_{n_j} \sum_{k_j = 0}^{m-N} \prod_{j=1}^{N+1} \frac{1}{k_j !} \frac{\partial^{k_j} A_{n_j}(t)}{\partial \tau_j^{k_j}} ,
$$

\[
\cdot \int_{T_{N+1}} (\tau_j - t)^{k_j} g_{n_j}(\tau_j) \sum_{p \in P^N} f_p \sigma[p, N + 1],
\]

(3.15)
where we set for notational convenience $f_p = (-1)^{d_p} d_p! (N - d_p)!$ and $\sum_{n_j}$ indicates summation over all possible $n_j$’s that appear in the formula: $n_1, n_2...n_{N+1}$. We also used the same convention for the sum over all possible $k_j$’s. Now we perform the standard change of variable for the integrals

$$
\int_{T_{N+1}} = \frac{1}{t_c} \int_{t_0}^{t_0+t_c} d\tau_1 \cdot \int_{t_0}^{TN} d\tau_{N+1} \rightarrow \frac{1}{\omega^N \beta_c} \int_{\beta_0}^{\beta_0+\beta_c} d\beta_1 \cdot \int_{\beta_0}^{\beta_N} d\beta_{N+1} = \frac{1}{\omega^N} \int_{B_{N+1}}^{N+1}(3.16)
$$

and so

$$
\tilde{H}^{(N,m-N)} = \frac{(-i)^N}{\omega^N (N + 1)!} \sum_{\forall n_j} \sum_{\forall k_j} \prod_{j=0}^{N+1} \frac{\partial^{k_j}}{k_j! \omega^{k_j}} \cdot \int_{B_{N+1}} (\beta_j - \beta)^{k_j} g_{n_j}(\beta_j) \sum_{p \in \mathbb{P}^N} f_p \sigma [p, N + 1] .
$$

(3.17)

In order to make this formula more compact we introduce some new definitions. We define the $N$-fold nested average as

$$
\left\langle \prod_{j=1}^{N+1} (\beta_j - \beta)^{k_j} g_{n_j}(\beta_j) \right\rangle_{N+1} = \frac{1}{\prod_{j=1}^{N+1} k_j!} \int_{B_{N+1}} \prod_{j=1}^{N+1} (\beta_j - \beta)^{k_j} g_{n_j}(\beta_j) \int_{B_{N+1}}^{N+1} \frac{\beta_j^n}{(N + 1)!}
$$

(3.18)

where the denominator integral is just a normalization volume

$$
\int_{B_{N+1}} = \frac{\beta_c^N}{(N + 1)!}
$$

(3.19)

and also the combinatorial sum operator

$$
S_{\hat{n}}(N) = \sum_{p \in \mathbb{P}^N} f_p \sigma [p, N + 1] = \sum_{p \in \mathbb{P}^N} (-1)^{d_p} d_p! (N - d_p)! \sigma [p, N + 1]
$$

(3.20)

where the index $\hat{n}$ is used to denote the dependence of this term on all the $n_j$’s that are being summed in Eq.(3.17), so $\hat{n} = (n_1, n_2,...,n_{N+1})$. Using these definitions, we can finally write our MTE formula as

$$
\tilde{H}^{(N,m-N)} = \frac{(-i)^N \beta_c^N}{[(N + 1)!]^2} \sum_{\forall n_j} \sum_{\forall k_j=0}^{N} \prod_{j=1}^{N+1} \frac{\partial^{k_j}}{k_j! \omega^{N+\sum_{j=1}^{N+1} k_j}} \left\langle \prod_{j=1}^{N+1} (\beta_j - \beta)^{k_j} g_{n_j}(\beta_j) \right\rangle_{N+1} S_{\hat{n}}(N).
$$

(3.21)

Before moving on we point out the advantages of this formula over the recursive formula we have seen before:

- With this formula any order of the MTE is directly accessible, meaning we do not need to calculate all orders up to $N - 1$ in order to calculate the $N$th order.
3.2 First Three Orders of the Effective Hamiltonian

• When calculating the MTE up to some specific order $m$ in $1/\omega$, there are a lot of “junk” terms being produced by the recursive formula that are $O(1/\omega^{m+1})$. With this formula it is completely straightforward to calculate only the required terms.

• This formula is much more generic. This stems from the fact that we made no claims about the form of the explicitly time dependent functions $g_n(\omega t)$ other than the condition in Eq. (3.2) and also the form of the $\sigma_n$ operators. They could be any kind of operator, Pauli’s, ladder operators, 2-qubit operators, N-qubit operators.

3.2 First Three Orders of the Effective Hamiltonian

Now that we have the formula for the $N$th order of the MTE we can attempt to find a formula for the $N$th order of the effective Hamiltonian, namely the $h_N(t; t_0)$ in

$$\mathcal{H}_{\text{eff}} = \sum_{N=0}^{\infty} \frac{h_N(t; t_0)}{\omega^N}. \quad (3.22)$$

To do this, we will use the recursive formula in Eq. (1.100)

$$h_N(t; t_0) = \frac{D^N\hat{H}}{D\mu^N} - \frac{D^N\hat{H}_{N-1}}{D\mu^N}, \quad (3.23)$$

with $\mu = 1/\omega$ and $D^k/D\mu^k$ is the PCO defined at the end of subsection 1.5.2, to calculate the first few orders in hope that a pattern will emerge. In zeroth order we obtain

$$h_0(t; t_0) = \frac{D^0\hat{H}}{D\mu^0} = \frac{D^0\hat{R}^{(0,0)}}{D\mu^0}$$

$$= \frac{D^0}{D\mu^0} \sum_{n_1} \langle (\beta_1 - \beta)^{k_1} g_{n_1}(\beta_1) \rangle_1 S_{n_1}(0)$$

$$= \sum_{n_1} A_{n_1}(t) \langle g_{n_1}(\beta_1) \rangle_1 S_{n_1}(0). \quad (3.24)$$

with $S_{n_1}(0) = \sum_{p \in P_0} (-1)^d_p d_p!(N - d_p)! \sigma [p, 1] = \sigma_{n_1}$, so

$$h_0(t; t_0) = \sum_{n_1} A_{n_1}(t) \langle g_{n_1}(\beta_1) \rangle_1 \sigma_{n_1}. \quad (3.25)$$

Two notes on this result:

• This term is time dependent only via the amplitude functions $A_{n_1}(t)$ as our effective Hamiltonian should be.

• This is exactly the definition of the RWA. Therefore our claim that the zeroth order of the effective Hamiltonian is the RWA becomes explicit in this formalism and also not just for the toy model but for a generic Hamiltonian.
Now we proceed with calculating the next order. The recursion formula for the first order of the effective Hamiltonian gives

$$h_1(t; t_0) = \frac{D\tilde{H}}{D\mu} - \frac{D\tilde{h}_0}{D\mu} = \frac{D\tilde{H}^{(0,1)}}{D\mu} + \frac{D\tilde{H}^{(1,0)}}{D\mu} - \frac{D\tilde{h}_0^{(0,1)}}{D\mu} - \frac{D\tilde{h}_0^{(1,0)}}{D\mu}. \quad (3.26)$$

We calculate each term separately

$$\frac{D\tilde{H}^{(0,1)}}{D\mu} = \frac{D}{D\mu} \sum_{n_1} \sum_{k_1=0}^1 \frac{\partial^k_1 A_{n_1}(t)}{\omega^k_1} \langle (\beta_1 - \beta)^k_1 g_{n_1}(\beta_1) \rangle_1 S_{n_1}(0) \quad (3.27)$$

$$= \sum_{n_1} \sum_{k_1=0}^1 \delta_{1,k_1} \partial^k_1 A_{n_1}(t) \langle (\beta_1 - \beta)^k_1 g_{n_1}(\beta_1) \rangle_1 \sigma_{n_1} \quad (3.28)$$

$$= \sum_{n_1} \partial_1 A_{n_1}(t) \langle (\beta_1 - \beta) g_{n_1}(\beta_1) \rangle_1 \sigma_{n_1}. \quad (3.29)$$

$$\frac{D\tilde{H}^{(1,0)}}{D\mu} = -\frac{i\beta_c}{4} \frac{D}{D\mu} \sum_{n_1,n_2} \frac{A_{n_1}(t) A_{n_2}(t)}{\omega} \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2 S_{n_1 n_2}(1) \quad (3.30)$$

$$= -\frac{i\beta_c}{4} \sum_{n_1,n_2} A_{n_1}(t) A_{n_2}(t) \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2 [\sigma_{n_1}, \sigma_{n_2}]. \quad (3.31)$$

For the last two terms we notice that \(h_0(t; t_0)\) has the same form as the original Hamiltonian with the difference that the explicitly time dependent functions are now constants. Therefore its MTE is completely equivalent under the substitution \(g_{n_j}(\beta_j) \rightarrow \langle g_{n_j}(\beta_j) \rangle_1\) which means

$$\frac{D\tilde{h}_0^{(0,1)}}{D\mu} = \sum_{n_1} \partial_1 A_{n_1}(t) \sigma_{n_1} \langle (\beta_1 - \beta) \langle g_{n_1}(\beta_1) \rangle_1 \rangle_1, \quad (3.32)$$

$$\frac{D\tilde{h}_0^{(1,0)}}{D\mu} = -\frac{i\beta_c}{4} \sum_{n_1,n_2} A_{n_1}(t) A_{n_2}(t) [\sigma_{n_1}, \sigma_{n_2}] \langle \langle g_{n_1}(\beta_1) \rangle_1 \rangle_1 \langle g_{n_2}(\beta_1) \rangle_1 \rangle_2. \quad (3.33)$$

According to the definition in Eq. (3.18) it is straightforward to see that

$$\langle (\beta_1 - \beta) g_{n_1}(\beta_1) \rangle_1 = \langle \beta_1 g_{n_1}(\beta_1) \rangle_1 - \beta \langle g_{n_1}(\beta_1) \rangle_1 \quad (3.34)$$

$$\langle (\beta_1 - \beta) \langle g_{n_1}(\beta_1) \rangle_1 \rangle_1 = \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) \rangle_1 - \beta \langle g_{n_1}(\beta_1) \rangle_1 \quad (3.35)$$

$$\langle \langle g_{n_1}(\beta_1) \rangle_1 \rangle_1 \langle g_{n_2}(\beta_1) \rangle_1 \rangle_1 = \langle g_{n_1}(\beta_1) \rangle_1 \langle g_{n_2}(\beta_1) \rangle_1 \quad (3.36)$$

and by recombining all these terms into Eq. (3.26) we get

$$h_1(t; t_0) = \sum_{n_1} \partial_1 A_{n_1}(t) \langle (\beta_1 g_{n_1}(\beta_1))_1 - \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) \rangle_1 \rangle_1 \sigma_{n_1} - \frac{i\beta_c}{4} \sum_{n_1,n_2} A_{n_1}(t) A_{n_2}(t) \langle (g_{n_1}(\beta_1) g_{n_2}(\beta_2))_2 - \langle g_{n_1}(\beta_1) \rangle_1 \langle g_{n_2}(\beta_1) \rangle_1 \rangle_1 \sigma_{n_1}, \sigma_{n_2}. \quad (3.37)$$
Note, however, that in the second term of the second sum we have terms that are symmetric with respect to the indices multiplied by terms that are antisymmetric

\[ \sum_{n_1,n_2} A_{n_1}(t) A_{n_2}(t) \langle g_{n_1}(\beta_1) \rangle_1 \langle g_{n_2}(\beta_1) \rangle_1 \left[ \sigma_{n_1}, \sigma_{n_2} \right] \]

\[ \sum_{n_1,n_2} A_{n_2}(t) A_{n_1}(t) \langle g_{n_2}(\beta_1) \rangle_1 \langle g_{n_1}(\beta_1) \rangle_1 \left[ \sigma_{n_2}, \sigma_{n_1} \right] = 0. \]

Therefore our first order term of the effective Hamiltonian is simplified to

\[ h_1(t; t_0) = \sum_{n_1} \partial_t A_{n_1}(t) (\langle \beta_1 g_{n_1}(\beta_1) \rangle_1 - \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) \rangle_1) \sigma_{n_1} - \frac{i\beta_c}{4} \sum_{n_1,n_2} A_{n_1}(t) A_{n_2}(t) \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2 \left[ \sigma_{n_1}, \sigma_{n_2} \right]. \]

With a procedure quite similar to the one followed for the calculation of the previous two orders of the effective Hamiltonian (see Appendix B) one can obtain the second order term

\[ h_2(t; t_0) = \sum_{n_1} \partial_t^2 A_{n_1}(t) \left( \langle \beta_1^2 g_{n_1}(\beta_1) \rangle_1 - \langle \beta_1 \rangle_1 \langle \beta_1 g_{n_1}(\beta_1) \rangle_1 + \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) \rangle_1 \right) \sigma_{n_1} - \frac{i\beta_c}{4} \sum_{n_1,n_2} A_{n_1}(t) \partial_t A_{n_2}(t) (\langle \beta_2 g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2 - \langle \beta_2 \rangle_1 \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2) \left[ \sigma_{n_1}, \sigma_{n_2} \right] - \frac{i\beta_c}{4} \sum_{n_1,n_2} \partial_t A_{n_1}(t) A_{n_2}(t) (\langle \beta_1 g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2 - \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2) \left[ \sigma_{n_1}, \sigma_{n_2} \right] - \frac{i\beta_c}{4} \sum_{n_1,n_2} \partial_t A_{n_1}(t) A_{n_2}(t) (\langle \beta_1 g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2 - \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2) \left[ \sigma_{n_1}, \sigma_{n_2} \right] - \frac{\beta_c^2}{36} \sum_{n_1,n_2,n_3} A_{n_1}(t) A_{n_2}(t) A_{n_3}(t) \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) g_{n_3}(\beta_3) \rangle_3 \left( 2 \left[ \sigma_{n_1}, \sigma_{n_2}, \sigma_{n_3} \right] - \left[ \sigma_{n_2}, \sigma_{n_1}, \sigma_{n_3} \right] \right). \]

It is very comforting that the explicitly time dependent terms have dropped even for the second order. Additionally, these formulas reproduce our results for the toy model. These few first orders are quite suggestive that there is indeed a pattern for the Nth term of the effective Hamiltonian. Namely, one should write down the MTE of the actual Hamiltonian and then throw out all terms that are of the wrong order in 1/\(\omega\), dependent on the FMI length \(\beta_c\) and non-periodic in the gauge parameter \(\beta_0\).

The periodicity with respect to \(\beta_0\) claim is also supported by the following observation. The \(N\)-fold nested integrals in the first few orders of the effective Hamiltonian are the unique combinations of decompositions of the \(N\)-fold nested integrals
originating from the MTE that are by definition periodic in $\beta_0$. For instance, consider
\begin{equation}
\langle \beta_1 g_n(\beta_1) \rangle_1 - \langle \beta_1 \rangle_1 \langle g_n(\beta_1) \rangle_1 = \langle (\beta_1 - \langle \beta_1 \rangle_1) g_n(\beta_1) \rangle_1 .
\end{equation}
The first term on the left side is the term that originates from the MTE and the second term was obtained via the recursion formula. We now replace the coefficient of the term originating from the recursion, in this 1-folded integral, with some unspecified parameter $a$
\begin{equation}
\langle (\beta_1 + a \langle \beta_1 \rangle_1 ) g_n(\beta_1) \rangle_1^{old} = \frac{1}{\beta c} \int_{\beta_0}^{\beta_0 + \beta_c} d\beta_1 \left( \beta_1 + \frac{a}{\beta c} \int_{\beta_0}^{\beta_0 + \beta_c} d\beta' \beta' \right) g_n(\beta_1) .
\end{equation}
and perform the change of variable $\beta_1 \to \beta'_1 + \beta_c$
\begin{equation}
\langle (\beta_1 + a \langle \beta_1 \rangle_1 ) g_n(\beta_1) \rangle_1^{new} = \frac{1}{\beta c} \int_{\beta_0}^{\beta_0 + 2\beta_c} d\beta_1 \left( \beta_1 + a\beta_0 + \frac{3a\beta_c}{2} \right) g_n(\beta_1) .
\end{equation}
By definition however
\begin{equation}
g_n(\beta'_1 + \beta_c) = g_n(\beta'_1)
\end{equation}
and therefore
\begin{equation}
\langle (\beta_1 + a \langle \beta_1 \rangle_1 ) g_n(\beta_1) \rangle_1^{new} = \frac{1}{\beta c} \int_{\beta_0}^{\beta_0 + 2\beta_c} d\beta_1 \left( \beta_1 + a\beta_0 + \frac{2 + 3a}{2} \beta_c \right) g_n(\beta_1) ,
\end{equation}
where we dropped the prime from the integration variable. If we now require that
\begin{equation}
\langle (\beta_1 + a \langle \beta_1 \rangle_1 ) g_n(\beta_1) \rangle_1^{old} = \langle (\beta_1 + a \langle \beta_1 \rangle_1 ) g_n(\beta_1) \rangle_1^{new}
\end{equation}
for any $\beta_0$, $\beta_c$ and $g_n(\beta_1)$ we obtain one unique solution $a = -1$ which is identical to the value of the parameter that we obtained from the recursion. If this is in fact the case then our effective Hamiltonian formula for a Hamiltonian $H(t)$ is
\begin{equation}
h_k(t; t_0) = \frac{D^0}{D^{\beta_0}_c} \frac{D^0}{D^{\beta_0}_0} \frac{D^k}{D^{\mu_k}} H
\end{equation}
Even if this formula is correct, one may still wonder why would this be an improvement in the calculation of the effective Hamiltonian. While it is true that the number of terms that need to be calculated still grows exponentially as we increase the order, the form of the effective Hamiltonian allows us to break the calculation into smaller more manageable sub-calculations. These include the calculation of the operator component
\begin{equation}
S_{\pi}(N) = \sum_{p \in \mathbb{P}^N} f_p \sigma [p, N + 1] = \sum_{p \in \mathbb{P}^N} (-1)^{d_p} d_p! (N - d_p)! \sigma [p, N + 1].
\end{equation}
3.3. A Simplification in the Recursive Calculation of the Effective Hamiltonian

and the $N$-fold integrals

$$\left\langle \prod_{j=1}^{N+1} (\beta_j - \beta)^{k_j} g_{n_j}(\beta_j) \right\rangle_{N+1} = \frac{1}{\prod_{j=1}^{N+1} k_j!} \int B_{N+1} \prod_{j=1}^{N+1} (\beta_j - \beta)^{k_j} g_{n_j}(\beta_j)$$

(3.51)

Calculating the operator component first, allows us to identify many vanishing components thus reducing the computation time considerably for the corresponding integrals.

Unfortunately proving this for any order is beyond the scope of this work. To make things worse, the procedure of calculating these terms gets severely more complicated and abstract with each additional order, therefore practically preventing us from reaching much higher orders. Even this small step, however, has pointed us to a few, so far, unnoticed properties of our effective Hamiltonian which we will elaborate on in the following sections.

3.3 A Simplification in the Recursive Calculation of the Effective Hamiltonian

Throughout the calculations of the previous section, one type of terms stood out because they were always vanishing, and these terms where

$$\frac{D^{N+1} \mathcal{H}_N^{(N+1,0)}}{D\mu^{N+1}}.$$  

As it turns out, this is not just a coincidence for the first three orders of the effective Hamiltonian and with some thorough considerations one can prove that this is a general pattern holding for any $N$. We shall now state the following theorem

**Theorem 3.3.1** The $(N + 1, 0)$ Magnus-Taylor expansion terms of the truncated effective Hamiltonian of order $N$ are at most of order $1/\omega^N$

$$\frac{D^{N+1} \mathcal{H}_N^{(N+1,0)}}{D\mu^{N+1}} = 0, \ \forall N \in [0, \infty) \cap \mathbb{Z}. \quad (3.52)$$

**Proof:** By construction, the effective Hamiltonian will have the same form as the original Hamiltonian under some relabeling/renaming of the involved terms

$$\mathcal{H}_N = \sum_{\tilde{n}} \tilde{A}_{\tilde{n}}(t) \tilde{g}_{\tilde{n}}(\omega t) \tilde{\sigma}_{\tilde{n}}.$$  

(3.53)

The difference is that all the explicitly time dependent functions $\tilde{g}_{\tilde{n}}(\omega t)$ are constants

$$\frac{d\tilde{g}_{\tilde{n}}(\omega t)}{dt} = 0, \ \forall \tilde{n} \in \mathbb{Z}. \quad (3.54)$$

With these simplifications in mind we can write

$$\frac{D^{N+1} \mathcal{H}_N^{(N+1,0)}}{D\mu^{N+1}} \propto \frac{D^{N+1}}{D\mu^{N+1}} \sum_{\forall \tilde{n}_j} \frac{\prod_{j=1}^{N+1} \tilde{A}_{\tilde{n}_j}(t) \tilde{g}_{\tilde{n}_j}}{\omega^{N+1}} \tilde{S}_{\tilde{n}}(N + 1). \quad (3.55)$$

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Chapter 3. Analytic Expression for the Effective Hamiltonian

In the effective Hamiltonian, however, powers of $1/\omega$ are included, which for the intents and purposes of the calculation would have to be absorbed into the definitions of either $\tilde{A}_{n_j}(t)$ or $\tilde{g}_{n_j}$. Thus, the only terms that are relevant for this proof are originating from $h_0(t; t_0)$ for which

$$\tilde{A}_{n_j}(t) = A_{n_j}(t), \quad \tilde{g}_{n_j} = \langle g_{n_j}(\beta_j) \rangle_1, \quad \tilde{\sigma}_{n_j} = \sigma_{n_j}$$ (3.56)

and so

$$\frac{D^{N+1}H_N^{(N+1,0)}}{D\mu^{N+1}} \propto \sum \prod_{j=1}^{N+1} A_{n_j}(t) \langle g_{n_j}(\beta_j) \rangle_1 S(N + 1) = 0.$$ (3.57)

This sum is trivially zero because the functions are all symmetric under any relabeling $n_j \leftrightarrow n_k$ while the operator component is always anti-symmetric in at least one of them.

This is a very useful result, because it means that we do not need to Magnus-Taylor expand the truncated effective Hamiltonian to the same order as the actual Hamiltonian as we have done so far, but one order lower. This is obviously a speed up in the calculation of the effective Hamiltonian using the recursive formula in Eq. (1.100).

3.4 Constant Amplitude Effective Hamiltonian

The pattern that the terms of the effective Hamiltonian follow, is not so trivial for the general case of time dependent amplitudes $A_{n_j}(t)$ due to the complexity of the terms that involve different order derivative products such as

$$\partial_t^{k_1} A_{n_1}(t) \partial_t^{k_2} A_{n_2}(t), \quad k_1 \neq k_2.$$ 

Fortunately, in the special case of a Hamiltonian with constant amplitudes only, $A_{n_j}(t) = A_{n_j}$, the problem is significantly simplified and our formula for the MTE becomes

$$\tilde{H} = \sum_{m=0}^{\infty} \frac{\beta^m \beta_c^m}{\omega^m [(m + 1)!]^2} \sum \prod_{j=1}^{m+1} A_{n_j} \left\langle \prod_{j=1}^{m+1} g_{n_j}(\beta_j) \right\rangle_{m+1} S_{\tilde{\sigma}}(m),$$ (3.58)

which is essentially just the ME. We proceed with calculating the effective Hamiltonian using our recursion equation in Eq. (1.100)

$$h_{N+1} = \frac{D^{N+1}H}{D\mu^{N+1}} - \frac{D^{N+1}H_N}{D\mu^{N+1}}.$$ (3.59)

The first term on the right side can be calculated using the previous relation

$$\frac{D^{N+1}H}{D\mu^{N+1}} = \frac{\beta(N+1) \beta_c^{N+1}}{[(N + 2)!]^2} \sum \prod_{j=1}^{N+2} A_{n_j} \left\langle \prod_{j=1}^{N+2} g_{n_j}(\beta_j) \right\rangle_{N+2} S_{\tilde{\sigma}}(N + 1).$$ (3.60)
3.4. **Constant Amplitude Effective Hamiltonian**

Fortunately, for the constant amplitude case, the second term in the recursions right hand side is identical to

\[
\frac{D^{N+1} \mathcal{H}_N}{D\mu^{N+1}} = \frac{D^{N+1} \mathcal{H}_N^{(N+1,0)}}{D\mu^{N+1}}
\]

which according to theorem (3.3.1) is vanishing. Therefore we obtain

\[
h_{N+1} = \frac{D^{N+1} \mathcal{H}}{D\mu^{N+1}} \Rightarrow \mathcal{H}_{\text{eff}} = \mathcal{H} = \sum_{N=0}^{\infty} \frac{j^{3N} \beta_c^N}{N!} \omega_N \left[\frac{(N + 1)!}{(N + 1)!}\right]^2 \sum_{\eta n_j} \prod_{j=1}^{N+1} A_{n_j} \left\langle \prod_{j=1}^{N+1} g_{n_j}(\beta_j) \right\rangle S_{\eta}(N),
\]

or in other words the effective Hamiltonian, ME and MTE are all identical for the case of constant amplitudes.
Summary and Outlook

In the second chapter we have seen that the utilization of a second order effective Hamiltonian succeeded to give an accurate description of the dynamics of the Cerfontaine gate (fidelity $\sim 97.8\%$). However, the accuracy of this effective Hamiltonian failed to surpass that of the RWA (fidelity $\sim 98.7\%$), which was of course one of the goals of this entire endeavor.

Although we cannot rule out the possibility that this non-achievement was due to a diverging effective Hamiltonian, there is also nothing to suggest it does besides the oscillatory behavior of the fidelity for the first three orders of the effective Hamiltonian, discussed in subsection 2.3.2. The Magnus series converges in the interval $[0, t_{\text{gate}}]$ according to the criterion given in Eq. (A.1). The Taylor expansions converge since our amplitude functions are analytic for the entire duration of the gate and the amplitude derivatives seem to decay for the first few orders.

The estimation of the required order of the effective Hamiltonian for which we would obtain an improved fidelity compared to the RWA is a nontrivial calculation. However, the increase of fidelity from first to second order suggests that perhaps even a treatment up to third order could yield an improvement over the RWA, but unfortunately we are currently not able of calculating any higher order for the Cerfontaine gate. This barrier motivated our search for an alternative way of calculating the effective Hamiltonian.

Using the ME formula by Arnal et al. [18] we obtained a formula for the MTE

$$\hat{H}^{(N,m-N)} = \frac{j^{3N} \beta_c^N}{[(N + 1)!]^2} \sum_{\forall n_j \forall k_j = 0}^m \prod_{j=1}^{N+1} \delta_{\epsilon}^{k_j} A_{n_j}(t) \left[ \prod_{j=1}^{N+1} (\beta_j - \beta)^{k_j} g_{n_j}(\beta_j) \right] \prod_{N+1} S(N).$$

By substituting this formula into the the recursion formula for the effective Hamiltonian, from [1], we obtained the first three orders of the effective Hamiltonian, see Eqs. (3.25), (3.39) and (3.40). However, at this point we are unable to write down a formula for an arbitrary order.

Nevertheless, we did noticed a pattern, namely the effective Hamiltonian is ”hidden” inside the MTE under a pile of redundant terms, and the above-mentioned recursion simply cancels these terms. At first glance, these terms seem to be random. Taking a closer look, we recognize the terms that are canceled to be all the non-periodic terms in the gauge parameter $\beta_0$ or directly dependent on the dimensionless FMI length $\beta_c$, as we demonstrated at the end of section 3.2.

To proceed with the idea presented in the previous paragraph, we suggest that one should try to prove that the definition of the effective Hamiltonian in [1] leads to a Hamiltonian which is periodic in the gauge parameter $\beta_0$ and independent of the
dimensionless FMI interval length $\beta_c$. Alternatively, one can axiomatically demand the last two conditions and try to prove that they lead to the same definition of an effective Hamiltonian as in [1].
Appendices
Appendix A

On the Convergence of the Magnus Expansion

This appendix serves as a brief review of the main results we know about the convergence of the Magnus expansion stripped off all their mathematical rigor. For a far more thorough and rigorous review of the information presented here we suggest [9].

Generally, the description of the time evolution of a system with some Hamiltonian $\mathcal{H}(t)$ using the Magnus expansion is not always possible. Specifically, three criteria need to be met which are presented in [9]. Most of them are either always met for finite dimensional Hilbert space systems or they require an a priori knowledge of the eigenvalues of the Magnus expansion, therefore they are irrelevant for practical application.

One of these criteria however requires that the Magnus expansion belongs in the same Lie algebra as the Hamiltonian of the system. This condition is met in the range $[0, r_c)$ as long as

$$\int_0^{r_c} dt \, \|\mathcal{H}(t)\|_2 < \pi$$  \hspace{1cm} (A.1)

where $\|\mathcal{H}(t)\|_2$ is the 2-norm

$$\|\mathcal{H}(t)\|_2 = \max_{\|\psi\|=1} \|\mathcal{H}(t)|\psi\rangle\|_2 \quad \text{and} \quad \|\psi\| = \sqrt{\langle \psi | \psi \rangle}.$$  \hspace{1cm} (A.2)

Therefore the maximum $r_c$ for which this inequality is satisfied determines the radius of convergence of the Magnus expansion. However this is only an estimate of the radius of convergence, which means that while the Magnus expansion will definitely converge in the interval $[0, r_c)$ where (A.1) is met, it could also converge for a larger radius $r'_c$ for which

$$\pi < \int_0^{r'_c} dt \, \|\mathcal{H}(t)\|_2 < \infty.$$  \hspace{1cm} (A.3)

An example of such a case is presented in [9]. Also in [9] an exact way of calculating the radius of convergence is presented, but once again it requires an a priori knowledge of the eigenvalues of the Magnus expansion, rendering it useless for practical applications.

In conclusion inequality (A.1) is our most efficient way of estimating the radius of convergence for the Magnus expansion but it should be taken with a grain of salt.
Appendix B

Calculation of the Second Order Effective Hamiltonian

Using Eqs. (3.25) and (3.39) we can now write the first order effective Hamiltonian, and relabel the involved terms

$$\mathcal{H}_1(t; t_0) = \frac{\mathcal{H}_1(t; t_0)}{\omega} + h_0(t; t_0) = \sum_n \tilde{A}_n(t) \tilde{g}_n \tilde{\sigma}_n.$$

(B.1)

The simplification for this Hamiltonian is that the $\tilde{g}_n$ are constants for the effective Hamiltonian since only the amplitudes carry the time dependence. We proceed with calculating

$$h_2(t; t_0) = \frac{D^2 \tilde{H}}{D\mu^2} - \frac{D^2 \tilde{H}_1}{D\mu^2} = \sum_{q=0}^2 \left( \frac{D^2 \tilde{H}_{(q,2-q)}}{D\mu^2} - \frac{D^2 \tilde{H}_{(q,2-q)}}{D\mu^2} \right)$$

(B.2)

where

$$\frac{D^2 \tilde{H}_{(0,2)}}{D\mu^2} = \frac{D^2}{D\mu^2} \sum_{n_1} \frac{2}{\omega^k_1} \partial^k_{n_1} \mathcal{A}_n(t) \langle \beta_{n_1} g_n(\beta_1) \rangle \sigma_{n_1}$$

(B.3)

$$\frac{D^2 \tilde{H}_{(1,1)}}{D\mu^2} = -\frac{i\beta_c}{4} \frac{D^2}{D\mu^2} \sum_{n_1,n_2} \frac{1}{\omega^{1+k_1+k_2}} \partial^k_{n_1} \mathcal{A}_n(t) \partial^k_{n_2} \mathcal{A}_n(t) \langle \beta_{k_1} g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle \sigma_{n_1} \sigma_{n_2}$$

(B.4)
$$\frac{D^2 \tilde{H}^{(2,0)}}{D\mu^2} = -\frac{\beta_c^2}{36} \sum_{n_1,n_2,n_3} A_{n_1}(t) A_{n_2}(t) A_{n_3}(t) \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) g_{n_3}(\beta_3) \rangle_3 S_{n_1 n_2 n_3}(2)$$

$$= -\frac{\beta_c^2}{36} \sum_{n_1,n_2,n_3} A_{n_1}(t) A_{n_2}(t) A_{n_3}(t) \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) g_{n_3}(\beta_3) \rangle_3 \cdot (2 [\sigma_{n_1}, [\sigma_{n_2}, \sigma_{n_3}]] - [\sigma_{n_2}, [\sigma_{n_1}, \sigma_{n_3}]])$$

(B.5)

$$\frac{D^2 \tilde{H}^{(0,2)}}{D\mu^2} = \frac{D^2}{D\mu^2} \sum_{\tilde{n}_1} \sum_{k_1=0}^{\frac{2}{3}} \frac{\partial}{\omega^k_1} \tilde{A}_{\tilde{n}_1}(t) \langle \beta_{1}^{k_1} \tilde{g}_{\tilde{n}_1}(0) \rangle_1 S_{\tilde{n}_1}(0)$$

$$= \frac{D^2}{D\mu^2} \sum_{\tilde{n}_1} \sum_{k_1=0}^{\frac{2}{3}} \frac{\partial}{\omega^k_1} \tilde{A}_{\tilde{n}_1}(t) \langle \beta_{1}^{k_1} \tilde{g}_{\tilde{n}_1}(0) \rangle_1 \tilde{g}_{\tilde{n}_1}(0)$$

(B.6)

$$\frac{D^2 \tilde{H}^{(1,1)}}{D\mu^2} = -\frac{i \beta_c}{4} \frac{D^2}{D\mu^2} \sum_{n_1, n_2, k_1, k_2=0}^{1} \frac{\partial}{\omega^{1+k_1+k_2}} \tilde{A}_{n_1}(t) \tilde{A}_{n_2}(t) \langle \beta_{1}^{k_1} \beta_{2}^{k_2} \tilde{g}_{n_1} \tilde{g}_{n_2} \rangle_2 \tilde{S}_{n_1 n_2}$$

$$= -\frac{i \beta_c}{4} \frac{D^2}{D\mu^2} \sum_{n_1, n_2, k_1, k_2=0}^{1} \frac{\partial}{\omega^{1+k_1+k_2}} \tilde{A}_{n_1}(t) \tilde{A}_{n_2}(t) \langle \beta_{1}^{k_1} \beta_{2}^{k_2} \tilde{g}_{n_1} \tilde{g}_{n_2} \rangle_2 \tilde{g}_{n_1} \tilde{g}_{n_2} \tilde{S}_{n_1 n_2}$$

(B.7)

$$\frac{D^2 \tilde{H}^{(2,0)}}{D\mu^2} = -\frac{\beta_c^2}{36} \frac{D^2}{D\mu^2} \sum_{n_1, n_2, n_3} \tilde{A}_{n_1}(t) \tilde{A}_{n_2}(t) \tilde{A}_{n_3}(t) \langle \tilde{g}_{n_1} \tilde{g}_{n_2} \tilde{g}_{n_3} \rangle_3 \tilde{S}_{n_1 n_2 n_3}$$

$$= -\frac{\beta_c^2}{36} \frac{D^2}{D\mu^2} \sum_{n_1, n_2, n_3} \tilde{A}_{n_1}(t) \tilde{A}_{n_2}(t) \tilde{A}_{n_3}(t) \langle \tilde{g}_{n_1} \tilde{g}_{n_2} \tilde{g}_{n_3} \rangle_3 \tilde{g}_{n_1} \tilde{g}_{n_2} \tilde{g}_{n_3} \times$$

$$\times (2 [\tilde{S}_{n_1}, [\tilde{S}_{n_2}, \tilde{S}_{n_3}]] - [\tilde{S}_{n_2}, [\tilde{S}_{n_1}, \tilde{S}_{n_3}]]])$$

(B.8)

Notice that the coefficient operator does not act trivially on these sums anymore as a result of our relabeling the terms of the effective Hamiltonian which in turn leads to an implicit $1/\omega$ dependence on the new amplitudes. In order to complete the calculation we now have to rewrite these terms for all possible combinations of terms involved in the first order Hamiltonian. From Eq. (B.6) we have the following cases

- Contribution from zeroth order terms

$$\tilde{A}_{n_1}(t) \rightarrow A_{n_1}(t), \tilde{g}_{n_1} \rightarrow \langle g_{n_1}(\beta_1) \rangle_1, \tilde{\sigma}_{n_1} \rightarrow \sigma_{n_1}$$

$$\downarrow$$

$$\left( \frac{D^2 \tilde{H}^{(0,2)}}{D\mu^2} \right)_1 = \sum_{n_1} \partial^2 \tilde{A}_{n_1}(t) \langle \beta_{1}^{2} \rangle_1 \langle g_{n_1}(\beta_1) \rangle_1 \sigma_{n_1}$$

(B.9)
APPENDIX B. CALCULATION OF THE SECOND ORDER EFFECTIVE HAMILTONIAN

- Contribution from first order 1-amplitude terms

\[ \tilde{\mathcal{A}}_{\tilde{n}_1}(t) \rightarrow \frac{\partial_t \mathcal{A}_{n_1}(t)}{\omega}, \tilde{g}_{\tilde{n}_1} \rightarrow \langle \beta_1 g_{n_1}(\beta_1) \rangle_1 - \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) \rangle_1, \tilde{\sigma}_{\tilde{n}_1} \rightarrow \sigma_{n_1} \]

\[
\left( \frac{D^2 \tilde{\mathcal{H}}^{(0,2)}}{D\mu^2} \right)_1 = -\frac{i\beta_c}{4} \sum_{n_1,n_2} \partial_t \mathcal{A}_{n_1}(t) \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2 [\sigma_{n_1}, \sigma_{n_2}] \]

(B.10)

- Contribution from first order 2-amplitude terms

\[ \tilde{\mathcal{A}}_{\tilde{n}_1}(t) \rightarrow \frac{\mathcal{A}_{n_1}(t)\mathcal{A}_{n_2}(t)}{\omega}, \tilde{g}_{\tilde{n}_1} \rightarrow -\frac{i\beta_c}{4} \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2, \tilde{\sigma}_{\tilde{n}_1} \rightarrow [\sigma_{n_1}, \sigma_{n_2}] \]

\[
\left( \frac{D^2 \tilde{\mathcal{H}}^{(0,2)}}{D\mu^2} \right)_3 = -\frac{i\beta_c}{4} \sum_{n_1,n_2} \partial_t \mathcal{A}_{n_1}(t) \mathcal{A}_{n_2}(t) \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2 [\sigma_{n_1}, \sigma_{n_2}] \\
= -\frac{i\beta_c}{4} \sum_{n_1,n_2} \partial_t \mathcal{A}_{n_1}(t) \mathcal{A}_{n_2}(t) \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2 [\sigma_{n_1}, \sigma_{n_2}] \\
- \frac{i\beta_c}{4} \sum_{n_1,n_2} \mathcal{A}_{n_1}(t) \partial_t \mathcal{A}_{n_2}(t) \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) g_{n_2}(\beta_2) \rangle_2 [\sigma_{n_1}, \sigma_{n_2}] \\
\]

(B.11)

And

\[
\frac{D^2 \tilde{\mathcal{H}}^{(0,2)}}{D\mu^2} = \sum_{i=1}^{3} \left( \frac{D^2 \tilde{\mathcal{H}}^{(0,2)}}{D\mu^2} \right)_i 
\]

(B.12)

From Eq. (B.7) we do not need to consider cases where both the amplitudes originate from first order terms since these would be \(O(1/\omega^3)\) therefore we have only the following cases

- Contribution from zero-zero order terms

\[ \tilde{\mathcal{A}}_{\tilde{n}_1}(t) \rightarrow \mathcal{A}_{n_1}(t), \tilde{g}_{\tilde{n}_1} \rightarrow \langle g_{n_1}(\beta_1) \rangle_1, \tilde{\sigma}_{\tilde{n}_1} \rightarrow \sigma_{n_1} \]

\[ \tilde{\mathcal{A}}_{\tilde{n}_2}(t) \rightarrow \mathcal{A}_{n_2}(t), \tilde{g}_{\tilde{n}_2} \rightarrow \langle g_{n_2}(\beta_1) \rangle_1, \tilde{\sigma}_{\tilde{n}_2} \rightarrow \sigma_{n_2} \]

\[
\left( \frac{D^2 \tilde{\mathcal{H}}^{(1,1)}}{D\mu^2} \right)_1 = -\frac{i\beta_c}{4} \sum_{n_1,n_2} \mathcal{A}_{n_1}(t) \partial_t \mathcal{A}_{n_2}(t) \langle \beta_2 \rangle_2 \langle g_{n_1}(\beta_1) \rangle_1 \langle g_{n_2}(\beta_1) \rangle_1 [\sigma_{n_1}, \sigma_{n_2}] \\
- \frac{i\beta_c}{4} \sum_{n_1,n_2} \partial_t \mathcal{A}_{n_1}(t) \mathcal{A}_{n_2}(t) \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) \rangle_1 \langle g_{n_2}(\beta_1) \rangle_1 [\sigma_{n_1}, \sigma_{n_2}] \\
\]

(B.13)
• Contribution form zero-first order 1-amplitude terms

\[ \tilde{A}_{\tilde{n}_1}(t) \rightarrow A_{n_1}(t), \tilde{g}_{\tilde{n}_1} \rightarrow \langle g_{n_1}(\beta_1) \rangle_1, \tilde{\sigma}_{\tilde{n}_1} \rightarrow \sigma_{n_1} \]

\[ \tilde{A}_{\tilde{n}_2}(t) \rightarrow \frac{\partial_t A_{n_2}(t)}{\omega}, \tilde{g}_{\tilde{n}_2} \rightarrow \langle \beta_1 g_{n_2}(\beta_1) \rangle_1 - \langle \beta_1 \rangle_1 \langle g_{n_2}(\beta_1) \rangle_1, \tilde{\sigma}_{\tilde{n}_2} \rightarrow \sigma_{n_2} \]

\[ \left( \frac{D^2 \mathcal{H}_{1}^{(1,1)}}{D\mu^2} \right)_2 = -\frac{i\beta_c}{4} \sum_{n_1,n_2} A_{n_1}(t) \partial_t A_{n_2}(t) \langle \beta_1 g_{n_1}(\beta_1) \rangle_1 \langle \beta_1 g_{n_2}(\beta_1) \rangle_1 - \langle \beta_1 \rangle_1 \langle \beta_1 \rangle_1 \langle g_{n_2}(\beta_1) \rangle_1 \left[ \sigma_{n_1}, \sigma_{n_2} \right] \quad (B.14) \]

• Same type of contribution as the previous one but with the order of substitutions reversed

\[ \tilde{A}_{\tilde{n}_1}(t) \rightarrow \frac{\partial_t A_{n_1}(t)}{\omega}, \tilde{g}_{\tilde{n}_1} \rightarrow \langle \beta_1 g_{n_1}(\beta_1) \rangle_1 - \langle \beta_1 \rangle_1 \langle g_{n_1}(\beta_1) \rangle_1, \tilde{\sigma}_{\tilde{n}_1} \rightarrow \sigma_{n_1} \]

\[ \tilde{A}_{\tilde{n}_2}(t) \rightarrow A_{n_2}(t), \tilde{g}_{\tilde{n}_2} \rightarrow \langle g_{n_2}(\beta_1) \rangle_1, \tilde{\sigma}_{\tilde{n}_2} \rightarrow \sigma_{n_2} \]

\[ \left( \frac{D^2 \mathcal{H}_{1}^{(1,1)}}{D\mu^2} \right)_3 = -\frac{i\beta_c}{4} \sum_{n_1,n_2} \partial_t A_{n_1}(t) A_{n_2}(t) \langle \beta_1 g_{n_1}(\beta_1) \rangle_1 \langle \beta_1 \rangle_1 \langle g_{n_2}(\beta_1) \rangle_1 \times \langle g_{n_2}(\beta_1) \rangle_1 \left[ \sigma_{n_1}, \sigma_{n_2} \right] \quad (B.15) \]

• Contribution form zero-first order 2-amplitude terms

\[ \tilde{A}_{\tilde{n}_1}(t) \rightarrow A_{n_1}(t), \tilde{g}_{\tilde{n}_1} \rightarrow \langle g_{n_1}(\beta_1) \rangle_1, \tilde{\sigma}_{\tilde{n}_1} \rightarrow \sigma_{n_1} \]

\[ \tilde{A}_{\tilde{n}_2}(t) \rightarrow \frac{A_{n_2}(t) A_{n_3}(t)}{\omega}, \tilde{g}_{\tilde{n}_2} \rightarrow -\frac{i\beta_c}{4} \langle g_{n_2}(\beta_1) g_{n_3}(\beta_2) \rangle_2, \tilde{\sigma}_{\tilde{n}_2} \rightarrow \left[ \sigma_{n_2}, \sigma_{n_3} \right] \]

\[ \left( \frac{D^2 \mathcal{H}_{1}^{(1,1)}}{D\mu^2} \right)_4 = -\frac{i\beta_c}{4} \sum_{n_1,n_2,n_3} A_{n_1}(t) A_{n_2}(t) A_{n_3}(t) \langle g_{n_1}(\beta_1) \rangle_1 \langle g_{n_2}(\beta_1) g_{n_3}(\beta_2) \rangle_2 \times \left[ \sigma_{n_1}, \left[ \sigma_{n_2}, \sigma_{n_3} \right] \right] \quad (B.16) \]

• Same type of contribution as the previous one but with the order of substitutions reversed

\[ \tilde{A}_{\tilde{n}_1}(t) \rightarrow \frac{A_{n_2}(t) A_{n_3}(t)}{\omega}, \tilde{g}_{\tilde{n}_1} \rightarrow -\frac{i\beta_c}{4} \langle g_{n_2}(\beta_1) g_{n_3}(\beta_2) \rangle_2, \tilde{\sigma}_{\tilde{n}_1} \rightarrow \left[ \sigma_{n_2}, \sigma_{n_3} \right] \]

\[ \tilde{A}_{\tilde{n}_2}(t) \rightarrow A_{n_1}(t), \tilde{g}_{\tilde{n}_2} \rightarrow \langle g_{n_1}(\beta_1) \rangle_1, \tilde{\sigma}_{\tilde{n}_2} \rightarrow \sigma_{n_1} \]
Appendix B. Calculation of the Second Order Effective Hamiltonian

\[
\left( \frac{D^2\mathcal{H}_1^{(1,1)}}{D\mu^2} \right)_5 = \frac{i\beta_c}{4} \sum_{n_1,n_2,n_3} A_{n_1}(t) A_{n_2}(t) A_{n_3}(t) \langle g_{n_2}(\beta_1) g_{n_3}(\beta_2) \rangle_2 \langle g_{n_1}(\beta_1) \rangle_1 \times \\
\times [\sigma_{n_1}, [\sigma_{n_2}, \sigma_{n_3}]]
\]

Note here that the last four terms add up to zero, the last two are opposite and the remaining two result in an antisymmetric sum. In total

\[
\frac{D^2\mathcal{H}_1^{(1,1)}}{D\mu^2} = \sum_{i=1}^5 \left( \frac{D^2\mathcal{H}_1^{(1,1)}}{D\mu^2} \right)_i = \left( \frac{D^2\mathcal{H}_1^{(1,1)}}{D\mu^2} \right)_1
\]  

(B.17)

Finally for Eq. (B.8) we know from Theorem (3.3.1) that

\[
\frac{D^2\mathcal{H}_1^{(2,0)}}{D\mu^2} = 0
\]

(B.19)

Notice that for this calculation we have set \( \beta = 0 \) because we know that it will drop out of our calculations. One can repeat these calculations without this substitution and see that indeed there are no \( \beta \) related terms in the end. This can also serve as a validity check for our calculations. Substitution of all these terms back into Eq. (B.2) yields Eq. (3.40).
Bibliography


