Research internship

Notes on project in DiVincenzo group

Jesse Slim

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Abstract

Magnus expansion

Contents

1. The truncated Magnus expansion

The Magnus expansion[1–4] for the time evolution under Hamiltonian $H(t)$ is defined as

$$\Omega(t,t_0) = \sum_{n=1}^{\infty} \Omega_n(t,t_0), \tag{1}$$

$$\Omega_1(t,t_0) = \int_{t_0}^{t} \mathrm{d}t_1 \tilde{H}(t_1), \tag{2}$$

$$\Omega_2(t,t_0) = -\frac{1}{2}\int_{t_0}^{t} \mathrm{d}t_1 \left[\Omega_1(t_1,t_0), \tilde{H}(t_1)\right] = \frac{1}{2}\int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \left[\tilde{H}(t_1), \tilde{H}(t_2)\right], \tag{3}$$

where $\tilde{H}(t) = -i/\hbar H(t)$. In the reminder of these notes, natural units with $\hbar = 1$ will be used.

We use this series to approximate the trajectory of a two-level qubit driven by an oscillating signal proportional to $\boldsymbol{\sigma}_x$ in the lab frame. To this end, we use the following rotating frame Hamiltonian:

$$\boldsymbol{H}(t) = \frac{E(t)}{4}\left(\boldsymbol{\sigma}_x + \cos(2\omega t)\boldsymbol{\sigma}_x - \sin(2\omega t)\boldsymbol{\sigma}_y\right), \tag{4}$$

where for now we have set the detuning Δ and phase offset ϕ of the drive both to zero.

1.1. First order Magnus expansion

Initially, we restrict ourselves to the first order Magnus term, which is equivalent to the rotating wave approximation for constant drive. We begin by studying the case of linear drive, given by

$$E(t) = E_0 + E_1 t. \tag{5}$$

We then integrate equation (2) over a full period $t_c = \pi/\omega$ of the drive Hamiltonian (4), starting from t_0:

$$\begin{aligned}
i\Omega_1(t_0+t_c,t_0) &= \int_{t_0}^{t_0+t_c} \frac{E(t)}{4}\left(\boldsymbol{\sigma}_x + \cos(2\omega t)\boldsymbol{\sigma}_x - \sin(2\omega t)\boldsymbol{\sigma}_y\right)\mathrm{d}t \\
&= \int_{t_0}^{t_0+t_c} \frac{E(t)}{4}\boldsymbol{\sigma}_x \,\mathrm{d}t + \int_{t_0}^{t_0+t_c} \frac{E(t)}{4}\left(\cos(2\omega t)\boldsymbol{\sigma}_x - \sin(2\omega t)\boldsymbol{\sigma}_y\right)\mathrm{d}t \\
&= \frac{E_0 t_c + E_1(t_0 t_c + t_c^2/2)}{4}\boldsymbol{\sigma}_x + \frac{E_1 t_c \sin(2\omega t_0)}{8\omega}\boldsymbol{\sigma}_x + \frac{E_1 t_c \cos(2\omega t_0)}{8\omega}\boldsymbol{\sigma}_y \\
&= t_c \frac{E_0 + E_1 t_0}{4}\boldsymbol{\sigma}_x + t_c^2 \frac{E_1}{8}\boldsymbol{\sigma}_x + \frac{t_c}{\omega}\left(\frac{E_1 \sin(2\omega t_0)}{8}\boldsymbol{\sigma}_x + \frac{E_1 \cos(2\omega t_0)}{8}\boldsymbol{\sigma}_y\right) \\
&= t_c\left[\frac{E_0 + E_1 t_0}{4}\boldsymbol{\sigma}_x + \frac{E_1}{8\omega}\left(\pi\boldsymbol{\sigma}_x + \sin(2\omega t_0)\boldsymbol{\sigma}_x + \cos(2\omega t_0)\boldsymbol{\sigma}_y\right)\right]
\end{aligned} \tag{6}$$

The first term of this evolution operator exponent,

$$t_c \frac{E_0 + E_1 t_0}{4}\boldsymbol{\sigma}_x = t_c \frac{E(t_0)}{4}\boldsymbol{\sigma}_x, \tag{7}$$

can be understood as the rotating wave evolution over a period t_c with constant drive given by the value of the driving envelope at the beginning of the evolution period $E(t_0)$. The second term,

$$t_c^2 \frac{E_1}{8}\boldsymbol{\sigma}_x = t_c \frac{\pi E_1}{8\omega}\boldsymbol{\sigma}_x, \tag{8}$$

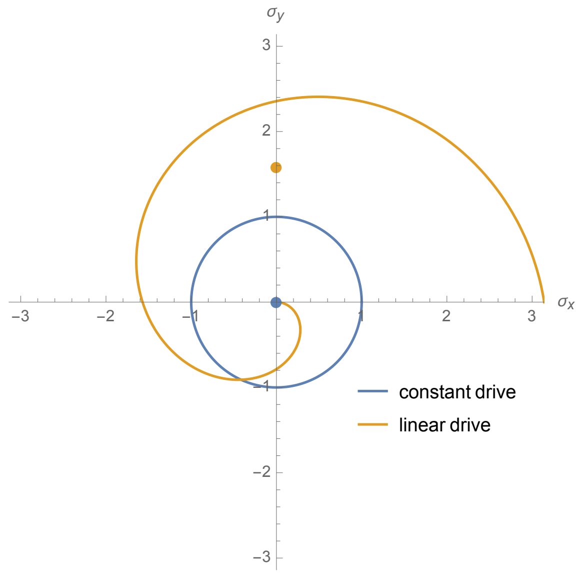

Figure 1 | Effect of the counter-rotating wave in the first order Magnus expansion. The $\boldsymbol{\sigma}_x$ and $\boldsymbol{\sigma}_y$ projections of the counter-rotating wave contribution, $E(t)\left[\cos(2\omega t)\boldsymbol{\sigma}_x + \sin(2\omega t)\boldsymbol{\sigma}_y\right]$, are traced for $t \in [t_0, t_0 + t_c]$ with $t_0 = 0$. Trajectories are shown both for constant drive $E(t) = 1$ and for a linearly increasing drive $E(t) = (t - t_0)$. The average projections are indicated with a dot. For constant drive, it can be seen that the average projection is zero, while for linear drive, the average is non-zero and directed $\pi/2$ radians from the initial (and final) projection. Choosing a different t_0 has the effect of rotating the trajectories and still leaves a non-zero average of equal magnitude in the linear drive case.

can still be understood in the rotating wave picture as the extra rotation brought about by the (linear) increase in driving strength during the evolution interval t_c. Keeping in mind that $t_c = \pi/\omega$, the effect of this term decreases if ω increases; i.e. the driving signal has less time to increase within one evolution interval.

The final two terms in equation (6),

$$t_c \frac{E_1}{8\omega} \left(\sin(2\omega t_0)\boldsymbol{\sigma}_x + \cos(2\omega t_0)\boldsymbol{\sigma}_y\right), \tag{9}$$

can no longer be understood in the rotating wave approximation. These terms constitute an average of the effect of the counter-rotating wave over a single evolution interval t_c, which is exactly the period of the counter-rotating wave. In the case of constant drive, i.e. $E_1 = 0$, this effect averages out to zero, but if the drive increases during the evolution interval, a non-zero average is obtained. The resulting “average counter-wave rotation axis” lies in the $x - y$ plane and has a constant magnitude, while the direction is determined by the start of the evolution interval t_0, as illustrated in Figure 1.

1.1.1 Effective Hamiltonian

Let’s see if we can find an effective Hamiltonian that corresponds to (6). Per the procedure described in Daniel’s notes, we proceed order by order of $1/\omega$, such that $H_{eff}^{(m)} = \sum_{n=0}^{m} (1/\omega)^n h_n$, where each h_n may not depend explicitly on t or ω and occurences of t_0 in (derivatives of) $H_1(t_0)$ are promoted to the instantaneous time t. We start with the trivial order $1/\omega^0 = 1$. In this case, h_0 is given by

$$h_0 = \left[\frac{E(t_0)}{4}\boldsymbol{\sigma}_x\right]_{t_0\to t} = \frac{H(t)}{4}\boldsymbol{\sigma}_x. \tag{10}$$

For the next order $1/\omega^1$ we use the iterative relation

$$h_{n+1} = C[\bar{H}(t_0), 1/\omega, n+1] - C[\bar{H}^{(n)}_{eff}(t_0), 1/\omega, n+1]. \tag{11}$$

The first term is readily extracted from (6) and equal to

$$C[\bar{H}(t_0), 1/\omega, 1] = \frac{E_1}{8\omega}\left(\pi\boldsymbol{\sigma}_x + \sin(2\omega t_0)\boldsymbol{\sigma}_x + \cos(2\omega t_0)\boldsymbol{\sigma}_y\right). \tag{12}$$

The second term is obtained by calculating the Magnus expansion of (10) up to first order in $1/\omega$. Noting that h_0 is proportional to $\boldsymbol{\sigma}_x$ for all times and $[h_0(t_1), h_0(t_2)] = 0$ for all t_1, t_2, the first order Magnus expansion is exact and given by

$$\bar{H}^{(0)}_{eff}(t_0) = \left[\frac{E(t_0)}{4} + \frac{E_1}{8\omega}\pi\right]\boldsymbol{\sigma}_x. \tag{13}$$

Therefore,

$$C[\bar{H}^{(0)}_{eff}(t_0), 1/\omega, 1] = \frac{E_1}{8\omega}\pi\boldsymbol{\sigma}_x, \tag{14}$$

leaving us with

$$h_1 = \frac{E_1}{8\omega}\left(\sin(2\omega t_0)\boldsymbol{\sigma}_x + \cos(2\omega t_0)\boldsymbol{\sigma}_y\right). \tag{15}$$

Let's see if taking the Magnus expansion of this effective Hamiltonian indeed matches the ME of the real Hamiltonian over an interval t_c. As per the notebook 'linear_drive_manual_integration.nb' it does, up to first order! There is however a third order term (and higher order terms) that explains the deviation of the trajectory of the effective Hamiltonian from the stroboscopic evolution given by repeated application of $\exp[-it_c\bar{H}(t_0+kt_c)]$ with increasing k, as observed in numerical simulations for large driving strengths.

1.2. Second order Magnus expansion

We now continue by investigating the second order term in the Magnus expansion, given by (3), to gain some intuition. We first focus on rewriting the commutator in the integrand:

$$\begin{aligned}
&\frac{1}{2}\left[\tilde{H}(t_1), \tilde{H}(t_2)\right] = \frac{1}{2}\left[-iH(t_1), -iH(t_2)\right] = -\frac{1}{2}\left[H(t_1), H(t_2)\right] \\
&= -\frac{E(t_1)E(t_2)}{32}\left[\,((1+\cos(2\omega t_1))\boldsymbol{\sigma}_x - \sin(2\omega t_1)\boldsymbol{\sigma}_y)\,, ((1+\cos(2\omega t_2))\boldsymbol{\sigma}_x - \sin(2\omega t_2)\boldsymbol{\sigma}_y)\,\right] \\
&= \frac{E(t_1)E(t_2)}{32}\Big((1+\cos(2\omega t_1))\sin(2\omega t_2)\,[\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y] + \sin(2\omega t_1)(1+\cos(2\omega t_2))\,[\boldsymbol{\sigma}_y, \boldsymbol{\sigma}_x]\Big) \\
&= i\frac{E(t_1)E(t_2)}{32}\Big((1+\cos(2\omega t_1))\sin(2\omega t_2) - \sin(2\omega t_1)(1+\cos(2\omega t_2))\Big)\boldsymbol{\sigma}_z \qquad (16) \\
&= -i\frac{E(t_1)E(t_2)}{4}\cos(\omega t_1)\cos(\omega t_2)\sin(\omega(t_1-t_2))\boldsymbol{\sigma}_z. \qquad (17)
\end{aligned}$$

A few important qualitative properties of the integrand and thus of the second order Magnus expansion term can be inferred from (17). Firstly, containing only the commutator $[\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y]$, the integrand is proportional to $\boldsymbol{\sigma}_z$ and represents the second order "composition effect" of non-commuting rotations around different axes in the $x-y$ plane. Furthermore, for $t_1 = t_2$ the final sine factor is zero, as is to be expected for the commutator at equal times.

Noting that this integrand is to be doubly integrated over t_1 and t_2, it is wise to make the integrand separable into factors only depending on t_1 or t_2. This yields the integrand

$$\begin{aligned}
&\frac{-iE(t_1)E(t_2)}{4}\cos(\omega t_1)\cos(\omega t_2)\left(\sin(\omega t_1)\cos(\omega t_2)-\cos(\omega t_1)\sin(\omega t_2)\right)\boldsymbol{\sigma}_z \\
=&\frac{-i}{8}\boldsymbol{\sigma}_z\left(E(t_1)\sin(2\omega t_1)E(t_2)\cos(\omega t_2)^2\right)+\frac{i}{8}\boldsymbol{\sigma}_z\left(E(t_1)\cos(\omega t_1)^2E(t_2)\sin(2\omega t_2)\right). \qquad (18)
\end{aligned}$$

We proceed by performing the inner integrals over $\mathrm{d}t_2$, resulting in

$$\begin{aligned}
\int_{t_0}^{t_1}\mathrm{d}t_2\,E(t_2)\cos(\omega t_2)^2 &= \int_{t_0}^{t_1}\mathrm{d}t_2\,(E_0+E_1t_2)\cos(\omega t_2)^2 \\
&= \frac{1}{4}(t_1-t_0)\left(E(t_0)+E(t_1)\right) \\
&+ \frac{1}{4\omega}\left(E(t_1)\sin(2t_1\omega)-E(t_0)\sin(2t_0\omega)\right) \\
&+ \frac{E_1}{8\omega^2}\left(\cos(2t_1\omega)-\cos(2t_0\omega)\right) \qquad (19)\\
\int_{t_0}^{t_1}\mathrm{d}t_2\,E(t_2)\sin(2\omega t_2) &= \int_{t_0}^{t_1}\mathrm{d}t_2\,(E_0+E_1t_2)\sin(2\omega t_2) \\
&= \frac{1}{2\omega}\left(E(t_0)\cos(2t_0\omega)-E(t_1)\cos(2t_1\omega)\right) \\
&+ \frac{E_1}{4\omega^2}\left(\sin(2t_1\omega)-\sin(2t_0\omega)\right). \qquad (20)
\end{aligned}$$

Plugging (19) and (20) into the integral of (18) over $\mathrm{d}t_2 \in [t_0, t_1]$ yields

$$\begin{aligned}
&-\frac{i}{8}\boldsymbol{\sigma}_zE(t_1)\sin(2\omega t_1)\Big(\frac{1}{4}(t_1-t_0)\left(E(t_0)+E(t_1)\right) \\
&\qquad+\frac{1}{4\omega}\left(E(t_1)\sin(2t_1\omega)-E(t_0)\sin(2t_0\omega)\right) \\
&\qquad+\frac{E_1}{8\omega^2}\left(\cos(2t_1\omega)-\cos(2t_0\omega)\right)\Big) \\
&+\frac{i}{8}\boldsymbol{\sigma}_zE(t_1)\cos(\omega t_1)^2\Big(\frac{1}{2\omega}\left(E(t_0)\cos(2t_0\omega)-E(t_1)\cos(2t_1\omega)\right) \\
&\qquad+\frac{E_1}{4\omega^2}\left(\sin(2t_1\omega)-\sin(2t_0\omega)\right)\Big), \qquad (21)
\end{aligned}$$

which thankfully can be simplified (by Mathematica, not by me...) to

$$\begin{aligned}
&\frac{i}{16}\boldsymbol{\sigma}_zE(t_1)\cos(\omega t_1)(t_0-t_1)(E(t_0)+E(t_1))\sin(\omega t_1) \\
&-\frac{i}{16\omega}\boldsymbol{\sigma}_zE(t_1)\cos(\omega t_1)(E(t_1)\cos(\omega t_1)-E(t_0)\cos(\omega(2t_0-t_1))) \\
&+\frac{iE_1}{32\omega^2}\boldsymbol{\sigma}_zE(t_1)\cos(\omega t_1)(\sin(\omega t_1)-\sin(\omega(2t_0-t_1))). \qquad (22)
\end{aligned}$$

Finally, we calculate the second order Magnus exponent term by integrating the previous expression with respect to $\mathrm{d}t_1$ over an evolution interval t_c, starting from t_0:

$$\begin{aligned}\frac{i}{t_c}\Omega_2(t_0+t_c,t_0) = &\frac{E(t_0)^2}{32\omega}\boldsymbol{\sigma}_z(1-2\cos(2\omega t_0)) \\ &+\frac{E_1 E(t_0)}{32\omega^2}\boldsymbol{\sigma}_z\left(\pi - 2\pi\cos(2\omega t_0) - 3\sin(2\omega t_0)\right) \\ &+\frac{E_1^2}{384\omega^3}\boldsymbol{\sigma}_z\left(3+4\pi^2+(18-6\pi^2)\cos(2\omega t_0)+18\pi\sin(2\omega t_0)\right).\end{aligned} \tag{23}$$

Direct calculation of the second order Magnus term using Daniel's scripts yields the same expression, which is comforting.

The first term of (23) represents the Bloch-Siegert shift and is the only term that survives for a constant drive with $E_1 = 0$. For $t_0 = kt_c$, we can understand the second term and the parts of third term that contain π^2 as the increase in Bloch-Siegert shift during the evolution interval t_c, similar to (8).

Noting that the expressions and integrals become increasingly complicated for higher order Magnus terms, we stop here with the manual integration and intuitive interpretation of the Magnus terms.

2. Impulse operators

The effective Hamiltonian generated from the Magnus expansion is applicable if the driving envelope is varied analytically. However, if the driving envelope experiences a non-analytical change, such as a sudden turn-on, an extra "impulse operator" is needed to describe the "jump" between the effective trajectory before and after the change. In this section we will work towards the development of such impulse operators.

2.1. Piecewise analytical driving envelopes

Once again, we start with a two-level system that is driven by a perpendicular ($\boldsymbol{\sigma}_x$) oscillating signal of frequency ω with a slowly (compared to ω) varying envelope $E(t)$. In the frame that rotates along with the driving frequency ω, the Hamiltonian is given by eq. (4) (for detuning $\Delta = 0$ and phase offset $\phi = 0$).

The stroboscopic Magnus trajectory, as defined in Section 1, approximates the evolution of a two-level system under perpendicular oscillating (frequency ω) drive by

2.2. Linear drive

References

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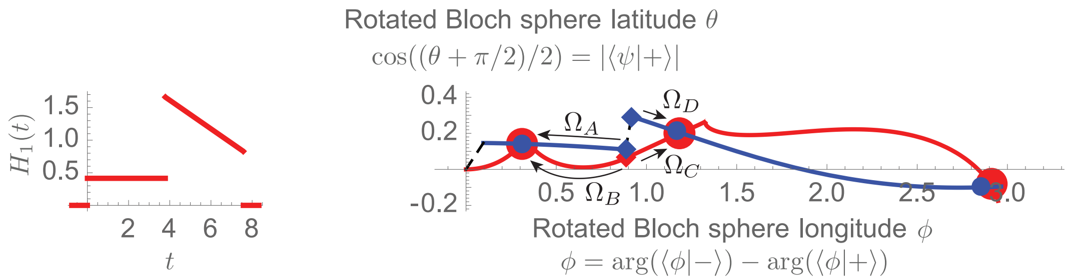

(a) | Piecewise analytical drive.

(b) | Trajectories.

Figure 2 | Effective Magnus trajectories under a piecewise analytical driving envelope. (a) | An exemplary piecewise analytical driving envelope is shown. This envelope, with a total pulse duration of $t_d = 7.57$, exhibits non-analyticities at $t = 0$ (turn-on time), $t = t_d/2$ and $t = t_d$ (turn-off time). The average drive strength over the total pulse duration is $\overline{H}_1 = 0.83$, such that the rotation induced by driving a two-level system with this particular pulse is $\theta_d = \overline{H}_1 t_d/2 = \pi$ in the rotating wave approximation. **(b)** | The evolution (red) of a system initially in the $|0\rangle$ state, driven by a sinusoidal signal with an envelope as given in Figure (a), is obtained through numerical integration. In addition, the stroboscopic Magnus trajectory of order $1/\omega^2$ (blue) is plotted. The actual and stroboscopic trajectories approximately coincide every $t_c = \pi/\omega$, starting at $t_0 = \alpha_0/\omega$ (red, blue dots). At each non-analytical point in the driving envelope, the stroboscopic trajectory shows a "jump". For the second discontinuity, at $t = t_d/2$, the corresponding point on each trajectory is indicated (diamond). Around this discontinuity, evolution operators along several sections of the actual and the stroboscopic trajectories are marked (Ω_i) and expanded upon in the main text. Relevant parameters are $\omega = 1$, $\alpha_0 = 1$.

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