

# Mølmer-Sørensen gate simulation

March 13, 2023

## 1 Goal

Derive the expression for simulating and optimizing a Mølmer-Sørensen gate pulse sequence.

## 2 Setup and scope

We'll discuss a simple two tone pulse sequence where the two tones are perfectly symmetric around the carrier. We'll ignore any error in the carrier frequency in this note. Crosstalk, coupling to carrier and other sideband orders are also ignored.

For a typical gate sequence, what we care about are

1. Ion motion:  
The MS interaction will drive each of the motional mode in a spin-dependent way. For a proper MS gate, we'd like the final motional state to be identical to where we started. Any deviation from this results in a closure error.
2. Spin operation:  
The enclosed area in phase-space from the driven motion results in a spin-dependent phase which is the main goal of the MS gate. Deviation in the control parameter could result in spin/angle error in the spin space.

## 3 Mølmer-Sørensen interaction

The effective Hamiltonian for a Mølmer-Sørensen gate sequence can be written as

$$H_{MS} = \frac{\Omega(t)}{2} \sum_{j=1,2} \sum_k \eta_{jk} \left( a_k e^{-i\theta_k(t)} + a_k^\dagger e^{i\theta_k(t)} \right) \sigma_x^j$$

where  $j$  is the ion index (simplified to 1 and 2) and  $k$  is the motional mode index. For the “fixed” parameters,  $\eta_{jk}$  is the Lamb-Dicke parameter for the  $j$ -th ion on the  $k$ -th mode.  $a_k$  and  $a_k^\dagger$  are the creation and annihilation operators for the  $k$ -th mode and the  $\sigma_x^j$  is the single qubit spin operator we are coupling to which we'll set as  $x$  in this note. (The error on the spin axis is ignored.) For the “variable” parameters in the pulse sequence,  $\Omega(t)$  is the time dependent two-photon Rabi frequency (controlled by laser power) and  $\theta_k(t)$  is the time-dependent phase offset between the laser and the  $k$ -th mode with,

$$\begin{aligned} \theta_k(t) &= \omega_k t - \theta(t) \\ &= \omega_k t - \int_0^t \delta(t') dt' \end{aligned}$$

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where  $\omega_k$  is the frequency of the  $k$ -th mode,  $\theta(t)$  is the half the phase difference of the two lasers and  $\delta(t')$  is the (symmetric) detuning of the lasers from the carrier. (If phase modulation is used,  $\theta(t)$  and  $\theta_k(t)$  may be discontinuous functions).

Using Magnus expansion, we can write down the unitary evolution of the system as

$$U_{MS}(\tau) = \exp \left[ \sum_{j=1,2} \sum_k \frac{\eta_{kj}}{2} \left( \alpha_k(\tau) a_k^\dagger - \alpha_k^*(\tau) a_k \right) \sigma_x^j \right] \exp(i\Theta(\tau) \sigma_x^1 \sigma_x^2)$$

where

$$\alpha_k(\tau) = \int_0^\tau \Omega(t) e^{i\theta_k(t)} dt$$

describes the displacement of the  $k$ -th mode, and

$$\Theta(\tau) = \frac{1}{2} \sum_k \eta_{k1} \eta_{k2} \int_0^\tau dt \int_0^t \Omega(t) \Omega(t') \sin(\theta_k(t) - \theta_k(t'))$$

is the angle of the two-qubit rotation. For a proper MS gate of length  $T$ , we need to have  $\alpha_k(T) = 0$  for all  $k$ s and the rotation angle at the end of the pulse  $\Theta(T)$  matching the angle we want.

For the purpose of optimization, the quantities we care about are.

1. Closure

$$\alpha_k(T) = \int_0^T \Omega(t) e^{i\theta_k(t)} dt$$

2. Gradient of closure w.r.t. mode frequencies

$$\begin{aligned} \frac{\partial \alpha_k(T)}{\partial \omega_k} &= \int_0^T \frac{\partial}{\partial \omega_k} \Omega(t) e^{i\theta_k(t)} dt \\ &= i \int_0^T \Omega(t) e^{i\theta_k(t)} \frac{\partial \theta_k(t)}{\partial \omega_k} dt \\ &= i \int_0^T \Omega(t) e^{i\theta_k(t)} t dt \end{aligned}$$

When closure is assumed, this can be re-written as,

$$\begin{aligned} \frac{\partial \alpha_k(T)}{\partial \omega_k} &= i \int_0^T \Omega(t) e^{i\theta_k(t)} t dt \\ &= i t \int_0^t \Omega(t') e^{i\theta_k(t')} dt' \Big|_0^T - i \int_0^T dt \int_0^t \Omega(t') e^{i\theta_k(t')} dt' \\ &= -i \int_0^T dt \int_0^t \Omega(t') e^{i\theta_k(t')} dt' \end{aligned}$$

which is proportional to average displacement. Moreover, if the pulse is symmetric, zeroing this value will also automatically zero the final displacement thus remove the need to optimize two values at the same time.

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3. Enclosed area

$$\begin{aligned}\mathcal{A}_k &= \text{Im} \left( \int_0^T dt \int_0^t dt' \Omega(t) \Omega(t') e^{i\theta_k(t) - i\theta_k(t')} \right) \\ &= \text{Im} \left( \int_0^T dt \Omega(t) e^{i\theta_k(t)} \int_0^t dt' \Omega(t') e^{-i\theta_k(t')} \right)\end{aligned}$$

4. Gradient of enclosed area w.r.t. mode frequencies

$$\frac{\partial \mathcal{A}_k}{\partial \omega_k} = \text{Re} \left( \int_0^T dt t \Omega(t) e^{i\theta_k(t)} \int_0^t dt' \Omega(t') e^{-i\theta_k(t')} - \int_0^T dt \Omega(t) e^{i\theta_k(t)} \int_0^t dt' t' \Omega(t') e^{-i\theta_k(t')} \right)$$

## 4 Segmented pulse

When parameterizing the pulse shape used to drive MS gate, the pulse is usually decomposed into a few segments (in time) and the pulse shape within each segment is only sensitive to few parameters. We can take advantage of this structure to reduce the computational complexity when optimizing for a large number of free parameters by only dealing with one segment (and therefore few parameters) at a time.

More specifically, during the optimization process, we care not only about the values listed above (closure, area, and their gradient w.r.t. mode frequency) but also their gradient w.r.t. the pulse shape parameters. By dealing with the effect of each segment properly, we can compute all the gradient within  $\mathcal{O}(N_p + N_s)$  instead of  $\mathcal{O}(N_p N_s)$ , where  $N_p$  is the number of parameters and  $N_s$  is the number of segments.

This is trivial to do for closure since it is a single integral and therefore is completely linear w.r.t. different segment of the integrand. The gradient of the integral on one segment is directly that on the final result and is independent of the functional form in any other segments.

The enclosed area, and the average displacement, is more complicated however, since they involve a double integral so the gradient of the integral within the segment is not the same as the effect on the final value. The change is still linear but does require a conversion factor caused by the later segments.

To calculate this, let's first consider a generic double integral

$$I = \int_0^T dt A(t) \int_0^t dt' B(t')$$

which should cover both cases we are interested above with the appropriate definition of the  $A$  and  $B$  functions.

Now let's assume that there are  $N_s$  segments. The  $n$ -th one starts at  $t_n$  and ends at  $t_{n+1}$  with

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$t_0 = 0$  and  $t_{N_s} = T$ .

$$\begin{aligned}
I &= \int_0^T dt A(t) \int_0^t dt' B(t') \\
&= \sum_{n=0}^{N_s-1} \int_{t_n}^{t_{n+1}} dt A(t) \int_0^t dt' B(t') \\
&= \sum_{n=0}^{N_s-1} \int_{t_n}^{t_{n+1}} dt A(t) \left( \sum_{n'=0}^{n-1} \int_{t_{n'}}^{t_{n'+1}} dt' B(t') + \int_{t_n}^t dt' B(t') \right) \\
&= \sum_{n=0}^{N_s-1} \sum_{n'=0}^{n-1} \int_{t_n}^{t_{n+1}} dt A(t) \int_{t_{n'}}^{t_{n'+1}} dt' B(t') + \sum_{n=0}^{N_s-1} \int_{t_n}^{t_{n+1}} dt A(t) \int_{t_n}^t dt' B(t') \\
&= \sum_{n=0}^{N_s-1} \sum_{n'=0}^{n-1} A_n B_{n'} + \sum_{n=0}^{N_s-1} C_n
\end{aligned}$$

where  $A_n \equiv \int_{t_n}^{t_{n+1}} A(t)dt$ ,  $B_n \equiv \int_{t_n}^{t_{n+1}} B(t)dt$ , and  $C_n \equiv \int_{t_n}^{t_{n+1}} dt A(t) \int_{t_n}^t dt' B(t')$ . All three of these values only depend on the value of the  $A$  and  $B$  functions within the corresponding segments and can be computed with  $\mathcal{O}(1)$  time. Moreover, by pre-computing the  $\sum_{n'=0}^{n-1} B_{n'}$  values ( $N_s - 1$  values in total), the two dimensional summation can be computed in  $\mathcal{O}(N_s)$  time and therefore the whole expression can be computed within  $\mathcal{O}(N_s)$  time.

As for the derivatives, the derivatives of  $A_n$ ,  $B_n$ ,  $C_n$  w.r.t. the corresponding parameters can be computed within  $\mathcal{O}(N_p)$  time. We then have

$$\begin{aligned}
\frac{\partial I}{\partial A_n} &= \sum_{n'=0}^{n-1} B_{n'} \\
\frac{\partial I}{\partial B_n} &= \sum_{n'=0}^{N_s-1} \sum_{n''=0}^{n'-1} A_{n'} \delta_{n,n''} \\
&= \sum_{n'=n+1}^{N_s-1} A_{n'} \\
\frac{\partial I}{\partial C_n} &= 1
\end{aligned}$$

which can be all computed within  $\mathcal{O}(N_s)$  time so the full set of all direvatives can be computed within  $\mathcal{O}(N_s + N_p)$  time.

#### 4.1 Segment evaluation

Let's limit the pulse shape we support within each segment to linear in terms of amplitude and phase (note that a linear phase ramp is a constant frequency shift, linear frequency ramp isn't currently supported). Under these assumptions, the most generic nontrivial form of  $A$  and  $B$  we need to deal with is

$$(a_0 t^2 + b_0 t + c_0) e^{i(\omega t + \varphi_0)}$$

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Combining  $A_i$ ,  $B_i$  and  $C_i$ , we actually care about the integral  $F_n(\omega, t) \equiv \int t^n e^{i\omega t} dt$  up to  $n = 4$  order (see below) (the phase factor  $\varphi_0$  is ignored since it's just a global multiplicity factor). From symbolic evaluation we have,

$$\begin{aligned}
F_0(\omega, t) &= \frac{-i}{\omega} e^{i\omega t} \\
F_1(\omega, t) &= \frac{-i\omega t + 1}{\omega^2} e^{i\omega t} \\
F_2(\omega, t) &= \frac{-i\omega^2 t^2 + 2\omega t + 2i}{\omega^3} e^{i\omega t} \\
F_3(\omega, t) &= \frac{-i\omega^3 t^3 + 3\omega^2 t^2 + 6i\omega t - 6}{\omega^4} e^{i\omega t} \\
F_4(\omega, t) &= \frac{-i\omega^4 t^4 + 4\omega^3 t^3 + 12i\omega t - 24\omega t - 24i}{\omega^5} e^{i\omega t}
\end{aligned}$$

We also have

$$\begin{aligned}
\frac{\partial F_n(\omega, t)}{\partial t} &= t^n e^{i\omega t} \\
\frac{\partial F_n(\omega, t)}{\partial \omega} &= i F_{n+1}(\omega, t)
\end{aligned}$$

For a pulse sequence where the amplitude and phase of the pulse are given by

$$\begin{aligned}
\Omega(t) &= \Omega_n + \Omega'_n(t - t_n) & (t_n \leq t < t_{n+1}) \\
\theta(t) &= \theta_n + \bar{\omega}_n(t - t_n) & (t_n \leq t < t_{n+1})
\end{aligned}$$

where  $\bar{\omega}_n$  is the motional drive frequency from the laser (half of red-blue sideband difference) during the  $n$ -th segment.

For closure, the shift within each segment is,

$$\begin{aligned}
\alpha_k^n &\equiv \int_{t_n}^{t_{n+1}} \Omega(t) e^{i\theta_k(t)} dt \\
&= \int_{t_n}^{t_{n+1}} (\Omega_n + \Omega'_n(t - t_n)) e^{i(\omega_k t - \theta_n - \bar{\omega}_n(t - t_n))} dt \\
&= \int_0^{\tau_n} (\Omega_n + \Omega'_n t) e^{i(\omega_k t + \varphi_k^n - \bar{\omega}_n t)} dt \\
&= e^{i\varphi_k^n} (\Omega_n F_0(\delta_k^n, \tau_n) + \Omega'_n F_1(\delta_k^n, \tau_n) - \Omega_n F_0(\delta_k^n, 0) - \Omega'_n F_1(\delta_k^n, 0)) \\
&= \frac{e^{i\varphi_k^n}}{\delta_k^{n2}} \left( (-i\Omega_n \delta_k^n + \Omega'_n) (e^{i\delta_k^n \tau_n} - 1) - i\Omega'_n \delta_k^n \tau_n e^{i\delta_k^n \tau_n} \right) \\
&= e^{i\varphi_k^n} \left( \Omega'_n \tau_n^2 \frac{\cos(\delta_k^n \tau_n) - 1}{\delta_k^{n2} \tau_n^2} + (\Omega_n \tau_n + \Omega'_n \tau_n^2) \frac{\sin(\delta_k^n \tau_n)}{\delta_k^n \tau_n} \right)
\end{aligned}$$

where  $\tau_n \equiv t_{n+1} - t_n$  is the length of the  $n$ -th segment,  $\delta_k^n \equiv \omega_k - \bar{\omega}_n$  is the detuning of the  $n$ -th segment from the  $k$ -th mode,  $\varphi_k^n \equiv \omega_k t_n - \theta_n$  is the initial phase difference with the  $k$ -th mode at the beginning of the  $n$ -th segment.

We can further transform this into a form that is easier to evaluate around  $\delta_k^n = 0$ ,

$$\begin{aligned}
\alpha_k^n &= e^{i\varphi_k^n} \left( \Omega'_n \tau_n^2 \frac{\cos(\delta_k^n \tau_n) - 1}{\delta_k^{n2} \tau_n^2} + (\Omega_n \tau_n + \Omega'_n \tau_n^2) \frac{\sin(\delta_k^n \tau_n)}{\delta_k^n \tau_n} \right. \\
&\quad \left. - i\Omega_n \delta_k^n \tau_n^2 \frac{\cos(\delta_k^n \tau_n) - 1}{\delta_k^{n2} \tau_n^2} - i\Omega'_n \tau_n^2 \frac{\delta_k^n \tau_n \cos(\delta_k^n \tau_n) - \sin(\delta_k^n \tau_n)}{\delta_k^{n2} \tau_n^2} \right) \\
&= e^{i\varphi_k^n} \left( (i\Omega_n \delta_k^n \tau_n^2 - \Omega'_n \tau_n^2) \frac{1 - \cos(\delta_k^n \tau_n)}{\delta_k^{n2} \tau_n^2} \right. \\
&\quad \left. + (\Omega_n \tau_n + \Omega'_n \tau_n^2) \text{sinc}(\delta_k^n \tau_n) - i\Omega'_n \tau_n^2 \text{cosec}(\delta_k^n \tau_n) \right)
\end{aligned}$$

The final closure is the sum of the value within each segment,

$$\alpha_k(T) = \sum_{n=0}^{N_s-1} \alpha_k^n$$

For the average displacement, the  $A_n$  terms are simply  $\tau_n$  and the  $B_n$  terms are  $\alpha_k^n$ . The  $C_n$  terms has to be computed,

$$\begin{aligned}
\bar{\alpha}_k^n &= \int_{t_n}^{t_{n+1}} dt \int_{t_n}^t dt' \Omega(t') e^{i\theta_k(t')} \\
&= \int_0^{\tau_n} dt \int_{t_n}^{t_n+t} dt' (\Omega_n + \Omega'_n(t' - t_n)) e^{i(\omega_k t' - \theta_n - \bar{\omega}_n(t' - t_n))} \\
&= e^{i\varphi_k^n} \int_0^{\tau_n} dt \int_0^t dt' (\Omega_n + \Omega'_n t') e^{i\delta_k^n t'} \\
&= \frac{e^{i\varphi_k^n}}{\delta_k^{n2}} \int_0^{\tau_n} dt \left( (\Omega'_n - i\Omega_n \delta_k^n - i\Omega'_n \delta_k^n t) e^{i\delta_k^n t} - (\Omega'_n - i\Omega_n \delta_k^n) \right) \\
&= \frac{e^{i\varphi_k^n}}{\delta_k^{n2}} \left( (\Omega'_n - i\Omega_n \delta_k^n) F_0(\delta_k^n, \tau_n) - i\Omega'_n \delta_k^n F_1(\delta_k^n, \tau_n) \right. \\
&\quad \left. - (\Omega'_n - i\Omega_n \delta_k^n) F_0(\delta_k^n, 0) + i\Omega'_n \delta_k^n F_1(\delta_k^n, 0) - (\Omega'_n - i\Omega_n \delta_k^n) \tau_n \right) \\
&= \frac{e^{i\varphi_k^n}}{\delta_k^{n2}} \left( \frac{-\Omega_n \delta_k^n - 2i\Omega'_n}{\delta_k^n} (e^{i\delta_k^n \tau_n} - 1) - \Omega'_n \tau_n e^{i\delta_k^n \tau_n} - (\Omega'_n - i\Omega_n \delta_k^n) \tau_n \right)
\end{aligned}$$

Again, for an better expression around  $\delta_k^n = 0$ ,

$$\begin{aligned}
\bar{\alpha}_k^n &= \frac{e^{i\varphi_k^n}}{\delta_k^{n2}} \left( -\Omega_n (\cos(\delta_k^n \tau_n) - 1) + \frac{2\Omega'_n \sin(\delta_k^n \tau_n)}{\delta_k^n} - \Omega'_n \tau_n \cos(\delta_k^n \tau_n) - \Omega'_n \tau_n \right. \\
&\quad \left. - i\Omega_n \sin(\delta_k^n \tau_n) - 2i \frac{\Omega'_n (\cos(\delta_k^n \tau_n) - 1)}{\delta_k^n} - i\Omega'_n \tau_n \sin(\delta_k^n \tau_n) + i\Omega_n \delta_k^n \tau_n \right) \\
&= e^{i\varphi_k^n} \tau_n \left( \Omega_n \tau_n \frac{1 - \cos(\delta_k^n \tau_n)}{\delta_k^{n2} \tau_n^2} + \Omega'_n \tau_n^2 \frac{2 \sin(\delta_k^n \tau_n) - \delta_k^n \tau_n \cos(\delta_k^n \tau_n) - \delta_k^n \tau_n}{\delta_k^{n3} \tau_n^3} \right. \\
&\quad \left. + i\Omega_n \tau_n \frac{\delta_k^n \tau_n - \sin(\delta_k^n \tau_n)}{\delta_k^{n2} \tau_n^2} - i\Omega'_n \tau_n^2 \frac{2 \cos(\delta_k^n \tau_n) - 2 + \delta_k^n \tau_n \sin(\delta_k^n \tau_n)}{\delta_k^{n3} \tau_n^3} \right)
\end{aligned}$$

For the enclosed area, the  $A_n$  and  $B_n$  terms are both the  $\alpha_k^n$  computed above. The  $C_n$  terms,

$$\begin{aligned}
\gamma_k^n &= \int_{t_n}^{t_{n+1}} dt \Omega(t) e^{i\theta_k(t)} \int_{t_n}^t dt' \Omega(t') e^{-i\theta_k(t')} \\
&= \int_{t_n}^{t_{n+1}} dt (\Omega_n + \Omega'_n(t - t_n)) e^{i(\omega_k t - \theta_n - \bar{\omega}_n(t - t_n))} \int_{t_n}^t dt' (\Omega_n + \Omega'_n(t' - t_n)) e^{-i(\omega_k t' - \theta_n - \bar{\omega}_n(t' - t_n))} \\
&= \int_0^{\tau_n} dt (\Omega_n + \Omega'_n t) e^{i\delta_k^n t} \int_0^t dt' (\Omega_n + \Omega'_n t') e^{-i\delta_k^n t'} \\
&= \int_0^{\tau_n} dt (\Omega_n + \Omega'_n t) e^{i\delta_k^n t} \left( \left( \frac{\Omega'_n + i\Omega_n \delta_k^n}{\delta_k^{n2}} + i \frac{\Omega'_n t}{\delta_k^n} \right) e^{-i\delta_k^n t} - \frac{\Omega'_n + i\Omega_n \delta_k^n}{\delta_k^{n2}} \right) \\
&= \frac{1}{\delta_k^{n2}} \int_0^{\tau_n} dt \left( (\Omega'_n + i\Omega_n \delta_k^n) \Omega_n + (\Omega'_n + 2i\Omega_n \delta_k^n) \Omega'_n t + i\Omega_n'^2 \delta_k^{n2} t^2 - (\Omega'_n + i\Omega_n \delta_k^n) (\Omega_n + \Omega'_n t) e^{i\delta_k^n t} \right) \\
&= \frac{1}{\delta_k^{n2}} \left( (\Omega'_n + i\Omega_n \delta_k^n) \Omega_n \tau_n + \frac{1}{2} (\Omega'_n + 2i\Omega_n \delta_k^n) \Omega'_n \tau_n^2 + \frac{1}{3} i\Omega_n'^2 \delta_k^{n2} \tau_n^3 \right. \\
&\quad \left. - (\Omega'_n + i\Omega_n \delta_k^n) \Omega_n (F_0(\delta_k^n, \tau_n) - F_0(\delta_k^n, 0)) - (\Omega'_n + i\Omega_n \delta_k^n) \Omega'_n (F_1(\delta_k^n, \tau_n) - F_1(\delta_k^n, 0)) \right) \\
&= \frac{1}{\delta_k^{n2}} \left( (\Omega'_n + i\Omega_n \delta_k^n) \Omega_n \tau_n + \frac{1}{2} (\Omega'_n + 2i\Omega_n \delta_k^n) \Omega'_n \tau_n^2 + \frac{1}{3} i\Omega_n'^2 \delta_k^{n2} \tau_n^3 \right. \\
&\quad \left. + \frac{i}{\delta_k^n} (\Omega'_n + i\Omega_n \delta_k^n) \Omega_n (e^{i\delta_k^n \tau_n} - 1) - (\Omega'_n + i\Omega_n \delta_k^n) \Omega'_n \left( \frac{-i\delta_k^n \tau_n + 1}{\delta_k^{n2}} e^{i\delta_k^n \tau_n} - \frac{1}{\delta_k^{n2}} \right) \right) \\
&= \frac{1}{\delta_k^{n2}} \left( (\Omega'_n + i\Omega_n \delta_k^n) \Omega_n \tau_n + \frac{1}{2} (\Omega'_n + 2i\Omega_n \delta_k^n) \Omega'_n \tau_n^2 + \frac{1}{3} i\Omega_n'^2 \delta_k^{n2} \tau_n^3 \right. \\
&\quad \left. - \frac{1}{\delta_k^{n2}} (\Omega_n^2 \delta_k^{n2} + \Omega_n'^2) (e^{i\delta_k^n \tau_n} - 1) + i(\Omega'_n + i\Omega_n \delta_k^n) \frac{\Omega'_n \tau_n}{\delta_k^n} e^{i\delta_k^n \tau_n} \right)
\end{aligned}$$