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January 13, 2025

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The harmony of the world is made manifest in Form and Number, and the heart and soul and all the poetry of Natural Philosophy are embodied in the concept of mathematical beauty.

– D’Arcy Wentworth Thompson

Contents

Publications

[1] Yaiza Aragonés-Soria, René Otten, Tobias Hangleiter, Pascal Cerfontaine, and David Gross. "Minimising Statistical Errors in Calibration of Quantum-Gate Sets." June 7, 2022. DOI: 10.48550/arXiv.2206.03417. (Visited on 06/08/2022). Pre-published.

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Software

The following open-source software packages were developed (at least partially) during the work on this thesis.

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A Python Welch's-method Spectrometer

Characterization and Improvements of a Millikelvin Confocal Microscope

Electrostatic Trapping of Excitons in Semiconductor Membranes

A Filter-Function Formalism For Quantum Operations

Parts of the results presented in this part have been published in Refs. 1 and 2. In Ref. 2, extensive use was made of Kubo's *cumulant expansion*. Due to an error in Kubo's paper which was only pointed out several years later [4] and the authors were not aware of, those results turned out to be not exact as claimed but approximate [5]. We investigate the accuracy of the expansion in Chapter 2.

[4]: Fox (1976), *Critique of the Generalized Cumulant Expansion Method*

[5]: Hangleiter, Cerfontaine, and Bluhm (2024), *Erratum: Filter-function Formalism and Software Package to Compute Quantum Processes of Gate Sequences for Classical Non-Markovian Noise [Phys. Rev. Research 3, 043047 (2021)]*

Monte Carlo and Lindblad master equation simulations 1

1.1 Validation of QFT fidelities

In this section, we perform Lindblad master equation and Monte Carlo simulations to verify the fidelities predicted for the QFT circuit in the main text. We focus on noise exclusively on the third qubit, entering through the noise operator $B_\alpha \equiv \sigma_y^{(3)}$.

To validate the fidelity for white noise, we use a Lindblad master equation [6, 7] in superoperator form. We represent linear maps $\mathscr{A} : \rho \to \mathscr{A}(\rho)$ by matrices in the Pauli transfer matrix representation as (see Ref. 2 for more details)

$$\mathscr{A}_{ij} := \operatorname{tr}\big(\sigma_i \mathscr{A}(\sigma_j)\big) \tag{1.1}$$

and operators as column vectors (*i. e.* generalized Bloch vectors) as

$$\rho_i := \operatorname{tr}(\sigma_i \rho), \tag{1.2}$$

allowing us to write the Lindblad equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\mathrm{i}[H(t), \rho(t)] + \sum_\alpha \gamma_\alpha \left(L_\alpha \rho(t) L_\alpha^\dagger - \frac{1}{2}\left\{ L_\alpha^\dagger L_\alpha, \rho(t) \right\} \right) \tag{1.3}$$

as a linear differential equation in matrix form,

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_i(t) = \sum_j \left(-\mathrm{i}\mathscr{H}_{ij}(t) + \sum_\alpha \gamma_\alpha \mathscr{D}_{\alpha,ij} \right) \rho_j(t). \tag{1.4}$$

Here, $\mathscr{H}_{ij}(t) = \operatorname{tr}\big(\sigma_i \big[H(t), \sigma_j\big]\big)$ and $\mathscr{D}_{\alpha,ij} = \operatorname{tr}\Big(\sigma_i L_\alpha \sigma_j L_\alpha^\dagger - \frac{1}{2}\sigma_i \big\{ L_\alpha^\dagger L_\alpha, \sigma_j \big\}\Big)$. By setting $L_\alpha \equiv \sigma_y^{(3)}$ as well as $\gamma_\alpha \equiv S_0/2$ with S_0 the amplitude of the one-sided noise power spectral density (PSD) so that $S(\omega) = S_0$, we can compare the fidelity obtained from the filter functions to that from the explicit simulation of Equation 1.4. The latter is computed as $F_{\mathrm{avg}} = 1/d^2 \operatorname{tr}\big(\mathscr{Q}^\dagger \mathscr{U}\big)$, where $\mathscr{Q}$ is the superpropagator due to the Hamiltonian evolution alone (*i. e.* the ideal evolution without noise).

For the Monte Carlo simulation, we explicitly generate time traces of $b_Q(t)$ (c.f. **??**) by drawing pseudo-random variables from a distribution whose PSD is $S(f) = S_0/f$. To do this, we draw complex, normally distributed samples in frequency space (*i. e.* white noise), scale it with the square root of the PSD, and finally perform the inverse Fourier transform. We choose an oversampling factor of 16, so that the time discretization of the simulation is $\Delta t_{\mathrm{MC}} = \Delta t/16 = 62.5\,\mathrm{ps}$ ($\Delta t = 1\,\mathrm{ns}$ is the time step of the pulses used in the FF simulation), leading to a highest resolvable frequency of $f_{\max} = 16\,\mathrm{GHz}$. Conversely, we increase the frequency resolution by sampling a time trace longer by a given factor, giving frequencies below $f_{\min}$ (16 kHz for pink, 0 Hz for white noise) weight zero, and truncating it to the number of time steps in the algorithm times the oversampling factor. This yields a time trace with frequencies $f \in [f_{\min}, f_{\max}]$ and a given resolution (we choose $\Delta f = 160\,\mathrm{Hz}$).

We then proceed to diagonalize the Hamiltonian $H(t) = H_c(t) + H_n(t)$ and compute the propagator for one noise realization as

$$U(t) = \prod_g V^{(g)} \exp\{-\mathrm{i}\Omega^{(g)}\Delta t_{\mathrm{MC}}\} V^{(g)\dagger}, \tag{1.5}$$

where $V^{(g)}$ is the unitary matrix of eigenvectors of $H(t)$ during time segment g and $\Omega^{(g)}$ the diagonal matrix of eigenvalues. Finally, we obtain an estimate for the average gate fidelity F_{avg} from the entanglement fidelity F_{e} as

$$\left\langle F_{\mathrm{avg}} \right\rangle = \left\langle \frac{dF_{\mathrm{e}} + 1}{d+1} \right\rangle = \left\langle \frac{\left|\mathrm{tr}\left(Q^\dagger U(\tau)\right)\right|^2 + d}{d(d+1)} \right\rangle. \tag{1.6}$$

Here, $Q \equiv U_{\mathrm{c}}(t = \tau)$ is the noise-free propagator at time τ of completion of the circuit and $\langle\cdot\rangle$ denotes the ensemble average over N Monte Carlo realizations of Equation 1.5, *i. e.*, $\langle A \rangle = \frac{1}{N}\sum_{i=1}^N A_i$. The standard error of the mean can be obtained as $\sigma_{\langle F_{\mathrm{avg}}\rangle} = \sigma_{F_{\mathrm{avg}}}/\sqrt{N}$ with $\sigma_{F_{\mathrm{avg}}}$ the standard deviation over the Monte Carlo traces.

2 Reconstruction by frequency-comb time-domain simulation

For a given interaction-picture quantum operation $\tilde{\mathcal{U}}$ resulting from the quantum system's evolution under the noise fully characterized by its one-sided power spectral density (PSD) $S(\omega)$, we define the filter function (FF) $\mathcal{F}(\omega;\tau)$ by

$$\tilde{\mathcal{U}}(\tau) = \exp\left\{-\int\frac{\mathrm{d}\omega}{2\pi}\mathcal{F}(\omega;\tau)S(\omega)\right\}. \tag{2.1}$$

Now, suppose that

$$S(\omega) = 2\pi\sigma_i^2\delta(\omega-\omega_i) =: S_i(\omega), \tag{2.2}$$

that is, the PSD of a monochromatic sinusoid of frequency ω_i and root mean square (RMS) σ_i. Then Equation 2.1 becomes

find factor 2π

Equation 2.2 discretizes $S(\omega)$ by sampling it at points ω_i, *i. e.*,

$$S(\omega) \sim \lim_{n\to\infty}\sum_{i=1}^{n} S_i(\omega).$$

$$\begin{aligned}\tilde{\mathcal{U}}_i(\tau) &= \exp\left\{-2\pi\sigma_i^2\int\frac{\mathrm{d}\omega}{2\pi}\mathcal{F}(\omega;\tau)\delta(\omega-\omega_i)\right\} \\ &= \exp\left\{-\sigma_i^2\mathcal{F}(\omega_i;\tau)\right\},\end{aligned} \tag{2.3}$$

where $\tilde{\mathcal{U}}_i(\tau)$ is the noisy quantum operation generated by monochromatic noise with PSD $S_i(\omega)$ according to Equation 2.2. It is now easy to invert Equation 2.3, and we obtain

$$\mathcal{F}(\omega_i;\tau) = -\sigma_i^{-2}\log\tilde{\mathcal{U}}_i(\tau). \tag{2.4}$$

Because we represent quantum operations as matrices in Liouville space, Equation 2.4 is easy to implement on a computer; to sample the exact FF at the set of discrete frequencies $\{\omega_i\}_i$ we simply need to compute $\tilde{\mathcal{U}}_i(\tau)$ using a time-domain simulation method of our choice and take the logarithm![1]

1: A similar approach was pursued by Geck in her PhD thesis to compare gate fidelities [8].

Indeed, we can go a step further and split apart the coherent and incoherent contributions to the noisy evolution. Since (in-)coherent quantum operations are represented by (anti-)symmetric matrices in Liouville space, we may define the incoherent and coherent FFs by

$$\begin{aligned}\mathcal{F}_\Gamma(\omega_i;\tau) &= \frac{1}{2}\left(\mathcal{F}(\omega_i;\tau)+\mathcal{F}(\omega_i;\tau)^\top\right) \\ &= \frac{1}{2\sigma_i^2}\left(\log\tilde{\mathcal{U}}_i(\tau)+\log\tilde{\mathcal{U}}_i(\tau)^\top\right),\end{aligned} \tag{2.5}$$

and

$$\begin{aligned}\mathcal{F}_\Delta(\omega_i;\tau) &= \frac{1}{2}\left(\mathcal{F}(\omega_i;\tau)-\mathcal{F}(\omega_i;\tau)^\top\right) \\ &= \frac{1}{2\sigma_i^2}\left(\log\tilde{\mathcal{U}}_i(\tau)-\log\tilde{\mathcal{U}}_i(\tau)^\top\right),\end{aligned} \tag{2.6}$$

respectively. This allows us to analyze in detail deviations of the closed-form expression obtained by means of the cumulant expansion , from the exact filter functions given by Equations 2.5 and 2.6. In the following, I will lay out explicitly how these can be computed in the time domain.

ref

To begin with, observe that from a Monte Carlo (MC) point of view, $\tilde{\mathcal{U}}$ is given by

$$\tilde{\mathcal{U}}(\tau) \equiv \left\langle \tilde{\mathcal{U}}_i(\tau) \right\rangle = \mathcal{Q}^\mathsf{T} \left\langle \mathcal{U}_i(\tau) \right\rangle, \tag{2.7}$$

where $\mathcal{U}_i(\tau)$ is the solution of the Schrödinger equation for a single realization of the noise and $\langle \cdot \rangle$ denotes the ensemble average. Inserting into Equation 2.3, we find

$$\begin{aligned} \mathcal{F}(\omega_i;\tau) =& \sigma_i^{-2} \log \left\langle \tilde{\mathcal{U}}_i(\tau) \right\rangle \\ =& \sigma_i^{-2} \log \mathcal{Q}^\mathsf{T} \left\langle \mathcal{U}_i(\tau) \right\rangle. \end{aligned} \tag{2.8}$$

For N realizations of the stochastic process underlying $b(t)$, the ensemble average of a quantity $A(t)$ that is a function of $b(t)$ is given by

$$\langle A \rangle (t) = \frac{1}{N} \sum_{i=1}^{N} A_i(t)$$

where i enumerates the realizations of the stochastic process. The relative error of this average scales as $N^{-1/2}$.

If we evaluate Equation 2.8 for a set of frequencies $\{\omega_i\}_i$ sampling the true spectrum $S(\omega)$ sufficiently well, we thus obtain the exact filter function $\mathcal{F}(\omega;\tau)$ (within the accuracy of MC), allowing us to compare the accuracy of the formalism developed in.

ref

So what does a single noise realization of Equation 2.2 in the time domain look like? It's a sinusoid with amplitude $A_i \sim \mathrm{Rayleigh}(\sigma_i)$,[2] frequency ω_i, and phase $\phi \sim U(0, 2\pi)$,[3]

tikz sketch?

$$b(t) = A_i \sin(\omega_i t + \phi). \tag{2.9}$$

Instead of taking the random sampling approach of MC, we can also compute the expectation value of $\mathcal{U}_i(t)$ over A_i and ϕ by integrating over the probability density functions,[4]

$$\mathbb{E}_{A_i,\phi}[\mathcal{U}] = \int \mathrm{d}x\, \rho_{A_i}(x) \int \mathrm{d}y\, \rho_\phi(y) \mathcal{U}[x,y], \tag{2.10}$$

where we wrote $\mathcal{U}[x,y]$ for the Liouville representation of the MC propagator for single x and y drawn from their respective distributions. Whether we choose the MC method or direct integration, in practice Equation 2.10 will be evaluated numerically, either by drawing random samples from the distributions $\mathrm{Rice}(0,\sigma_i)$ and $U(0,2\pi)$ or by discretizing Equation 2.10.

2: $\mathrm{Rayleigh}(\sigma)$ is the Rayleigh distribution with probability density function [**RayleighDistributionWiki**]

$$\rho(x) = \frac{x}{\sigma^2} \exp\left\{-\frac{x^2}{2\sigma^2}\right\}.$$

It describes the probability distribution of the distance from the origin of a point drawn from a bivariate normal distribution with mean 0 and standard deviation σ.

3: The probability density function of the uniform distribution $U(a,b)$ is

$$\rho(y) = \begin{cases} (b-a)^{-1} & \text{if} \quad a \le y < b, \\ 0 & \text{else} \end{cases}$$

4: We write the expectation value of an observable A with respect to a random variable X with the probability density function ρ_X as $\mathbb{E}_X[A]$.

Appendix

Filter Functions A

A.1 Second-order concatenation

In this appendix, I lay out how the second-order filter functions of atomic pulse segments can be re-used to compute the filter function of the concatenated sequence. While it is not possible, due to the nested time integral, to perform the calculation entirely without concern for the internal structure of the individual segments, it is also not necessary to compute everything from scratch.

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Special Terms

F

FF filter function. 8

M

MC Monte Carlo. 8, 9

P

PSD power spectral density. 8

R

RMS root mean square. 8