Optimal calibration of qubit detuning and crosstalk

Supplemental Materials

SM1. NUMBER OF SHOTS PER MEASUREMENT TIME

In this work, we use the Fisher information to establish the optimal strategy to perform a Ramsey interference experiment. To find this strategy, we assume that the measurement scheme includes N_{times} measurements at times $T = (t_1, ..., t_{N_{\text{times}}})$, each with a different number of shots $S = (s_1, ..., s_{N_{\text{times}}})$. We then optimize the Cramér-Rao bound (CRB) with respect to both T and S, while keeping a total number of shots $\sum_i s_i = N_{\text{tot}}$. Finally, we inspect the final result and, whenever two times are closer than an arbitrarily small margin, we merge them into a single time.

Algorithm 1 Optimal Allocation of Measurement Times and Shots

Require: Maximal number of measurement times N_{times} (default $N_T = 10$)
Require: Total shots N_{tot} (default 1000)
Require: Merge tolerance δ (default 0.01)
Ensure: Optimised times and shots $(\widehat{T}, \widehat{S})$

1: **Optimise:** $(\widehat{T}, \widehat{S}) = \arg\min_{\{t_i, s_i\}} \big[\, \mathrm{CRB}_\omega(T,S) + \mathrm{CRB}_\gamma(T,S) \big]$
   s.t. $\sum_i s_i = N_{\text{tot}},\ s_i \in \mathbb{N}_{\geq 0},\ t_i > 0$
2: **Group:** merge any two times with $|t_i - t_j| < \delta$
   by $(t_i, t_j) \longrightarrow \big((t_i + t_j)/2\big)$ and $(s_i, s_j) \longrightarrow s_i + s_j$.
3: **return** $(\widehat{T}, \widehat{S})$

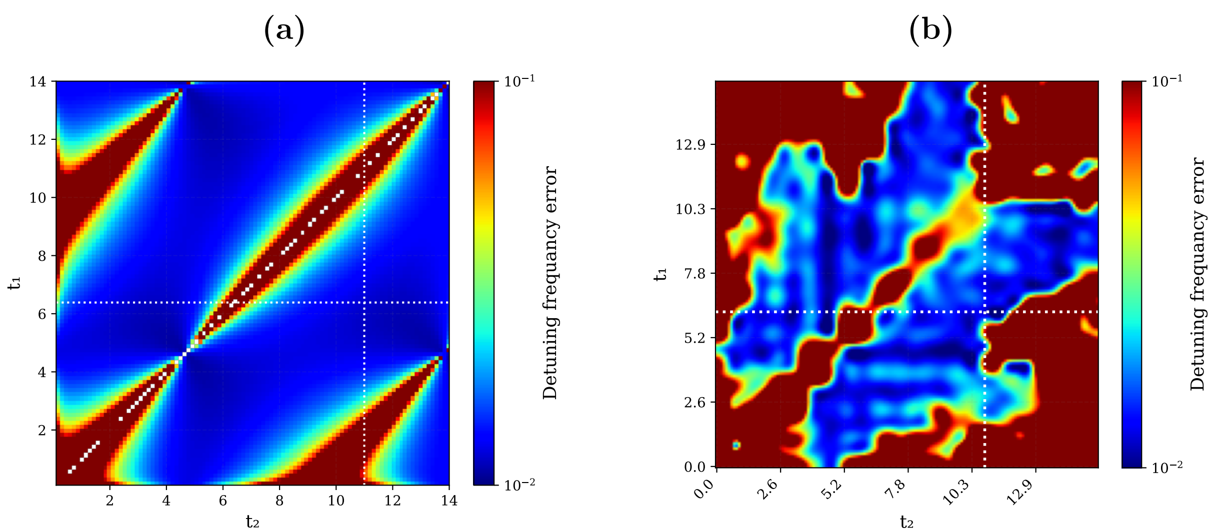

FIG. 1. Cramér-Rao bound as a function of the measurement times in (a) the theoretical calculation and (b) IQCC experiment (IQCC), for $\omega = 0.34$ and $\gamma = 0.135$. The dashed lines denote the optimal times.

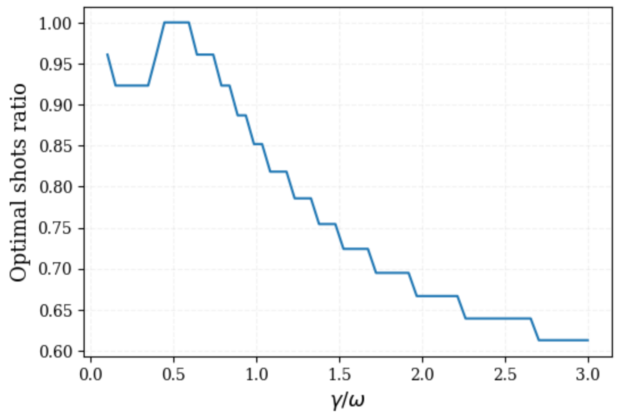

FIG. 2. Ratio of the number of shots between the first and second measurements, as a function of γ/ω. The discrete steps are related to the total number of measurements used in the optimization algorithm: the curve becomes continuous for $N_{\text{shots}} \to \infty$.

In all cases we considered, the algorithm converged to two measurement times only, consistently with the number of free parameters in the theoretical result (see Fig. 1 for an example). In contrast, the number of shots in each measurement depended on ω and γ. Figure 2 shows the ratio of the number of measurements between the first and second time as a function of γ/ω. The ratio changes from approximately one for $\gamma < \omega$ to 0.6 for $\gamma = 3\omega$. Intuitively, for large values of γ, later times provide less information about the system, and are probed with a smaller number of shots. To simplify our presentation, in the main text, we fixed this ratio to 1, such that both times are measured with the same number of shots.

SM2. DERIVATION OF EQ. (5) FOR THE CRAMÉR-RAO BOUND IN THE GAUSSIAN APPROXIMATION.

Under the Gaussian approximation, the result of each measurement is given by the normal distribution

$$x_n \sim \mathcal{N}\big(\langle X(t_n)\rangle\,,\,\sigma^2\big). \tag{1}$$

In this case, the likelihood and log-likelihood functions are respectively defined by

$$L(\boldsymbol{\theta}) = \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \, \exp\Big[-\tfrac{\left(x_n - \langle X(t_n)\rangle\right)^2}{2\sigma^2}\Big] \tag{2}$$

$$= (2\pi\sigma^2)^{-N/2} \, \exp\Big[-\frac{1}{2\sigma^2} \sum_{n=1}^{N} \big(x_n - \langle X(t_n)\rangle\big)^2\Big] \tag{3}$$

and

$$\ell(\boldsymbol{\theta}) = \ln L(\boldsymbol{\theta}) = -\frac{N}{2} \ln\!\big(2\pi\sigma^2\big) - \frac{1}{2\sigma^2} \sum_{n=1}^{N} \big(x_n - \langle X(t_n)\rangle\big)^2. \tag{4}$$

By differentiating l with respect to the fit parameters θ_i, we obtain

$$\frac{\partial \ell}{\partial \theta_j} = \frac{1}{\sigma^2} \sum_{n=1}^{N} \big(x_n - \langle X(t_n)\rangle\big) \, \frac{\partial \langle X(t_n)\rangle}{\partial \theta_j}. \tag{5}$$

By definition, the Fisher information is given by

$$\mathcal{I}_{jk}(\boldsymbol{\theta}) = \mathbb{E}\Big[\frac{\partial \ell}{\partial \theta_j} \, \frac{\partial \ell}{\partial \theta_k}\Big] \tag{6}$$

and equals

$$\mathcal{I}_{jk}(\boldsymbol{\theta}) = \frac{1}{\sigma^4} \sum_{n=1}^{N} \sum_{m=1}^{N} \underbrace{\mathbb{E}\big[\big(x_n - \langle X(t_n)\rangle\big)\big(x_m - \langle X(t_m)\rangle\big)\big]}_{\sigma^2 \, \delta_{nm}} \, \frac{\partial \langle X(t_n)\rangle}{\partial \theta_j} \, \frac{\partial \langle X(t_m)\rangle}{\partial \theta_k} \tag{7}$$

$$= \frac{1}{\sigma^4} \sum_{n=1}^{N} \sigma^2 \, \frac{\partial \langle X(t_n)\rangle}{\partial \theta_j} \, \frac{\partial \langle X(t_n)\rangle}{\partial \theta_k} \tag{8}$$

$$= \frac{1}{\sigma^2} \sum_{n=1}^{N} \frac{\partial \langle X(t_n)\rangle}{\partial \theta_j} \, \frac{\partial \langle X(t_n)\rangle}{\partial \theta_k}. \tag{9}$$

SM3. RAW DATA FROM EXPERIMENTAL SYSTEMS

To benchmark our optimization strategies, we performed Ramsey-interference measurements on a superconducting transmon and an NV centre. Fig. 3 shows representative raw traces together with damped-cosine fits, from which we extract the “true” parameters used

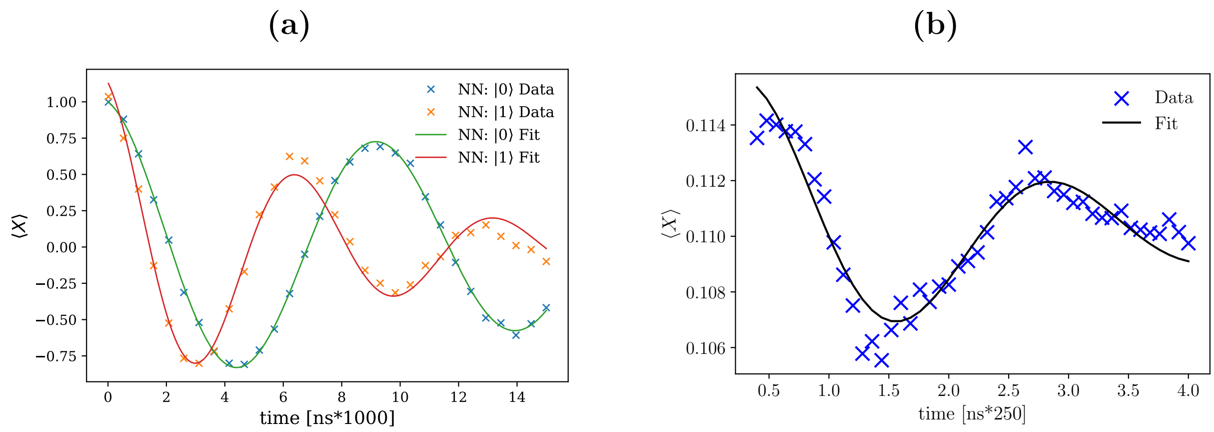

FIG. 3. Raw Ramsey-interference data (crosses) and least-squares fits to $A\cos(\omega t+\phi)\,e^{-\gamma t}+c$ (solid lines). **(a)** Superconducting circuit: $\langle X\rangle$ vs. time[ns$\times$1000] for a target qubit whose nearest neighbour (NN) is prepared in $|0\rangle$ (blue/green) or $|1\rangle$ (orange/red), revealing a state-dependent frequency shift (crosstalk). **(b)** NV centre: $\langle X\rangle$ vs. time[ns$\times$250]. The extracted fit parameters serve as ground truth for error estimation.

to compare estimation errors.

SM4. OPTIMAL MEASUREMENT TIME FOR THE X, Y STRATEGY

In the case of measuring X and Y at a single time, one can find the optimal time analytically:

$$\mathcal{I}_{\omega\omega}=\frac{1}{\sigma^2}\Big[\big(-t\,e^{-\gamma t}\sin(\omega t)\big)^2+\big(-t\,e^{-\gamma t}\cos(\omega t)\big)^2\Big]=\frac{t^2e^{-2\gamma t}}{\sigma^2}\big[\sin^2(\omega t)+\cos^2(\omega t)\big]=\frac{t^2e^{-2\gamma t}}{\sigma^2}, \tag{10}$$

$$\mathcal{I}_{\gamma\gamma}=\frac{1}{\sigma^2}\Big[\big(-t\,e^{-\gamma t}\cos(\omega t)\big)^2+\big(t\,e^{-\gamma t}\sin(\omega t)\big)^2\Big]=\frac{t^2e^{-2\gamma t}}{\sigma^2}\big[\cos^2(\omega t)+\sin^2(\omega t)\big]=\frac{t^2e^{-2\gamma t}}{\sigma^2}, \tag{11}$$

$$\mathcal{I}_{\omega\gamma}=\frac{1}{\sigma^2}\Big[\big(-t\,e^{-\gamma t}\sin(\omega t)\big)\big(-t\,e^{-\gamma t}\cos(\omega t)\big)+\big(-t\,e^{-\gamma t}\cos(\omega t)\big)\big(t\,e^{-\gamma t}\sin(\omega t)\big)\Big]=0 \tag{12}$$

We find that the Fisher Information matrix is

$$\mathcal{I}(t)=\frac{t^2e^{-2\gamma t}}{\sigma^2}\begin{pmatrix}1&0\\0&1\end{pmatrix}, \tag{13}$$

leading to the Cramér-Rao Bound (CRB)

$$CRB_\theta = \left[\mathcal{I}^{-1}(t)\right]_{jj} = \frac{\sigma^2 e^{2\gamma t}}{t^2} \qquad (\theta = \omega, \gamma), \qquad (j = 1, 2). \tag{14}$$

To optimize the CRB we take a derivative with respect to t of the function $f(t) := e^{2\gamma t}/t^2$ and demand it to be equal to zero: $f'(t) = e^{2\gamma t}\big(2\gamma t - 2\big)/t^3 = 0$, leading to

$$t_{\text{opt}} = \frac{1}{\gamma}, \tag{15}$$

One can check that this is indeed a maximum by taking the second derivative: $f''(t_{\text{opt}}) = 2e^2/t_{\text{opt}}^4 > 0$.

SM5. SIMULTANEOUS RAMSEY INTERFERENCE EXPERIMENT ON ALL QUBITS

Theoretically, to estimate all parameters, one could initialize the entire system into a global superposition state $|+\rangle^{\bigotimes n}$, allow it to evolve over time, and subsequently measure all qubits simultaneously. The resulting data would then be fitted to the analytical model to deduce the system's parameters, including both individual qubit detunings and crosstalk effects. In practice, this is not so simple. To get a sense of the complexity of the problem, let us find the $\langle X \rangle$ value of the middle qubit in a simple one-dimensional 3-qubit model that is initiated in a global superposition:

$$\begin{aligned} \psi(t) &= e^{-iHt}|+++\rangle, \\ \langle \psi(t)|IXI|\psi(t)\rangle &= \frac{1}{4}\Big(\cos(t\omega_{i+1}) + \cos(t(j_i + \omega_{i+1})) \\ + \cos(t(j_{i+1} + \omega_{i+1})) &+ \cos(t(j_i + j_{i+1} + \omega_{i+1}))\Big)e^{-t\gamma_i} \end{aligned} \tag{16}$$

After the fitting process, we are left with a set of parameters that are vastly different than the correct ones. Moreover, the loss function value is lower for the wrong parameters than for the true ones.

$$\sum (y_i - f(x_i, \theta_{wrong}))^2 \leq \sum (y_i - f(x_i, \theta_{correct}))^2 \tag{17}$$

where y_i is the measured value and $f(x_i, \theta)$ is the value of the expectation value function given a set of parameters θ. Since we have a finite amount of shots, we have an inevitable uncertainty in our data that is governed by $\frac{1}{\sqrt{N}}$. This creates the problem of overfitting the noisy data to a completely different set of parameters.

This results in estimation errors approximately an order of magnitude higher than those obtained from the single-qubit methods.

SM6. TILING OF IBM QUANTUM COMPUTERS

In the main text, we demonstrated how to calculate the crosstalk of a one-dimensional system using two experiments. Here, we extend the same approach to the two-dimensional topology of IBM quantum computers.

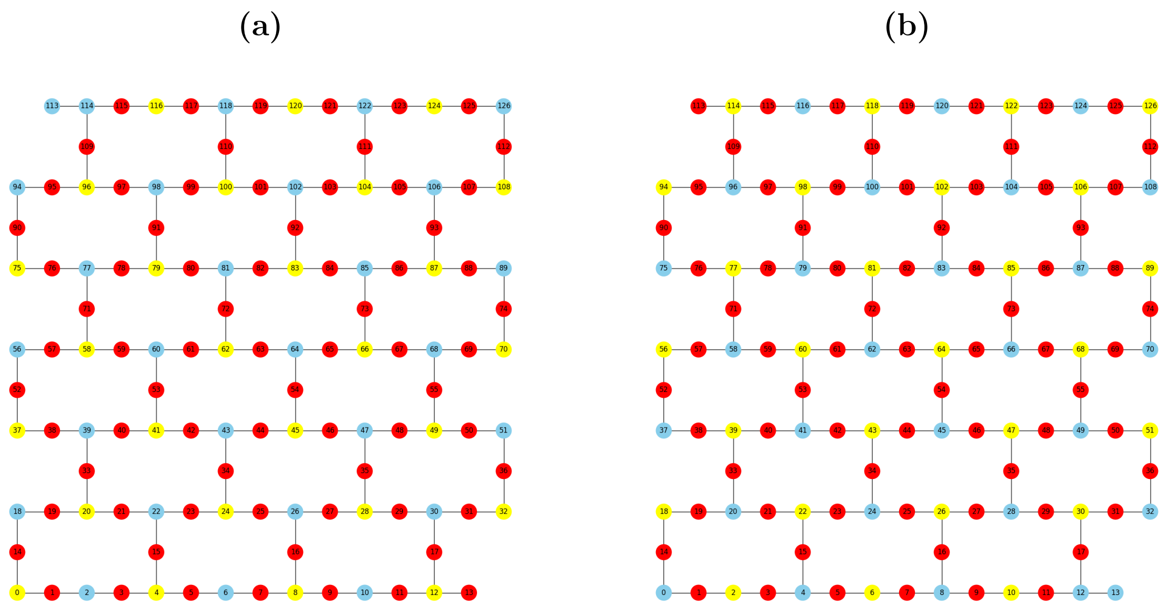

FIG. 4. IBM tiling for probing crosstalk effects. The red nodes represent qubits in the $|+\rangle$ state where the Ramsey interference is performed, and blue (yellow) nodes represent qubits in the $|0\rangle$ ($|1\rangle$) state.