## Simulation of SNI for Bias Estimation

We cannot compute  $\hat{\mathcal{N}}_{st}^{-1}$  exactly, and using Monte Carlo to directly estimate  $\hat{\mathcal{N}}_{st}^{-1}\mathcal{N}_{st}$  introduces statistical errors due to the finite size of samples M, which may obscure the information about the bias. Therefore, we use a small trick in the SNI.py: we simulate the relative error between  $\hat{\mathcal{N}}_{st}$  and the true  $\mathcal{N}_{st}$ , as shown below:

$$\hat{\mathcal{N}}_{st}^{-1} \mathcal{N}_{st} = \frac{1}{(1 - \hat{P})\mathcal{I} + \hat{P}\mathcal{E}} \{ (1 - P)\mathcal{I} + P\mathcal{E} \} 
= \frac{1}{(1 - \hat{P})\mathcal{I} + \hat{P}\mathcal{E}} \{ (1 - \hat{P})\mathcal{I} + \hat{P}\mathcal{E} + (P - \hat{P})(\mathcal{E} - \mathcal{I}) \} 
= \mathcal{I} + \frac{1}{(1 - \hat{P})\mathcal{I} + \hat{P}\mathcal{E}} \{ (P - \hat{P})(\mathcal{E} - \mathcal{I}) \} 
= \mathcal{I} + \sum_{k=0}^{\infty} \frac{(-1)^k \hat{P}^k}{(1 - \hat{P})^{k+1}} \mathcal{E}^k \{ (P - \hat{P})(\mathcal{E} - \mathcal{I}) \} 
= \mathcal{I} + (P - \hat{P}) \sum_{k=0}^{\infty} \{ \frac{(-1)^k \hat{P}^k}{(1 - \hat{P})^{k+1}} \mathcal{E}^{k+1} - \frac{(-1)^k \hat{P}^k}{(1 - \hat{P})^{k+1}} \mathcal{E}^k \} 
= (1 + \frac{P - \hat{P}}{1 - \hat{P}}) \mathcal{I} + (P - \hat{P}) \sum_{k=1}^{\infty} \frac{(-1)^{k-1} \hat{P}^{k-1}}{(1 - \hat{P})^{k+1}} \mathcal{E}^k$$
(1)

We can use Monte Carlo simulation to estimate the second term,  $\sum_{k=1}^{\infty} \frac{(-1)^{k-1} \hat{P}^{k-1}}{(1-\hat{P})^{k+1}} \mathcal{E}^k$ , which yield the estimate of  $\langle O \rangle_{circuit}$ , ultimately allows us to approximate the absolute value of the bias:

$$|Bias| = |\frac{P - \hat{P}}{1 - \hat{P}} \langle O \rangle_I + (P - \hat{P}) \langle O \rangle_{circuit}|$$
(2)