

Dual-Frequency Quantum Phase Estimation Mitigates the Spectral Leakage of Quantum Algorithms

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Abstract—Quantum phase estimation is an important component in diverse quantum algorithms. However, it suffers from spectral leakage, when the reciprocal of the record length is not an integer multiple of the unknown phase, which incurs an accuracy degradation. For the existing single-sample estimation scheme, window-based methods have been proposed for spectral leakage mitigation. As a further advance, we propose a dual-frequency estimator, which asymptotically approaches the Cramér-Rao bound, when multiple samples are available. Numerical results show that the proposed estimator outperforms the existing window-based methods, when the number of samples is sufficiently high.

I. INTRODUCTION

QUANTUM PHASE ESTIMATION [1]–[3] is a key enabler of quantum computational speedup over classical computers. It is a widely used component of quantum algorithms providing substantial acceleration over their best classical counterpart, including Shor’s factoring algorithm [4], the quantum clock synchronization algorithm [5], [6], the Harrow-Hassidim-Lloyd (HHL) algorithm [7], [8] conceived for solving linear systems, and the quantum counting algorithm [9], [10]. Recently, iterative quantum phase estimators have also been proposed for potential application in near-term noisy intermediate-scale quantum (NISQ) computers [11]–[13].

The circuit diagram of quantum phase estimation is portrayed in Fig. 1, where the initial state $|\psi\rangle$ of the data register is an eigenstate of the unitary operator \mathcal{U} satisfying $\mathcal{U}|\psi\rangle = e^{j\varphi}|\psi\rangle$, and QFT_M^{-1} denotes the inverse quantum Fourier transform [14, Sec. 5.1] applied to M qubits, which is a quantum-domain version of the classical discrete Fourier transform [15, Sec. 8]. This algorithm aims for estimating the phase φ . Broadly speaking, the $2^M - 1$ controlled unitaries produce a 2^M -point sinusoidal signal in the control register, whose frequency corresponds exactly to the desired phase φ . This may be viewed as the quantum-domain version of the power method of eigendecomposition [16]. When efficient implementations of the power of the unitary operator \mathcal{U} are available, exponential speedup over classical algorithms is possible, as seen in Shor’s algorithm [4].

Quantum phase estimation yields the exact result, when the recording length 2^M is an integer multiple of the period of the sinusoidal signal [14, Sec. 5.2.1]. When this is not the case, the spectral leakage problem [17] arises, which is an important topic in classical signal processing methods related to the discrete Fourier transform. The quantum-domain version of this problem is somewhat more grave, since the measurement outcome would assume erroneous values at non-negligible probabilities, hence the information about the correct phase is lost.

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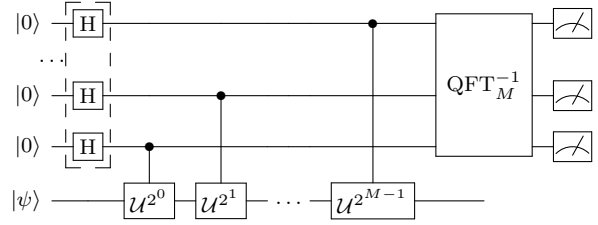


Fig. 1. The circuit diagram of quantum phase estimation.

One of the conventional solutions to the spectral leakage issue is to multiply the time-domain signal by a smooth “window function” [17]. This idea has been applied to the quantum phase estimation problem in [18], where the authors show that the cosine window [15, Sec. 7] is optimal in terms of the mean-squared error (MSE) of single-sample-based estimation. An efficient quantum circuit-based implementation of the cosine window has later been proposed in [19], also showing that it has satisfactory performance in terms of the error probability.

While existing treatises focus on single-sample-based estimation, in this letter, we consider the spectral leakage mitigation attained by multiple samples (i.e. measurement outcomes). This is motivated by the fact that the coherence time of NISQ computers is limited [20], hence classical computing power may be harnessed, by appropriately fusing multiple samples. Explicitly, our contributions are as follows:

- We derive the Cramér-Rao bound (CRB) of the quantum phase estimation problem, which sheds light upon the asymptotic multiple-sample performance of practical estimators.
- We propose a dual-frequency estimator that asymptotically attains the CRB upon increasing the number of samples. We term this as the asymptotic regime.
- Using numerical simulations, we demonstrate that the proposed dual-frequency estimator outperform the cosine window-based solution, when the number of samples is sufficiently large.

The rest of this letter is organized as follows. We first formulate the spectral leakage problem and discuss the existing countermeasures in Section II. Next, we derive the CRB and propose the dual-frequency estimator in Section III. The numerical results are then presented in Section IV, and we conclude in Section V.

II. PROBLEM FORMULATION AND RELATED WORKS

According to Fig. 1, the quantum state of the control register at the output of QFT_M^{-1} may be expressed as

$$|\phi\rangle_{\text{out}} = \frac{1}{N} \sum_{m=0}^{N-1} \sum_{n=0}^{N-1} e^{jn(\varphi - \frac{2\pi m}{N})} |m\rangle, \quad (1)$$

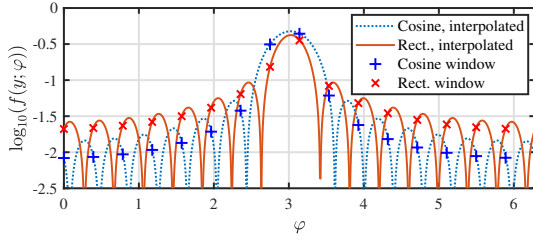


Fig. 2. Illustration of the observation probability distribution $f(y; \varphi)$ for rectangular and cosine windows, respectively.

where $N = 2^M$ is the record length. The probability of observing the outcome $|y\rangle$ is thus given by

$$f(y; \varphi) = |\langle y | \phi \rangle_{\text{out}}|^2 = \frac{1}{N^2} \left| \sum_{n=0}^{N-1} e^{jn(\varphi - \frac{2\pi y}{N})} \right|^2. \quad (2)$$

When $\varphi = 2\pi k/N$, $k \in \mathbb{Z}$, we see that the probability $f(y; \varphi)$ takes the maximum value of 1 at $y = k$, hence the phase estimation yields the exact solution. However, when φ is not an integer multiple of $2\pi/N$, $f(y; \varphi)$ is non-zero for almost all $0 \leq y \leq N-1$, causing large estimation errors. This phenomenon is referred to as “spectral leakage” in the literature of classical signal processing [17], [21].

The spectral leakage issue can be mitigated using the classic windowing method [22], multiplying the input signal by a “window” function defining a weighting vector α . This results in the following observation probability distribution

$$f(y; \varphi) = \frac{1}{N} \left| \sum_{n=0}^{N-1} \alpha_n e^{jn(\varphi - \frac{2\pi y}{N})} \right|^2, \quad (3)$$

where α_n is the n -th entry of α , and $\|\alpha\| = 1$. Upon comparing (2) to (3), we see that the original quantum phase estimation corresponds to a rectangular window of $\alpha = \frac{1}{\sqrt{N}} \mathbf{1}$. This weighting procedure may be implemented upon replacing the Hadamard gates in the dashed box of Fig. 1 by customized state preparation circuits [19].

It has been shown that in terms of the lowest MSE, the optimal window is the cosine window [18], [23], given by

$$\alpha_n^{(\cos)} = \sqrt{\frac{2}{N}} \sin \left[\frac{\pi(n-1)}{N} \right]. \quad (4)$$

The authors of [19] have designed an efficient state preparation circuit for the cosine window. The effect of the window may be intuitively interpreted by considering the corresponding observation probability distribution, as portrayed in Fig. 2. Observe that the “sidelobes” of the cosine window are much lower than those of the rectangular window, hence the probability that extremely large errors occur is substantially reduced. However, it is also seen that the cosine window has a wider mainlobe. If the sidelobes can be suppressed without widening the mainlobe, we may achieve better performance than that of the cosine window. This motivates our dual-frequency estimator, which will be detailed in Section III.

When multiple samples are available, it is possible to further improve the accuracy by simply taking the average of these samples, which we refer to as the “sample-mean estimator”. The sample-mean estimator has a time complexity on the order of $O(N_s)$, where N_s is the number of samples. In fact, when the sidelobes are effectively suppressed, the sample-mean estimator is sufficient for obtaining a near-optimal performance (in the sense of CRB), as will be detailed in Section III.

III. PROPOSED ESTIMATOR

In this section, we first derive the CRB of the quantum phase estimation problem, which will be used as a performance benchmark in the numerical simulations of Section IV. Moreover, it also motivates us to propose the dual-frequency estimator detailed in Section III-B, which asymptotically approaches the CRB upon increasing the number of samples.

A. CRB Analysis

The CRB is a lower bound on the mean-squared error of estimators [24], which is tight, when the noise is weak or the number of observations is large. In light of this, it may be used as the metric for determining the optimal window function for a large number of samples. The generic CRB of the quantum phase estimation problem has been derived in the literature [25], [26]. In this section, we take into account the effect of the window function on the phase estimation performance.

In general, given the likelihood function $f(y; \theta)$ of an observation y , the CRB of the parameter θ is given by

$$\mathbb{E}\{(\theta - \hat{\theta})^2\} \geq 1/\text{FI}(\theta), \quad (5)$$

where $\text{FI}(\theta) = \mathbb{E} \left\{ \left[\frac{\partial \ln f(y; \theta)}{\partial \theta} \right]^2 \right\}$ is the Fisher information of θ [24]. When there are multiple independent and identical distributed observations, the total Fisher information is the sum of the Fisher information of all individual observations.

In the context of quantum phase estimation, the likelihood function of a single observation is given by (3), which may be rewritten in a more compact form as

$$f(y; \varphi) = \frac{1}{N} |e_y^H \alpha|^2 = \frac{1}{N} e_y^H \alpha \alpha^H e_y, \quad (6)$$

where $e_y := [1, e^{j(\varphi - \frac{2\pi y}{N})}, \dots, e^{j(N-1)(\varphi - \frac{2\pi y}{N})}]^T$. The Fisher information may also be obtained using the following alternative form

$$\text{FI}(\varphi) = \sum_y \frac{1}{f(y; \varphi)} \cdot \left(\frac{\partial}{\partial \varphi} f(y; \varphi) \right)^2, \quad (7)$$

where the partial derivative may be expressed as

$$\begin{aligned} \frac{\partial}{\partial \varphi} f(y; \varphi) &= \frac{1}{N} \left[\left(\frac{\partial e_y}{\partial \varphi} \right)^T \alpha^* \alpha^T e_y^* + \left(\frac{\partial e_y^*}{\partial \varphi} \right)^T \alpha \alpha^H e_y \right] \\ &= \frac{j}{N} e_y^H (\alpha \alpha^H \mathbf{N} - \mathbf{N} \alpha \alpha^H) e_y, \end{aligned} \quad (8)$$

where we have $\mathbf{N} = \text{diag}\{0, 1, \dots, N-1\}$. Upon introducing $\mathbf{A} = \alpha \alpha^H$, the Fisher information may be expressed as

$$\begin{aligned} \text{FI}(\varphi) &= \frac{1}{N} \sum_{y=0}^{N-1} \frac{|e_y^H (\alpha \alpha^H \mathbf{N} - \mathbf{N} \alpha \alpha^H) e_y|^2}{e_y^H \alpha \alpha^H e_y} \\ &= \frac{4}{N} \sum_{y=0}^{N-1} \frac{\text{Im}^2 \{ e_y^H \mathbf{A} \mathbf{N} e_y \}}{e_y^H \mathbf{A} e_y}. \end{aligned} \quad (9)$$

When there are N_s samples, due to their mutual independence, the total Fisher information is simply formulated as $N_s \cdot \text{FI}(\varphi)$.

We may use (9) to obtain an intuition about the optimal window in the asymptotic regime. In Fig. 3, we compare the square-root CRB of various windows, where we set the record length to $N = 128$, corresponding to 7 control qubits. Observe that the rectangular window (equivalent to no windowing over a finite interval) corresponds to the lowest CRB. This indicates

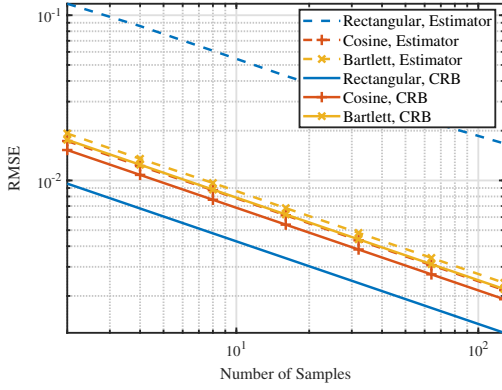


Fig. 3. The square-root CRB vs. number of samples of various window functions, compared with the RMSE of corresponding sample-mean estimators.

that it should have the best asymptotic performance. However, we see that the naive sample-mean-based estimator operates far from the CRB. By contrast, the sample-mean estimators of cosine and Bartlett windows exhibit near-CRB performances. We will further address this issue in Section III-B.

B. The Dual-Frequency Estimator

Let us commence our discussion from constructing an approximate maximum likelihood estimator based on the rectangular window with the aid of N_s samples. We first denote the samples as $\mathbf{y} = [y_1, y_2, \dots, y_{N_s}]^T$. From (2), the exact maximum likelihood estimator is given by

$$\hat{\varphi}_{\text{ML}} = \underset{\varphi}{\operatorname{argmax}} \sum_{i=1}^{N_s} \ln \left| \sum_{n=0}^{N-1} e^{jn(\varphi - \frac{2\pi y_i}{N})} \right|^2. \quad (10)$$

Since the samples only take integer values between 0 and $N-1$, we may use an alternative parametrization of $\mathbf{z} \in \mathbb{R}^N$, whose n -th entry z_k represents the number of times that $n-1$ occurs in the samples \mathbf{y} . Thus we may rewrite (10) as

$$\hat{\varphi}_{\text{ML}} = \underset{\varphi}{\operatorname{argmax}} \sum_{k=1}^N z_k \ln \left| \sum_{n=0}^{N-1} e^{jn(\varphi - \frac{2\pi k}{N})} \right|^2. \quad (11)$$

A naive strategy of solving (11) is an exhaustive search of φ in $[0, 2\pi)$, which is computationally expensive. To simplify the problem, we first obtain a rough estimate of φ as

$$\hat{\varphi}_{\text{rough}} = \frac{2\pi}{N} \left[\left(\underset{k}{\operatorname{argmax}} z_k \right) - 1 \right]. \quad (12)$$

Note that the worst-case complexity of this step is on the order of $O(N_s)$ when $N_s \ll N$. Next we conduct a refined search within $\mathcal{F} := [\hat{\varphi}_{\text{rough}} - 2\pi/N, \hat{\varphi}_{\text{rough}} + 2\pi/N]$. Although more sophisticated optimization techniques may have better performance, here we consider the simple approach of a uniform grid search over $O(\sqrt{N_s})$ grid points, inspired by the fact that the Fisher information is on the order of $O(N_s)$. To avoid the summation over n in (11), we consider the following approximation for large N :

$$\frac{1}{N} \left| \sum_{n=0}^{N-1} e^{jn(\varphi - \frac{2\pi k}{N})} \right| \approx \left| \operatorname{sinc} \left(\frac{N\varphi}{2\pi} - k \right) \right|. \quad (13)$$

Using the above approximation, the worst-case complexity of the grid search is reduced to $O(N_s^{1.5})$. We denote the final estimate as $\hat{\varphi}_{\text{AML}}$, which may be obtained as

$$\hat{\varphi}_{\text{AML}} = \underset{\varphi \in \mathcal{F}}{\operatorname{argmax}} \sum_{k=1}^N z_k \ln \left| \operatorname{sinc} \left(\frac{N\varphi}{2\pi} - k \right) \right|, \\ \varphi = \hat{\varphi}_{\text{rough}} + \frac{4k\pi}{N N_s}, \quad k \in \mathbb{Z}$$

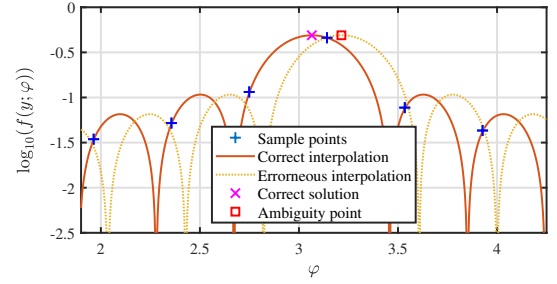


Fig. 4. Illustration of the ambiguity problem associated with the approximate maximum likelihood estimator when φ is close to $2\pi k/N$, $k \in \mathbb{Z}$.

where N_g is the number of grid points. The correction term is denoted as $e_{\text{AML}} = \hat{\varphi}_{\text{AML}} - \hat{\varphi}_{\text{rough}}$.

This estimator, however, does not in general yield satisfactory performance. We may develop some further intuition concerning this issue by revisiting Fig. 2. Observe that most of the information about φ is contained in the pair of sample points within the mainlobe. When φ is near $(2\pi k + 1)/N$, $k \in \mathbb{Z}$, the largest and the second largest entries in \mathbf{z} may be used as reliable estimates of the two sample points. However, when φ is close to $2\pi k/N$, $k \in \mathbb{Z}$, it is likely that the second largest entry in \mathbf{z} corresponds to the first sidelobe, causing an unexpected estimation error. As portrayed in Fig. 4, the difficulty of distinguishing the highest sidelobe from the sample point in the mainlobe having smaller likelihood incurs an ambiguity problem for the maximum likelihood estimator.

To tackle this problem, we split the samples into two sets, each having $N_s/2$ samples. For the first set, we compute the aforementioned approximate maximum likelihood estimator, and obtain $\hat{\varphi}_{\text{rough},1}$ and $e_{\text{AML},1}$. For the second set, we apply a frequency offset of $1/2N$ (one half of a frequency resolution unit) to the control register, resulting in the following maximum likelihood problem

$$\hat{\varphi}_{\text{ML},2} = \frac{\pi}{N} + \underset{\varphi}{\operatorname{argmax}} \sum_{k=1}^N z_k \ln \left| \sum_{n=0}^{N-1} e^{jn(\varphi - \frac{2\pi k}{N} + \frac{\pi}{N})} \right|^2. \quad (14)$$

Similarly, we may obtain $\hat{\varphi}_{\text{rough},2}$ and $e_{\text{AML},2}$. Based on these results, we construct four candidate intermediate estimates, contained in a vector as follows:

$$\mathbf{u} = [\hat{\varphi}_{\text{rough},1} + e_{\text{AML},1}, \hat{\varphi}_{\text{rough},1} - e_{\text{AML},1}, \\ \hat{\varphi}_{\text{rough},2} + e_{\text{AML},2}, \hat{\varphi}_{\text{rough},2} - e_{\text{AML},2} + 2\pi/N]^T. \quad (15)$$

Finally, we find the pair of entries in \mathbf{u} that are the closest to each other, meaning that

$$(i, j) = \underset{(i,j)}{\operatorname{argmax}} (u_i - u_j)^2, \quad (16)$$

and the final estimate is given by

$$\hat{\varphi}_{\text{DF}} = \frac{1}{2}(u_i + u_j). \quad (17)$$

The overall complexity of the dual-frequency estimator is at most $O(N_s^{1.5})$, which is comparable to the $O(N_s)$ complexity of the simple sample-mean estimator.

The rationale of the dual-frequency estimator may be intuitively understood as follows. To circumvent the difficulty of distinguishing the correct solution from the ambiguity point, we include both points into the set of candidate estimates, and also apply the same technique to the set of samples associated with the $(1/2N)$ -frequency offset. Since the ambiguity points of both sets are unlikely to be the same due to the frequency

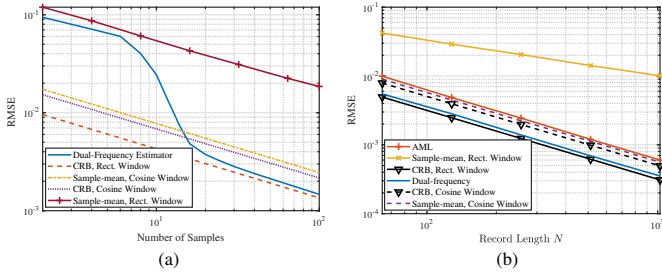


Fig. 5. The phase estimation RMSE vs. (a) the number of samples, (b) the record length N , of both the proposed dual-frequency estimator and the cosine window method, compared to the corresponding CRBs.

offset, we may then identify the correct solution by finding the matching pair of candidate solutions using (16).

Finally, we show that the $(1/2N)$ -frequency offset exploited in the estimator may be implemented using single-qubit phase rotation gates, hence the computational overhead of state preparation is negligible. Note that this offset may be obtained by initializing the input state of the control register as

$$|\phi\rangle_{\text{in}} = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{j\frac{\pi n}{N}} |n\rangle. \quad (18)$$

This state admits the following simple tensor-product form

$$|\phi\rangle_{\text{in}} = \bigotimes_{m=1}^M \frac{1}{\sqrt{2}} \left(|0\rangle + e^{j\frac{\pi 2^{m-1}}{N}} |1\rangle \right), \quad (19)$$

which may be implemented by applying the phase rotation gate $\mathcal{R}_z(\pi N^{-1} 2^{m-1})$ to each m -th qubit in the control register. This implies that the qubit complexity of the dual-frequency estimator is $\lceil \log_2 N \rceil$, which is the same as that of the windowing methods.

IV. NUMERICAL RESULTS

In this section, we characterize the performance of the proposed estimator using numerical simulations. We first consider the relationship between the root-mean-squared error (RMSE) of the estimators and the number of samples. In this example, we set the number of control qubits to $M = 7$, corresponding to $N = 128$. The number of samples N_s varies from 2 to 100. The unknown phase φ is randomly chosen from $(0, 2\pi)$ in each of the 10^5 Monte Carlo trials. The RMSE of the dual-frequency estimator as well as that of the sample-mean estimator based on the cosine window is portrayed in Fig. 5a, where the corresponding CRBs are also incorporated as benchmarks.

Observe that all curves in Fig. 5a exhibit the same linear trend in the asymptotic regime on the log-log scale. This implies that both estimators have the same asymptotic error scaling as the CRB, which scales on the order of $O(1/\sqrt{N_s})$ (in terms of RMSE). When N_s is insufficiently large, the dual-frequency estimator exhibits a performance similar to that of the sample-mean estimator. But as N_s increases, the performance of the dual-frequency estimator “switches” to near-CRB operation. Observe furthermore that it outperforms the cosine window-based method for $N_s \geq 16$. The relatively low accuracy of the dual-frequency estimator in the small- N_s regime originates from the fact that the number of samples is too small for us to construct any reliable candidate estimate (as given in (15)). Consequently, the sample points that are far away from the true value of φ (i.e., the “outliers”) cannot be reliably identified, hence would cause large estimation errors.

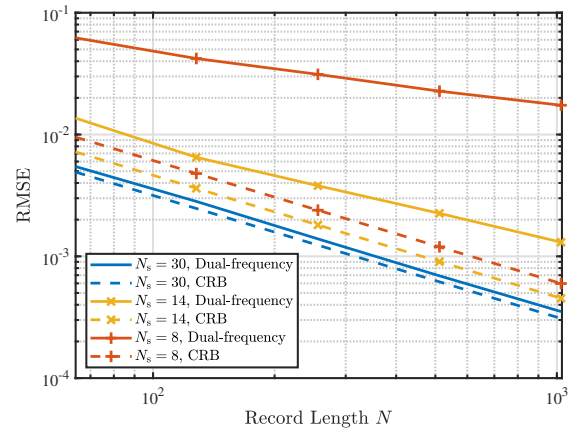


Fig. 6. The RMSE of the dual-frequency estimator vs. the record length, for N_s values in different regions.

Next we consider the dependence of the RMSE on the record length N . We set the number of samples to $N_s = 30$. The number of control qubits varies from 6 to 10, corresponding to $N = 64, 128, 256, 512, 1024$. The corresponding results are portrayed in Fig. 5b. We also incorporate the approximate maximum likelihood estimator in Fig. 5b for a better illustration.

Observe that the sample-mean estimator based on the rectangular window exhibits an $O(1/\sqrt{N})$ scaling, while the others exhibit $O(1/N)$ scaling. This is a phenomenon that has also been observed in [18], which suggests that the rectangular window does not provide a substantial quantum speedup in the sense of RMSE scaling, since the $O(1/N)$ scaling (i.e., the “Heisenberg limit [27]”) is an important characteristic of quantum algorithms conceived for phase estimation.

We also observe that the dual-frequency estimator does not exhibit the aforementioned bimodal phenomenon with respect to N . This suggests that for large N , we may still use a constant number of samples (for example, $N_s \geq 20$ as indicated by Fig. 5a) to achieve a near-CRB performance.

In Fig. 6, we portray the dependence of the RMSE on the record length N for different values of N_s . Specifically, we pick three values of N_s from the *ambiguity region* ($N_s \leq 10$), the *transition region* ($10 < N_s \leq 20$), and the *asymptotic region* ($N_s > 20$). We observe that in the asymptotic region ($N_s = 30$), the dual-frequency estimator exhibits a near-CRB performance, and has an order of $O(1/N)$ RMSE scaling. By contrast, in the ambiguity region, the estimator exhibits an order of $O(1/\sqrt{N})$ RMSE scaling. Finally, in the transition region, the order of RMSE scaling is between $O(1/\sqrt{N})$ and $O(1/N)$.

V. CONCLUSIONS

A dual-frequency phase estimator was proposed for mitigating the spectral leakage-induced error in quantum phase estimation algorithm based on multiple samples. We have presented its CRB analysis in the asymptotic regime. This CRB also inspires the design of our dual-frequency estimator. Compared to the naive sample-mean estimator, the proposed estimator attains the Heisenberg limit in the sense of exhibiting RMSE scaling on the order of $O(1/N)$. Furthermore, the estimator is capable of outperforming the cosine window, which is shown to be optimal for single-sample estimation, when the number of samples is sufficiently large (but constant with respect to N). A promising future research direction would be extending the proposed dual-frequency estimator for

mitigating the spectral leakage of the iterative quantum phase estimators [28], [29] designed for near-term hybrid quantum classical computation. Our method may also inspire future research on the algorithmic error mitigation for a broader range of quantum algorithms.

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