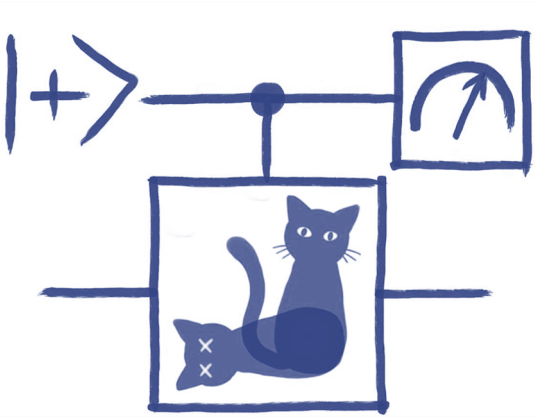
Heisenberg-limited quantum phase estimation of multiple eigenvalues with a single control qubit



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Heisenberg-limited quantum phase estimation of multiple eigenvalues with a single[1] control qubit

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Abstract

Quantum phase estimation is a cornerstone in quantum algorithm design, allowing for the inference of eigenvalues of exponentially-large sparse matrices. The maximum rate at which these eigenvalues may be learned, –known as the Heisenberg limit–, is constrained by bounds on the circuit depth required to simulate an arbitrary Hamiltonian. Single-control qubit variants of quantum phase estimation have garnered interest in recent years due to lower circuit depth and minimal qubit overhead. In this work we show that these methods can achieve the Heisenberg limit, *also* when one is unable to prepare eigenstates of the system. Given a quantum subroutine which provides samples of a 'phase function' $g(k) = \sum_j A_j e^{i\phi_j k}$ with unknown eigenvalue phases ϕ_j and probabilities A_j at quantum cost $O(k)$, we show how to estimate the phases $\{\phi_j\}$ with accuracy (root-mean-square) error δ for total quantum cost $T = O(\delta^{-1})$. Our scheme combines the idea of Heisenberg-limited multi-order quantum phase estimation for a single eigenvalue phase [1, 2] with subroutines with so-called dense quantum phase estimation which uses classical processing via time-series analysis for the QEEP problem [3] or the matrix pencil method. For our algorithm which adaptively fixes the choice for k in $g(k)$ we prove Heisenberg-limited scaling when we use the time-series/QEEP subroutine. We present numerical evidence that using the matrix pencil technique the algorithm can achieve Heisenberg-limited scaling as well.

[1] Technically, we might need up to two qubits – see the note under Lem. 2.3.2.

Contents

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Chapter 1

Introduction

Quantum computers should be used to simulate nature efficiently. This idea was suggested by Feynman as early as 1980s [4], long before quantum computers came to be. We now live the exciting times that see the first quantum computers come to life. In the last year we reached the milestone of a quantum device running a calculation that could not be performed using any classical algorithm at the time [5]. This comes with a promise of quantum advantage – solving unsolved practical problems in e.g. chemistry and condensed matter physics.

To achieve quantum advantage in the near term, it is crucial to focus on designing clever quantum algorithms. This is because current "Noisy Intermediate Scale Quantum" (NISQ) devices are limited in size and subject to noise, which limits the depth of practically realisable algorithms [6]. Thus, problems to solve must be carefully selected and the algorithms have to be tailored to the (prospectively) available quantum processors.

Quantum Phase Estimation (QPE) has been a cornerstone of quantum computing since the beginning of the field. It is the foundation of the quantum part of Shor's ground-breaking algorithm [7] and other known algorithms that provide exponential speedup over their classical analogues [8, 9]. While the original algorithm is thought to be infeasible on NISQ devices, in the last years a lot of interest has been drawn to its less costly versions. In this work, we focus on an algorithm that is more suited for near-term use. We design a classical post-processing scheme that is provably asymptotically optimal in the estimation precision.

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1.1 Digital Quantum Simulation

The term quantum simulation refers to using a quantum computer to study a model quantum system. It was the first task suggested for quantum computers [4] and remains one of the most promising directions for quantum computing nowadays. This suggestion was motivated by the fact that the number of parameters needed to describe the state of a quantum system grows exponentially with the number of particles. As a consequence, systems larger than around 50 particles cannot be classically simulated on even the world's largest supercomputers [6]. In contrast, because quantum computers store data as quantum states, the number of qubits needed scales linearly with the simulated system size.

A fundamental problem in quantum simulation is mimicking the dynamics of another quantum system. More precisely, *Hamiltonian simulation* is defined as the task of approximating the unitary evolution generated by a Hamiltonian H, given a classical description of H. As even merely writing down the matrix elements of the unitary operation is exponentially difficult, this task is expected to be in general intractable for classical computers. Conversely, in 1996 Lloyd showed that any open or closed system whose dynamics is determined by local interactions can be efficiently modeled on digital quantum computers [10]. The core of the method is time-slicing (dividing the evolution into discrete time steps) and noting that for sufficiently short times the unitary can be easily approximated (e.g. using the Trotter-Suzuki decomposition [11] or randomised compilation [12]). The method was improved in the next few years [13, 14]. It was shown that computation time has to scale at least linearly with the evolution time [15]. In 2017, Low and Chuang formulated lower bounds on the cost of Hamiltonian simulation and designed an optimal algorithm using the framework of quantum signal processing [16].

After successfully implementing time evolution, we need to find a way to extract relevant physical information. Hamiltonian simulation on its own is not practically useful, as its output is a quantum state that takes exponential space to store on a classical computer. Algorithms have been described and experimentally implemented to obtain many different quantities. In the field of quantum chemistry, important properties include molecular energies [17–25] and their derivatives such as polarisability or magnetisability [26], with which we can classically calculate activation energies, equilibrium bond lengths, and reaction paths. In condensed matter, we wish to learn e.g. dynamic properties such as correlators [27], expectation values at finite energies and for micro- or macrocanonical ensembles [28]. The main focus of high energy physics is on scattering amplitudes

[29] and cross sections [30].

Digital quantum simulation has promising applications to many fields of science. Before the year 2000, Lloyd's scheme was adapted to simulate non-interacting fermions [31], nonrelativistic many-body systems [13, 32] and equilibration to the Gibbs state [33]. Subsequently, it was applied to electronic structure Hamiltonians [17, 18], and experimentally implemented for small molecules [22–26, 34–36], condensed matter systems [27, 37, 38] and quantum magnets [34, 39]. One of the holy grails in the field, that could result in reducing the world energy usage by up to 3%, is simulation of FeMoCo (FeMo cofactor of the Nitrogenase enzyme) and so far remains beyond our reach [21, 40]. We hope that in the future quantum computers will help to improve efficiency of chemical reactions of industrial importance, design new pharmaceuticals, and efficiently collect solar energy [6].

1.2 Complexity theory

Computational complexity theory aims to classify computational problems based on their difficulty – the amount of resources, such as computational time, needed to solve them on a particular computational model. *Problem* refers to the abstract task to be solved, that can be viewed as an infinite set of *instances* – inputs of variable size, with solutions for every instance. For example, the instances of the Hamiltonian simulation problem are particular local Hamiltonians, whose size is measured by the number of particles they describe, and the solutions are descriptions of quantum circuits that implement the time evolution up to the desired precision. There are many types of computational problems: search problems, optimisation problems, sampling problems. A collection of problems of the same type that require similar resources is called a *complexity class*.

The fundamental complexity classes, P (Polynomial time) and NP (Nondeterministic Polynomial time), consist of *decision problems*, for which the answer is either yes or no. They are usually represented as *formal languages*. A language L over an alphabet Σ is a subset of the set Σ^* of all finite strings of symbols from Σ (usually $\Sigma = \{0, 1\}$ and Σ^* are binary representations of integers). Every element of Σ^* represents an instance of the problem, and the problem is encoded as the set $L \subset \Sigma^*$ of all instances for which the answer is yes. This type of problems is particularly important because every computational problem can be reformulated as a number of decision problems (for example, if the answer to the original problem is an integer, we may ask for each bit of its binary representation).

The class of problems thought to be feasible on a quantum computer is called BQP (Bounded-error Quantum Polynomial time). It is a set of decision problems such that there exists a polynomial size quantum circuit that decides whether $x \in L$ with probability at least $2/3$. We often use an equivalent generalised definition, including all types of computational problems that can be solved by a quantum computer in polynomial time with a fixed probability of error [41, 42].

While BQP can be thought of as a quantum equivalent of the class P, a quantum analog of NP is called Quantum Merlin Arthur (QMA). It is defined as a set of decision problems for which there exist polynomial-time *quantum verifiers*: quantum circuits that take as an input x and an additional quantum state (called a *quantum proof*), such that if $x \in L$ there exists a proof for which the verifier outputs 1 with high probability, and if $x \notin L$ the verifier outputs 0 with high probability for any proof [42]. It is known that P $\subseteq$ BQP $\subseteq$ QMA $\subseteq$ PSPACE [43].

Every complexity class contains the subset of "hardest" problems, such that finding a polynomial-time algorithm for any of them gives polynomial-time algorithms for all problems in the class. More precisely, a problem L is called BQP-hard if every problem in BQP can be reduced to it, i.e an algorithm that solves L can be adapted to solve any problem in BQP with a small overhead. If moreover $L \in$ BQP, then L is called BQP-complete.

Identifying which problems are easy or hard to solve on a quantum device is crucial to understand the power and limitations of quantum computing. A problem that is well known to be feasible is Hamiltonian simulation [10], described in section 1.1. On the other hand, the first problem proven to be hard (more specifically QMA-complete) was the local Hamiltonian problem – finding the ground energy of a local Hamiltonian [44]. Further research in this area could determine whether quantum computers are strictly more powerful than classical computers and help to prove important conjectures in complexity theory, such as P$\neq$NP.

Complexity theory is mostly concerned with polynomial versus exponential separation. On the contrary, in practice polynomial improvements, or even reduction of constant factors, may be significant in the field. In particular, the focus of this thesis is on a quadratic speedup. It was recently shown that quantum algorithms that only quadratically outperform their classical counterparts are unlikely to lead to quantum advantage [45]. However, in this thesis we compare two quantum algorithms and therefore achieving quadratic speedup is certainly worthwhile.

1.3 Quantum Metrology

Quantum metrology is the study of making optimal measurements by exploiting quantum phenomena such as entanglement [46]. It seeks to find fundamental limits on what precision is achievable when our resources, such as computation time or number of samples, are finite – bounded by N, and design experiments that saturate these limits. Specifically, the focus is often on the estimation rate i.e. the scaling of precision with N in the limit of large N and the goal is to achieve accuracy beyond the $O(N^{-1/2})$ bound imposed by the central limit theorem, termed *sampling noise limit* or *standard quantum limit* (SQL). The best achievable scaling is known to be $O(N^{-1})$; it is called the *quantum metrology limit* (QML) or *Heisenberg limit* [47] as it is derived from the generalised Heisenerg uncertainty relations.

Uncertainty relations are intrinsic to the formalism of quantum mechanics, the most celebrated example being the position-momentum uncertainty principle. In the early days of quantum mechanics, time and energy were believed to be related in the same way. That would mean that to estimate energy up to precision ΔE we need our experiment to last at least $O(1/\Delta E)$ – the Heisenberg limit. This reasoning is not rigorous, as time is not an operator in quantum mechanics. Already in 1960 Aharonov and Bohm gave an example of a situation where this principle can be violated to an arbitrary extent [48].

The term "Heisenberg limit" has been used since the 1990s in the field of interferometry [49]. In this context, it relates two conjugate variables: the number of photons N and the accuracy of estimation of the phase of light ϕ, introduced when the light passes through the studied sample. It can be easily derived from the uncertainty principle for these variables $\Delta\phi\Delta N \geq 1/2$: if the number of photons in an experiment is bounded by N, then clearly $\Delta N \leq N/2$ and so $\Delta\phi \geq N^{-1}$ [50–52]. This scaling can be achieved, for instance, by using squeezed states of light, while for classical states such as coherent light we get the sampling limit $\Delta\phi \in O(N^{-1/2})$ [50, 51]. However, this derivation is again not strict due to the phase operator being ill-defined. In fact, there exist states of light for which $\Delta\phi \in O(N^{-2})$ – seemingly enabling sub-Heisenberg estimation [51, 53].

These discrepancies revealed the need for a more precise framework [50, 54, 55]. In Ref. [50], conditions were defined on validity of the Heisenberg limit. Firstly, appropriate accuracy measures have to be chosen that correctly take into account contributions from unlikely data [1, 50, 55]. Secondly, no prior information about the phase can be used [49, 50]. If either of those conditions is breached, sub-Heisenberg limits can be achieved [49, 52, 53].

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The aforementioned studies revealed that temporal and physical resources can be exchanged: using N photons is the equivalent of a single photon passing through the sample N times. These ideas can be unified by counting 'total number of passes' as a resource, allowing physical system that give mathematically identical results to be treated by the same formula. [1, 54]. This framework also encompasses digital quantum phase estimation (which is the main focus of this thesis and described in Sec. 1.4) – a single pass through the phase shift is equivalent to a single application of the unitary operator whose parameters we aim to estimate. In Ref. [47], Atia and Aharonov show that the time-energy uncertainty relation holds for unknown Hamiltonians, if the time is replaced by the computational complexity of simulating the measurement, linking back to the origins of the formula.

Optimal algorithms for phase estimation have been proposed in the late 2000s, both in the framework of interferometry [50, 56] and digital quantum computing [55]. Unfortunately, these algorithms were difficult to implement in practice. Quantum metrology in the last 10 years has been focused on designing algorithms that are both practical and efficient. A lot of research has been done on how to beat the classical limit without using entanglement [1, 24, 28, 57–59], as entangled states are usually very costly to prepare. It was shown that this goal does not require not only entangled states, but also pure states [60, 61]. Another obstacle is decoherence induced by the environment; surprisingly, it was demonstrated that in some cases it can be used to enhance measurement accuracy [62, 63]. Other studies have shown that the presence of depolarising noise decreases the precision, but can be compensated for [2, 19, 64]. Realistic noise, however, might degrade our ability to measure [19].

1.4 Quantum Phase Estimation

The task of Quantum Phase Estimation (QPE) is to estimate the eigenphases of unitary operator U, given access to a quantum circuit that implements U. Most QPE algorithms are based on *phase kickback* – introducing an additional qubit register (called the *ancillary register* or *control register*), that can control U's action on the original register (called the *system register*). Controlled operations are used to encode information about U on the control register, so that the eigenphases can be learned by tomography of the ancillary qubits.

QPE is a basic building block of quantum algorithms. Many of them, including Shor's ground-breaking factoring algorithm [7] consist only of

QPE and classical calculations. QPE plays a central role in quantum simulation. It has mostly been proposed to determine eigenenergies [17, 18, 21–24, 65], but can also be adapted to calculate mean values [66] and energy derivatives [26] or prepare thermal equilibrium states [33, 67]. Most known quantum algorithms that achieve exponential speedups, such as order finding, period finding, discrete logarithm, Deutsch-Jozsa algorithm, quantum counting, linear equations [43], use QPE as their quantum subroutine.

QPE was from the very beginning described as a universal framework to design quantum algorithms. The first paper formally introducing QPE [8] in fact describes the much more general Hidden Subgroup Problem (HSP) [43]. Instances of the HSP include many important problems in Mathematics and Computer Science, such as graph isomorphism and prime factorization [8, 43]. It has even been suggested that all problems for which exponential quantum speedup is possible can be reduced to the HSP [43]. In Ref. [8] Kitaev gave an efficient algorithm to solve the HSP for all abelian groups – the Abelian Stabiliser Problem (ABS), which can be easily mapped to phase estimation [9]. The idea of QPE's universality was formalised later by proving that a sampling variant of phase estimation is a BQP-complete problem [41], as described in detail in Sec. 2.1.

The first algorithm for QPE was proposed by Kitaev in 1995 [8] in the context of ABS. In 1998, Cleve, Ekert, Macchiavello and Mosca adapted it to the task of estimating arbitrary phases [9] and formulated in the way that is commonly used to this day [43]. This standard algorithm uses an n-qubit control register to estimate the first n bits of the phase. As the correct estimate is returned with high probability, the algorithm appears to achieve the Heisenberg limit. However, as first pointed out in Ref. [1], if contributions from outlying data are correctly included, one only gets the sampling noise limit.

Although the standard algorithm uses an n-qubit register, Kitaev suggested in 1997 that one can use multiple preparations of a single control qubit and classical calculations instead (so-called iterative QPE) [44, 68]. This class of QPE algorithms is much more practical – the first works focused on it, published in 2000s by Higgins et al., already included experimental demonstrations [1, 57]. Moreover, these schemes were proven to be Heisenberg-limited. They were further improved [2, 64, 69] and shown to be robust against noise [2, 64]. Recently, it was found that, for certain classes of Hamiltonians, no ancillary qubits or control operations are needed [28, 59].

Most analyses of single-control QPE were done with an unpractical assumption that we can prepare exact eigenstates of the unitary U. In

Ref. [19] it was demonstrated numerically that this requirement is unnecessary; one may infer single eigenvalues from mixed or superposed initial eigenstates using a single ancilla qubit and standard classical signal processing techniques [70]. By a clever adjustment of the quantum phase estimation problem to target estimation of the spectral function, Eq. (2.14), of the input state, Ref. [3] was able to prove rigorous results, with bounds that were subsequently improved in Ref. [71]. Due to the need to 'densely sample' the phase function $g(k) = \sum_j A_j e^{i\phi_j k}$ (i.e. drawing samples at $k = 0, 1, \ldots, K$ as opposed to $k = 2^d$ used by textbook QPE), and a lack of optimization of the classical post-processing techniques, these schemes failed to achieve the Heisenberg limit. This year, the first algorithms were published that aim to estimate multiple phases with a single ancilla qubit at Heisenberg limit – Ref. [72] demonstrated numerical evidence for accomplishing this task, and the algorithm of Ref. [73] was shown to achieve Heisenberg scaling up to polylog factors. However, providing a rigorous solution that removes these log factors remains an open problem.

1.5 In this work

In this work, we demonstrate single-control qubit quantum phase estimation at the Heisenberg limit. We extend the methods used in Refs. [1, 2] that obtain Heisenberg-limited scaling for single eigenphases to the multiple-phase setting by the use of a multi-order scheme and phase matching subroutines between different orders. We show that to make this phase matching unambiguous requires the sampling scheme to be adaptive, i.e. the next choice for k of $g(k)$ depends on the current phase estimates. At each order the multi-order algorithm requires input from a dense phase estimation method: for a given order k we use samples from $g(k\mathsf{k})$ with $\mathsf{k} = 0, 1, \ldots, K$. Using the time-series or QEEP analysis of Ref. [3] as classical processing subroutine, we are able to obtain a rigorous proof of Heisenberg-limited scaling of our multi-order scheme. Using the matrix pencil method analysed in Ref. [19], as such a dense subroutine, we are able to show numerical results consistent with the Heisenberg limit, with a performance improvement over the time-series analysis results.

In essence, our work is concerned with what choices of k in $g(k)$ and what classical processing are needed to enable Heisenberg-limited scaling, i.e. scaling which minimizes the total number of applications T of (controlled) U given a targeted error δ with which to estimate multiple eigenvalue phases of U present in some input state $|\Psi\rangle$. It can thus be viewed as purely solving a problem of classical signal processing. This

does not mean that such questions are trivial: for example, the question of how to estimates phases if one is allowed to only get single samples from $g(k)$ for a set of randomly chosen k relates to the dihedral hidden subgroup problem in quantum information theory [74].

1.5.1 Outline

Chapter 2 provides the necessary background to understand our new results. It is concerned with the case we only wish to estimate a single eigenphase. We describe in detail the textbook QPE algorithm of Ref. [9, 43] and evaluate its performance. We split phase estimation into quantum and classical parts and give quantum circuits to perform the quantum part with a single control qubit. We calculate information theoretic bounds on the estimation precision with given resources. We present the algorithm of Ref. [2] that estimates a single eigenvalue with one ancilla qubit at Heisenberg limit.

In chapter 3 we present our results. We begin by defining the problem that we aim to solve, i.e. estimation of multiple eigenvalues. We present the algorithm of Ref. [3] that targets a similar task and adapt it to serve as a subroutine for our multi-order scheme. We discuss the problems with estimating multiple phases and how we circumvent them. We define our algorithm and prove that it achieves the Heisenberg scaling. We demonstrate the scaling numerically for two different subroutines – the rigorous one based on Ref. [3], and a more practical one using matrix pencil method of Ref. [19].

In chapter 4 we discuss the results and propose possible ways to improve our scheme.

Chapter 2

Quantum Phase Estimation

The goal of this chapter is to present the known results about Quantum Phase Estimation. In Sec. 2.1 we define a sampling variant of phase estimation (Def. 2.1.1) and show that it is a BQP-hard problem (Thm. 2.1.3). In Sec. 2.2, we present the best known algorithm for QPE and its performance in the case where we want to estimate a single phase and are able to prepare the corresponding eigenstate. We show the naive reasoning that suggests this algorithm achieves the Heisenberg scaling, and that with a correct choice of accuracy measure it only achieves the sampling-noise scaling. In Sec. 2.3 we separate the quantum part of a phase estimation problem, namely sampling of the phase function $g(k)$ (Eq. (2.13)) given an input unitary U and input state $|\Psi\rangle$ in Definition 2.3.3 through running some quantum circuits, and the classical processing of samples from $g(k)$ to extract the eigenvalue data of U. We prove several Cramer-Rao bounds on the scaling of the error versus the total quantum cost for the estimation of a single eigenvalue phase (Thm. 2.4.1). We state the previous result on getting Heisenberg-limited scaling for a single eigenvalue phase (Alg. 2.5.1).

2.1 BQP-hardness

The problem of phase estimation is BQP-hard – every problem in BQP can be reduced to this problem. In order to prove this, we define a sampling variant of phase estimation, as in Ref. [41]:

Definition 2.1.1 (Phase Estimation Sampling, PES)**.** *Let U be a unitary acting on an n-qubit register, described by a $poly(n)$-size quantum circuit. Suppose the eigenvalues of U are $\lambda_j = e^{i\phi_j}$ and the corresponding eigenstates are $|\phi_j\rangle$.*

Given an estimation precision $\epsilon = \Omega(1/poly(n))$, a sampling error probability $1 - p = \Omega(1/poly(n))$ and a polynomial size circuit that prepares an initial state $|\Psi\rangle$, return an estimate of ϕ_j up to ϵ with probability at least $p|\langle\Psi|\phi_j\rangle|^2$.

We also need a rigorous definition of BQP-hardness.

Definition 2.1.2 (BQP [42])**.** *A language L is in BQP if and only if there exists a polynomial-time generated family of quantum circuits $\{Q_n : n \in \mathbb{N}\}$, such that*

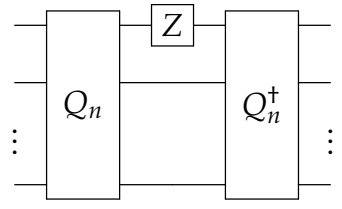
1. *for all $n \in \mathbb{N}$, Q_n takes n input qubits (the circuit $Q_{|x|}$ is applied to the state $|x0...0\rangle$) and produces one output qubit.*
2. *For all $x \in L$, the probability of measuring 0 on $Q_{|x|}(x)$ is $< \frac{1}{100}$.*
3. *For all $x \notin L$, the probability of measuring 1 on $Q_{|x|}(x)$ is $< \frac{1}{100}$.*

We note that BQP is usually defined for error probability $1/3$ instead of $1/100$. However, it is a standard result from complexity theory that these definitions are equivalent [42]. We use the above definition for convenience.

Theorem 2.1.3. *[PES is BQP-hard] For every $L \in$ BQP there exists a polynomial-time generated family of quantum circuits $\{U_n : n \in \mathbb{N}\}$, $\epsilon, p \in (0,1)$ such that running PES with $U = U_{|x|}(x)$, $|\Psi\rangle = |0\rangle^{\otimes n}$, precision ϵ and sampling error probability $1 - p$ decides whether $x \in L$ with probability at least $2/3$.*

Proof. Let $L \in$ BQP, and let $\{Q_n\}$ be as described in Def. 2.1.2. Without the loss of generality, we can assume the decision is made by measuring the first qubit. We can write the state $Q_{|x|}|x0...0\rangle$ as $\alpha_0|0\rangle|\psi_0\rangle + \alpha_1|1\rangle|\psi_1\rangle$ for some α_0, α_1 and $|\psi_i\rangle$ – some state on the other qubits. Then $|\alpha_i|^2$ is the probability of measuring $i = 0, 1$ on the first qubit. If $x \in L$, then $|\alpha_0|^2 < 1/100$, and if $x \notin L$, then $|\alpha_1|^2 < 1/100$.

Now we construct the following circuit U_n:



It is obvious that since $\{Q_n\}$ is polynomial-time generated, $\{U_n\}$ is also polynomial-time generated. We have

$$U_{|x|}|x0...0\rangle = Q^\dagger_{|x|}(\alpha_0|0\rangle|\psi_0\rangle - \alpha_1|1\rangle|\psi_1\rangle) = \tag{2.1}$$

$$= +|x0...0\rangle - 2\alpha_1|1\rangle|\psi_1\rangle \tag{2.2}$$

$$= -|x0...0\rangle + 2\alpha_0|0\rangle|\psi_0\rangle\,. \tag{2.3}$$

Hence $|x0...0\rangle$ is almost an eigenstate of $U_{|x|}$, with an eigenvalue $+1$ or -1 depending on whether $x \in L$. We can determine which is the case by running PES with $U = U_{|x|}$, $|\Psi\rangle = |x0...0\rangle$, $\epsilon = 1/8$ and $p = 3/4$. We accept x if the output value $\varphi \in [1/4, 3/4]$, and reject otherwise. From the calculation in Ref. [41] we have

$$P(\text{correct outcome}) \geq p\left(1 - \frac{|\alpha_{x,1}|^2}{\sin^2(\pi/8)}\right) \geq \frac{2}{3}. \tag{2.4}$$

□

The phase estimation problem turns out to be feasible – it can be solved on a quantum computer in polynomial time. In the next sections we present some algorithms that accomplish this task. We evaluate the performance of these algorithms for a simpler problem than PES. Namely, in the rest of this chapter we focus on the case where the register is prepared in an eigenstate of the unitary and we are only trying to estimate a single eigenvalue corresponding to this state.

2.2 Quantum Phase Estimation Algorithm

The most well-known phase estimation algorithm is usually referred to simply as Quantum Phase Estimation Algorithm (QPEA) [9, 43]. The algorithm uses an n-qubit control register, coupled to the system register (on which the oracle U acts). It consists of 3 steps, as presented by the quantum circuit in figure 2.1. First, we create a uniform superposition of all states of the ancillary register by applying Hadamard gates. Then, we perform a number of controlled U operations to encode information about U on the ancillary register. The total number of applications of U is

$$T = \sum_{k=0}^{n-1} 2^k = 2^n - 1. \tag{2.5}$$

Finally, we perform inverse Fourier transform on the control register and measure in the computational basis. If the initial state of the system register is an eigenstate of U $|\phi\rangle$, the state of the ancillary register before the measurement is $\sum_{l=0}^{2^n-1} \alpha_l |l\rangle$, where

$$\alpha_l = \frac{1 - e^{i2^n\phi}}{2^n} \frac{1}{1 - e^{i(\phi - \frac{2\pi l}{2^n})}} \tag{2.6}$$

(see Ref. [43] for details). Measuring the register in state $|l\rangle$ results in an estimate $\tilde{\phi}_l = 2\pi l/2^n$ and happens with probability

$$|\alpha_l|^2 = \frac{1-\cos 2^n\phi}{4^n}\frac{1}{1-\cos(\tilde{\phi}_l-\phi)}. \tag{2.7}$$

For the optimal outcome l^*, we have

$$\frac{1}{2\pi}|\tilde{\phi}_{l^*}-\phi| < 2^{-(n+1)}. \tag{2.8}$$

As we always have $1-\cos(x) < x^2/2$, the probability of obtaining this result is

$$|\alpha_{l^*}|^2 \geq \frac{1-\cos 2^n\phi}{4^n}\frac{4^n}{\pi^2} = \frac{1-\cos 2^n\phi}{\pi^2}. \tag{2.9}$$

The probability averaged over all possible values of ϕ is π^{-2}. So with fixed probability we get an estimate with error $< \pi T^{-1}$. This claim can be made more precise – by using extra qubits we can make this probability arbitrarily close to 1, while still preserving the $O(T^{-1})$ scaling [43].

However, as first pointed out in Ref. [57], other uncertainty measures fail to reach this optimal scaling. To talk about the Heisenberg limit, the error δ should be quantified by an expectation value of some error function $C(\tilde{\phi}-\phi)$ over the distribution $P(\mathbf{x}|\phi)$ of possible measurement outcomes $\mathbf{x}$, averaged over all possible values of the phase ϕ:

$$\delta^2 = \sum_{\mathbf{x}}\int_0^{2\pi} d\phi P(\mathbf{x}|\phi)C(\tilde{\phi}(\mathbf{x})-\phi). \tag{2.10}$$

Other measures do not take into account the contribution of outliers or make use of pre-existing information about the phase, and therefore do not necessarily translate into a correspondingly small standard deviation (on the other hand, the standard deviation can be used to bound all other commonly used uncertainty measures). Admittedly, if they give a small value, results from multiple separate measurements can be combined in an estimate with small standard deviation. However, if the number of the separate measurements needed is not constant, the scaling is not preserved [50, 55].

Following Ref. [57], we quantify the error by the square root of the

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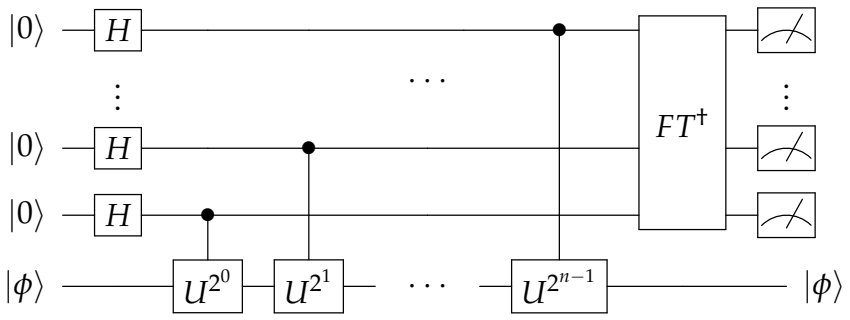
Holevo variance

$$\begin{aligned} V_H &= |\langle e^{i(\tilde{\phi}-\phi)}\rangle|^{-2} - 1 \approx 2\langle 1 - \cos(\tilde{\phi}-\phi)\rangle \\ &= 2\sum_{l=0}^{2^n-1} |\alpha_l|^2 [1-\cos(\tilde{\phi}_l - \phi)] \\ &= 2\,\frac{1-\cos 2^n\phi}{4^n} \sum_{l=0}^{2^n-1} 1 \\ &= \frac{1-\cos 2^n\phi}{2^{n-1}}. \end{aligned} \tag{2.11}$$

The average phase uncertainty $\sqrt{\langle V_H\rangle} = 2^{(n-1)/2}$ scales as $O(T^{-1/2})$, which is the Standard Quantum Limit. QPEA clearly does not achieve the Heisenberg limit.

It turns out a similar scheme can achieve not only the optimal scaling, but even optimal accuracy [55]. The encoding (second) and measurement (third) steps of QPEA are optimal; we only need to change the first step. Instead of preparing an equal superposition we need to prepare an optimal initial state. The way to find this state for any cost function C is described in Ref. [55]. However, for commonly used cost functions, this states are highly entangled and therefore very difficult to prepare. Alternatively, we can accomplish the same goal with repeated measurements of a much simpler circuit, as we will show in the next section.

Figure 2.1: *Quantum circuit for QPEA*



2.3 Single-ancilla QPE

The QPEA calls for one extra qubit in the control register for each bit of the estimate and requires operations controlled by this large entangled regis-

ter, which makes it infeasible on near-term devices. It has been known since the 1990s that the control register can be replaced by a single qubit using classical feedback and re-preparation of the control state [75], also known as iterative QPE [8, 44]. The algorithms that use a single ancilla qubit are particularly promising for the NISQ era. They require smaller quantum processors and circuit depths, and instead off-load part of the computation to a classical computer. In this section we describe how the task can be split into the quantum and classical part.

2.3.1 The classical and quantum tasks of phase estimation

One may separate quantum phase estimation into the extraction of a signal which consists of oscillations at eigenvalue frequencies ϕ_j at a chosen time k, and the processing of this signal to resolve the frequencies. Let us first define the following:

Notation 2.3.1 (Signal or Phase Function)**.** *Let $U \in U(2^N)$ be an N-qubit unitary operator, and $|\Psi\rangle \in \mathbb{C}^{2^N}$ an N-qubit state. We label the eigenstates $|\phi_j\rangle$ of U by their phase — $U|\phi_j\rangle = e^{i\phi_j}|\phi_j\rangle$. We can decompose $|\Psi\rangle$ in terms of these eigenstates,*

$$|\Psi\rangle = \sum_j a_j |\phi_j\rangle, \tag{2.12}$$

and write the probability $A_j := |a_j|^2$. We define the phase function – also called the signal– $g(k)$ for $k \in \mathbb{R}$ of a state $|\Psi\rangle$ under U as

$$g(k) = \sum_j A_j e^{ik\phi_j}. \tag{2.13}$$

The spectral function $A(\phi)$ is defined as

$$A(\phi) = \sum_j A_j \delta(\phi - \phi_j). \tag{2.14}$$

Note that $\int_0^{2\pi} d\phi A(\phi) = 1$, and $g(k) = \int_0^{2\pi} d\phi e^{ik\phi} A(\phi)$; i.e. the phase function sets the Fourier coefficients of the spectral function.

Note that one may change seamlessly between the description of a unitary U and its eigenvalues and a Hermitian operator H and its eigenvalues using the transform $U = e^{iHt}$ for an appropriate choice of t.

One may consider algorithms estimating $g(k)$ at integer $k \in \mathbb{Z}$, which require the quantum circuits using controlled-U^k in Fig. 2.2 with $k \in \mathbb{Z}$. In

our final Alg. 3.2.1 we will however use $k \in \mathbb{R}$. This generalization can be pulled back to $k \in \mathbb{Z}$ without additional overhead in a query-based model via a result from [76]:

Lemma 2.3.2. *[76] Fix $k \in \mathbb{R}$. Given a quantum circuit that implements a unitary U with circuit depth t_U, one may construct a quantum circuit to implement U^k with error ε with circuit depth $\lfloor k \rfloor t_U + O\left(\frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)} t_U\right)$.*

Crucially, the additional term is additive, and does not affect the scaling in k. However, the gadget required to implement U^k does require an additional control bit. (In the case of performing Hamiltonian simulation $U = e^{iHt}$ this additional control is typically not needed.)

The following task summarizes the quantum subroutine for phase estimation which is to be executed with the quantum circuits in Fig. 2.2:

Definition 2.3.3 (Phase Function Estimation, PFE)**.** *Let U be an N-qubit unitary operator and $|\Psi\rangle$ an N-qubit quantum state. Assume*

1. *A polynomial-size (in N) quantum circuit implementation of U (conditional on a control qubit) and,*

2. *A polynomial-size (in N) quantum circuit that prepares $|\Psi\rangle$.*

Given a parameter $k \in \mathbb{Z}$, error $\epsilon > 0$, and confidence $0 < p \leq 1 \in \mathbb{R}$, PFE *outputs an estimate $\tilde{g}(k)$ of the phase function $g(k)$ of $|\Psi\rangle$ under U, with $\mathbb{P}(|\tilde{g}(k) - g(k)| \leq \epsilon) \geq 1 - p$ with quantum cost $T = \mathrm{poly}(N) M |k|$ where M is the number of repetitions of both experiments in Fig. 2.2 and $M = \Theta(\log(1-p)\epsilon^{-2})$ via a Chernoff bound. Lemma 2.3.2 shows that an identical statement holds when $k \in \mathbb{R}$ with cost T scaling as $\mathrm{poly}(N) M(\lfloor k \rfloor + O(1))$.*

Note that estimating the quantum cost of the subroutine in Def. 2.3.3 as linear in k is consistent with general no-fast forwarding statements [15] which state that for general Hamiltonians one cannot implement $U^t = \exp(itH)$ in time sublinear in t. It is expected that phase function estimation is hard to do efficiently on a classical computer.

The quantum subroutine for PFE proceeds by executing the circuits in Fig. 2.2 for a given k. The control qubit is prepared in the $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ state, and is used to control k applications of the unitary U on the system register prepared in $|\Psi\rangle$. The reduced density matrix of the control qubit then takes the form

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & g(k) \\ g^*(k) & 1 \end{pmatrix}. \tag{2.15}$$

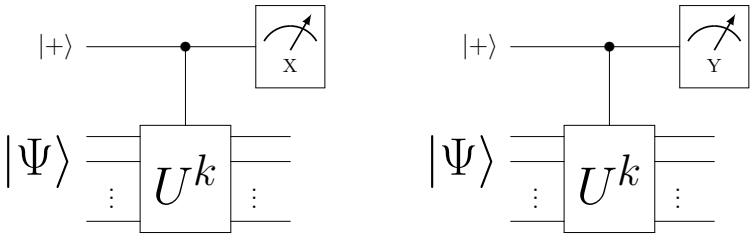


Figure 2.2: *For an input state* $|\Psi\rangle = \sum_j a_j |\phi_j\rangle$ *the probability for the ancilla measurement outcome to be* ± 1 *is* $\mathbb{P}(\pm 1) = \frac{1}{2}\sum_j A_j[1 \pm \cos(k\phi_j)]$ *(left circuit measuring in the X-basis) and* $\mathbb{P}(\pm 1) = \frac{1}{2}\sum_j A_j[1 \mp \sin(k\phi_j)]$ *(right circuit measuring in the Y-basis).*

The phase function $g(k)$ can thus be extracted by state tomography of the control qubit: one estimates the real and imaginary parts of $g(k) = g^{(r)}(k) + ig^{(i)}(k)$ by M repetitions of the circuit in Fig. 2.2 and measurements of the control qubit in the X- or Y-basis respectively. We will ignore any dependence of phase function estimation on N in the rest of the thesis.

2.4 Limits for single-eigenvalue phase estimation

In the previous section we have shown how to accomplish the quantum part of phase estimation, the generation of the signal function $g(k)$. Now we approach the classical part – constructing the optimal estimator of the phase ϕ given access to the quantum subroutine 2.3.3. We are interested in how accurately we can estimate the phase with given quantum resources T, which we quantify by total number of applications of the unitary U – so a single realisation of the circuit in Fig. 2.2 has quantum cost k. In particular, we focus on the rate of phase estimation – the rate of convergence of the estimation error δ as a function of the quantum resources used. We will see that to complete this task efficiently, we need to split our resources wisely, i.e. carefully select the values of k to sample $g(k)$ at. The following theorem introduces and proves the Heisenberg limit (the optimal rate at which the phases can be learnt), the sampling limit, and the dense signal limit, which hold depending on how we decide to distribute our resources.

Theorem 2.4.1 (The Heisenberg, Dense Signal and Sampling Limits)**.** *The (root-mean-square) error* δ *of an estimator* $\tilde{\phi}$ *of the eigenvalue phase* ϕ *employing*

the circuits in Fig. 2.2 on a eigenstate of U is always lower bounded as

$$\text{Heisenberg Limit: } \delta \geq cT^{-1} \tag{2.16}$$

where T is the quantum cost of implementing the circuits. If we choose to use only quantum circuits with $k = 1$, the sampling noise limit holds:

$$\text{Sampling Noise Limit: } \delta \geq T^{-1/2} \tag{2.17}$$

If we choose circuits with $k = 0, 1, \ldots, K$ with a fixed number of repetitions M for each circuit we are bound by a so-called 'dense signal' limit:

$$\text{Dense Signal Limit: } \delta \geq cT^{-3/4} \tag{2.18}$$

In these statements c is some constant.

Proof. Let $\tilde{\phi}$ be an estimator of ϕ which is inferred from the data $\mathbf{x}$. Here the data $\mathbf{x}$ is the string of outcomes of the ancilla qubit measurements for all the experiments using the left and right circuits in Fig. 2.2. We have

$$\delta^2 = \sum_{\mathbf{x}} \mathbb{P}(\mathbf{x}|\phi)(\phi - \tilde{\phi}(\mathbf{x}))^2 \geq I^{-1}(\phi), \tag{2.19}$$

by the Cramer-Rao theorem [77, 78] where the Fisher information is defined as

$$I(\phi) = \sum_{\mathbf{x}} \mathbb{P}(\mathbf{x}|\phi) \left\{ \frac{\partial}{\partial \phi} \ln \left[\mathbb{P}(\mathbf{x}|\phi) \right] \right\}^2. \tag{2.20}$$

Thus $I(\phi)$ limits the information we may learn about ϕ given a dataset $\mathbf{x}$ drawn from $\mathbb{P}(\mathbf{x}|\phi)$ and we can calculate $I(\phi)$. Let M_k^r be the number of experiments, using the circuit with the X measurement, and M_k^i be the number of experiments using the circuit with the Y measurement with a certain chosen k. The Fisher information for all independent experiments together is additive, i.e. $I(\phi) = \sum_k [M_k^r I(\phi|k, r) + M_i^r I(\phi|k, i)]$ with $I(\phi|k, r)$ and $I(\phi|k, i)$ the Fisher information of a single experiment. For a single experiment we can calculate, using Eq. (2.20) and the probability for the output bit given in Fig. 2.2, that $I(\phi|k, r) = I(\phi|k, i) = k^2$ and thus

$$I(\phi) = \sum_k k^2 (M_k^r + M_k^i). \tag{2.21}$$

At the same time the total quantum cost of all experiments is

$$T = \sum_k k(M_k^r + M_k^i). \tag{2.22}$$

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The key insight here is that the relative dependence on k is different between T and I and this implies that the trend of the number of experimental runs $M_k^{r/i}$ as a function of k will affect the maximum rate of estimation. If we choose only $k = 1$ and $M_{k=1}^r = M_{k=1}^i$, we see that $\delta^2 \geq \frac{1}{T}$ which is the sampling noise limit.

Clearly the biggest value for $I(\phi)$ for a given T is obtained when choosing a single largest possible $k = K$ so that $T = KM_K$ and $I(\phi) = K^2 M_K = T^2/M_K$. This implies the Heisenberg limit, i.e. $\delta \geq cT^{-1}$ where c is some constant. If we however make the 'dense signal' choice, that is, $M_k^r = M_k^i = M$ for $k = 0, 1 \ldots K$, then

$$I(\phi) = \frac{M}{3} K(K+1)(1+2K), \tag{2.23}$$

while the total quantum cost is $T = MK(K+1)$. To leading order in K we then have $\delta \geq I(\phi)^{-\frac{1}{2}} = \sqrt{\frac{3}{2}} M^{\frac{1}{4}} T^{-\frac{3}{4}}$, which is the dense signal limit. □

Remark: We note that a randomized version of the dense signal choice can potentially scale in Heisenberg-limited fashion [69]. In this method, one would draw k at random from $1, \ldots, K$ and repeat this S times to generate random variables $k_1, \ldots, k_S$ and repeat experiments with fixed M for each such k_i. With the right choice of $S \times M = \text{polylog}(K)$, one can argue, using the Cramer-Rao lower bound analysis above, that the expected error $\mathbb{E}(\delta) \geq \frac{\text{polylog}(\mathbb{E}(T))}{\mathbb{E}(T)}$ where $\mathbb{E}(T)$ is the expected quantum cost.

2.5 Heisenberg-limited algorithm for a single phase

Clearly, the sampling noise limit can be achieved by choosing $k = 1$ in the circuits of Fig. 2.2. However, one can ask whether the dense signaling limit or the Heisenberg limit can also be achieved, in particular when we demand that the efficient classical post-processing is efficient. For the dense signaling limit one needs a classical method to process the estimations of $g(k)$ at $k = 0, 1, \ldots, K$ to estimate $\tilde{\phi}$. Using perturbation theory in the noise, the matrix pencil method has been claimed to achieve this for a single eigenvalue [79].

Achieving the Heisenberg limit is non-trivial due to phase aliasing: the phase function $g(k)$ obtained by the experiments using U^k remains invariant if any phase ϕ is shifted by $\frac{2\pi}{k}$. This implies that a strategy of estimating ϕ from a single point $g(k)$ at large k will fail unless ϕ is already known to sit within a window of width $\frac{2\pi}{k}$. This issue may circumvented

by sampling $g(k)$ at multiple orders $k = 2^d$ to gradually zoom in on ϕ. To get Heisenberg scaling, one takes the number of samples M and thus the confidence to depend on the order, so that the most significant bits of ϕ are determined with highest confidence. Methods for doing this were first introduced in Ref. [1], and improved in Ref. [2] for the purpose of gate calibration. Here we state the result:

Algorithm 2.5.1 (Heisenberg Algorithm For Single Eigenvalue [1, 2])**.** *Given an targeted error $\delta > 0$, and numbers $\alpha, \gamma \in \mathbb{Z}^+$. The Heisenberg algorithm outputting an estimate $\tilde{\phi}$ for ϕ proceeds as follows:*

1. *Fix $d_f = \lceil \log_2(1/\delta) \rceil$.*
2. *For $d = 0, 1 \ldots, d_f$:*
   (a) *Use the* PFE *subroutine, Def. 2.3.3, circuits in Fig. 2.2, to obtain an estimate $\tilde{g}(k)$ of $g(k)$ for $k = 2^d$ using $M_d = \alpha + \gamma(d_f + 1 - d)$ repetitions of both experiments.*
   (b) *Compute $\tilde{\theta}^{(d)} = \mathrm{Arg}[\tilde{g}(2^d)] \in [0, 2\pi)$*
   (c) *If $d = 0$, set $\tilde{\phi}^{(0)} = \tilde{\theta}^{(0)}$.*
   (d) *Else, set $\tilde{\phi}^{(d)}$ to be the (unique) number in $[\tilde{\phi}^{(d-1)} - \frac{\pi}{2^d}, \tilde{\phi}^{(d-1)} + \frac{\pi}{2^d}]$ such that*
   $$2^d \tilde{\phi}^{(d)} = \tilde{\theta}^{(d)} \mod 2\pi. \tag{2.24}$$
3. *Return $\tilde{\phi} = \tilde{\phi}^{(d_f)}$ as an estimate for ϕ.*

It was proved in [2] that for some choices of α and γ the root-mean-square error δ on the final estimate $\phi^{(d_f)}$ is at most cT^{-1} for a constant c and total cost $T = 2\sum_{d=0}^{d_f} 2^d M_d$, thus reaching the Heisenberg limit.

Chapter 3

Heisenberg-limited algorithm for multiple phases

So far we have discussed the phase estimation of a single eigenvalue, when the system register is prepared in the eigenstate. However, in realistic setting this is not possible – preparing exact eigenstates is typically very costly on a quantum device, and something we would want to avoid. In this chapter we consider the case where the initial state has significant overlap with multiple eigenstates, and aim to estimate all the corresponding eigenphases.

In Sec. 3.1 we properly define a multi-eigenvalue phase estimation problem (with assumptions). We state the algorithm that can accomplish this task (Alg. 3.1.4) without the optimal scaling, that we will use as a subroutine. In Section 3.2 we present our Heisenberg-limited algorithm (Alg. 3.2.1). We discuss a critical aliasing problem to be solved which occurs when estimating multiple eigenvalues. We show that an adaptive choice for k in $g(k)$ can solve this issue and we prove that such adaptive choice always exists (Lem. 3.2.2). We prove that our algorithm achieves Heisenberg-limited scaling (Thm. 3.2.5), which is the main result of this work. In Sec. 3.3 we numerically compare this rigorous implementation to an implementation using the matrix pencil method, used in Ref. [19], for which we are unable to find a rigorous proof of Heisenberg scaling.

3.1 Defining the task of multiple-eigenvalue phase estimation

In this section we define the goal of estimating multiple eigenvalue phases of some unitary U. When the input state $|\Psi\rangle$ is supported on multiple eigenstates, choosing a single k does not suffice, simply since knowing Eq. (2.13) at a single point k does not give a unique solution $\{A_j, \phi_j\}$ [19]. A simple way to circumvent this problem is thus to estimate densely — estimating $g(k)$ for all integers $0 \leq k \leq K$ would allow us to fit up to $O(K)$ (ϕ_j, A_j) pairs. However, this does not saturate the Heisenberg limit as shown in Theorem 2.4.1, hence we need to come up with a different method.

Separate from this, the full eigenspectrum of an arbitrary N-qubit unitary U has up to 2^N unique values, making it impossible to describe in polynomial time in N. In addition, the spectral content of the input state $|\Psi\rangle$ could be very dense, with many eigenvalues clustered together instead of separated by gaps, and the probability for these eigenvalues, A_j, could be sharply concentrated or uniformly spread. To deal with general input states, Ref. [3] thus formulated the quantum eigenvalue estimation problem (QEEP): instead of estimating individual phases, the focus is on estimating the spectral function $A(\phi)$ in Eq. (2.14) with some resolution.

Definition 3.1.1 (Quantum Eigenvalue Estimation Problem, QEEP)**.** *Let $A(\phi)$ be the spectral function defined in Eq.* (2.14) *for a unitary U and $|\Psi\rangle$. Given an error bound $\epsilon > 0$ and a confidence bound $p > 0$, and a set of nonnegative (approximate indicator) functions $f^l(\phi)$ for $\phi \in [0, 2\pi)$ for $l = 0, \ldots L-1$, $L = \lceil \frac{2\pi}{\epsilon} \rceil$, where $f^l(.)$ has support on only the interval bin*

$$\mathcal{V}_l = [(l-1)\epsilon, (l+1)\epsilon]_T, \tag{3.1}$$

and $f^l(\phi) + f^{(l-1)}(\phi) = 1$ for all $\phi \in \mathcal{V}_l \cap \mathcal{V}_{l-1}$. Assuming access to the PFE *subroutine, Def. 2.3.3, the goal is to output an approximation $\tilde{b}_l$ for $l = 0, \ldots, L-1$ to the integral*

$$b_l = \int_0^{2\pi} d\phi A(\phi) f^l(\phi), \tag{3.2}$$

which satisfies

$$\sum_{l=0}^{L-1} |\tilde{b}_l - b_l| \leq \epsilon, \tag{3.3}$$

with probability at least p.

Note that the bins $\mathcal{V}_l$ have width 2ϵ and overlap on a region of width ϵ and $\sum_{l=0}^{L-1} b_l = 1$.

3.1.1 Methods of dense signal phase estimation

For estimating multiple phases there are two dense signal methods using estimates of $g(k)$ with $k = 0, 1, \ldots, K$. These are the matrix pencil method first studied for QPE in Ref. [19], see Algorithm 3.3.1, and the 'time series analysis' proposed in Ref. [3] to solve the QEEP problem above. We can examine the scaling of the total cost in light of the dense signal limit of Theorem 2.4.1. Ref. [3] proved the following

Theorem 3.1.2 (QEEP Algorithm [3])**.** *One can solve the QEEP problem in Definition 3.1.1 with $\{f^l(.)\}$ a set of 'bump' functions*

$$f^l(\phi) = \frac{2a}{\epsilon} \int_{l\epsilon-\frac{\epsilon}{2}}^{l\epsilon+\frac{\epsilon}{2}} \exp\left\{ -\left[1 - \frac{4}{\epsilon^2}(\phi - \phi')^2\right]^{-1} \right\} d\phi', \tag{3.4}$$

with normalization constant $a \approx 2.252$, using PFE *in Def. 2.3.3 with $k = 0, \ldots, K-1$ with $K = O\left(\epsilon^{-1} \ln^2(\epsilon^{-1})\right)$. The total quantum cost is $T = O(|\ln(1-p)|\epsilon^{-6})$.*

We note that the approximate indicator functions $f^l(.)$ are designed to have a quickly decaying Fourier series, which is required to achieve polynomial-time scaling. We also refer the reader to Ref. [71], which has extended the result by relaxing the requirement that $f^l(\phi) + f^{(l-1)}(\phi) = 1$ on the interval $\mathcal{V}_l \cap \mathcal{V}_{l-1}$. The idea of the QEEP algorithm is as follows. Since $b_l = \sum_j A_j f^l(\phi_j)$, using Eq. (2.14), periodically extending $f^l(\phi)$ beyond $[0, 2\pi)$ and Fourier decomposing gives $b_l = \sum_j A_j \sum_{k\in\mathbb{Z}} e^{ik\phi_j} \tilde{f}^l(k) = \sum_{k\in\mathbb{Z}} g(k)\tilde{f}^l(k)$. At the same time, the fact that $f^l(.)$ is an indicator function ensures that $b_l \approx \sum_{\phi_j \in \mathcal{V}_l} A_l$. Thus knowledge of $g(k)$ for a range of k allows one to estimate the weights b_l. The requirement to estimate the spectral function to within a 1-norm ϵ, Eq. (3.3), is very stringent, hence the scaling of T with error ϵ is quite costly, $T = O(\epsilon^{-6})$. It is possible that one can improve the scaling by re-examining the analysis in [3].

Given estimates of $g(k)$ for $k = 0, \ldots, K$ (dense signal), one can ask for error bounds of processing this data to estimate phases ϕ_j and their associated probabilities A_j using the matrix pencil technique. Bounding the error of the matrix pencil method naturally requires a gap Δ between these phases, namely a necessary condition to get convergent estimates for ϕ_j and A_j is that $K \geq 1/\Delta$ [80]. We do however not want to impose the presence of a gap in this work.

Here is our precise definition of the problem to be solved and achieving the Heisenberg limit for multiple eigenvalues requires solving this problem with a total quantum cost $T = O(\delta^{-1})$:

Definition 3.1.3 (Multiple eigenvalue estimation problem)**.** *Fix an error bound $\delta > 0$, a probability bound A, and a number of phases $n_\phi > 0$. For a unitary U and state $|\Psi\rangle$, we assume that $A_j > A$ for exactly n_ϕ phases ϕ_j and $A_j = 0$ for all other phases so that $n_\phi \leq A^{-1}$. Let $g(k) = \sum_j A_j e^{ik\phi_j}$ be the phase function in Def. 2.3.1 and assume access to the PFE quantum subroutine in Def. 2.3.3 for any $k \in \mathbb{R}$. The task is to output a set $\{\tilde{\phi}_l\}$ of n_ϕ or fewer estimates of the phases $\{\phi_j\}$ such that, if we take the closest estimate $\tilde{\phi}_j^{(\text{closest})}$ of each phase ϕ_j,*

$$\tilde{\phi}_j^{(\text{closest})} = \arg\min_{\tilde{\phi}_l}(|\tilde{\phi}_l - \phi_j|_T), \tag{3.5}$$

the accuracy error

$$\delta_j = \sqrt{\sum_{\mathbf{x}} \mathbb{P}\left(\mathbf{x}|\{\phi_l, A_l\}\right) \left|\tilde{\phi}_j^{(\text{closest})}(\mathbf{x}) - \phi_j\right|_T^2}, \tag{3.6}$$

is bounded by $\delta_j \leq \delta$ for all $j = 1, \ldots, n_\phi$.

Remarks: Def. 3.1.3 allows us the freedom to assign a single estimate to multiple phases when calculating the final mean-square-error.

The accuracy error that we target is uses the distance measure $|.|_T$ – a natural distance on the circle that respects the 2π periodicity. The precise definition of this metric and some of its properties that are used in the proofs later in this chapter are given in App A.

We intend to solve the problem considered in Def. 3.1.3 by identifying phases from the output of the QEEP problem in Def. 3.1.1 that have probability above the minimum A. To extend this to the Heisenberg limit we will use this QEEP algorithm in Theorem 3.1.2 for a unitary $V = U^k$ with exponentially growing k, thus with eigenphases

$$\theta_j = k\phi_j \mod 2\pi. \tag{3.7}$$

Hence in Algorithm 3.1.4 and Lemma 3.1.5 below we refer to estimating eigenvalue phases θ of such $V = U^k$.

Algorithm 3.1.4 is an extension to the QEEP algorithm allowing us to output maximally n_ϕ phases by solving the QEEP problem. Lemma 3.1.5

then states what error is obtained on the estimates for θ when the QEEP algorithm 3.1.2 succeeds with probability p.

Let us first motivate Algorithm 3.1.4. One may identify phases with sufficient probability in the output of the QEEP algorithm as the bins l with $b_l > b_{\text{cutoff}}$ with b_l in Eq. (3.2). Then to convert this into an estimate of a phase θ_j, for each such bin we could yield an estimate ϵl in the middle of the corresponding bin $\mathcal{V}_l$.

We calculate appropriate values of b_{cutoff} and the QEEP error ϵ to guarantee an estimate for each θ_j with $A_j > A$ with a provable confidence, and to guarantee no estimate in the absence of any θ_j. Def. 3.1.1 states that when there exists such a $\theta_j \in \mathcal{V}_l \cap \mathcal{V}_{l-1}$, we are guaranteed with confidence p that $\tilde{b}_l + \tilde{b}_{l-1} + \epsilon > A$ (as $b_l + b_{l-1} > A$). To guarantee that at least one of $\tilde{b}_l$ or $\tilde{b}_{l-1}$ is larger than b_{cutoff} with the same confidence, we thus require $b_{\text{cutoff}} \leq (A - \epsilon)/2$.

Similarly, Def. 3.1.1 states that when there exists no $\theta_j \in \mathcal{V}_l$ with $A_j > 0$, we are guaranteed with confidence p that $b_l < \epsilon$. To prevent a spurious estimate in this case, we require $b_{\text{cutoff}} \geq \epsilon$. Solving this to maximise ϵ (which minimizes the cost of the QEEP routine) yields $b_{\text{cutoff}} = \epsilon = A/3$.

A further small complication exists in solving the problem posed in Def. 3.1.3: we require that one outputs at most n_ϕ phases. This will be satisfied if we can guarantee at most one phase estimate per θ_j with $A_j > A$, as we know there are $n_\theta = n_\phi$ such estimates. As the bins $\mathcal{V}_l$ (Def. (3.1)) overlap, a phase θ_j may participate in up to two neighbouring bins — corresponding to amplitudes $b_l, b_{l+1} > A/3$. To ensure that this does not result in two estimates being generated, one could take all contiguous sets $b_{l_1}, b_{l_1+1}, \ldots, b_{l_2} > A/3$ and prune away every second index l. In doing this we need to respect the periodicity of the $\mathcal{V}_l$: $\mathcal{V}_{L-1} \cap \mathcal{V}_0 \neq \emptyset$, so these contiguous sets may wrap around the circle. Pruning every second index when starting from the middle of one of these contiguous sets may result in two neighbouring $l, l+1$ being removed, which is not what we desire. Instead, in the following pseudocode, after generating the set of all l with sufficient b_l, we find the first gap (in l) between these regions (corresponding to the first $b_l < A/3$). We then iterate (from this point $l_{\min}$ to $L-1$ and then from 0 to $l_{\min}$) over the b_l, and remove each l from our set if $b_{l-1} > A/3$ and $l-1$ was not itself removed.

Algorithm 3.1.4 (Conservative QEEP Eigenvalue Extraction)**.** *Fix a probability bound A, an error bound $0 < \epsilon < \frac{A}{3}$, and a confidence bound $0 < p < 1$. Assume access to a QEEP Algorithm 3.1.2 for a unitary V. Define $+_L$ and $-_L$ as addition and subtraction modulo L (so $0 -_L 1 = L - 1$). The algorithm proceeds as follows:*

1. *Use the QEEP subroutine with error ϵ, Alg. 3.1.2, and confidence p to generate an estimate $\tilde{b}_l$ for b_l as defined in Eq.* (3.2)
2. *Construct the set*
$$S = \{l \in \{0, \ldots, L-1\} | \tilde{b}_l \geq A/3\}. \tag{3.8}$$
3. *Find the smallest $l \in \{0, \ldots, L\}$ with $l \notin S$ and call it $l_{\min}$.*
4. *For $l' = l_{min}, \ldots, l_{min} +_L (L-1)$:*
   (a) *if $l' \in S$ and $l' -_L 1 \in S$, remove l' from S.*
5. *Return the set $\{\tilde{\theta}_l = l\epsilon\}_{l \in S}$ as a set of estimates of eigenphases of V.*

The following Lemma then relates the performance of Alg. 3.1.4 to the performance of the QEEP subroutine. Here $\{\theta_j\}$ is an ordered list of n_ϕ phases, while $\{\tilde{\theta}_l\}$ is an (ordered) list of at most n_ϕ phases.

Lemma 3.1.5. *Fix a confidence bound $0 < p < 1$, a probability bound A, a number of phases $n_\theta \geq A^{-1}$, and an error bound $0 < \epsilon < \frac{A}{3}$. Let $g(k) = \sum_j A_j e^{ik\theta_j}$ be the phase function Def. 2.3.1 for a unitary V. Let $\{\tilde{\theta}_l\}$ be a set of estimates of $\{\theta_j\}$ generated by Alg. 3.1.4 with error ϵ and confidence bound p. With probability at least p, the following statements are true:*

1. *For each phase θ_j with $A_j > 0$, there exists at least one estimate $\tilde{\theta}_l$ such that $|\theta_j - \tilde{\theta}_l|_T \leq 2\epsilon$.*
2. *For each estimate $\tilde{\theta}_l$ there exists at least one phase θ_j with $A_j > 0$ such that $|\theta_j - \tilde{\theta}_l|_T \leq 2\epsilon$.*
3. *The number of estimates $|\{\tilde{\theta}_l\}| \leq n_\theta$.*

Proof. Our proof follows by showing that the output from Alg. 3.1.4 satisfies these statements whenever Eq. (3.3) holds. This yields our confidence bound as Eq. (3.3) holds with probability p by Def. 3.1.1.

To see that statement 2 holds when Eq. (3.3) is satisfied, note that if $\mathcal{V}_l$ contains no phases θ_j with $A_j > A$ and Eq. (3.3) is satisfied, $\tilde{b}_l < \epsilon < A/3$, and l will not be added to the set S in Alg. 3.1.4. This implies that when Eq. (3.3) holds, if $l \in S$ there exists some $\theta_j \in \mathcal{V}_l$ with $A_j > A$, in which case $|\theta_j - \tilde{\theta}_l|_T = |\theta_j - \epsilon l|_T \leq 2\epsilon$. To see that statement 3 holds when Eq. (3.3) is satisfied, note that $\theta_j \in \mathcal{V}_l \cap \mathcal{V}_{l+_L 1}$ for exactly one l (and $\theta_j \notin \mathcal{V}_m$ for $m \neq l, l +_L 1$). Then, when Eq. (3.3) holds, $\tilde{b}_l + \tilde{b}_{l+_L 1} > 2A/3$, so

$\max(\tilde{b}_l, \tilde{b}_{l+_L 1}) > A/3$, and either l, $l +_L 1$ or l and $l +_L 1$ will be added to the set S during step 2 of Alg. 3.1.4 for each phase θ_j. Then, step 4 of Alg. 3.1.4 will remove $l +_L 1$ if l remains in S, so each phase θ_j can contribute to only one final estimate $\tilde{\theta}_l = l\epsilon$, and the number of estimates is bounded from above by the number of phases.

To see that statement 1 holds, we use the point in the previous paragraph that, when Eq. (3.3) is satisfied, each phase θ_j with $A_j > A$ adds either l, $l +_L 1$, or l and $l +_L 1$ to the set S during step 2. of Alg. 3.1.4. Then in step 4. of Alg. 3.1.4, l is removed from S only if $l -_L 1$ remains in S, and $l +_L 1$ is removed from S only if l remains in S. This implies that the distance from θ_j to an estimate is bounded by

$$\max_{\theta_j \in \mathcal{V}_l \cap \mathcal{V}_{l+_L 1}} \max_{l'=l-_L 1, l, l+_L 1} |\theta_j - \epsilon l'|_T = \epsilon(l +_L 1) - \epsilon(l -_L 1) = 2\epsilon, \quad (3.9)$$

as required. □

3.2 Multiple eigenvalues: multi-order estimation and the phase matching problem

To achieve Heisenberg-limited scaling for multiple phases, we combine the dense signal algorithms of the previous section which can resolve multiple phases with the single-phase Heisenberg limited algorithm, Algorithm 2.5.1, which achieves the correct scaling.

A natural way to achieve such combination is to estimate phases $\{\theta_j^{(d)}\}$ of U^{2^d} for multiple orders $d = 0, 1 \ldots, d_f$ via a dense signal method (e.g. Alg. 3.1.4), and then combine them in the same manner as in Algorithm 2.5.1. If we would manage to get an estimate of $\theta_j^{(d)} = \phi_j 2^d$ at each order d with error ϵ *and* be able to combine these estimates in an unequivocal manner, then reaching the Heisenberg limit for multiple phases may be feasible. Note that the error in the final d_fth estimate in this case would be $\delta \sim \epsilon/2^{d_f}$; one may achieve arbitrarily small δ for fixed ϵ by thus making d_f arbitrarily large. This allows us to use (possibly non-optimal) routines such as the QEEP algorithm since the scaling with ϵ does not propagate to a scaling in δ for a sufficiently small ϵ.

However, this may not be feasible when we use only U^{2^d} for increasing d. Consider the binary expansion of $\phi_j = 2\pi \times 0.b_1^j b_2^j \ldots$ with bits $b_i^j = 0, 1$. Consider two phases with probabilities $A_j \geq A$ which differ in their most significant bits, are identical in a next set of bits and differ again

in lesser significant bits. Based on using the lowest d, we estimate these phases as different, hence we keep two separate estimates. However, for somewhat larger k, we get identical $\theta_j^{(d)}$ estimates as there is no sensitivity to the initial differing bit string segment and very little sensitivity to the least significant bits. Hence we improve the separate estimates with this information in identical manner. However, at some point we reach a d such that we measure two different $\theta_j^{(d)}$ again, but how do we match these two different estimates to the previous estimates and avoid swapping the last bit string segment between the phases?

Instead, we will not focus on the estimation of subsequent binary digits of the phases ϕ_j, but we will estimate the eigenphases of $V = U^{k_d}$ for $k_d = \prod_{d'=1}^{d} \kappa_d$ with $\kappa_d \geq 2$ a, possibly non-integer, multiplier. We can make use of non-integer κ_d efficiently by virtue of Lem. 2.3.2. Still this algorithm needs a means of associating the dth order estimates $\tilde{\theta}_j^{(d)}$ with estimates $\{\tilde{\phi}_j^{(d)}\}$ made at previous orders, and as it turns out this requires an adaptive strategy for choosing the next multiplier κ_d in Alg. 3.2.1. A key part of this scheme is that we need to determine κ_d based on only the estimates $\tilde{\phi}_j^{(d-1)}$ from the previous round. Although this scheme requires some classical processing of the experimental data before the experiment is finished, it is not an adaptive scheme in the same sense as iterative QPE [8], as we do not require feedback within the coherent lifetime of a single experiment.

The generalization from estimating U^{2^d} to U^{k_d} for $k_d \in \mathbb{R}$ presents one small additional complication. In order to prove bounds on the estimation at each order we will require invoking Lemma A.0.2. However, this requires that our phases ϕ_j satisfy Eq. (A.3) (unless $k_d \in \mathbb{N}$). If a phase ϕ_j does not satisfy Eq. (A.3), one can construct a situation where two corresponding estimates $\tilde{\phi}_j^{(d)}$ are found on either side of the branch cut at 2π, and where we cannot guarantee that our algorithm would choose the 'correct' one (without knowledge of the hidden ϕ_j). To solve this issue, we note that one may shift the phases of U by a constant χ by performing phase estimation on $Ue^{-i\chi}$ instead of U. This need not even be done on the quantum device, as one simply multiplies estimates of $g(k)$ by $e^{-ik\chi}$. As we assume the existence of only n_ϕ phases, we can always find some $Ue^{i\chi}$ with phases in some window $[\phi_{\min}, \phi_{\max})$ with $\phi_{\min} \geq \frac{\pi}{k}$, $\phi_{\max} \leq \frac{\pi(2\lfloor k \rfloor - 1)}{k}$ when $k \geq 3n_\phi$. This will allow us to invoke Lem. A.0.2 to match estimates of eigenphases of $Ue^{i\chi}$ and estimates of eigenphases of $(Ue^{i\chi})^k$ as we require. We also note that the above issue can be circumvented when

$U = e^{iHt}$ by a suitable choice of t.

3.2.1 Heisenberg-limited algorithm for multiple phases

We now describe our Heisenberg-limited phase estimation algorithm. This algorithm targets a final error $\delta = O(\delta_c)$, where δ_c is a fixed input to the algorithm itself (We will calculate the constant of proportionality in the proof of Theorem 3.2.5). The Heisenberg limit will be achieved by making this δ_c smaller while keeping the error ϵ of the phase extraction subroutine, Alg. 3.1.4, constant.

Algorithm 3.2.1. *[Adaptive multi-order phase estimation algorithm] We assume access to the conservative QEEP eigenvalue extraction algorithm, Alg. 3.1.4 for a unitary $V = U^k$ (for arbitrary $k > 0 \in \mathbb{R}$), and an initial state $|\Psi\rangle$. Fix a final error δ_c, a probability bound A, a number of phases $n_\phi \leq A^{-1}$, and error parameters ϵ_0 and ϵ bounded as*

$$\epsilon_0 \leq \epsilon_{\text{crit},0} \equiv \frac{2\pi}{300 n_\phi^4} \tag{3.10}$$

and

$$\epsilon \leq \epsilon_{\text{crit}} \equiv \frac{2\pi}{300 n_\phi^2}. \tag{3.11}$$

Let the confidence parameter p_d be

$$p_d = 1 - e^{-\alpha} \left(\frac{k_d \delta_c}{\pi} \right)^\gamma, \tag{3.12}$$

given some real numbers $\alpha > 0$ and $\gamma > 2$ (which can be further specified in the proof of Theorem 3.2.5). The algorithm proceeds as follows:

1. *Let $d = 0$ and $k_{d=0} = 1$. Use Alg. 3.1.4 to find a set of first estimates $\{\tilde{\phi}_j^{(0)}\}$ of eigenvalues of U with error parameter ϵ_0 in Eq. (3.10), probability bound A, and confidence $p_{d=0}$ in Eq. (3.12). If this set is empty or has more than n_ϕ elements, return $\{0\}$.*

2. *Find the point $\zeta \in [0, 2\pi)$ defined by*

$$\zeta = \underset{\zeta' \in [0,2\pi]}{\arg\max} \min_j \left| \tilde{\phi}_j^{(0)} - \zeta' \right|_T, \tag{3.13}$$

i.e. ζ is the midway point in the largest gap between the phase estimates $\tilde{\phi}_j^{(0)}$. Let

$$d_\zeta = \min_j \left| \tilde{\phi}_j^{(0)} - \zeta \right|_T, \tag{3.14}$$

i.e. d_ζ is half the size of the largest gap. Shift the unitary $U \to Ue^{-i(\zeta + \frac{1}{2}d_\zeta - 8\epsilon_0)}$, $\tilde{\phi}_j^{(0)} \to \tilde{\phi}_j^{(0)} - \zeta - d_\zeta/2 + 8\epsilon_0 \mod 2\pi$.

3. *Choose $\kappa_1 = k_1$ with $k_1 \in [3n_\phi, 3n_\phi + 1]$ such that for all $\tilde{\phi}_j^{(0)} \neq \tilde{\phi}_l^{(0)}$, either*

$$|\tilde{\phi}_j^{(0)} k_1 - \tilde{\phi}_l^{(0)} k_1|_T > 4(\epsilon_0 + k_1). \tag{3.15}$$

or

$$|\tilde{\phi}_j^{(0)} - \tilde{\phi}_l^{(0)}|_T < \frac{\pi}{k_1}. \tag{3.16}$$

4. *While $k_d < \frac{2\epsilon}{\delta_c}$:*

   (a) *Set $d \to d + 1$.*

   (b) *Use Alg. 3.1.4 to find a set of estimates $\{\tilde{\theta}_l^{(d)}\}$ of eigenvalues of $V = U^{k_d}$ with error parameter ϵ in Eq.* (3.11)*, probability bound A, and confidence p_d in Eq.* (3.12)*.*

   (c) *If there exists some $\tilde{\phi}_j^{(d-1)}$ such that*

$$\min_l |k_d \tilde{\phi}_j^{(d-1)} - \tilde{\theta}_l^{(d)}|_T > 2\epsilon(1 + \kappa_d), \tag{3.17}$$

   or there exists some $\tilde{\theta}_l^{(d)}$ such that

$$\min_j |k_d \tilde{\phi}_j^{(d-1)} - \tilde{\theta}_l^{(d)}|_T > 2\epsilon(1 + \kappa_d), \tag{3.18}$$

   or the number of estimates $|\{\tilde{\theta}_l^{(d)}\}| > n_\phi$, return $\{\tilde{\phi}_j^{(d-1)} + \zeta + d_\zeta/2 - 8\epsilon_0 \mod 2\pi\}$. This is a failure mode.

   (d) *If not, for each $\tilde{\theta}_l^{(d)}$, find the estimate $\tilde{\phi}_j^{(d-1)}$ and an integer $n \in [0, k_d)$ which minimizes*

$$|\tilde{\phi}_j^{(d-1)} - (\tilde{\theta}_l^{(d)} + 2\pi n)/k_d|_T, \tag{3.19}$$

   and set $\{\tilde{\phi}_l^{(d)}\} = \{(\tilde{\theta}_l^{(d)} + 2\pi n)/k_d\}$.

(e) *If any* $\tilde{\phi}_j^{(d)} \in [0, \frac{\pi}{k_d}) \cup (\frac{\pi(2\lfloor k_d \rfloor - 1)}{k_d}, 2\pi]$, *return* $\{\tilde{\phi}_j^{(d-1)} + \zeta + d_\zeta/2 - 8\epsilon_0 \mod 2\pi\}$. *This is a failure mode.*

(f) *Choose the multiplier* $\kappa_{d+1} \in [2,3]$ *such that for all* $\tilde{\phi}_j^{(d)} \neq \tilde{\phi}_l^{(d)}$, *either*

$$|\tilde{\phi}_j^{(d)} k_d \kappa_{d+1} - \tilde{\phi}_l^{(d)} k_d \kappa_{d+1}|_T > 4\epsilon(1+\kappa_{d+1}). \tag{3.20}$$

or

$$|\tilde{\phi}_j^{(d)} - \tilde{\phi}_l^{(d)}|_T < \frac{\pi - 2\epsilon(1+\kappa_{d+1})}{k_d \kappa_{d+1}}, \tag{3.21}$$

and set $k_{d+1} = k_d \kappa_{d+1}$.

5. *Return* $\{\tilde{\phi}_j^{(d)} + \zeta + d_\zeta/2 - 8\epsilon_0 \mod 2\pi\}$.

In the rest of this section, we prove that Alg. 3.2.1 can achieve the Heisenberg limit. We note that Alg. 3.1.4 which is invoked in this algorithm assumes that the error parameter ϵ or ϵ_0 is at most $A/3 \leq 1/(3n_\phi)$ which is fulfilled by Eq. (3.10) and Eq. (3.11).

We note that the first use of the QEEP subroutine possibly needs to use a smaller error parameter, called ϵ_0, bounded by Eq. (3.10) than subsequent uses where ϵ needs to be only bounded by Eq. (3.11). This relates to a technical issue, namely $k_1 \geq 3n_\phi$ in order for Lemma C.0.1 in Appendix C and thus Lemma A.0.2 to apply. For later rounds $k_d \geq 3n_\phi$ automatically, not putting a constraint on the multiplier κ_d, and indirectly allowing to relax the region of valid choices for ϵ. The first step in proving the performance of Algorithm 3.2.1 is to show that the multipliers can be chosen in the first (step 3 in Alg. 3.2.1), and subsequent rounds (step 4f in Alg. 3.2.1), which obey the desired conditions. This is accomplished by the following Lemma which is proved in Appendix B.

Lemma 3.2.2. *Let* $\{\tilde{\phi}_j^{(0)}\} \in [0, 2\pi)$ *be a set of at most* n_ϕ *phases. Assuming Eq.* (3.10), *for a randomly chosen* $k_1 \in [3n_\phi, 3n_\phi + 1]$ *with probability at least* $1/2$, *either Eq.* (3.15) *or Eq.* (3.16) *for all* $\tilde{\phi}_j^{(0)} \neq \tilde{\phi}_l^{(0)}$. *Fix a* k_d. *Let* $\{\tilde{\phi}_j^{(d)}\} \in [0, 2\pi)$ *be a set of at most* n_ϕ *phases. Assuming Eq.* (3.11), *for a randomly chosen* $\kappa_{d+1} \in [2,3]$ *with probability at least* $3/4$, *either Eq.* (3.20) *or Eq.* (3.21) *for all* $\tilde{\phi}_l^{(d)} \neq \tilde{\phi}_j^{(d)}$.

Remarks: The probability with which a multiplier can be found which obeys the desired property is rather arbitrary in this Lemma and can be increased by choosing a smaller ϵ. Note that it is easy to verify whether

for a randomly chosen multiplier the desired conditions hold or not. The validity of this Lemma importantly does not depend on whether the phase estimates are actually accurate, it only depends on the number of phases n_ϕ. In practice, we do not generate a random multiplier κ_{d+1} through this Lemma, but simply exhaustively search for a valid κ_{d+1} starting at the maximal value.

The reason to adaptively choose the multiplier κ_{d+1} for $d = 0, \ldots$ is that two (estimated) phases in principle need to lead to separate estimates at the next order: this is expressed in Eq. (3.20). An exception to this occurs when the (estimated) phases are still close enough, as in Eq. (3.21), so that their next-order refined estimates could merge at the next order, see Fig. 3.1. Phase estimates can thus split and merge over the multiple orders. They split when sufficient accuracy is available at the next order to distinguish them, they can stay or are allowed to merge when such accuracy is not yet needed at the given order.

In what follows below we will assume, just for simplicity of the proof, that the error parameter ϵ is bounded by $\epsilon_{\text{crit},0}$ in Eq. (3.10) for all rounds, and ϵ is the same for all rounds, including the first one.

3.2.2 Bounding the error with and without failures

In this section we state and prove the two key intermediate lemmas, Lemma 3.2.3 and Lemma 3.2.4 on our way towards proving that Alg. 3.2.1 reaches the Heisenberg-limit. Together, these lemmas allow us to bound the error in Alg. 3.2.1, –assuming that the phase extraction subroutine succeeds for the first d rounds–, to within $O(\epsilon/k_d)$.

These Lemmas deal with the issue of 'aliasing' or the correct matching of new estimates with older estimates which is solved by the specific choice of κ_{d+1} in step 4f of Alg. 3.2.1, see also Fig. 3.1. It is important to note that there is no 1-1 relation between these estimates and the actual phases as the number of estimates is at most the number of phases.

Let d_f be the last order executed in Alg. 3.2.1, i.e. the last order for which we go through step 4b, construct the estimates $\{\tilde{\theta}_l^{(d_f)}\}$ and pass the tests at step 4c and 4e and output $\{\tilde{\phi}_l^{(d_f)}\}$. When none of the failure modes is encountered, d_f is set by the first k_d such that $k_d \geq \frac{\epsilon}{\delta_c}$ (since the next $k_{d+1} \geq 2\epsilon/\delta_c$ as $\kappa_{d+1} \geq 2$). Since $\kappa_d \geq 2$, we observe that

$$d_f \leq \log_2\left(\frac{2\epsilon}{\delta_c}\right). \tag{3.22}$$

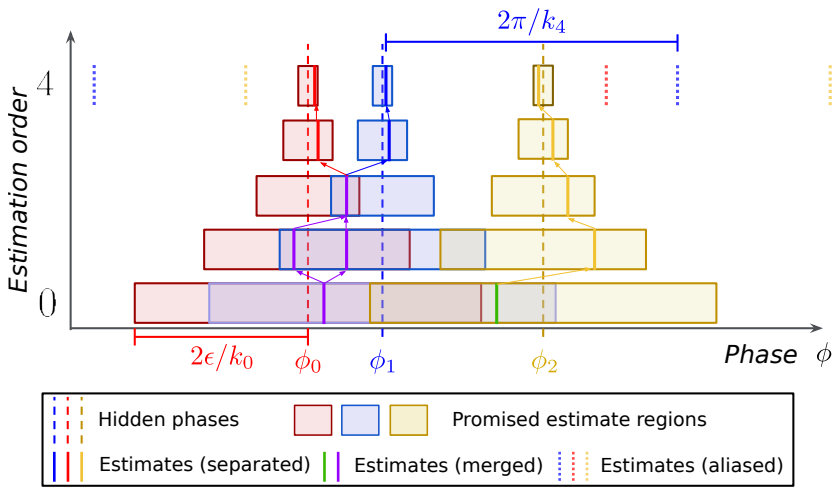

Figure 3.1: *Schematic of the execution of Alg. 3.2.1 to estimate three hidden phases, ϕ_0, ϕ_1 and ϕ_2 (dashed lines). The algorithm progresses from bottom to top as the estimation order d increases. At each order d, the phase extraction subroutine (Alg. 3.1.4) promises to return an estimate $\tilde{\theta}^{(d)}_{\to j}$ of each $\theta^{(d)}_j = k_d\phi_j \mod 2\pi$ that corresponds to an estimate $\tilde{\phi}^{(d)}_{\to j}$ (solid lines) lying within the promised estimate region about ϕ_j (coloured boxes). By matching phases at subsequent orders (arrows), the algorithm is able to converge to an ever-more accurate estimate of each ϕ_j. The phase extraction subroutine only promises that each region will contain at least one phase (and that the total number of estimates at each order is bounded by n_ϕ) - when two regions overlap, the subroutine may merge the phases to give a single estimate (green and purple lines). Estimates at subsequent orders may continue to separate and even re-merge until the regions separate, at which point the algorithm promises with high confidence a separate estimate for each hidden phase. The estimate $\tilde{\phi}^{(d)}_{\to j}$ at each order is only known $\mod (2\pi)/k_d$, leading to a set of potential aliases (dotted lines at $d = 4$) for each phase. We do not know a priori which alias is correct, and must rely on the fact that the true estimate $\tilde{\phi}^{(d)}_{\to j}$ needs to be close to a previous estimate $\tilde{\phi}^{(d-1)}_{\to j}$. By carefully choosing each k_d, we can guarantee that no alias will satisfy this condition (so long as Alg. 3.1.4 succeeds), and our phase matching will be unambiguous.*

In Corollary 3.2.3.1 we argue that when the QEEP subroutines, Alg. 3.1.4, succeed up to order d_f, we indeed never exit via these failure modes.

Lemma 3.2.3. *If each invocation of the QEEP subroutine, Alg. 3.1.4, succeeds in Alg. 3.2.1 up to order d_f, then in this last round d_f in step 4d it holds that*

- *(Property 1a) For every phase ϕ_j there exists an estimate $\tilde{\phi}^{(d_f)}_l$ such that*

$$|\phi_j - \tilde{\phi}_l^{(d_f)}|_T \leq 2\epsilon/k_{d_f}.$$

- *(Property 1b) For every estimate $\tilde{\phi}_l^{(d_f)}$ there exists a phase ϕ_j such that* $|\phi_j - \tilde{\phi}_l^{(d_f)}|_T \leq 2\epsilon/k_{d_f}$.

Proof. We prove this Lemma by induction. Consider the first round $d = 0$ ($k_{d=0} = 1$), i.e. step 1 of Alg. 3.2.1. If the QEEP subroutine, Alg. 3.1.4, succeeds (with probability p_0) then Lemma 3.1.5 holds, namely for each ϕ_j there exists an estimate $\tilde{\phi}_l^{(0)}$ such that

$$|\phi_j - \tilde{\phi}_l^{(0)}|_T \leq 2\epsilon. \tag{3.23}$$

and for each estimate $\tilde{\phi}_l^{(0)}$ there exists at least one ϕ_j such that

$$|\phi_j - \tilde{\phi}_l^{(0)}|_T \leq 2\epsilon. \tag{3.24}$$

Hence the statement to be proven holds at $d = 0$. Now consider step 2 of Alg. 3.2.1 and invoke Lemma C.0.1 for which the assumptions are fulfilled by Eqs. (3.23),(3.24). This implies that with the choice of $k_1 \geq 3n_\phi$ in step 3 in Alg. 3.2.1 the shifted phases and their 0th-order estimates obey the technical condition in Lemma A.0.2 and we can use Eq. (A.4). In the next steps we work with these shifted phases but for simplicity we don't use any new notation.

Now assume the statement to be proven holds at order d i.e. let $\{\tilde{\phi}_l^{(d)}\}$ be a set of at most n_ϕ estimates of the phases $\{\phi_j\}$ with

- (Assumption 1a) For every phase ϕ_j there exists an estimate $\tilde{\phi}_l^{(d)}$ such that $|\phi_j - \tilde{\phi}_l^{(d)}|_T \leq 2\epsilon/k_d$.
- (Assumption 1b) For every estimate $\tilde{\phi}_l^{(d)}$ there exists a phase ϕ_j such that $|\phi_j - \tilde{\phi}_l^{(d)}|_T \leq 2\epsilon/k_d$.

Note that these assumptions certainly imply that one can apply Lemma A.0.2 to the estimates $\tilde{\phi}_l^{(d)}$. That is, given that the real phases ϕ_j are $2\epsilon/k_d$ close to these estimates and that the (shifted) ϕ_j obey Eq. (C.2), it implies that Eq. (A.4) can be used with $k \geq 3n_\phi$ (which is the case for all rounds $d \geq 1$).

We consider the QEEP subroutine, Alg. 3.1.4, with a given choice of κ_d obeying the conditions in step 3 (for $d = 1$) and 4f (for higher d), executed

in step 4b with confidence p_d. In the math below we refer to conditions on $\kappa_{d>1}$, namely Eq. (3.20) and Eq. (3.21), but the conditions on κ_1 in Eq. (3.15) and Eq. (3.16) are of identical form (so we don't make a separate argument for the $d = 0 \to d = 1$ induction step).

Let thus $\{\tilde{\theta}_l^{(d+1)}\}$ be a set of estimates of the eigenphases $\{\theta_j^{(d+1)}\}$ of $U^{k_{d+1}}$ corresponding to the set $\{\phi_j\}$, that is,

$$\theta_j^{(d+1)} = k_{d+1}\phi_j \mod 2\pi. \tag{3.25}$$

and $k_{d+1} = k_d\kappa_{d+1}$. By assuming that Alg. 3.1.4 succeeds we can invoke Lemma 3.1.5, namely

- (Assumption 2a) For every phase $\theta_j^{(d+1)}$ there exists an estimate $\tilde{\theta}_l^{(d+1)}$ such that $|\theta_j^{(d+1)} - \tilde{\theta}_l^{(d+1)}|_T \leq 2\epsilon$.
- (Assumption 2b) For every estimate $\tilde{\theta}_l^{(d+1)}$ there exists a phase $\theta_j^{(d+1)}$ such that $|\theta_j^{(d+1)} - \tilde{\theta}_l^{(d+1)}|_T \leq 2\epsilon$.

To prove the induction step, we thus need to show that the set $\tilde{\phi}_j^{(d+1)}$ generated by step 4d of Alg. 3.2.1 satisfies the following two properties

- (Property 1a) For every phase ϕ_j there exists an estimate $\tilde{\phi}_l^{(d+1)}$ such that $|\phi_j - \tilde{\phi}_l^{(d+1)}|_T \leq 2\epsilon/k_{d+1}$.
- (Property 1b) For every estimate $\tilde{\phi}_l^{(d+1)}$ there exists a phase ϕ_j such that $|\phi_j - \tilde{\phi}_l^{(d+1)}|_T \leq 2\epsilon/k_{d+1}$.

First consider Assumption 2a. Assumption 2a implies that for every phase ϕ_j there exists a $\tilde{\theta}_l^{(d+1)}$ such that

$$|k_{d+1}\phi_j - \tilde{\theta}_l^{(d+1)}|_T \leq 2\epsilon. \tag{3.26}$$

In this proof we will use the label $l =\!\!\to j$ for this $\tilde{\theta}_l^{(d+1)}$ associated with ϕ_j. Thus, also using Eq. (A.4), the last inequality is equivalent to

$$\min_{n\in\{0,\ldots,\lfloor k_{d+1}\rfloor-1\}} |\phi_j - (\tilde{\theta}_{\to j}^{(d+1)} + 2\pi n)/k_{d+1}|_T \leq \frac{2\epsilon}{k_{d+1}}, \tag{3.27}$$

with

$$n_{j,\to j}^{\text{ideal}} = \operatorname*{arg\,min}_{n\in\{0,\ldots,\lfloor k_{d+1}\rfloor-1\}} |\phi_j - (\tilde{\theta}_{\to j}^{(d+1)} + 2\pi n)/k_{d+1}|_T. \tag{3.28}$$

Similarly, by Assumption 1a, there is some $\tilde{\phi}^{(d)}_{l=\to j}$ which is $2\epsilon/k_d$-close to ϕ_j, again using a label which shows this association.

Consider the optimization at step 4d in Alg. 3.2.1

$$\xi_l = \min_j \xi_{j,l},\ \xi_{j,l} \equiv \left|\tilde{\phi}^{(d)}_j - (\tilde{\theta}^{(d+1)}_l + 2\pi n_{jl})/k_{d+1}\right|_T \tag{3.29}$$

in Eq. (3.19) with

$$n_{j,l} = \underset{n\in\{0,\ldots,\lfloor k_{d+1}\rfloor -1\}}{\arg\min} \left|\tilde{\phi}^{(d)}_j - (\tilde{\theta}^{(d+1)}_l + 2\pi n)/k_{d+1}\right|_T,\ \ n_l = \underset{n_{j,l}}{\arg\min}\, \xi_{j,l}. \tag{3.30}$$

The goal is thus to prove that for each ϕ_j, using the corresponding $\tilde{\theta}^{(d+1)}_{\to j}$, we have $n_{\to j} = n^{\text{ideal}}_{j,\to j}$ which directly implies Property 1a.

We can bound using Eq. (A.2) and then Eq. (A.4), Assumptions 1a and 2a and optimality of $n_{\to j,\to j}$

$$\begin{aligned}
\xi_{\to j,\to j} &= \left|\tilde{\phi}^{(d)}_{\to j} - (\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n_{\to j,\to j})/k_{d+1}\right|_T \\
&\le \left|\tilde{\phi}^{(d)}_{\to j} - \phi_j\right|_T + \left|\phi_j - (\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n^{\text{ideal}}_{j,\to j})/k_{d+1}\right|_T \\
&\le \frac{2\epsilon}{k_d} + \frac{1}{k_{d+1}}\left|k_{d+1}\phi_j - \tilde{\theta}^{(d+1)}_{\to j}\right|_T \\
&= \frac{2\epsilon}{k_d} + \frac{1}{k_{d+1}}\left|\theta^{(d+1)}_j - \tilde{\theta}^{(d+1)}_{\to j}\right|_T \le \frac{2\epsilon(1+\kappa_{d+1})}{k_{d+1}}.
\end{aligned} \tag{3.31}$$

Now if Eq. (3.20) holds for some other $m \not\to j$, we claim on the other hand that

$$\xi_{m,\to j} > \frac{2\epsilon(1+\kappa_{d+1})}{k_{d+1}}, \tag{3.32}$$

hence matching $\theta^{(d+1)}_{\to j}$ with such $\tilde{\phi}^{(d)}_m$, with $m \not\to j$ is non-optimal and will not be chosen in the Algorithm. To indeed see that Eq. (3.20) implies

Eq. (3.32), we can calculate

$$\begin{aligned}
\frac{4\epsilon(1+\kappa_{d+1})}{k_{d+1}} &< \frac{1}{k_{d+1}}\left|k_{d+1}\tilde{\phi}^{(d)}_{\to j} - k_{d+1}\tilde{\phi}^{(d)}_{m}\right|_T \\
&\leq \frac{1}{k_{d+1}}\left|k_{d+1}\tilde{\phi}^{(d)}_{\to j} - \tilde{\theta}^{(d+1)}_{\to j}\right|_T + \frac{1}{k_{d+1}}\left|\tilde{\theta}^{(d+1)}_{\to j} - k_{d+1}\tilde{\phi}^{(d)}_{m}\right|_T \\
&\leq \frac{2\epsilon(1+\kappa_{d+1})}{k_{d+1}} \\
&\quad + \min_{n\in\{0,\dots,\lfloor k_{d+1}\rfloor-1\}}\left|\tilde{\phi}^{(d)}_{m} - (\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n)/k_{d+1}\right|_T \\
\Rightarrow \frac{2\epsilon(1+\kappa_{d+1})}{k_{d+1}} &< \min_{n\in\{0,\dots,\lfloor k_{d+1}\rfloor-1\}}\left|\tilde{\phi}^{(d)}_{m} - (\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n)/k_{d+1}\right|_T = \xi_{m,\to j}.
\end{aligned} \tag{3.33}$$

Here we have used that Eq. (A.4) holds for the estimate $\tilde{\phi}^{(d)}_m$.

Alternatively, for those $m \not\to j$ for which Eq. (3.21) holds, we claim that

$$n_{m,\to j} = n_{\to j,\to j}, \tag{3.34}$$

hence for those $\tilde{\phi}^{(d)}_m \neq \tilde{\phi}^{(d)}_{\to j}$ the algorithm produces a single new estimate equal to $(\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n_{\to j,\to j})/k_{d+1}$.

To see that Eq. (3.21) implies Eq. (3.34) indeed, note that it is sufficient to prove that

$$\left|\tilde{\phi}^{(d)}_{m} - (\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n_{\to j,\to j})/k_{d+1}\right|_T < \frac{\pi}{k_{d+1}}, \tag{3.35}$$

as one can then show that for $n' \neq n_{\to j,\to j} \in \{0,\dots,\lfloor k_{d+1}\rfloor - 1\}$ that

$$\begin{aligned}
\frac{2\pi}{k_{d+1}} &\leq \left|\frac{2\pi}{k_{d+1}}(n_{\to j,\to j} - n')\right|_T \\
&= \left|(\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n_{\to j,\to j})/k_{d+1} - (\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n')/k_{d+1}\right|_T \\
&\leq \left|(\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n_{\to j,\to j})/k_{d+1} - \tilde{\phi}^{(d)}_{m}\right|_T \\
&\qquad + \left|\tilde{\phi}^{(d)}_{m} - (\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n')/k_{d+1}\right|_T \\
&< \frac{\pi}{k_{d+1}} + \left|\tilde{\phi}^{(d)}_{m} - (\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n')/k_{d+1}\right|_T \\
\Rightarrow \frac{\pi}{k_{d+1}} &< \left|\tilde{\phi}^{(d)}_{m} - (\tilde{\theta}^{(d+1)}_{\to j} + 2\pi n')/k_{d+1}\right|_T,
\end{aligned} \tag{3.36}$$

so $n_{\to j,\to j}$ is optimal. Using Eq. (A.2), Eq. (3.21) and Eq. (3.40), we can prove Eq. (3.35) since

$$\begin{aligned}\left|\tilde{\phi}_m^{(d)} - (\tilde{\theta}_{\to j}^{(d+1)} + 2\pi n_{\to j,\to j})/k_{d+1}\right|_T \leq& \left|\tilde{\phi}_m^{(d)} - \tilde{\phi}_{\to j}^{(d)}\right| \\ &+ \left|\tilde{\phi}_{\to j}^{(d)} - (\tilde{\theta}_{\to j}^{(d+1)} + 2\pi n_{\to j,\to j})/k_{d+1}\right|_T \\ <& \frac{\pi - 2\epsilon(1+\kappa_{d+1})}{k_{d+1}} + \frac{2\epsilon(1+\kappa_{d+1})}{k_{d+1}} \\ =& \frac{\pi}{k_{d+1}}. \end{aligned} \tag{3.37}$$

We have thus shown that for each ϕ_j, there is a $\tilde{\theta}_{\to j}^{(d+1)}$, such that step 4d will output $(\tilde{\theta}_{\to j}^{(d+1)} + 2\pi n_{\to j,\to j})/k_{d+1}$ with $n_{\to j,\to j}$ defined in Eq. (3.30), related to the previous order estimate $\phi_{\to j}^{(d)}$ which was already close to $\phi_j^{(d)}$. The last step is to show that $n_{\to j,\to j} = n_{j,\to j}^{\text{ideal}}$ using Property 1a. It holds that

$$\begin{aligned}|\phi_j - (\tilde{\theta}_{\to j}^{(d+1)} + 2\pi n_{\to j,\to j})/k_{d+1}|_T \leq& |\phi_j - \tilde{\phi}_{\to j}^{(d)}|_T \\ &+ |\tilde{\phi}_{\to j}^{(d)} - (\tilde{\theta}_{\to j}^{(d+1)} + 2\pi n_{\to j,\to j})/k_{d+1}|_T \\ \leq& \frac{2\epsilon}{k_d} + \frac{2\epsilon(1+\kappa_{d+1})}{k_{d+1}} < \frac{\pi}{k_{d+1}}, \end{aligned} \tag{3.38}$$

where we used that $4\epsilon(\kappa_{d+1}+1) < \pi$. Indeed for $d > 1$, $\epsilon < \frac{\pi}{16}$ ($\kappa_{d+1} \leq 3$) and for $d = 0$, $\epsilon < \frac{\pi}{4(3n_\phi+2)}$ ($\kappa_1 \leq 3n_\phi + 1$) given the upper bounds on ϵ in Eqs. (3.11) and (3.10). This implies through the same argument as in Eq. (3.36) that $n_{j,\to j}^{\text{ideal}}$ achieving the minimum in Eq. (3.27) equals $n_{\to j,\to j}$ and hence we obtain Property 1a.

Now let's prove Property 1b. Given a $\tilde{\theta}_l^{(d+1)}$, let $\phi_{j=\to l}$ be the real phase for which, by Assumption 2b, it holds that

$$|k_{d+1}\phi_{\to l} - \tilde{\theta}_l^{(d+1)}|_T = k_{d+1}|\phi_{\to l} - (\tilde{\theta}_l^{(d+1)} + 2\pi n_{\to l,l}^{\text{ideal}})/k_{d+1}|_T \leq 2\epsilon. \tag{3.39}$$

To prove Property 1b, we need to show that $n_l = n_{\to l,l}^{\text{ideal}}$ with n_l defined in Eq. (3.30). Let also $\tilde{\phi}_{\to j}^{(d)}$ be the previous order $2\epsilon/k_d$-close estimate to $\phi_{j=\to l}$ by Assumption 1a. The idea is that $\tilde{\phi}_{\to j}^{(d)} = \tilde{\phi}_{\to(\to l)}^{(d)}$ is matched to $\tilde{\theta}_l^{(d+1)}$ in the optimization step of the algorithm, so that this leads to a better estimate for the phase $\phi_{j=\to l}$.

Given a $\tilde{\theta}_l^{(d+1)}$ we can deduce, as before, that

$$\begin{aligned}\xi_{\to j,l} &= \left|\tilde{\phi}_{\to j}^{(d)} - (\tilde{\theta}_l^{(d+1)} + 2\pi n_{\to j,l})/k_{d+1}\right|_T \\ &\leq \left|\tilde{\phi}_{\to j}^{(d)} - \phi_{\to l}\right|_T + \left|\phi_{\to l} - (\tilde{\theta}_l^{(d+1)} + 2\pi n_{\to l,l}^{\text{ideal}})/k_{d+1}\right|_T \\ &\leq \frac{2\epsilon}{k_d} + \frac{1}{k_{d+1}}\left|k_{d+1}\phi_{\to l} - \tilde{\theta}_l^{(d+1)}\right|_T \\ &= \frac{2\epsilon}{k_d} + \frac{1}{k_{d+1}}\left|\theta_{\to l}^{(d+1)} - \tilde{\theta}_l^{(d+1)}\right|_T \leq \frac{2\epsilon(1+\kappa_{d+1})}{k_{d+1}}. \end{aligned} \tag{3.40}$$

Using previous arguments, all other $\xi_{m,l}$ are either larger or give the same integer $n_{\to j,l}$ and thus $n_l = n_{\to j,l}$. In addition, we can bound, using this equality and Assumption 1a

$$\begin{aligned}|\phi_{\to l} - (\tilde{\theta}_l^{(d+1)} + 2\pi n_{\to j,l})/k_{d+1}|_T \leq \\ |\phi_{\to l} - \tilde{\phi}_{\to j}^{(d)}|_T + |\tilde{\phi}_{\to j}^{(d)} - (\tilde{\theta}_l^{(d+1)} + 2\pi n_{\to j,l})/k_{d+1}|_T \\ \leq \frac{2\epsilon}{k_d} + \frac{2\epsilon(1+\kappa_{d+1})}{k_{d+1}} < \frac{\pi}{k_{d+1}}, \end{aligned} \tag{3.41}$$

implying that $n_l = n_{\to j,l} = n_{\to l,l}^{\text{ideal}}$ as desired. □

Algorithm 3.2.1 has a few failure modes, namely steps 1, 4c and 4e where we exit and return an estimate of lower order. Arguments in Lemma 3.2.3 show that these failure modes are only encountered when the QEEP subroutine, Alg. 3.1.4, fails at some order. For clarity, we collect these observations in a single Corollary:

Corollary 3.2.3.1. *If each invocation of the QEEP subroutine, Alg. 3.1.4, succeeds in Alg. 3.2.1, we never exit at step 1, 4c or 4e.*

Proof. Consider step 1 in Alg. 3.2.1 applying Alg. 3.1.4 which obeys Lemma 3.1.5, showing that success of Alg. 3.1.4 implies that the number of phases is at most n_ϕ. By assumption there is at least one phase with $A_j > 0$, and hence success means that Alg. 3.1.4 cannot return the empty set due to 1. in Lemma 3.1.5. Hence if Alg. 3.1.4 succeeds we do not exit at step 1. Now consider step 4c: again success of Alg. 3.1.4 implies that the number of estimates does not exceed n_ϕ. Consider Eq. (3.17) and Eq. (3.18). If Alg. 3.1.4 succeeds up to order $d-1$, the phase estimates $\tilde{\phi}_j^{(d-1)}$ obey Eq. (A.4) for k_d, hence the condition in Eq. (3.18) equals, for each $\tilde{\theta}_l^{(d)}$

$$\min_j \min_n |\tilde{\phi}_j^{(d-1)} - (\tilde{\theta}_l^{(d)} + 2\pi n)/k_d|_T > \frac{2\epsilon(1+\kappa_d)}{k_d}. \tag{3.42}$$

As we argued, via induction, this does not happen when Alg. 3.1.4 succeeds up to order d, as $\min_j \xi_{j,l}$ is upper-bounded as in Eq. (3.40) for all $d' \leq d$. Similarly, Eq. (3.17) implies the existence of a $\tilde{\phi}_j^{(d-1)}$ with

$$\min_l \min_n |\tilde{\phi}_j^{(d-1)} - (\tilde{\theta}_l^{(d)} + 2\pi n)/k_d|_T > \frac{2\epsilon(1+\kappa_d)}{k_d}. \tag{3.43}$$

which can not happen due to the success of Alg. 3.1.4 which implies the bound in Eq. (3.31). Consider lastly step 4e which exits if the current dth order estimates do not lie in the region for which Eq. (A.3) holds with given k_d. We have argued in Lemma 3.2.3 that, assuming success of the subroutines implementing Alg. 3.1.4, that Eq. (A.3) holds for the phase estimates at all orders. □

Now let us consider failures of the QEEP subroutine, Alg. 3.1.4, which do not lead to exiting. Let's imagine that the first failure occurs at some order d_0. Now we want to make sure that continuing with higher orders after such failure still leads to an error of order $\sim \epsilon/k_{d_0-1}$, even though the failure (or any subsequent failure) is not detected.

To show this, we check that if Alg. 3.2.1 exits at some later round, namely during $d = d_f + 1$ and outputs estimates $\tilde{\phi}_j^{(d_f)}$ that these will be sufficiently close to the estimates right before failure, that is, the set of phases $\tilde{\phi}_j^{(d_0-1)}$.

Then, by Lem. 3.2.3, these estimates will also be sufficiently close to the true phases ϕ_j.

Lemma 3.2.4. *Let Alg. 3.2.1 exit at order $d = d_f + 1$ and let the QEEP subroutine, Alg. 3.1.4, of step 4b first fail at $d = d_0 \leq d_f + 1$. For each ϕ_j, there will be an estimate $\tilde{\phi}_l^{(d_f)}$, produced at step 4d in Alg. 3.2.1 which satisfies*

$$\left|\phi_j - \tilde{\phi}_l^{(d_f)}\right|_T \leq \frac{14\epsilon}{k_{d_0-1}}. \tag{3.44}$$

Vice-versa, for each estimate $\tilde{\phi}_l^{(d_f)}$ there exists a phase ϕ_j such that

$$\left|\phi_j - \tilde{\phi}_l^{(d_f)}\right|_T \leq \frac{14\epsilon}{k_{d_0-1}}. \tag{3.45}$$

Proof. Since each QEEP subroutine, Alg. 3.1.4, in Alg. 3.2.1 succeeds up to order $d_0 - 1$, Lemma 3.2.3 garantees that

- (Property 1a) For every phase ϕ_j there exists an estimate $\tilde{\phi}_l^{(d_0-1)}$ such that $|\phi_j - \tilde{\phi}_l^{(d_0-1)}|_T \leq \frac{2\epsilon}{k_{d_0-1}}$.

- (Property 1b) For every estimate $\tilde{\phi}_l^{(d_0-1)}$ there exists a phase ϕ_j such that $|\phi_j - \tilde{\phi}_l^{(d_0-1)}|_T \leq \frac{2\epsilon}{k_{d_0-1}}$.

Then, since the algorithm does not exit at step 4c through Eqs. (3.17) or step 4e for any order $d = d_0, \dots d_f$, it implies that for each estimate $\tilde{\phi}_l^{(d-1)}$ we can associate some $\tilde{\theta}_{m_l}^{(d)}$ that satisfies

$$\frac{1}{k_d}\left|k_d\tilde{\phi}_l^{(d-1)} - \tilde{\theta}_{m_l}^{(d)}\right|_T = \min_{n\in\{0,\dots,\lfloor k_{d+1}\rfloor-1\}} |\tilde{\phi}_l^{(d-1)} - (\tilde{\theta}_{m_l}^{(d)} + 2\pi n)/k_d|_T \leq \frac{2\epsilon(1+\kappa_d)}{k_d}, \quad (3.46)$$

where the second equality follows from being allowed to apply Eq. (A.4) (which is validated by passing the test at step 4e). This implies that in step 4d of Alg. 3.2.1 at round d, for a given $\tilde{\theta}_{m_l}^{(d)}$, the optimization of ξ_{n,m_l} over n will pick the integer n_{l,m_l}, i.e. the integer associated with matching $\tilde{\theta}_{m_l}^{(d)}$ with $\tilde{\phi}_l^{(d-1)}$. Indeed, similar as in the proof of Lemma 3.2.3, we can argue about other estimates $\tilde{\phi}_k^{(d)} \neq \tilde{\phi}_l^{(d)}$. Since κ_{d+1} is chosen in step 4f of Alg. 3.2.1, we claim that either Eq. (3.20) holds, in which case

$$\min_{n\in\{0,\dots,\lfloor k_{d+1}\rfloor-1\}} \left|\tilde{\phi}_k^{(d)} - \frac{2\pi n + \tilde{\theta}_{m_l}^{(d+1)}}{k_{d+1}}\right|_T > \frac{2\epsilon}{k_{d+1}}(1+\kappa_{d+1}), \quad (3.47)$$

hence this ξ_{k,m_l} is not optimal, or that Eq. (3.21) holds, in which case

$$n_{l,m_l} = \operatorname*{arg\,min}_{n\in\{0,\dots,\lfloor k_{d+1}\rfloor-1\}} \left|\tilde{\phi}_k^{(d)} - \frac{2\pi n + \tilde{\theta}_{m_l}^{(d+1)}}{k_{d+1}}\right|_T = n_{k,m_l}. \quad (3.48)$$

The proofs of these claims are exactly the same as in the proof of Lemma 3.2.3, i.e. using Eqs. (3.35), (3.36),(3.37).

Now let's us prove Eq. (3.44). Given a phase ϕ_j, we can use Property (1a) to find an associated estimate $\tilde{\phi}_{\to j}^{(d_0-1)}$ within $2\epsilon/k_{d_0-1}$. Then for this estimate let $\theta_{m_{\to j}}^{(d_0)}$ be the matched estimate in the next round for

which Eq. (3.46) holds, so that the round produces a new estimate $\tilde{\phi}_{\to j}^{(d_0)} = \frac{\tilde{\theta}_{m_{\to j}}^{(d_0)} + 2\pi n_{\to j, m_{\to j}}}{k_{d_0}}$ (which we label with $\to j$ again) for which

$$|\tilde{\phi}_{\to j}^{(d_0-1)} - \tilde{\phi}_{\to j}^{(d_0)}|_T \leq \frac{2\epsilon}{k_{d_0}}(1 + \kappa_{d_0}). \tag{3.49}$$

Then again for $\tilde{\phi}_{\to j}^{(d_0)}$ there exists some matching $\theta_{m_{\to j}}^{(d_0+1)}$ etc. and this generates a series of estimates $\tilde{\phi}_{\to j}^{(d)}$ up to order d_f. For a given ϕ_j we can then bound, using this series of estimates and $\kappa_d \geq 2$ for all d,

$$\begin{aligned}
\left|\tilde{\phi}_j^{(d_f)} - \phi_j\right|_T &\leq \left|\tilde{\phi}_{\to j}^{(d_0-1)} - \phi_j\right|_T + \sum_{d=d_0}^{d_f} \left|\tilde{\phi}_{\to j}^{(d-1)} - \tilde{\phi}_{\to j}^{(d)}\right|_T \\
&\leq \frac{2\epsilon}{k_{d_0-1}} + \sum_{d=d_0}^{d_f} \frac{2\epsilon(1+\kappa_d)}{k_d} \\
&= \frac{2\epsilon}{k_{d_0-1}} \left(1 + \sum_{d=d_0}^{d_f} \frac{1+\kappa_d}{\kappa_{d_0}\kappa_{d_0+1}\ldots\kappa_d}\right) \\
&\leq \frac{2\epsilon}{k_{d_0-1}} \left(1 + \sum_{n=0}^{\infty} \frac{3}{2^n}\right) = \frac{14\epsilon}{k_{d_0-1}}.
\end{aligned} \tag{3.50}$$

Now let's prove Eq. (3.45) and start with an estimate $\tilde{\phi}_l^{(d_f)}$ which was obtained from some $\tilde{\theta}_l^{(d_f)}$ matched with a previous estimate $\tilde{\phi}_l^{(d_f-1)}$ (just for convenience we again use the same label) such that $|\tilde{\phi}_l^{(d_f)} - \tilde{\phi}_l^{(d_f-1)}|_T \leq \frac{2\epsilon}{k_{d_f}}(1 + \kappa_{d_f})$, using that we do not exit through Eq. (3.18). Then again for this previous estimate $\tilde{\phi}_l^{(d_f-1)}$ we can repeat the argument and create a sequence of estimates up to $\tilde{\phi}_l^{(d_0-1)}$. For the last estimate, we invoke Property (1b), namely that there is a nearby ϕ_j. Then we can upperbound for this ϕ_j: $|\tilde{\phi}_l^{(d_f)} - \phi_j|_T \leq |\tilde{\phi}_l^{(d_0-1)} - \phi_j|_T + \sum_{d=d_0}^{d_f} |\tilde{\phi}_l^{(d)} - \tilde{\phi}_l^{(d-1)}|_T$ etc., exactly as in Eq. (3.50), leading to Eq. (3.45). □

3.2.3 Algorithm 3.2.1 achieves the Heisenberg limit

We have seen that the success of the QEEP subroutines in Alg. 3.2.1 leads to an error scaling as $\epsilon/k_{d_f} \sim \delta_c$. Now we must choose the success proba-

bility p_d of these subroutines in Eq. (3.12), depending on α, γ so that the total mean-square-error is bounded by some $\delta^2 = O(\delta_c^2)$ while the quantum cost $T = O(\delta^{-1})$. We note that the next theorem contains no logarithmic factors in δ^{-1}, as in [73], but achieves pure Heisenberg scaling.

Theorem 3.2.5. *Algorithm 3.2.1 solves the multiple eigenvalue estimation problem in Def. 3.1.3 with accuracy error δ and total quantum cost $T = O(\delta^{-1})$, given A, n_ϕ and a fixed ϵ_0 and ϵ obeying Eqs.* (3.11) *and* (3.10)*, and some choice for the constants $\alpha > 0$ and $\gamma > 2$.*

Remarks: Note that the dependence on the number of phases n_ϕ is not made explicit in the statement of this Theorem, but this dependence will be polynomial in n_ϕ, not necessarily a very low-order polynomial. This dependence comes through the choice for ϵ_0 (and ϵ) via Eq. (3.10) which sets the error and thus the running time of the QEEP Algorithm 3.1.2.

Proof. Our proof is motivated by the analysis in [2] for a single phase ϕ leading to Theorem 2.5.1. The idea is to bound the mean-square-error in the final estimation of ϕ by summing over error contributions at each order d at which the phase extraction subroutine may fail (with probability $1 - p_d$). By the right choice of p_d depending on d and parameters α and γ, the idea is that $\delta^2 = O(\delta_c^2)$ where δ_c is a final targeted error and δ^2 is mean-square-error of the phase estimate. The point is then to show that the quantum cost T scales as δ_c^{-1} and thus $\delta = O(T^{-1})$, reaching the Heisenberg limit.

In our case the multipliers at each order are not fixed (as in Theorem 2.5.1) but depend on phase estimates at previous orders and thus measurement data at previous orders. Our confidence parameter p_d in Eq. (3.12), which determines the number of repeats of experiments, and hence the cost, in Alg. 3.1.4, depends on k_d and is thus a random variable depending on previous measurement data. All measurement data are denoted by $\mathbf{x}$ and thus we have random variables $k_d(\{\kappa_{d'}(\mathbf{x})\}_{d'=1}^{d})$ and $p_d(\{\kappa_{d'}(\mathbf{x})\}_{d'=1}^{d})$.

Consider the mean-square-error δ_j^2 for the jth phase ϕ_j in Eq. (3.27) in Definition 3.1.3.

We have three error contributions to consider given a choice for the random variable k_d.

1. With probability $1 - p_0$ the subroutine Alg. 3.1.4 in Alg. 3.2.1 fails at step 1 ($d = 0$). In this case, as we always return *some* estimate, δ_j is bounded for all j by π.

2. With probability at most $(1 - p_{d_0}) \prod_{d=0}^{d_0-1} p_d \leq 1 - p_{d_0} = e^{-\alpha} \left(\frac{k_{d_0}\delta_c}{\pi}\right)^{\gamma}$, the subroutine Alg. 3.1.4 in Alg. 3.2.1 fails for the first time at some

order $1 \leq d_0 \leq d_f$, and the algorithm proceeds in any way afterwards (by possibly exiting or not). In this case, Lemma 3.2.4 bounds δ_j for all j by $\frac{14\epsilon}{k_{d_0-1}}$ or Lemma 3.2.3 bounds δ_j for all j by $\frac{2\epsilon}{k_{d_0-1}} \leq \frac{14\epsilon}{k_{d_0-1}}$.

3. With probability less than $\prod_{d=0}^{d_f} p_d < 1$ the subroutine Alg. 3.1.4 in Alg. 3.2.1 succeeds up to the final round d_f, and Lemma 3.2.3 implies that $\delta_j \leq 2\epsilon/k_{d_f} \leq 2\delta_c$ for all j as $k_{d_f} \geq \epsilon/\delta_c$.

We can now bound the mean-square-error as a sum over the above three contributions weighted by their relevant probabilities:

$$\begin{aligned}
\delta_j^2 &\leq (1-p_0)\pi^2 + \sum_{\mathbf{x}} \mathbb{P}(\mathbf{x}) \left[\sum_{d_0=1}^{d_f-1} \mathbb{P}(\kappa_1, \ldots, \kappa_{d_0}|\mathbf{x})(1 - p_{d_0}(\{\kappa'_d\}_{d'=1}^{d_0})) \left[\frac{14\epsilon}{k_{d_0-1}(\{\kappa'_d\}_{d'=1}^{d_0-1})} \right]^2 \right] + 4\delta_c^2 \\
&= \pi^2 e^{-\alpha} \left(\frac{\delta_c}{\pi} \right)^\gamma + \sum_{\mathbf{x}} \mathbb{P}(\mathbf{x}) \left[\sum_{d_0=1}^{d_f-1} \mathbb{P}(\kappa_1, \ldots, \kappa_{d_0}|\mathbf{x}) e^{-\alpha} \left(\frac{k_{d_0}\delta_c}{\pi} \right)^\gamma \frac{196\epsilon^2}{k_{d_0-1}^2} \right] + 4\delta_c^2 \\
&\leq \pi e^{-\alpha} \left(\frac{\delta_c}{\pi} \right)^\gamma + 0.15 \times \delta_c^2 \sum_{\mathbf{x}} \mathbb{P}(\mathbf{x}) \mathbb{P}(\kappa_1, \ldots, \kappa_{d_0}|\mathbf{x}) \sum_{d_0=1}^{d_f-1} \left(\frac{k_{d_0}\delta_c}{\pi} \right)^{\gamma-2} + 4\delta_c^2. \qquad (3.51)
\end{aligned}$$

Here we have removed the dependency of k_{d_0} and k_{d_0-1} on the previous multipliers for notational simplicity. For $d = 1$ we have

$$e^{-\alpha}\kappa_{d_0}^2 196(\epsilon/\pi)^2 = e^{-\alpha}k_1^2 196(\epsilon_0/\pi)^2 \leq \frac{196 \times 16 \times 4}{(300)^2} \leq 0.15 \qquad (3.52)$$

due to Eq. (3.10). For $d > 1$, $e^{-\alpha}\kappa_{d_0}^2 196(\epsilon/\pi)^2 \leq \frac{9\times196\times4}{(300)^2} = 0.08$, due to Eq. (3.11).

To evaluate the middle term, we write $k_{d_0} = k_{d_f}\frac{k_{d_0}}{k_{d_f}}$, and note that as $k_d = \prod_{d'=1}^{d} \kappa_{d'}$, we have $\frac{k_{d_0}}{k_{d_f}} \leq 2^{d_0-d_f}$ as the multiplier $\kappa_d \geq 2$. As $k_{d_f} \leq \frac{2\epsilon}{\delta_c} < \frac{\pi}{2\delta_c}$, we have

$$\sum_{d_0=1}^{d_f-1} \left(\frac{k_{d_0}\delta_c}{\pi} \right)^{\gamma-2} \leq \frac{1}{2^{\gamma-2}} \sum_{d_0=1}^{d_f-1} (2^{\gamma-2})^{(d_0-d_f)} \leq \frac{2^{4-\gamma}}{2^\gamma - 4}, \qquad (3.53)$$

where the last inequality holds since $\gamma > 2$. By letting the upperbound be independent of the κ_ds, we can remove the dependence on $\mathbf{x}$ in Eq. (3.51) using that $\sum_{\mathbf{x}} \mathbb{P}(\mathbf{x})\mathbb{P}(\kappa_1, \ldots, \kappa_{d_0}|\mathbf{x}) = 1$. This yields a final bound on δ_j of

$$\delta_j^2 \leq \delta_c^2 \left[\pi^{1-\gamma} e^{-\alpha} \delta_c^{\gamma-2} + \frac{0.15 \times 2^{4-\gamma}}{2^\gamma - 4} + 4] \right]. \qquad (3.54)$$

As $\gamma > 2$, this scales as δ_c^2 as $\delta_c \to 0$.

Let us now calculate the cost of executing Alg. 3.2.1 in terms of the number of unitary applications. Again this depends on the choice of multiplier κ_d at each step. Let us fix a sequences of k_ds, and let d_f be the final round of estimation in this algorithm, i.e. the final round for which we invoked the quantum subroutine in Alg. 3.1.4. At each order d we use $V^{\mathsf{k}} = U^{k_d \mathsf{k}}$, where $\mathsf{k} = 0, 1, \ldots, K$, with $2M_d$ samples where K is a function of ϵ as in Theorem 3.1.2. By Lemma 2.3.2 the cost of each experiment is $\lfloor k_d \mathsf{k} \rfloor + O(M_d)$. We can calculate

$$\begin{aligned} T = \sum_{\mathbf{x}} \mathbb{P}(\mathbf{x}) \mathbb{P}(\kappa_1, \ldots, \kappa_{d_0} | \mathbf{x}) \sum_{d=0}^{d_f} \sum_{\mathsf{k}=1}^{K} (2M_d \lfloor k_d \mathsf{k} \rfloor + O(M_d^2)) \\ \leq \sum_{d=0}^{d_f} M_d k_d K(K+1) + (d_f + 1) K O(M_{d=0}^2) \end{aligned} \tag{3.55}$$

where we have used $M_{d=0} \geq M_d$. The QEEP algorithm in Theorem 3.1.2 requires $M_d = O(|\ln(1-p_d)|\epsilon^{-b_1})$ with p_d in Eq. (3.12) and $K = O(\epsilon^{-b_2})$ for some integers $b_1 > 0$ and $b_2 > 0$. (We keep these integers free to account for any polylog factors.). Let the constant of proportionality in this scaling be b_3. The last term in Eq. (3.55) only has $\mathrm{poly}(\ln \delta_c^{-1})$ dependence, using Eq. (3.22) for d_f and the expression of M_0 in terms of δ_c, and we ignore it in the rest of the proof. We may bound

$$\begin{aligned} T &\leq b_3 \epsilon^{-b_1 - 2b_2} \sum_{d=0}^{d_f} k_d \left| -\alpha + \gamma \ln\left(\frac{k_d \delta_c}{\pi}\right) \right| \\ &= b_3 \epsilon^{-b_1 - 2b_2} \sum_{d=0}^{d_f} k_d \left[\alpha - \gamma \ln\left(\frac{k_d \delta_c}{\pi}\right) \right]. \end{aligned} \tag{3.56}$$

We again bound $k_d = \frac{k_d}{k_{d_f}} k_{d_f} \leq 2^{d-d_f} \frac{\pi}{2\delta_c}$, which yields

$$\begin{aligned} T &\leq \delta_c^{-1} \left[\frac{\pi b_3}{2} \epsilon^{-b_1 - 2b_2} \sum_{d=0}^{d_f} 2^{d-d_f} \left[\alpha - \gamma (d - d_f - 1) \ln(2) \right] \right] \\ &\leq \delta_c^{-1} \pi b_3 \epsilon^{-b_1 - 2b_2} (\alpha + 2\gamma \ln(2)). \end{aligned} \tag{3.57}$$

Combining our bounds then yields

$$\begin{aligned}\delta &\leq \delta_c \left[e^{-\alpha}\pi^{1-\gamma} + 4 + \frac{0.15 \times 2^{4-\gamma}}{2^\gamma - 4}\right]^{\frac{1}{2}} \\ &\leq T^{-1} \left[e^{-\alpha}\pi^{1-\gamma} + 4 + \frac{0.15 \times 2^{4-\gamma}}{2^\gamma - 4}\right]^{\frac{1}{2}} \pi b_3 \epsilon^{-b_1-2b_2}[\alpha + 2\gamma \ln(2)] \\ &= O(T^{-1}), \end{aligned} \tag{3.58}$$

which is the Heisenberg limit. □

3.3 Numerical implementation

Thm. 3.2.5 requires using the QEEP algorithm (Theorem 3.1.2 and Algorithm 3.1.4) in order to obtain provable bounds. Instead of analytic bounds, we now turn to a numerical demonstration, giving the opportunity to implement and test Algorithm 3.2.1 with a few modifications. We test the algorithm using two different sub-routines, one based on the matrix pencil method [79], and one based on the QEEP time-series analysis of Theorem 3.1.2, as described in Algorithm 3.1.4. Code to implement all simulations can be found at `https://github.com/alicjadut/qpe`.

To improve the practical performance of Alg. 3.2.1, we make the following two small changes. Firstly, instead of choosing κ_{d+1} in step 4f in the ranges declared in Lem. 3.2.2, we choose the largest κ_{d+1} consistent with Eq. (3.20) and Eq. (3.21) for all $\tilde{\phi}_j^{(d)}, \tilde{\phi}_l^{(d)}$. We note that the maximum such κ_{d+1} is bounded above by $\frac{\pi}{2\epsilon} - 1$, as the left-hand side of Eq. (3.20) is bounded above by 2π and the left-hand side of Eq. (3.21) is bounded below by 0. (In practice, tighter bounds can be found by checking the boundaries of the regions $R_{jl}^{(n)}$ defined in Eq. (B.5), and we find the largest possible κ_{d+1} by iterating backwards through these boundaries till a gap is found.) Secondly, as the bounds for ϵ and ϵ_0 in Lem. 3.2.2 are rather loose, and our performance scales rather badly in both, we choose the largest $\epsilon = \epsilon_0$ that allows all simulations to find a value of $\kappa_{d+1} > 2$ at each order.

When using the matrix pencil processing subroutine, we follow the implementation described in Ref. [19]:

Algorithm 3.3.1. *The matrix pencil method takes as input estimates of the phase function $g(k) = \sum_j A_j e^{ik\theta_j}$ for a unitary V at points $k = 0, 1, \ldots K$ and a probability bound A, and proceeds as follows:*

1. *Construct the* $L_K \times (2K - L_K + 1)$ *Hankel matrices* $G^{(0)}$, $G^{(1)}$, *where* $G^{(a)}_{i,j} = g(i + j + a - K)$ *for* $i \in \{0, 1, ...L_K - 1\}, j \in \{0, 1, ..., 2K - L_K\}$, $a = 0, 1$, *with* $L_K = \lfloor (K + 1)/2 \rfloor$, *and using* $g(-k) = g^*(k)$.

2. *Construct the* $L_K \times L_K$ *shift matrix* T *by least-squares minimization of the matrix* 2*-norm* $\|TG^{(0)} - G^{(1)}\|$.

3. *Calculate the eigenvalues of* T, $\lambda_j = |\lambda_j| e^{i\tilde{\theta}_j}$ *and from there the phase estimates* $\tilde{\theta}_j$.

4. *Calculate the probability estimates* $\tilde{A}_j$ *by least-squares minimization of the vector* 2*-norm* $\|BA - g\|$, *where* B *is the* $(K + 1) \times L_K$ *matrix*

$$B_{k,j} = \lambda_j^k, \tag{3.59}$$

   and $g = [g(0), ...g(K)]^T$.

5. *Return the phase estimates* $\tilde{\theta}_j$ *for which the corresponding probability estimate* $\tilde{A}_j \geq A$.

To use this algorithm as a subroutine in Alg. 3.2.1 (in place of Alg. 3.1.4), we implement it on the matrix $V = U^{k_d}$, which requires implementing $V^{\mathsf{k}} = U^{\mathsf{k}k_d}$ for a range of integer k on a quantum device.

To isolate the performance of the estimation routine from the generation of the signal itself, we do not test our protocols on data generated from simulating or approximating a particular unitary. Instead, we test the ability of the protocols to estimate $n_\phi = 2$ and $n_\phi = 4$ randomly-chosen phases $\phi_j \in [0, 2\pi]$ when sampling from the true phase function $g(k)$. We take all phases with equal weight — $A_j = 1/n_\phi$. We simulate the sampling from $g(k)$ in Algorithm 3.3.1 or Algorithm 3.1.2 for some $V = U^{k_d}$ by simulating the readout of a control qubit with the reduced density matrix of Eq. (2.15). (In practice this would be generated by the quantum circuit in Fig. 2.2.) We first draw M_d i.i.d. samples from the two Bernoulli distributions

$$\mathbb{P}^r_k(+1) = \frac{1}{2} \sum_{j=1}^{n_\phi} A_j (1 + \cos(\theta_j k)), \tag{3.60}$$

$$\mathbb{P}^i_k(+1) = \frac{1}{2} \sum_{j=1}^{n_\phi} A_j (1 - \sin(\theta_j k)), \tag{3.61}$$

where $\theta_j = k_d \phi_j \mod 2\pi$ are the eigenvalues of V. Then, we return the fraction of $+1$s drawn as estimates for the real and imaginary parts of $g(k)$

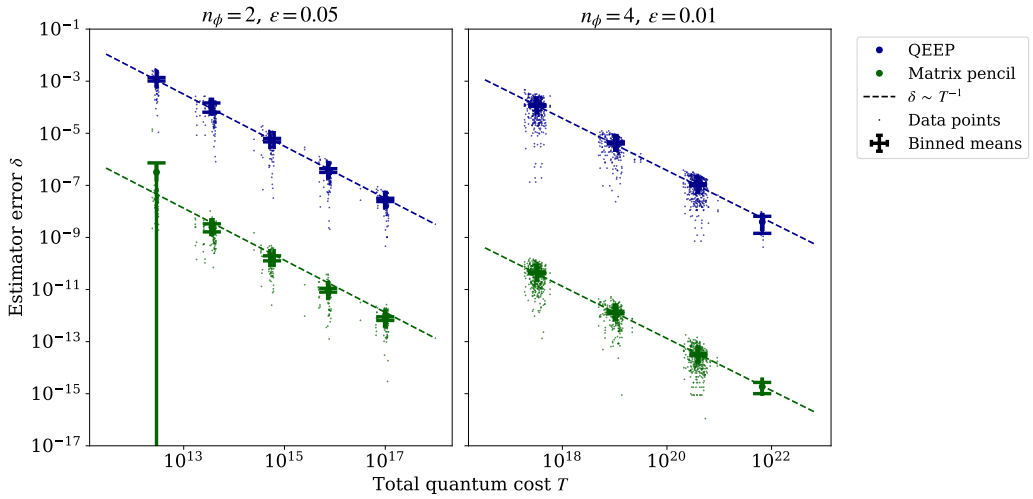

Figure 3.2: *Convergence of the algorithm with total quantum cost T. Phase estimates were obtained with either QEEP (blue) or matrix pencil (green) subroutines with parameters described in the text. Individual points show the error $\delta = |\tilde{\phi}_j - \phi_j|_T$ on individual phases in each simulation. This data is binned in the x-axis, and for each bin a root-mean-square error and standard deviation (error bars) are plotted in the x- and y-direction. Dotted lines show a fit of these means to $\delta \sim T^{-1}$.*

respectively. This is then repeated at all points $k = k_d \mathsf{k}$ for $\mathsf{k} = 0, 1, \ldots, K$. Following the discussion in Sec. 2.4 and using the notation from Eq. (3.55), we sum the total quantum cost for the algorithm over all requested $g(k)$ queries; $T = 2\sum_d \sum_{\mathsf{k}=1}^{K} \mathsf{k} k_d M_d$. (We ignore the sub-leading correction from the final term in Eq. (3.55) as this will not affect the scaling of our result.) For the signal length K and number of points M_d to sample each $g(k)$ at, we follow the bounds given in Ref. [3] (both when using the QEEP and matrix pencil subroutines):

- signal length: $K = \lceil 0.1 L \ln^2 L \rceil$, with $L = \lceil \frac{2\pi}{\epsilon} \rceil$ the number of bins used in the QEEP subroutine (Def. 3.1.1).
- number of measurements of each circuit: $M_d = \left\lceil |\ln(1 - p_d)|\, \epsilon^{-4} \right\rceil$.

Here, p_d is given in Eq. (3.12) for a given k_d. This equation requires fixing a choice of α and γ — across all experiments we take $\alpha = 2$ and $\gamma = 2.1$.

To demonstrate that our methods achieve the Heisenberg limit, in Fig. 3.2 we plot the error as a function of the total quantum cost for a set of simulations using the methods described above. Each simulation draws a

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different set of n_ϕ random phases, and a final error $\delta_c \in [10^{-5}, 10^{-2}]$ (for each choice of δ_c we use the same 50 sets of phases). We plot the error for each phase estimate separately in Fig. 3.2 (i.e. each simulation corresponds to n_ϕ points in the plot). As both the total quantum cost and the error is different between simulations, we bin all experiments within a range of T values, and calculate the root mean square error and root mean square total quantum cost. This gives a good approximation to the accuracy error defined in Def. 3.1.3 for the restricted data set used. For the QEEP subroutine, we observe a clear fit of the data (blue points) to a $\delta \sim T^{-1}$ trend, as expected from Thm. 3.2.5, but with a rather large constant factor; we find $T \sim 10^{10}\delta^{-1}$ for estimating 2 phases and $T \sim 10^{15}\delta^{-1}$ for estimating 4. Further optimization of the QEEP algorithm for these purposes may yet improve this constant factor. However, as the methods of Ref. [3] were not designed for estimating individual phases, it may be expected that this method performs somewhat badly for this purpose, so we have not pursued this further. Simulations using the matrix pencil subroutine outperform simulations using the QEEP subroutine by a factor of $10^4 - 10^6$, and clearly demonstrate Heisenberg-limited scaling $\delta \sim T^{-1}$ as well. We take this result instead of an analytic proof as strong numerical evidence for Heisenberg-limited scaling when a version of Alg. 3.2.1 is constructed using the matrix pencil method as a subroutine. We notice that the error in two phase estimates the first bin of the matrix pencil method is significantly above the remainder of the population (by about a factor $100\times$). Further investigation shows that the two phases in question are from the same simulation, and separated by only 1.5×10^{-4}. By contrast, for the simulation in question (at $d = 1$) our algorithm sets $k_1 K \sim 3 \times 10^3 < (1.5 \times 10^{-4})^{-1}$ (where $k_1 K$ is the largest value of the phase function $g(k)$ sampled during this simulation). This implies that our signal lies within the region where improving our estimation accuracy by increasing the number of shots M_d is exponentially hard [80]. In latter simulations with the two phases we see that our estimation error regresses to similar results as all other estimates.

Chapter 4

Future outlook and conclusions

In this work we studied Heisenberg-limited quantum phase estimation using a single control qubit. In this form of phase estimation, we rely on classical signal processing to extract eigenvalue data from the phase function $g(k)$ in Eq. (2.13).

It has been an open question whether these methods can achieve the Heisenberg limit in the case of multiple phases: Ref. [73] answered this question up to log factors with a Heisenberg-limited Monte Carlo algorithm, providing a sampling of the spectral function $A(\phi)$ in Eq. (2.14) from which to estimate the phases. In this work we also answered this question in the affirmative exactly with a new adaptive multi-order phase estimation algorithm, for which we prove Heisenberg scaling if the algorithm uses a QEEP phase extraction subroutine. We numerically show the performance of this algorithm, also when instead of using a QEEP subroutine, one uses the matrix pencil method to extract phase estimates from the phase function $g(k)$.

In obtaining our results we encountered at least two details of quantum phase estimation that we have not seen discussed in the literature. The first is the dense signal limit, Eq. (2.18) in Thm. 2.4.1: sampling $g(k)$ at *all* integer point $k = 1, \ldots, K$ is sub-optimal regardless of what method is used to process the data. However, we also briefly argued that by picking points among $k = 1, \ldots, K$ at random one may go beyond this, and one could interpret this as allowing the results obtained in [73] in which such randomized choices for k are taken.

The second is the need for adaptive choices of k_d to solve the phase matching problem. It is unclear to us how far this problem extends; although Lemma 3.2.2 provides a practical solution, others may still exist. Another open question with respect to Algorithm 3.2.1 is whether one can

remove the need to choose real-valued multipliers κ_d and restrict to integer choices. Restricting $\kappa_d \in \mathbb{N}$ would significantly simplify some technical issues, i.e. the applicability of Lemma A.0.2 and the need for shifting phases in step 2 of Alg. 3.2.1, but we don't know how to prove a version of Lemma 3.2.2 for $k_d \in \mathbb{Z}^+$. In fact, we don't know whether there is a fundamental difference in performance between only using data obtained with integer k in $g(k)$ versus data obtain with real-valued, –in practice rational–, k in $g(k)$.

We have assumed in our problem description, Def. 3.1.3, that the spectrum in the input state is discrete consisting of n_ϕ phases with probability above some cut-off. In practice this condition may not be fulfilled and thus studying the performance of the algorithms on more typical spectra induced by many-body Hamiltonians and easy-to-prepare input states will be of interest.

A direction for future research is to make this algorithm efficient in practice (i.e. improve the parameter dependence and the practical run time) or devise yet-different Heisenberg-scaling algorithms and examine their performance in the presence of experimentally-noisy signals $g(k)$.

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Appendix A

Properties of the metric $|.|_T$

Quantum phase estimation describes a series of protocols to estimate the eigenphases ϕ_j. As these eigenvalues are defined on the circle $[0, 2\pi)$, we need a notion of distance which respects this periodicity:

Definition A.0.1. *For $x \in \mathbb{R}$ we define the distance $|\cdot|_T \in [0, \pi]$ as*

$$|x|_T := \min_{m\in\mathbb{Z}}(|\Delta|), \textit{with } \; x = \Delta + 2\pi m, \textit{ with } \Delta \in [-\pi, \pi). \tag{A.1}$$

Clearly, the distance obeys the triangle inequality: for $x_1, x_2 \in \mathbb{R}$

$$|x_1 + x_2|_T \leq |x_1|_T + |x_2|_T. \tag{A.2}$$

The following Lemma addresses a technical issue in the proof of performance of Algorithm 3.2.1. For integer k, we have $|kx|_T = \min_{m\in\mathbb{Z}} |k\Delta + 2\pi m| = |k| \min_{m\in\mathbb{Z}} |\Delta + \frac{2\pi m}{k}|_T$, implying Eq. (A.4) directly. However, for $k \in \mathbb{R}$ (or rational numbers $k \in \mathbb{Q}$) we need to specify a range of x for which such a statement holds, i.e.

Lemma A.0.2. *Suppose $k \in \mathbb{R} > 1$, $\theta, \phi \in [0, 2\pi)$. If*

$$\frac{\pi}{k} \leq \phi \leq \frac{\pi(2\lfloor k\rfloor - 1)}{k}, \tag{A.3}$$

we have for any θ

$$\min_{n\in\{0,\ldots,\lfloor k\rfloor -1\}} \left|\phi - \frac{\theta}{k} - \frac{2\pi n}{k}\right|_T = \frac{1}{k} |k\phi - \theta|_T . \tag{A.4}$$

Proof. Let $x = \phi - \frac{\theta}{k}$, then Eq. (A.3) and $\theta \in [0, 2\pi)$ imply that

$$-\pi \leq kx \leq 2\pi\lfloor k\rfloor - \pi. \tag{A.5}$$

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and thus $kx = \Delta + 2\pi m$ with $m \in \{0, \dots \lfloor k \rfloor - 1\}$ and $\Delta \in [-\pi, \pi)$ and $|k\phi - \theta|_T = |\Delta|$. Hence $x = \frac{\Delta}{k} + \frac{2\pi m}{k}$ with $m \in \{0, \dots \lfloor k \rfloor - 1\}$, implying Eq. (A.4) where the minimum can be achieved by $m = n$. □

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Appendix B

Proof of Lemma 3.2.2

Let us first prove the existence of $\kappa_{d+1} \in [2, \kappa_{\max}]$ with $\kappa_{\max} = 3$ that satisfies our conditions (the proof for k_1 is similar), for small enough ϵ in Eq. (3.11). Note that Eq. (3.11) implies

$$\epsilon \leq \frac{\pi}{300} \approx 0.01. \tag{B.1}$$

Given some pair $\tilde{\phi}_j^{(d)} \neq \tilde{\phi}_l^{(d)}$, $j < l$, let $\Delta_{j,l} = |\tilde{\phi}_j^{(d)} - \tilde{\phi}_l^{(d)}|$ and let $R_{j,l}$ be a set of κ_{d+1} such that neither Eq. (3.21) nor Eq. (3.20) hold for the chosen phases, that is,

$$R_{j,l} = \Big\{ \kappa_{d+1} \in [2, \kappa_{\max}] : |\Delta_{j,l}|_T \geq \frac{\pi - 2\epsilon(1+\kappa_{d+1})}{k_d \kappa_{d+1}} \\ \wedge |k_d \kappa_{d+1} \Delta_{j,l}|_T \leq 4\epsilon(1+\kappa_{d+1}) \Big\}. \tag{B.2}$$

We call $\cup_{j,l} R_{j,l}$ the forbidden region and want to show that we can choose a value for $\kappa_{d+1} \in [2,3]$ outside this forbidden region if ϵ is sufficiently small. We do this by bounding the size of the forbidden region above and showing that this is smaller than the region $[2,3]$, leaving room to choose κ_{d+1}.

Note that $R_{j,l}$ is nonempty only if

$$k_d \Delta_{j,l} \geq k_d |\Delta_{j,l}|_T \geq \frac{\pi - 2\epsilon(1+\kappa_{d+1})}{\kappa_{d+1}} \geq \frac{\pi - 2\epsilon(1+\kappa_{\max})}{\kappa_{\max}} > \frac{73\pi}{225}, \tag{B.3}$$

using Eq. (B.1).

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We may write the set $R_{j,l}$ as

$$R_{j,l} = \left[\max\left(2, \frac{\pi - 2\epsilon}{k_d|\Delta_{j,l}|_T + 2\epsilon}\right), \kappa_{\max}\right] \cap \bigcup_{n\in\mathbb{N}} R_{j,l}^{(n)}, \tag{B.4}$$

where $R_{j,l}^{(n)}$ is the set of κ_{d+1} for which

$$|k_d\kappa_{d+1}\Delta_{j,l}|_T = \left|k_d\kappa_{d+1}\Delta_{j,l} - 2\pi n\right| \leq 4\epsilon(1+\kappa_{d+1}), \tag{B.5}$$

for some $n \in \mathbb{N}$.

Solving this equation for κ_{d+1} yields

$$R_{j,l}^{(n)} = \left[\frac{2\pi n - 4\epsilon}{k_d\Delta_{j,l} + 4\epsilon}, \frac{2\pi n + 4\epsilon}{k_d\Delta_{j,l} - 4\epsilon}\right]. \tag{B.6}$$

The size of each interval $R_{j,l}^{(n)}$ can then be calculated

$$\left|R_{j,l}^{(n)}\right| = \frac{8\epsilon(2n\pi + k_d\Delta_{j,l})}{k_d^2\Delta_{j,l}^2 - 16\epsilon^2}. \tag{B.7}$$

We can bound

$$\left|R_{j,l}\right| \leq \left|\bigcup_{n=1}^{n_{\max}} R_{j,l}^{(n)}\right| \leq \sum_{n=1}^{n_{\max}} \left|R_{j,l}^{(n)}\right| = \frac{8\epsilon}{k_d^2\Delta_{j,l}^2 - 16\epsilon^2}(\pi n_{\max}(n_{\max}+1) + k_d\Delta_{j,l}n_{\max}). \tag{B.8}$$

Here, $n_{\max} = n_{\max}(j,l)$ is the largest index of a set $R_{j,l}^{(n)}$ in Eq. (B.5) for which $\kappa_{d+1} \in [2, \kappa_{\max}]$. Since $\kappa_{d+1} \leq 3$, Eq. (B.5) implies that

$$n_{\max} \leq \frac{3(k_d\Delta_{j,l} + 4\epsilon) + 4\epsilon}{2\pi}, \tag{B.9}$$

Now using Eq. (B.3) and Eq. (B.1) gives

$$\begin{aligned}\left|R_{j,l}\right| &\leq \frac{1}{1-(4\epsilon/k_d\Delta_{j,l})^2}\left(\frac{30\epsilon(864000\epsilon^2 + 248160\epsilon\pi + 11899\pi^2)}{5329\pi^3}\right) \\ &\leq \frac{3\epsilon(864000\epsilon^2 + 248160\epsilon\pi + 11899\pi^2)}{532\pi^3} \leq 0.24,\end{aligned} \tag{B.10}$$

where the last inequality used Eq. (B.1). As there are $n_\phi \geq 2$ phases the length of the total forbidden region $\cup_{j,l} R_{j,l}$ is bounded from above by

$\frac{n_\phi^2}{2}\left|R_{j,l}\right|$. We want to this interval to be, say, at most $1/4$, so that by choosing κ_{d+1} randomly we have a 75% change of not landing in the forbidden interval. For larger n_ϕ we thus should use

$$\epsilon \leq \epsilon_{\text{crit}} = \frac{2\pi}{300 n_\phi^2}, \tag{B.11}$$

leading to Eq. (3.11).

We now repeat the above approach for the special case of finding the multiplier in the first round $\kappa_1 = k_1$. Consider thus $k_1 \in [3n_\phi, \kappa_{\max}]$ with $\kappa_{\max} = 3n_\phi + 1$. The key difference here is that there is a stricter lower bound on this multiplier $\kappa_{\max}$ so that ϵ needs to be chosen smaller, depending on n_ϕ, namely we choose

$$\epsilon_0 \leq \epsilon_{\text{crit},0} = \frac{2\pi}{300 n_\phi^4}, \tag{B.12}$$

as expressed in Eq. (3.10).

Given some pair $\tilde{\phi}_j^{(0)} \neq \tilde{\phi}_l^{(0)}$, $j < l$, and again let $\Delta_{j,l} = |\tilde{\phi}_j^{(0)} - \tilde{\phi}_l^{(0)}|$. Then, let $R_{j,l}$ be the set of k_1 such that neither Eq. (3.21) nor Eq. (3.20) holds for the chosen phases. That is,

$$R_{j,l} = \left\{ k_1 \in \left[3n_\phi, \kappa_{\max}\right] : |\Delta_{j,l}|_T \geq \frac{\pi - 2\epsilon_0(1+k_1)}{k_1} \wedge |k_1 \Delta_{j,l}|_T \leq 4\epsilon_0(1+k_1) \right\}. \tag{B.13}$$

We again call $\cup_{j,l} R_{j,l}$ the forbidden region and want to show that we can choose a value for $k_1 \in [3n_\phi, 3n_\phi + 1]$ outside this forbidden region, assuming that ϵ_0 is chosen small enough. Note that the logic of the first few inequalities in Eq. (B.3) still holds in this new calculation, leading to

$$\Delta_{j,l} \geq \frac{\pi - 2\epsilon_0(1+\kappa_{\max})}{\kappa_{\max}} \geq \frac{\pi(1 - \frac{2+3n_\phi}{75 n_\phi^4})}{1+3n_\phi}, \tag{B.14}$$

where the second inequality used Eq. (B.12) and the value for $\kappa_{\max}$. Note that for large n_ϕ this allows $\Delta_{j,l}$ to decrease like $\sim 1/n_\phi$, while previously $\Delta_{j,l}$ was lowerbounded by a constant, Eq. (B.3).

This time, we may write the set $R_{j,l}$ as

$$R_{j,l} = \left[\max\left(3n_\phi, \frac{\pi - 2\epsilon_0}{|\Delta_{j,l}|_T + 2\epsilon_0}\right), \kappa_{\max} \right] \cap \bigcup_{n \in \mathbb{N}} R_{j,l}^{(n)}, \tag{B.15}$$

where $R_{j,l}^{(n)}$ is the set of k_1 satisfying

$$\left| k_1 \Delta_{j,l} - 2\pi n \right| \leq 4\epsilon_0 (1 + k_1), \tag{B.16}$$

for some $n \in \mathbb{N}$. Solving this equation for k_1 yields

$$R_{j,l}^{(n)} = \left[\frac{2\pi n - 4\epsilon_0}{\Delta_{j,l} + 4\epsilon_0}, \frac{2\pi n + 4\epsilon_0}{\Delta_{j,l} - 4\epsilon_0} \right]. \tag{B.17}$$

with length

$$\left| R_{j,l}^{(n)} \right| = \frac{8\epsilon_0 (2n\pi + \Delta_{j,l})}{\Delta_{j,l}^2 - 16\epsilon_0^2}. \tag{B.18}$$

We can then bound

$$\begin{aligned} \left| R_{j,l} \right| &\leq \left| \bigcup_{n=n_{\min}}^{n_{\max}} R_{j,l}^{(n)} \right| \leq \sum_{n=n_{\min}}^{n_{\max}} \left| R_{j,l}^{(n)} \right| \\ &= \frac{8\epsilon_0 \left[\pi (n_{\max}^2 - n_{\min}^2) + (\Delta_{j,l} + \pi)(n_{\max} - n_{\min}) + 2\pi n_{\min} + \Delta_{j,l} \right]}{\Delta_{j,l}^2 - 16\epsilon_0^2}. \end{aligned} \tag{B.19}$$

Here, $n_{\max} = n_{\max}(j,l)$ and $n_{\min} = n_{\min}(j,l)$ are the largest and smallest indices of sets $R_{j,l}^{(n)}$ in Eq. (B.16) for which $k_1 \in [3n_\phi, 3n_\phi + 1]$. Finding the minimal and the maximal value for n in Eq. (B.16) given the bounds on k_1 gives

$$\frac{3n_\phi(\Delta_{j,l} - 4\epsilon_0) - 4\epsilon_0}{2\pi} \leq n_{\min} \leq n_{\max} \leq \frac{(3n_\phi + 1)(\Delta_{j,l} + 4\epsilon_0) + 4\epsilon_0}{2\pi}. \tag{B.20}$$

As there are n_ϕ phases, the length of the total forbidden region $\cup_{j,l} R_{j,l}$ is bounded from above by $\frac{n_\phi^2}{2} \left| R_{j,l} \right|$. By plugging the bounds for ϵ_0 in Eq. (B.12) and $\Delta_{j,l}$ in Eq. (B.14) in Eq. (B.19), one can verify that

$$|R_{j,l}| \frac{n_\phi^2}{2} \leq \frac{-16 - 168n_\phi - 621n_\phi^2 + 552n_\phi^4 + 14400n_\phi^5 + 44550n_\phi^6 + 40500n_\phi^7 + 73125n_\phi^8 + 270000n_\phi^9 + 202500n_\phi^{10}}{450n_\phi^3(-4 - 9n_\phi - 100n_\phi^3 - 150n_\phi^4 + 1875n_\phi^7)}, \tag{B.21}$$

which can be verified to be less than 0.5 for all n_ϕ. Hence a random choice for k_1 in the interval $[3n_\phi, 3n_\phi + 1]$ gives at least a 50% chance to not land in the forbidden region. □

Appendix C

Range of shifted phase estimates

In this Appendix we prove that when the unitary U is shifted in step 2 of Alg. 3.2.1, and as long as the output of the phase extraction subroutine (Alg. 3.1.4) meets the promises given in Lem. 3.1.5, all phase estimates of U^{k_d} will lie in the region for which Lem. A.0.2 holds. This allows us to invoke Lem. A.0.2 as required during Lem. 3.2.3 and Lem. 3.2.4. Note that if we were to shift the spectrum such that the middle of the largest gap would sit at 0, we would do $U \to Ue^{-i\zeta}$. However, the 'stay-away-from-the-boundary' condition of Lem. A.0.2 is not symmetric, hence we shift by a different amount which also depends on the error ϵ_0 in the phase estimates.

Lemma C.0.1. *Let $\{\phi_j\}$ be the list of eigenphases of unitary U, and let n_ϕ, $\{\tilde{\phi}_l^{(0)}\}$, ζ, d_ζ be as defined in steps 1 and 2 of Alg. 3.2.1. Assume:*

- *(Assumption 1a) For every phase ϕ_j, there exists an estimate $\tilde{\phi}_l^{(0)}$ such that $|\phi_j - \tilde{\phi}_l^{(0)}|_T \leq 2\epsilon_0$.*
- *(Assumption 1b) For every estimate $\tilde{\phi}_l^{(0)}$, there exists a phase ϕ_j such that $|\phi_j - \tilde{\phi}_l^{(0)}|_T \leq 2\epsilon_0$.*

Then for all $k \geq 3n_\phi$, for the estimated shifted eigenphases $\{\tilde{\varphi}_l^{(0)}\}$ it holds that

$$\frac{\pi}{k} + 16\epsilon_0 \leq \tilde{\varphi}_l^{(0)} \leq \frac{\pi(2\lfloor k \rfloor - 1)}{k} - 16\epsilon_0. \tag{C.1}$$

which implies Eq. (A.4) *for $\tilde{\varphi}_l^{(0)} = \phi$. In addition, the eigenphases $\{\varphi_j\}$ of the*

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shifted unitary $Ue^{-i(\zeta+d_\zeta/2-8\epsilon_0)}$ *satisfy*

$$\frac{\pi}{k} + 14\epsilon_0 \leq \varphi_j \leq \frac{\pi(2\lfloor k \rfloor - 1)}{k} - 14\epsilon_0. \tag{C.2}$$

which again implies Eq. (A.4) *for* $\varphi_j = \phi$.

Proof. Let

$$\tilde{\varphi}_l^{(0)} = \left(\tilde{\phi}_l^{(0)} - \zeta - \frac{d_\zeta}{2} + 8\epsilon_0\right) \bmod 2\pi. \tag{C.3}$$

Let us first show that

$$\tilde{\varphi}_l^{(0)} \in \left[\frac{\pi}{2n_\phi} + 8\epsilon_0, 2\pi - \frac{3\pi}{2n_\phi} + 8\epsilon_0\right]. \tag{C.4}$$

By definition of ζ (as the midway point in the largest gap) and d_ζ (as half the largest gap) we have

$$\left(\tilde{\phi}_l^{(0)} - \zeta - \frac{d_\zeta}{2}\right) \bmod 2\pi \in \left[\frac{d_\zeta}{2}, 2\pi - \frac{3d_\zeta}{2}\right]. \tag{C.5}$$

We have $d_\zeta \geq \pi/n_\phi$ (with equality corresponding to n_ϕ uniformly distributed estimates). By Eq. (3.10) it follows that

$$\epsilon_0 \leq \frac{\pi}{48n_\phi}, \tag{C.6}$$

and thus $\epsilon_0 < \frac{d_\zeta}{16}$, leading to Eq. (C.4). By the assumptions the shifted phases φ_j lie within $2\epsilon_0$ from the estimates $\tilde{\varphi}_l^{(0)}$. Thus for each φ_j there exists a $\tilde{\varphi}_l^{(0)}$ such that

$$\varphi_j - 14\epsilon_0 \geq \tilde{\varphi}_l^{(0)} - 16\epsilon_0 \geq \frac{\pi}{2n_\phi} - 8\epsilon_0 \geq \frac{\pi}{2n_\phi} - \frac{8\pi}{48n_\phi} = \frac{\pi}{3n_\phi} \geq \frac{\pi}{k}. \tag{C.7}$$

and

$$\varphi_j + 14\epsilon_0 \leq \tilde{\varphi}_l^{(0)} + 16\epsilon_0 \leq 2\pi - 3\left(\frac{\pi}{2n_\phi} - 8\epsilon_0\right) \leq 2\pi - \frac{3\pi}{k} \leq \frac{\pi(2\lfloor k \rfloor - 1)}{k}. \tag{C.8}$$

where we have used Eq. (C.4), Eq. (C.6), $k \geq 3n_\phi$ and $\lfloor k \rfloor > k - 1$. This implies Eq. (C.2) and also Eq. (C.1). □

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