Quantum phase estimation for a class of generalized eigenvalue problems

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Quantum computing has been recognized for its potential to solve currently intractable physics problems, such as quantum many-body problems [1]. The ability to process information in a fundamentally quantum way is also being explored for physics problems more broadly. For example, a quantum algorithm for the wave equation has been recently proposed [2]. Montanaro and Pallister proposed a quantum method of solving boundary-value problems via finite-element discretization [3]. A quantum algorithm for linear initial-value differential equations has been proposed by Berry et al. [4, 5]. These algorithms are based in some way on quantum linear system solvers [6, 7].

Another problem that arises frequently in physics and engineering is computation of spectra. It is often the case that a few eigenvalues are of primary interest, such as the calculation of the ground state and first few excited states. Another example is the determination of whether a system is linearly stable, and if unstable, what the growth rate is.

Quantum phase estimation (QPE) is a core quantum algorithm that offers quantum speedups for this problem. Fundamentally, QPE provides a technique for finding eigenvalues of unitary matrices. Moreover, QPE forms an important quantum subroutine in other algorithms, such as Shor’s algorithm [8] and HHL [6]. Abrams and Lloyd [9] realized that QPE could be used to calculate eigenvalues and eigenstates of Hamiltonians, in effect providing a quantum algorithm to solve the eigenvalue problem \( H \psi = \lambda \psi \). QPE could be used to find, for example, the electronic ground state in atomic physics or quantum chemistry problems [10]. In such problems that stem from quantum physics, the number of degrees in the Schrödinger equation increases exponentially with the number of particles, and thus a numerical solution is intractable via classical computation for many particles. As a result, QPE may become a key algorithm for solving ground states in a future error corrected, digital quantum computer.

In this paper, we show that QPE can also be usefully applied for calculating eigenvalues and eigenvectors of a certain class of generalized eigenvalue problems that arise naturally in physical applications. Generalized eigenvalue problems take the form \( Av = \lambda Bv \) where \( A \) and \( B \) are matrices. We assume that \( A \) is Hermitian and \( B \) is positive definite. Examples within this restricted class include regular Sturm–Liouville problems. Another important example is linear ideal MHD, which is an important model for determining stability of magnetically confined plasmas such as those used in fusion reactors. We demonstrate that generalized eigenvalue problems within the restricted class may be reduced to a standard eigenvalue problem in such a way that the effective Hamiltonian is still sparse, and thus potentially efficiently implementable. Then one can apply the standard procedure of Abrams and Lloyd [9].

Our motivating problems of interest arise from partial differential equations in classical physics, such as continuum dynamics, rather than quantum problems. These problems typically involve polynomial growth with respect to a parameter such as the number of grid points, rather than exponential growth. For instance, if some physical quantity is represented on a \( d \)-dimensional grid with \( N \) points per dimension, the total number of grid points required is \( N^d \). Yet these problems can pose great challenges in three dimensions in complex geometry when extremely high resolution is required. Computing eigenvalues classically requires \( O(\text{poly}(N^d)) \) arithmetic operations. For grid-based discretizations of partial differential equations, it has not been established that an exponential speedup is possible; estimates have given a possible polynomial speedup [11]. We return to this point in the discussion.

An outline for the rest paper is as follows. Section II provides a brief overview of quantum phase estimation. In Sec. III, we describe how QPE can be applied to a restricted class of generalized eigenvalue problems. In Sec. IV, we apply this idea to the Sturm–Liouville eigenvalue and discuss different discretizations. In Sec. V, we describe a problem of some practical importance, the determination of stability of magnetized plasmas, that this technique could be applied to. Finally, we give our con-
II. QUANTUM PHASE ESTIMATION

We briefly recall the main facets of quantum phase estimation. Phase estimation is a technique that, given an eigenvector \( v \) of a unitary matrix \( U \), can provide the eigenvalue. Since the eigenvalues of a unitary matrix have magnitude one, the eigenvalue is often written as \( e^{i\pi\phi} \) with \( 0 \leq \phi < 1 \).

QPE can be applied to solving for eigenvalues of a Hermitian eigenvalue problem,

\[
Hv = \lambda v.
\]  

(1)

For the moment, we assume the unitary gate \( U_H = e^{-iHt} \) can be efficiently applied. For example, assume \( 0 \leq \lambda < 1 \) and let \( t = 2\pi \). If the desired eigenvalue \( \lambda \) is not between 0 and 1, \( H \) can be shifted by a multiple of identity and scaled by modifying \( t \) to bring the eigenvalue into this range. If \( v \) is an eigenvector of \( H \) with eigenvalue \( \lambda \), then \( v \) is also an eigenvector of \( U_H \), with \( U_Hv = e^{-2\pi i\lambda} v \).

The critical components of the algorithm are state preparation, Hamiltonian simulation, and measurement of the phase. We mention state preparation and measurement of the phase here, and we return to Hamiltonian simulation in the discussion.

State preparation is an important part for phase estimation. The desired eigenfunction is typically not known in advance, and the input state must be sufficiently close to an eigenvector. If the normalized eigenvectors of \( H \) are \( v_j \), and the input state is \( v \), the probability of determining the eigenvalue of state \( j \) is the overlap \( P_j = |\langle v|v_j \rangle|^2 \), and thus to measure a specific eigenvalue \( \lambda_j \) requires on average \( 1/P_j \) trials. We will not delve into state preparation in any further depth here. We merely remark that the best way to approximate the desired eigenvector is problem-dependent. Knowledge of the specific physics of the problem can often be used to vastly narrow the space of interest. For instance, the WKB method can provide first approximations to partial differential equations, as could classically computed approximations on a coarser grid [12]. Adiabatic evolution is another method by which to prepare states [13].

The textbook approach to phase estimation uses the inverse quantum Fourier transform, where each bit of precision requires an additional ancilla qubit [14]. Because quantum computers in the near term will have constrained numbers of qubits, there is an active research area into variants of phase estimation to improve the practical performance. The Kitaev method, for instance, requires only one additional qubit [15]. Other QPE variants offer reductions in the required circuit depth, coherence time, and number of samples [16, 17]. Additionally, algorithms resilient to error from experimental imperfections have been explored [18, 19].

III. GENERALIZED EIGENVALUE PROBLEM

Consider the generalized eigenvalue problem,

\[
Av = \lambda Bv.
\]  

(2)

Although \( \lambda \) and \( v \) are sometimes referred to as generalized eigenvalues and generalized eigenvectors, we follow a typical physics convention of simply calling them eigenvalues and eigenvectors. We assume \( A \) is Hermitian, \( A_B = A_B^\dagger \). We also restrict to considering cases where \( B \) is positive definite. In general, \( A \) and \( B \) need not commute. Under these conditions, just like Hermitian eigenvalue problems, the eigenvalues are real, and eigenvectors with distinct eigenvalues are orthogonal when weighted by \( B \). That is, if \( v \) and \( w \) are eigenvectors with different eigenvalues, then \( v^\dagger Bw = 0 \).

Since quantum phase estimation can compute eigenvalues for the standard eigenvalue problem, it is natural to ask whether the same technique can be applied to the generalized eigenvalue problem. We answer this question affirmatively: that for at least some cases, generalized eigenvalue problems can be solved as efficiently as standard eigenvalue problems. Since our primary motivation comes from discretization of differential equations, we think of \( A \) as arising from a differential operator which will be local and sparse. Typically \( A \) will have a banded structure. In many problems of interest, \( B \) will also be sparse.

In considering Eq. (2), even if we assume we can apply \( U_A = e^{-iAt} \) and \( U_B = e^{-iBt} \) efficiently, it does not appear the techniques of QPE can straightforwardly provide a solution to yield the eigenvalues. That is because QPE relies on the fact that \( H \) or \( U_H \) applied to an eigenvector \( v \) produces a multiple of \( v \). In the generalized eigenvalue problem, it is not true that applying \( U_A \) to \( v \) produces a multiple of \( v \), as can be seen from Eq. (2).

One could rewrite Eq. (2) as \( B^{-1}Av = \lambda v \), however one runs into the immediate problem that the matrix \( B^{-1}H \) in general will not be Hermitian. Instead we use the fact that a positive definite matrix \( B \) has a unique positive definite square root \( B^{1/2} \). We introduce the change of variables

\[
u = B^{1/2}v,
\]  

(3)

which transforms (2) into

\[
\tilde{H} = B^{-1/2}AB^{-1/2}u = \lambda u,
\]  

(4)

and \( \tilde{H} \) is Hermitian. The problem has thus been reduced to standard Hermitian eigenvalue form to which QPE could in principle be applied.

A potential issue with Eq. (4) is that in general, even if \( B \) is sparse, \( B^{-1/2} \) is not sparse and \( \tilde{H} \) will be full. For example, the inverse of a tridiagonal matrix is dense. When \( \tilde{H} \) is full and in the absence of some other special structure, it is not likely that the unitary gate \( U_{\tilde{H}} \) required for QPE can be implemented efficiently.
For a restricted class of matrices $B$, however, $B^{-1/2}$ will be sparse. In particular, if in addition to being positive definite $B$ is also diagonal or block diagonal, its inverse retains the same sparseness pattern, and therefore $\tilde{H}$ will also be sparse. In the case where $B$ is diagonal, $B_{ij} = b_j \delta_{ij}$, then $\tilde{H}_{ij} = b_j^{-1/2} A_{ij} b_j^{-1/2}$. Therefore, $U \tilde{H} = e^{-iRt}$ could be efficiently implementable as a unitary gate, enabling phase estimation as described in Sec. II for this class of generalized eigenvalue problems.

### IV. STURM–LIOUVILLE PROBLEM

#### A. Finite-difference discretization

The Sturm–Liouville problem presents a paradigmatic example of a generalized eigenvalue problem. It takes the form

$$\frac{d}{dx} \left( p(x) \frac{dy}{dx} \right) + q(x)y(x) = \lambda r(x)y(x), \quad (5)$$

where $\lambda$ is the eigenvalue, and for boundary conditions we assume $y(0) = y(1) = 0$. We assume a regular Sturm–Liouville problem, for which $p > 0$ and $r > 0$ on $[0,1]$.

Quantum phase estimation for a restricted form of the Sturm–Liouville example employed a finite-difference discretization with a position basis, in which the weight function $r(x)$ turned into a diagonal mass matrix. Let us consider other discretizations, such as the finite element method. In a Galerkin procedure using a set of basis functions $\phi_i$, the matrix $B$ arises as

$$B_{ij} = \int dx \phi_i^*(x) \phi_j(x) \quad (10)$$

Some classes of finite-element methods, including discontinuous Galerkin, can turn the weight function into a block diagonal mass matrix. This can occur when a discretization uses disjoint cells, with each cell spanned by multiple basis functions, which may be orthogonal or non-orthogonal. If the basis functions within a cell are non-orthogonal, the matrix $B$ is block diagonal rather than diagonal. In fact, even if $r(x) = 1$ and there is no weight function, this choice of basis functions will lead to block diagonal positive-definite $B$. When $B$ is block diagonal, so is $B^{-1}$, and hence $B^{-1}$ is sparse. Then, for positive definite $B$, one can find $B^{-1/2}$ which is also block diagonal positive-definite.
diagonal. Therefore, $B^{-1/2}AB^{-1/2}$ will be sparse as well, allowing its time evolution operator to be implemented efficiently.

In contrast, other common finite-element discretizations may not lead to sparse $B^{-1/2}$. For example, consider the linear tent functions $\phi_j$ in one dimensions, where each basis function has finite support and overlaps with each of its two neighbors. The matrix $B$ is then tridiagonal. For this discretization, $B^{-1}$ and $H$ will not be sparse.

V. LINEAR IDEAL MHD

Another important example of a nontrivial generalized eigenvalue problem to which phase estimation might be fruitfully applied arises from plasma physics. Magnetohydrodynamics (MHD) describes the self-consistent motion of a conducting fluid with a magnetic field. MHD can describe the macroscopic behavior of a plasma, at a fluid level that coarse grains over the motion of individual particles, and it has found applications in stellar physics, astrophysical disks, planetary magnetism. When describing magnetically confined plasmas, such as those used in tokamak fusion reactors, ideal MHD has proven essential for calculations of macroscopic plasma stability [21–23].

In linear ideal MHD, the task of solving normal mode stability of a static plasma equilibrium takes the form of a generalized eigenvalue problem. The normal mode equation is

$$F(\xi(x)) = -\omega^2 \rho(x) \xi(x),$$

where $\xi$ is the Lagrangian fluid displacement, $\omega^2$ is the eigenvalue, $\rho(x)$ is the equilibrium mass density of the MHD fluid, and $F$ is the force operator, given by [24]

$$F(\xi) = -\nabla p_1 - B_0 \times (\nabla \times B_1) + (\nabla \times B_0) \times B_1 + (\nabla \Phi) \nabla \cdot (\rho \xi).$$

(12)

Here, $\Phi$ is an external potential, and $p_1$ and $B_1$ are the perturbed pressure and magnetic field and are linear in $\xi$. Here, $F$ is a differential operator, and therefore local.

It is a fundamental result of MHD theory that $F$ is a self-adjoint operator [24]. That is, given any two allowed displacements $\xi$ and $\eta$,

$$\int dx \eta^* \cdot F(\xi) = \int dx \xi^* \cdot F(\eta).$$

(13)

From the self-adjointness property, it follows that $\omega^2$ is real. One has normal-mode instability if there are any modes for which $\omega^2 < 0$, which corresponds to an imaginary frequency and an exponentially growing solution.

Discretization of Eq. (11) in the position basis, e.g., through finite-difference discretization, yields a sparse Hermitian matrix on the LHS and a diagonal, positive matrix on the RHS. Thus, the method described in Sec. III is in applicable. There are subtleties associated with singularities of the MHD spectrum, which are beyond the scope of this work, although methods have been developed to deal with them in classical computation [25].

VI. DISCUSSION

We have shown that quantum phase estimation can be applied to certain generalized eigenvalue problems of the form $Av = \lambda Bv$, where $A$ is a Hermitian matrix and $B$ is a positive definite matrix. This is accomplished by reducing this problem to a standard eigenvalue problem by defining $\tilde{H} = B^{-1/2}AB^{-1/2}$. For this reduction to lead to a sparse Hamiltonian whose time evolution can be implemented efficiently, $B^{-1/2}$ must be sparse. For example, $B$ can be diagonal or block diagonal. Many classes of physics problems arise where the fundamental continuous equations, when discretized, produce a diagonal or block-diagonal matrix $B$ that is positive definite. Some examples are Sturm–Liouville eigenvalue problems and the normal-mode formulation of the spectral equation in ideal MHD.

Even for problems whose continuous formulation is in standard Hermitian eigenvalue form, such as the time-independent Schrödinger equation, some choices of non-orthogonal basis functions lead to a generalized eigenvalue problem where $B$ is block diagonal, and for which these techniques can again be used to reduce the problem to standard form on which phase estimation can be applied.

Because the problem has been reduced to the standard form of phase estimation, the same practical considerations and error estimates that have been discussed elsewhere apply [9, 11]. One aspect that merits further comment is whether exponential speedup is attainable for the types of partial differential equations we have used as motivation. So far, it has not been established that any discretization based on a real-space uniform grid can lead to exponential speedup [11]. At most polynomial speedup has been shown in a fixed number of dimensions. The problem is not unique to phase estimation but arises with any Hamiltonian simulation [26].

This is a result of the spectral norm problem, which is that the error associated with digital quantum simulation of a Hamiltonian $H$, which scales with the norm $|H|$. For simplicity, consider simulation based on first-order Trotterization of $H = H_1 + H_2$. To simulate for a time $t$ in $m$ Trotter steps, an error estimate using the Baker–Campbell–Hausdorff formula is [27]

$$\varepsilon = O\left(\frac{|[H_1, H_2]|^2}{m}\right)$$

(14)

As one refines a grid, the norm of the discrete differential operator grows as the inverse of the grid spacing. Taking the case of one dimension for simplicity and a second-order derivative in $H_1$, one has $|H_1| \sim N^2$. Thus, with
\[ [H_1, H_2] \sim N^2, \text{ to simulate for a given time } t \text{ with constant error, } m \text{ must grow as } N^2, \text{ which is exponential in the number of qubits } n = \log N. \text{ Thus, Hamiltonian simulation may require so many Trotter steps to ensure accuracy that there is no exponential speedup} \ [11, 28]. \text{ Other algorithms for Hamiltonian simulation besides Trotterization produce similar conclusions; Ref.} [29] \text{ provides an algorithm with complexity scaling in the worst case as } |H|_{\text{max}} \text{, the largest entry of } H \text{ in absolute value. As in the Hamiltonian of Eq. (8), this norm also scales inversely with the grid size when there is a discrete differential operator.}

However, for certain applications, the actual error may be much smaller than the above error estimates of Hamiltonian simulation \ [28, 30, 31]. In particular, phase estimation of a smooth ground-state eigenfunction \( v \) or a vector approximating \( v \) that has little projection onto highly oscillatory modes should have much smaller error than the worst case because \[ |[H_1, H_2]v| \] \text{ will be much smaller than } |[H_1, H_2]|. \text{ Because grid-based discretizations of partial differential equations are common in classical computing, this issue deserves further investigation.}

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