

Solving feed forward partial differential equations with the quantum singular value transformation

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Abstract

We state eight partial differential equations which can be solved with the quantum singular value transformation, one quantum algorithm which is dependent upon two Hamiltonians and a unitary transformation.¹

1 Introduction

1.1 Overview

Quantum algorithms have garnered significant attention over the past few years, resulting in speedups using industrially developed, intermediate noisy scale, hardware available from Google Quantum AI [1], to other areas of research surrounding quantum chemistry computations for investigating properties of electronic structures [2], with several potential applications in the future as improvements to hardware are achieved. To demonstrate the prospects of applying quantum algorithms for solving partial differential equations, rather than fifteen which have previously been investigated by extending the approach of a variational quantum algorithm proposed by Lubasch et al, [4], which is dependent upon interfacing quantum, and classical, methods of computation for optimizing cost functions under a broad ensemble of initial conditions, each of which is prepared with the ZGR-QFT ansatz, we provide an overview of the quantum singular value transform (QSVT), which the authors of [5] propose is a viable candidate for solving feed forward differential equations. The QSVT is dependent upon a Hamiltonian formulation, in which a matrix is embedded in the block of a unitary transformation. As one application of such a transformation, it is possible to solve feed forward differential equations, upon having prepared an initial state that is acted upon by the matrix which is embedded into the unitary transformation, which could be of interest to implement on future hardware if novel error correcting codes are continually developed for mitigating errors caused by noise. With a runtime that is dependent upon the probability of selecting a suitably prepared state that is dependent on properties of the matrix, we identify eight differential equations which could be solved with this method, including the Heat equation, Reaction-diffusion equation, Heat kernel equation, Cole-Hopf transformation, Hartree equation, and Mason-Weaver equation. In comparison to gate-based quantum computation that is reliant upon executing operations on noisy qubits after an initial state of the solution is prepared, the QSVT is implemented through the action of two Hamiltonians, H and Z which are provided below in the next section. Each Hamiltonian for implementing the QSVT is dependent upon the action of the unitary U_f , which can be examined more closely, and analyzed in more detail, after having determined an appropriate function f which is dependent upon the singular values of the matrix. Following this overview, in the next subsection we describe the QSVT.

1.2 Algorithm

We describe an overview of the transform provided in [3], and then state eight partial differential equations which can be solved with the transformation after having identified conditions on the matrices A and B that we define later in the section. First, define,

$$U_f \equiv i \begin{bmatrix} \sqrt{\mathbf{I} - f(A^\dagger)f(A)} & f(A^\dagger) \\ f(A) & -\sqrt{\mathbf{I} - f(A)f(A^\dagger)} \end{bmatrix},$$

corresponding to the unitary transformation, for a matrix A . In order to simulate the time evolution of some Hamiltonian H , which takes the form,

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$$\begin{bmatrix} \cdot & A^\dagger \\ A & \cdot \end{bmatrix} ,$$

with $A^\dagger A \leq \mathbf{I}$, for arbitrary entries along the diagonal of the matrix above, we must be able to apply the Hamiltonian to,

$$Z \equiv \begin{bmatrix} 0 & A^\dagger \\ A & 0 \end{bmatrix} .$$

From a decomposition of the Hilbert space into left and right components, $\mathcal{H}_L \oplus \mathcal{H}_R$, the eigenvectors of the Hamiltonian can be determined from the system of equations,

$$H \begin{bmatrix} |r_j\rangle \\ \pm |l_j\rangle \end{bmatrix} \equiv \pm \sigma_j \begin{bmatrix} |r_j\rangle \\ \pm |l_j\rangle \end{bmatrix}$$

From the form of the unitary U_f defined at the beginning of the section, one can achieve inverse block encoding by taking $f(\sigma) \equiv \sigma$, from which the unitary would take the form,

$$i \begin{bmatrix} \sqrt{\mathbf{I} - A^\dagger A} & A^\dagger \\ A & -\sqrt{\mathbf{I} - AA^\dagger} \end{bmatrix} .$$

Under the assumption that there exists a function for which $f(\sigma) \equiv \sigma$, the previous system of equations for the eigenvalues and eigenvectors of the Hamiltonian allows one to also determine the eigenvalues and eigenvectors for the unitary transformation, from the system of equations,

$$U \begin{bmatrix} |\psi\rangle \\ 0 \end{bmatrix} = i \begin{bmatrix} (\sqrt{\mathbf{I} - A^\dagger A}) |\psi\rangle \\ A |\psi\rangle \end{bmatrix}$$

for some $\psi \in \mathcal{H}$. To solve feed forward differential equations, implement, for a square matrix A , the time-dependent construction,

$$\begin{bmatrix} (\sqrt{\mathbf{I} - A^\dagger A}) |\psi\rangle \\ (\sqrt{\mathbf{I} - A^\dagger A}) A |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - A^\dagger A}) A^{n-1} |\psi\rangle \\ A^n |\psi\rangle \end{bmatrix} \equiv \sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - A^\dagger A}) A^k |\psi\rangle |k\rangle \right) + A^n |\psi\rangle |n\rangle ,$$

of the state ψ , which is dependent upon repeated application of the matrix A to the first entry of the row vector given above, $(\sqrt{\mathbf{I} - A^\dagger A}) |\psi\rangle$. Another crucial quantity B , from the equality,

$$\frac{A - \mathbf{I}}{\Delta t} = B \iff A = B\Delta t + \mathbf{I} ,$$

for some duration of time Δt , and also that,

$$A^\dagger A = \mathbf{I} + (B + B^\dagger)\Delta t + B^\dagger B \Delta t^2 \leq \mathbf{I} ,$$

where B satisfies the time-evolution,

$$\frac{d}{dt} |\psi\rangle = B |\psi\rangle .$$

1.3 Paper organization

With the overview of the singular value transform, and its properties, in the next section we provide seven partial differential equations that can be solved using the transform. To apply the QSVT to each PDE of interest, we must identify the matrices A and B , which are related by the identity provided above. In each case, we express the ensemble of quantum states that are prepared by the QSVT as a summation.

1.4 Singular values of PDEs

We list each of the eight PDEs.

1.4.1 Heat equation

From solutions u for,

$$\frac{\partial u}{\partial t} = \Delta u \quad ,$$

write,

$$B \equiv \Delta \quad ,$$

which we denote as,

$$B^{\text{HE}} \equiv \Delta \quad .$$

We obtain the following expression for the A matrix,

$$A^{\text{HE}} = B^{\text{HE}} \Delta t + \mathbf{I} = \Delta \Delta t + \mathbf{I} \quad ,$$

from which the desired state that must be prepared is of the form,

$$\begin{bmatrix} (\sqrt{\mathbf{I} - (A^{\text{HE}})^\dagger A^{\text{HE}}}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (A^{\text{HE}})^\dagger A^{\text{HE}}}) A^{\text{HE}} |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (A^{\text{HE}})^\dagger A^{\text{HE}}}) (A^{\text{HE}})^{n-1} |\psi\rangle \\ (A^{\text{HE}})^n |\psi\rangle \end{bmatrix} \equiv \begin{bmatrix} (\sqrt{\mathbf{I} - (\Delta \Delta t + \mathbf{I})^\dagger (\Delta \Delta t + \mathbf{I})}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (\Delta \Delta t + \mathbf{I})^\dagger (\Delta \Delta t + \mathbf{I})}) (\Delta \Delta t + \mathbf{I}) |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (\Delta \Delta t + \mathbf{I})^\dagger (\Delta \Delta t + \mathbf{I})}) (\Delta \Delta t + \mathbf{I})^{n-1} |\psi\rangle \\ (\Delta \Delta t + \mathbf{I})^n |\psi\rangle \end{bmatrix} \quad ,$$

which is equivalent to the summation of states,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (\Delta \Delta t + \mathbf{I})^\dagger (\Delta \Delta t + \mathbf{I})}) (\Delta \Delta t + \mathbf{I})^k |\psi\rangle |k\rangle \right) + (\Delta \Delta t + \mathbf{I})^n |\psi\rangle |n\rangle \quad ,$$

from the summation,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (A^{\text{HE}})^\dagger A^{\text{HE}}}) (A^{\text{HE}})^k |\psi\rangle |k\rangle \right) + (A^{\text{HE}})^n |\psi\rangle |n\rangle \quad .$$

1.4.2 Reaction-diffusion equation

From solutions u for,

$$\partial_t \tilde{u} = D \partial_x^2 \tilde{u} - U(x) \tilde{u} \quad ,$$

given a pertubation of the solution,

$$u \equiv u_0(x) + u(\tilde{x}, t) \quad ,$$

write,

$$B \equiv D \partial_x^2 - U(x) \quad ,$$

which we denote as,

$$B^{\text{RD}} \equiv D\partial_x^2 - U(x) \quad .$$

We obtain the following expression for the A matrix,

$$A^{\text{RD}} = B^{\text{RD}} \Delta t + \mathbf{I} =_{\Delta} \Delta t + \mathbf{I} \quad ,$$

from which the desired state that must be prepared is of the form,

$$\begin{bmatrix} (\sqrt{\mathbf{I} - (A^{\text{RD}})^{\dagger} A^{\text{RD}}}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (A^{\text{RD}})^{\dagger} A^{\text{RD}}}) A^{\text{RD}} |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (A^{\text{RD}})^{\dagger} A^{\text{RD}}}) (A^{\text{RD}})^{n-1} |\psi\rangle \\ (A^{\text{RD}})^n |\psi\rangle \end{bmatrix} \equiv \begin{bmatrix} (\sqrt{\mathbf{I} - (A^{\text{HE}})^{\dagger} A^{\text{HE}}}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (A^{\text{HE}})^{\dagger} A^{\text{HE}}}) A^{\text{HE}} |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (A^{\text{HE}})^{\dagger} A^{\text{HE}}}) (A^{\text{HE}})^{n-1} |\psi\rangle \\ (A^{\text{HE}})^n |\psi\rangle \end{bmatrix} \quad ,$$

which is equivalent to the summation of states,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (\Delta t + \mathbf{I})^{\dagger} (\Delta t + \mathbf{I})}) (\Delta t + \mathbf{I})^k |\psi\rangle |k\rangle \right) + (\Delta t + \mathbf{I})^n |\psi\rangle |n\rangle \quad ,$$

from the summation,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (A^{\text{RD}})^{\dagger} A^{\text{RD}}}) (A^{\text{RD}})^k |\psi\rangle |k\rangle \right) + (A^{\text{RD}})^n |\psi\rangle |n\rangle \quad .$$

1.4.3 Heat kernel

From solutions K for,

$$\frac{\partial K}{\partial t}(t, x, y) =_{\Delta} K(t, x, y) \quad ,$$

defined for $t > 0$, satisfying the condition,

$$\lim_{t \rightarrow 0} K(t, x, y) = \delta_x(y) \quad ,$$

for x, y belonging to some finite volume, write,

$$B \equiv_{\Delta} \quad ,$$

which we denote as,

$$B^{\text{HK}} \equiv_{\Delta} \quad .$$

We obtain the following expression for the A matrix,

$$A^{\text{HK}} = B^{\text{HK}} \Delta t + \mathbf{I} =_{\Delta} \Delta t + \mathbf{I} \quad ,$$

from which the desired state that must be prepared is of the form,

$$\begin{bmatrix} (\sqrt{\mathbf{I} - (A^{\text{HK}})^\dagger A^{\text{HK}}}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (A^{\text{HK}})^\dagger A^{\text{HK}}}) A^{\text{HK}} |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (A^{\text{HK}})^\dagger A^{\text{HK}}}) (A^{\text{HK}})^{n-1} |\psi\rangle \\ (A^{\text{HK}})^n |\psi\rangle \end{bmatrix} \equiv \begin{bmatrix} (\sqrt{\mathbf{I} - (A^{\text{RD}})^\dagger A^{\text{RD}}}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (A^{\text{RD}})^\dagger A^{\text{RD}}}) A^{\text{RD}} |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (A^{\text{RD}})^\dagger A^{\text{RD}}}) (A^{\text{RD}})^{n-1} |\psi\rangle \\ (A^{\text{RD}})^n |\psi\rangle \end{bmatrix},$$

which is equivalent to the summation of states,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (\Delta \Delta t + \mathbf{I})^\dagger (\Delta \Delta t + \mathbf{I})}) (\Delta \Delta t + \mathbf{I})^k |\psi\rangle |k\rangle \right) + (\Delta \Delta t + \mathbf{I})^n |\psi\rangle |n\rangle, \quad ,$$

from the summation,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (A^{\text{HK}})^\dagger A^{\text{HK}}}) (A^{\text{HK}})^k |\psi\rangle |k\rangle \right) + (A^{\text{HK}})^n |\psi\rangle |n\rangle.$$

1.4.4 Cole-Hopf transformation

From solutions w for,

$$w_t = a \Delta w, \quad ,$$

write,

$$B \equiv a \Delta, \quad ,$$

which we denote as,

$$B^{\text{CH}} \equiv a \Delta.$$

We obtain the following expression for the A matrix,

$$A^{\text{H-C}} = B^{\text{H-C}} \Delta t + \mathbf{I} = a \Delta \Delta t + \mathbf{I}, \quad ,$$

from which the desired state that must be prepared is of the form,

$$\begin{bmatrix} (\sqrt{\mathbf{I} - (aA^{\text{H-C}})^\dagger aA^{\text{H-C}}}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (aA^{\text{H-C}})^\dagger aA^{\text{H-C}}}) aA^{\text{H-C}} |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (aA^{\text{H-C}})^\dagger aA^{\text{H-C}}}) (aA^{\text{H-C}})^{n-1} |\psi\rangle \\ (aA^{\text{H-C}})^n |\psi\rangle \end{bmatrix} \equiv \begin{bmatrix} (\sqrt{\mathbf{I} - (A^{\text{HK}})^\dagger A^{\text{HK}}}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (A^{\text{HK}})^\dagger A^{\text{HK}}}) A^{\text{HK}} |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (A^{\text{HK}})^\dagger A^{\text{HK}}}) (A^{\text{HK}})^{n-1} |\psi\rangle \\ (A^{\text{HK}})^n |\psi\rangle \end{bmatrix}, \quad ,$$

which is equivalent to the summation of states,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (a \Delta \Delta t + \mathbf{I})^\dagger (a \Delta \Delta t + \mathbf{I})}) (a \Delta \Delta t + \mathbf{I})^k |\psi\rangle |k\rangle \right) + (a \Delta \Delta t + \mathbf{I})^n |\psi\rangle |n\rangle, \quad ,$$

from the summation,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (A^{\text{H-C}})^\dagger A^{\text{H-C}}}) (A^{\text{H-C}})^k |\psi\rangle |k\rangle \right) + (A^{\text{H-C}})^n |\psi\rangle |n\rangle.$$

1.4.5 Hartree equation

From solutions u over \mathbf{R}^{d+1} for,

$$i\partial_t + \nabla^2 u = V(u)u \quad ,$$

for a potential,

$$V(u) \equiv \pm |x|^{-n} |u|^2 \quad ,$$

write,

$$B \equiv \frac{1}{i} (V(u) - \nabla^2 u) \quad ,$$

which we denote as,

$$B^H \equiv \frac{1}{i} (V(u) - \nabla^2 u) \equiv \frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u) \quad .$$

We obtain the following expression for the A matrix,

$$A^H = B^H \Delta t + \mathbf{I} = \left(\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u) \right) \Delta t + \mathbf{I} \quad ,$$

from which the desired state that must be prepared is of the form,

$$\begin{bmatrix} (\sqrt{\mathbf{I} - (A^H)^\dagger A^H}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (A^H)^\dagger A^H}) A^H |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (A^H)^\dagger A^H}) (A^H)^{n-1} |\psi\rangle \\ (A^H)^n |\psi\rangle \end{bmatrix}$$

which is equivalent to the row vector,

$$\begin{bmatrix} (\sqrt{\mathbf{I} - (\frac{1}{i} \pm |x|^{-n} |u|^2 - \nabla^2 u)^\dagger (\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u))}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (\frac{1}{i} \pm |x|^{-n} |u|^2 - \nabla^2 u)^\dagger (\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u))}) (\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u)) |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (\frac{1}{i} \pm |x|^{-n} |u|^2 - \nabla^2 u)^\dagger (\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u))}) (\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u))^{n-1} |\psi\rangle \\ (\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u))^n |\psi\rangle \end{bmatrix} \quad ,$$

which is equivalent to the summation of states,

$$\sum_{0 \leq k \leq n-1} \left(\left(\sqrt{\mathbf{I} - (\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u))^\dagger (\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u))} \right) \left(\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u) \right)^k |\psi\rangle |k\rangle \right) + \dots \\ \left(\frac{1}{i} (\pm |x|^{-n} |u|^2 - \nabla^2 u) \right)^n |\psi\rangle |n\rangle \quad ,$$

from the summation,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (A^H)^\dagger A^H}) (A^H)^k |\psi\rangle |k\rangle \right) + (A^H)^n |\psi\rangle |n\rangle \quad .$$

1.4.6 Mason-Weaver equation

From solutions c for,

$$D \frac{\partial c}{\partial z} = -sgc \ ,$$

write,

$$B \equiv -sgc \ ,$$

which we denote as,

$$B^{\text{MW}} \equiv -sgc \ .$$

We obtain the following expression for the A matrix,

$$A^{\text{MW}} = B^{\text{MW}} \Delta t + \mathbf{I} = (-sgc) \Delta t + \mathbf{I} \ ,$$

from which the desired state that must be prepared is of the form,

$$\begin{bmatrix} (\sqrt{\mathbf{I} - (A^{\text{MW}})^\dagger A^{\text{MW}}}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (A^{\text{MW}})^\dagger A^{\text{MW}}}) A^{\text{MW}} |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (A^{\text{MW}})^\dagger A^{\text{MW}}}) (A^{\text{MW}})^{n-1} |\psi\rangle \\ (A^{\text{MW}})^n |\psi\rangle \end{bmatrix}$$

which is equivalent to the row vector,

$$\begin{bmatrix} (\sqrt{\mathbf{I} - (((-sgc)\Delta t + \mathbf{I}))^\dagger ((-sgc)\Delta t + \mathbf{I})}) |\psi\rangle \\ (\sqrt{\mathbf{I} - (((-sgc)\Delta t + \mathbf{I}))^\dagger ((-sgc)\Delta t + \mathbf{I})}) ((-sgc)\Delta t + \mathbf{I}) |\psi\rangle \\ \vdots \\ (\sqrt{\mathbf{I} - (((-sgc)\Delta t + \mathbf{I}))^\dagger ((-sgc)\Delta t + \mathbf{I})}) ((-sgc)\Delta t + \mathbf{I})^{n-1} |\psi\rangle \\ ((-sgc)\Delta t + \mathbf{I})^n |\psi\rangle \end{bmatrix} \ .$$

which is equivalent to the summation of states,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (((-sgc)\Delta t + \mathbf{I}))^\dagger ((-sgc)\Delta t + \mathbf{I})}) ((-sgc)\Delta t + \mathbf{I})^k |\psi\rangle |k\rangle \right) + ((-sgc)\Delta t + \mathbf{I})^n |\psi\rangle |n\rangle \ ,$$

from the summation,

$$\sum_{0 \leq k \leq n-1} \left((\sqrt{\mathbf{I} - (A^{\text{MW}})^\dagger A^{\text{MW}}}) (A^{\text{MW}})^k |\psi\rangle |k\rangle \right) + (A^{\text{MW}})^n |\psi\rangle |n\rangle \ .$$

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