Hamiltonian singular value transformation and inverse block encoding

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Abstract: The quantum singular value transformation is a powerful quantum algorithm that allows one to apply a polynomial transformation to the singular values of a matrix that is embedded as a block of a unitary transformation. This paper shows how to perform the quantum singular value transformation for a matrix that can be embedded as a block of a Hamiltonian. The transformation can be implemented in a purely Hamiltonian context by the alternating application of Hamiltonians for chosen intervals: it is an example of the Quantum Alternating Operator Ansatz (generalized QAOA). We also show how to use the Hamiltonian quantum singular value transformation to perform inverse block encoding to implement a unitary of which a given Hamiltonian is a block. Inverse block encoding leads to novel procedures for matrix multiplication and for solving differential equations on quantum information processors in a purely Hamiltonian fashion.
The quantum singular value transformation (QSVT) [1] shows that if one can embed a matrix $A$ in a block of a performable unitary transformation, one can also implement a transformation with the same singular vectors as $A$, but whose singular values are polynomial functions of the singular values of $A$. The quantum singular value transformation is a powerful quantum algorithm that encompasses other quantum algorithms such as quantum simulation and matrix inversion as subcases. The methods of the QSVT are based on the technique of qubitization [2], a state-of-the-art method for simulating a Hamiltonian evolution given the ability to perform block encoding.

This paper presents a purely Hamiltonian version of the quantum singular value transformation. We show that if one has the ability to apply a Hamiltonian $H$ of which $A$ is a block, then we can perform the full quantum singular value transformation using the Quantum Alternating Operator Ansatz (generalized QAOA): we alternate application of the Hamiltonian $H$ with a second, readily applied Hamiltonian, for a chosen set of times. Our motivation in developing Hamiltonian QSVT is simple: quantum information processing is generically implemented via the application of semiclassical control fields, which apply time-dependent Hamiltonians to the quantum information bearing degrees of freedom. In the gate model of quantum computing, these control fields are used to implement unitary quantum logic gates, which are applied to the qubits/qudits/qumodes in the quantum computer. But many more possible Hamiltonians can be applied, including global Hamiltonians, as in the Quantum Approximate Optimization Algorithm (original QAOA) [3]. In general, the ability to apply a set of Hamiltonians governed by the application of time varying control fields allows one to apply any effective Hamiltonian in the algebra generated by the set. Different coherent quantum information processors, e.g., coherent diabatic quantum annealers [4], allow the application of the Hamiltonian quantum singular value transformation to the set of Hamiltonians that are ‘native’ to those processors – i.e., those that can be efficiently applied. By introducing a purely Hamiltonian version of the quantum singular value transformation that bypasses the gate model of quantum computing, we hope to expand the power of near term quantum information processors.

**Main result:**

In this paper we show that if one can apply a Hamiltonian of which a matrix $A$ is an
off-diagonal block, we can deterministically implement the unitary transformation
\[
U_f = i \left( \sqrt{I - f(A) f(A)} \begin{pmatrix} f(A) \\ f(A) \end{pmatrix} - f(A) \begin{pmatrix} f(A) \\ f(A) \end{pmatrix} \right),
\]
(1)
where \( f(A) \) is the matrix with the same singular vectors as \( A \), and singular values that are a function \( f \) of the singular values of \( A \).

\( U_f \) is easily verified to be unitary as long as \( f(A) f(A) \leq I \). (For example, expand the square root as a power series.) Note that \( U \) is anti-Hermitian as well as unitary, and so has eigenvalues \( \pm i \). Like the unitary QSVT, the Hamiltonian singular value transformation takes time \( O(\sigma_{\min}^{-1} \log(1/\epsilon)) \) to perform the transformation to accuracy \( \epsilon \), where \( \sigma_{\min} \) is the smallest singular value of \( A \).

Setting \( f(x) = x \) yields inverse block encoding, or inverse qubitization [2]: the ability to apply a Hamiltonian of which a matrix is a block allows one to apply a unitary of which the matrix is a block. Below, we apply inverse block encoding to give Hamiltonian versions of matrix multiplication and the quantum solution of differential equations.

**Preliminaries:**

Assume the ability to apply a Hamiltonian \( \pm H \), where
\[
H = \begin{pmatrix} \bullet & A^\dagger \\ A & \bullet \end{pmatrix},
\]
(2)
and the on-diagonal blocks are arbitrary. We assume that \( A^\dagger A \leq I \). We also assume the ability to apply the Hamiltonian \( \pm Z \), where
\[
Z = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.
\]
(3)
As shown in [5], by applying \( \pm H \) in alternation with \( \pm Z \), we can average out/refocus the on-diagonal terms of \( H \) in time \( O(1) \), so without loss of generality we take \( H \) to be of the form
\[
H = \begin{pmatrix} 0 & A^\dagger \\ A & 0 \end{pmatrix}.
\]
(4)

Write \( A = \sum_j \sigma_j |\ell_j\rangle\langle r_j| \), where \( \sigma_j \) are the singular values of \( A \) and \( |r_j\rangle, |\ell_j\rangle \) are the corresponding right and left singular vectors. The Hamiltonian \( H \) acts on the Hilbert space \( \mathcal{H}_R \oplus \mathcal{H}_L \) consisting of the direct sum of the the Hilbert spaces for the right and left singular vectors. The eigenvectors of \( H \) take the form
\[
H \left( \begin{pmatrix} |r_j\rangle \\ \pm|\ell_j\rangle \end{pmatrix} \right) = \pm \sigma_j \left( \begin{pmatrix} |r_j\rangle \\ \pm|\ell_j\rangle \end{pmatrix} \right),
\]
(5)
That is, within the two-dimensional subspace $\mathcal{H}_j$ spanned by $|r_j\rangle \pm |\ell_j\rangle$, $H$ acts as $\sigma_j X$, where $X$ is the $x$ Pauli matrix in this subspace.

Note that we can also apply the transformation

$$e^{i\phi Z/2}e^{-iHt}e^{i\phi Z/2} \equiv e^{-iG_\phi t}, \quad (6)$$

where

$$G_\phi \equiv \begin{pmatrix} 0 & e^{i\phi} A^\dagger \\ e^{-i\phi} A & 0 \end{pmatrix}. \quad (7)$$

$G_\phi$ acts within $\mathcal{H}_j$ as $\sigma_j$ times a Pauli matrix for a rotation about an axis at angle $\phi$ in the $xy$ plane.

Hamiltonian quantum singular value transformation:

From the results of the previous section, we can apply transformations of the form

$$e^{-iG_{\phi_k} t_k} \ldots e^{-iG_{\phi_1} t_1}. \quad (8)$$

Equation (8) shows that we can generate unitary transformations that act in each of the $\mathcal{H}_j$ as polynomials in $\cos(\sigma_j t_i)$, $\sin(\sigma_j t_i)$. The coefficients of these polynomials are determined by tuning the $\phi_i$. Qubitization [2] shows how to generate a broad class of such polynomial unitary transformations. Note that because of the Hamiltonian nature of our construction, we have greater flexibility than the transformations applied in qubitization [2] and the quantum singular value transformation [1]: there, because $H$ is applied as a block of a unitary, the times $t_i$ are all fixed to be equal. Here, we can vary the times $t_i$ as well as the angles $\phi_i$. This feature could prove useful for optimizing the transformation using variational methods.

The theorems of [1-2] show that the ability to perform transformations of the form (8) allows us to apply transformations of the form

$$U = \bigoplus_j \begin{pmatrix} P(\cos \sigma_j) & i \sin \sigma_j Q(\cos \sigma_j) \\ i \sin \sigma_j Q^*(\cos \sigma_j) & P^*(\cos \sigma_j) \end{pmatrix}, \quad (9)$$

where the degree of the polynomial $P$ is less than or equal to $k$, and the degree of the polynomial $Q$ is less than or equal to $k - 1$. The polynomials $P$ and $Q$ can be determined at will by choosing the angles $\phi_i$, subject to the constraint that $P$ has parity $k \mod 2$, $Q$
has parity \( k - 1 \mod 2 \), and that \(|P(\cos \sigma)|^2 + \sin^2 \sigma|Q(\cos \sigma)|^2 = 1 \). The first of these constraints comes from the product form of equation (8), and the second from unitarity.

To perform the Hamiltonian singular value transformation, we choose \( Q \) so that

\[
\sin \sigma_j Q^*(\cos \sigma_j) = f(\sigma_j) \pm \epsilon
\]

Equivalently, \( \sqrt{1-x^2}Q^*(x) \approx f(\arccos(x)) \): as in [1-2] we are effectively decomposing the function \( f(\arccos(x)) \) in terms of Chebyshev polynomials. For suitably smooth functions \( f \) the decomposition achieves accuracy \( \epsilon \) for Chebyshev polynomials of degree \( O(\log(1/\epsilon)) \). Similarly, take

\[
-iP(\cos(\sigma_j)) = \sqrt{I - f^*(\sigma_j)f(\sigma_j)} \pm \epsilon.
\]

To within accuracy \( \epsilon \), the resulting unitary transformation is

\[
U_f = i \left( \begin{array}{cc} \sqrt{I - f(A\dagger)f(A)} & f(A\dagger) \\ f(A) & -\sqrt{I - f(A)f(A\dagger)} \end{array} \right),
\]

which is the desired Hamiltonian singular value transformation of equation (1).

Inverse block encoding is obtained by taking \( f(\sigma) = \sigma \), which gives

\[
U = i \left( \begin{array}{cc} \sqrt{I - A\dagger A} & A\dagger \\ A & -\sqrt{I - AA\dagger} \end{array} \right).
\]

Because the derivative of \( \arccos \) diverges at \( \pm 1 \), we require \( |\sigma| < 1 - \delta \) in order to obtain an error scaling of \( \epsilon = O(e^{-\sqrt{2\delta k}}) \) in the \( k \)-th order Chebyshev polynomial expansion of \( \arccos(x) \) [6-7].

The error scaling for the Hamiltonian quantum singular value transformation is the same as for the unitary QSVT, and the number of alternating steps required to perform the transformation goes as \( \# = O(\sigma_{\text{min}}^{-1} \log(1/\epsilon)) \). In comparison with performing the same procedure using the generalized quantum linear systems algorithm [5,8], which relies on quantum phase estimation, we see that the dependence of the time has gone from \( 1/\epsilon \) to \( \log(1/\epsilon) \).

Since in practice the alternating Hamiltonians are applied by turning on and off semi-classical control fields, we also need to address the question of how accurately these control fields need to be applied. If each Hamiltonian application consists of a time-dependent term of the form \( \gamma(t)H \), then the key figure of merit is the total integral of \( \gamma(t) \) over the period during which the control is turned on and off: this integral needs to be precise to
accuracy $O(\epsilon/\#)$ in order for the accumulated error over the overall alternating sequence to be less than $\epsilon$. Note that in existing high-coherence quantum information processors such as ion traps, the semiclassical control error is the dominant source of error over the quantum computation. Current superconducting and ion-trap quantum computers have pulse control errors on the order of $2 \times 10^{-3} - 5 \times 10^{-3}$, with a next-generation goal of $1 \times 10^{-3}$. Given the favorable error scaling, the Hamiltonian QSVT should be performable on current NISQ devices.

The Hamiltonian quantum singular value transformation is implemented solely through the alternating application of the Hamiltonian $H$ and the Hamiltonian $Z$. That is, it is an application of the Quantum Alternating Operator Ansatz or generalized QAOA. As in the original QAOA (Quantum Approximate Optimization Algorithm) [3], this feature makes the Hamiltonian QSVT ripe for the application of variational methods: we set some task for the unitary $U_f$ to accomplish and try to find an optimal $f$ by varying the parameters $t_i, \phi_i$ in equation (8).

Applications:

Inverse block encoding provides a novel method for quantum matrix multiplication [9-10]: from equation (13) we have

$$U \left( \begin{array} {c} \psi \\ 0 \end{array} \right) = i \left( \begin{array} {c} (\sqrt{I - A^\dagger A})\psi \\ A^\dagger \psi \end{array} \right),$$

which allows one to implement $A|\psi\rangle$ with probability

$$\langle \psi|A^\dagger A|\psi\rangle.$$  

Amplitude amplification provides a quadratic improvement, allowing the state $A|\psi\rangle$ to be prepared in time $\sqrt{\langle \psi|A^\dagger A|\psi\rangle}$.

When $A$ is square, applying this procedure first to the first and second components of the state $(|\psi\rangle, 0, \ldots, 0)^T$, then to the second and third components, then to the third and fourth, etc. allows one deterministically to construct the state

$$\begin{pmatrix} \langle \sqrt{I - A^\dagger A}\psi \rangle \\ \langle \sqrt{I - A^\dagger A}A|\psi\rangle \\ \vdots \\ \langle \sqrt{I - A^\dagger A}A^{n-1}|\psi\rangle \\ A^n|\psi\rangle \end{pmatrix} = \sum_{k=0}^{n-1} (\sqrt{I - A^\dagger A}A^k|\psi\rangle|k\rangle + A^n|\psi\rangle|n\rangle).$$

(16)
Measuring the value of the second register yields the state $A^n|\psi\rangle$ with probability

$$\langle \psi | A^\dagger A^n | \psi \rangle.$$  \hfill (17)

Again, amplitude amplification provides a quadratic speed up in the preparation of this state.

Note that the requirement $A^\dagger A \leq I$ means that the probability of obtaining $A^n|\psi\rangle$ will be asymptotically exponentially suppressed except for components corresponding to the singular value $\sigma_j = 1$. Since $\sigma_j = 1$ corresponds to subspaces on which $H$ acts in a unitary fashion, this method allows us to identify ‘hidden’ unitaries in $H$.

When $A = I + B\Delta t$, then the state (16) yields the Euler forward solution of the differential equation

$$\frac{d|\psi\rangle}{dt} = B|\psi\rangle.$$ \hfill (18)

The requirement that

$$A^\dagger A = I + (B + B^\dagger)\Delta t + B^\dagger B\Delta t^2 \leq I$$ \hfill (18)

means that the eigenvalues of $B$ must have negative real part, so that the differential equation (18) is dissipative. If $B$ is sparse or low rank, then we can implement the Hamiltonian $H$ via conventional methods of quantum Hamiltonian simulation [11-13]. This method of solving the forward differential equation allows one to obtain the (unnormalized) state $|\psi(t)\rangle = e^{Bt}|\psi(0)\rangle$ that is the solution to the differential equation (18) by projecting onto the final component of the state in (16), which succeeds with probability $\langle \psi(t) | \psi(t) \rangle$.

That is, one can use inverse block encoding to solve dissipative differential equations on a quantum computer without having to resort to matrix inversion, a potential savings in computational complexity over conventional quantum differential equation solvers [14-15].

**History states:**

The Hamiltonian version of the quantum singular value transformation can be used to perform quantum matrix inversion to apply $(\sqrt{I - A^\dagger A})^{-1}$ to the first $n$ components of the vector (16) to obtain the state

$$\begin{pmatrix} |\psi\rangle \\ A|\psi\rangle \\ \ldots \\ A^n|\psi\rangle \end{pmatrix} = \sum_{k=0}^{n} A^k |\psi\rangle |k\rangle.$$ \hfill (20)
In the case that $A = I + B\Delta t$, this state is the ‘history state’ for the solution of the differential equation (18). The matrix inversion is non-deterministic, and succeeds with probability $O(1/\tilde{\kappa})$, where $\tilde{\kappa}$ is the condition number of $\sqrt{I - A^\dagger A}$.

Multiple Hamiltonians:

When building quantum computers, we implement unitary transformations by applying time dependent Hamiltonians $\sum_j \gamma_j(t) H_j$ governed by semiclassical control fields $\gamma_j(t)$. This ability allows us to implement effective Hamiltonians in the Lie algebra $A$ generated by the $H_j$, and to implement the corresponding embedding unitaries. The Hamiltonian QSVT then allows us deterministically to implement the $U_f$ of equation (1) for any $A$ that can be embedded in a block of a Hamiltonian $\in A$. Note that even systems where the applied Hamiltonians are quite simple, as in QAOA [3] where one alternates the application of an Ising Hamiltonian with identical rotations of the qubits about the $X$ axis, the algebra generated by the Hamiltonians is typically the full algebra of all possible Hamiltonians – QAOA is universal for quantum computation [16]. The set of effective Hamiltonians that can be generated efficiently by any given coherently controllable quantum system depends on the nature of the control Hamiltonians. Since Hamiltonian QSVT can be applied to any coherently controllable Hamiltonian system, we hope that our results will encourage experimentalists to investigate novel architectures for Hamiltonian quantum information processing. For example, Hamiltonian QSVT is a natural procedure to implement on the next generation of coherent diabatic quantum annealers.

Discussion:

This paper showed how to perform a Hamiltonian version of the quantum singular value transformation solely by the alternating application of Hamiltonians for different lengths of time. The method is an example of the quantum alternating operator ansatz (generalized QAOA), and allows the direct construction of the unitary transformations of the QSVT, without the application of quantum logic gates. Our goal in presenting this construction is straightforward: quantum information processing is typically implemented by the application of semiclassical control fields to implement time-varying Hamiltonians, which can be applied globally as well as locally. For experimentally accessible Hamiltonians, the Hamiltonian QSVT represents a direct and simple way to perform the powerful quantum singular value transformation.
As a simple example of Hamiltonian QSVT, we showed how to perform inverse block encoding: given the ability to apply a Hamiltonian, deterministically implement a unitary transformation in which the Hamiltonian is embedded as the off-diagonal blocks. Inverse block encoding provides novel methods for quantum matrix multiplication and the quantum solution of forward differential equations. Given the ability to apply multiple Hamiltonians, inverse block encoding allows one to embed any transformation in the algebra generated by the set of accessible Hamiltonians in a deterministically constructed unitary transformation.
References

[1] A. Gilyén, Y. Su, G.H. Low, N. Wiebe, *STOC 2019: Proceedings of the 51st Annual ACM SIGACT Symposium on Theory of Computing*, 193204 (2019).

[2] G.H. Low, I.L. Chuang, *Quantum* **3**, 163 (2019); arXiv: 1610.06546v3.

[3] E. Farhi, J. Goldstone, S. Gutmann, ‘A quantum approximate optimization algorithm,’ arXiv: 1411.4028 (2014).

[4] E.J. Crosson, D.A. Lidar, ‘Prospects for Quantum Enhancement with Diabatic Quantum Annealing,’ arXiv: 2008.09913 (2020).

[5] S. Lloyd, S. Bosch, G. De Palma, B. Kiani, Z.-W. Liu, M. Marvian, P. Rebentrost, D.M. Arvidsson-Shukur ‘Quantum polar decomposition algorithm,’ arXiv: 2006.00841 (2020).

[6] J.P. Boyd, *Chebyshev and Fourier Spectral Methods*, Dover Books on Mathematics, Dover (2001).

[7] A. Gil, J. Segura, N.M. Temme, *Numerical Methods for Special Functions*, Society of Industrial and Applied Mathematics (2007).

[8] A.W. Harrow, A. Hassidim, S. Lloyd, *Phys. Rev. Lett.* **103**, 150502 (2009).

[9] C. Shao, ‘Quantum Algorithms to Matrix Multiplication,’ arXiv: 1803.01601.

[10] L. Zhao, Z. Zhao, P. Rebentrost, J. Fitzsimons ‘Compiling basic linear algebra subroutines for quantum computers,’ arXiv: 1902.10394.

[11] S. Lloyd, *Science* **273**, 1073-1078 (1996).

[12] I.M. Georgescu, S. Ashhab, F. Nori, *Rev. Mod. Phys.* **86**, 153 (2014).

[13] A.M. Childs, A. Ostrander, Y. Su, *Quantum* **3**, 182 (2019); arXiv: 1805.08385v2.

[14] D.W. Berry, *J. Phys. A: Math. Theor.* **47** 105301 (2014).
[15] D.W. Berry, A.M. Childs, A. Ostrander, G. Wang, Comm. Math. Phys. 356, 1057-1081 (2017).

[16] S. Lloyd, ‘Quantum approximate optimization is computationally universal,’ arXiv: 1812.11075 (2018).