Quantum algorithm for total least squares data fitting

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The total least squares (TLS) method is widely used in data-fitting. Compared with the least squares fitting method, the TLS fitting takes into account not only observation errors, but also errors from the measurement matrix of the variables. In this work, the TLS problem is transformed to finding the ground state of a Hamiltonian matrix. We propose quantum algorithms for solving this problem based on quantum simulation of resonant transitions. Our algorithms can achieve at least polynomial speedup over the known classical algorithms.

I. INTRODUCTION

One basic problem in applied mathematics is to create a theoretical model and make a reliable prediction according to the observed data [1]. This problem appears in a broad class of fields such as signal processing, automatic control, physics, astronomy, biology, statistics, economics, etc [1][2]. The linear model with some parameters is most widely used, and the key is to determine these unknown parameters from the measurement data of certain variables. Let \( x = (x_1, \ldots, x_N)^T \) be the parameter vector that characterizes the model. Suppose that the observed data can be expressed by a linear combination as \( a_1 x_1 + \ldots + a_N x_N = b_i \), where \( a_1, \ldots, a_N \) and \( b_i \) stand for the observed data of variables. Such a data-fitting problem usually gives rise to an overdetermined linear system of equations with \( N \) unknowns \( x \) and \( M > N \). Our task is to find an optimal estimate of the parameter vector \( x \) under some constraints.

The well-known least squares (LS) method is one of the most widely used methods in data-fitting. It finds the vector \( x \) that minimizes \( \|Ax - b\|_2 \), where \( \| \cdot \|_2 \) denotes the matrix 2-norm. The LS solution can be expressed by Moore-Penrose inverse, and when \( A \) is of full column rank, it reads \( x_{LS} = (A^T A)^{-1} A^T b \). There exist two types of classical methods for the LS solution [3].

The direct method based on QR factorization is the standard one, while the iterative method utilizes the CG-like solvers. The sampling method is popular for large scale problems, which reduces the problem size under appropriate assumptions on the sampling probabilities, and achieves an approximate LS solution efficiently and accurately.

In the LS method, the matrix \( A \) is fixed and assumed to be free from error, while the vector \( b \) is contaminated by errors. However, this assumption is usually unrealistic in some cases, since the matrix \( A \) may not be accurate as well due to sampling errors, human errors, modeling errors and instrument errors, etc [4]. Page 5]. The total least squares (TLS) method gives a better estimate than the LS method [1] when there exist errors in both the vector \( b \) and the matrix \( A \), and especially when these errors are independent random variables with zero mean and equal variance, i.e., independent and identically distributed random variables.

Fitting a large amount of data is in fact a difficult task for a classical computer. For example, the computational complexity of the TLS method depends on the singular value decomposition (SVD), which costs about \( 26N^3 \) by using the R-bidiagonalization [5], where \( N \) is the data size. Even the partial SVD via the s-step Lanczos procedure or randomized SVD needs about \( O(N^2) \) flops [1,7]. Quantum computers can outperform classical computers in solving a number of problems [8–11]. In Ref. [12], a quantum data-fitting algorithm was proposed for the least squares method.

In this work, we propose a quantum algorithm for the TLS method of data-fitting based on the quantum simulation of resonant transitions. In Sec. II, we introduce the TLS fitting method; in Sec. III, we present a quantum algorithm for the TLS method, and in Sec. IV, we simulate the algorithms through a numerical example, and we conclude in Sec. V.

II. TOTAL LEAST SQUARES FITTING

The TLS data fitting problem can be formulated as

\[
\{ x_{TLS}, \ E_{TLS}, \ f_{TLS} \} : = \arg \min_{x, E, f} \| E, f \|_F \quad \text{s.t.} \ (A + E)x = b + f, \ \\
\]

where \( E \) denotes the errors in the observation matrix \( A \), \( f \) denotes the errors in the observation vector \( b \), and \( \| \cdot \|_F \) stands for the Frobenius matrix norm. The TLS method is also known as errors-in-variables model, measurement error modeling or orthogonal regression in the statistical literature [2][13]. The classical solver for the TLS problem is based on SVD [1]. For an overdetermined linear system of equations \( Ax \approx b \), suppose that \( A \) and its
algorithms based on the quantum simulation of resonant Hermitian matrix whose eigenvalues and the corresponding eigenvectors are state of the matrix.

The problem of TLS fitting is transformed to finding the ground state vectors of the matrix $S$. The TLS solution can also be expressed as

$$x_{\text{TLS}} = (A^\dagger A - \sigma_{N+1}^2 I)^{-1} A^\dagger b,$$

following Ref. [1] Theorem 2.7.

III. QUANTUM ALGORITHMS FOR TLS FITTING

From the above analysis, we can see that obtaining TLS solution to a data-fitting problem can be reduced to finding the singular vector $v_{N+1}$, which corresponds to the smallest singular value of the augmented matrix $C$. The vector $v_{N+1}$ can be obtained by solving the eigenproblem of an extended matrix

$$D = C^\dagger C,$$

whose eigenvalues and the corresponding eigenvectors are $\sigma_j^2$ and $v_j$, respectively. The approach we introduced can be applied for the extended matrix directly. The problem of TLS fitting is transformed to finding the ground state of the matrix $D$. In this work, we propose quantum algorithms based on the quantum simulation of resonant transitions and apply them for the TLS fitting.

We have proposed quantum algorithms for solving eigenproblems of a physical system [16, 17]. When the transition frequency between two energy levels of the system matches the frequency of a probe qubit coupled to the system, the probe qubit exhibits a dynamical response. By varying the frequency of the probe qubit and identifying the locations of resonance peaks, the energy spectrum of the system can be determined. And the system can be controllably evolved to the eigenstate with any desired eigenvalue. Therefore the energy spectrum and the corresponding eigenstates of the system can be obtained. In this work, we optimize the previous algorithms and apply them for TLS fitting. The present algorithm requires $(n + 1)$ qubits, with one probe qubit and $n$ qubits representing the matrix $D$, and $2^n \geq N + 1$. Details of the algorithms are described as follows.

A. Algorithm I

The Hamiltonian of the algorithm is constructed as

$$H^{(1)} = -\frac{1}{2} \omega \sigma_z \otimes I + H^{(1)}_R + c \sigma_x \otimes F,$$

where

$$H^{(1)}_R = \varepsilon_0 |1\rangle \langle 1| \otimes |\psi\rangle \langle \psi| + |0\rangle \langle 0| \otimes D,$$

and $I$ is the identity operator, $\sigma_{x,z}$ are the Pauli matrices, and $\omega$ is the frequency of the probe qubit. The first term in Eq. (6) is the Hamiltonian of the probe qubit, the matrix $D$ is encoded in the second term as shown in Eq. (7), and the third term describes the coupling between the probe qubit and the $n$-qubit quantum register that represents the system. Here, $\varepsilon_0$ is a reference parameter, and $c \ll 1$ is the coupling strength. In the algorithm, we set the probe qubit in its excited state $|1\rangle$ and the $n$-qubit register in a reference state $|\psi\rangle$ that can be easily prepared, then the initial state of the circuit is an eigenstate of $H^{(1)}_R$ with eigenvalue $\varepsilon_0$. The operator $F$ acts as a transition operator that transforms the reference state $|\psi\rangle$ to an eigenstate of the matrix $D$ with the desired eigenvalue. Its form depends on the eigenstate of interest. We give a detailed form of the operator $F$ for TLS fitting in Sec. III.C.

In order to obtain the eigenstate $|v_{N+1}\rangle$ of the matrix $D$, we need to obtain its corresponding eigenvalue first. By varying the frequency of the probe qubit $\omega$ or the reference parameter $\varepsilon_0$, we can locate the transition frequencies between the reference state and the eigenstates of $D$ through the quantum simulation of resonant transitions, thus the ground state eigenvalue of the matrix $D$ can be obtained. The procedures of the algorithm are briefly summarized as follows.

First, we make a guess on the range of the ground state eigenvalue of the matrix $D$ as $[\lambda_{\text{min}}, \lambda_{\text{max}}]$. Set the reference parameter $\varepsilon_0 < \lambda_{\text{min}}$, and the transition frequency between the reference state and the eigenstates of $D$ is $[\omega_{\text{min}}, \omega_{\text{max}}]$ with $\omega_{\text{min}} = \lambda_{\text{min}} - \varepsilon_0$ and
\[ \omega_{\text{max}} = \lambda_{\text{max}} - \varepsilon_0 \] (Here we use atomic units). We discretize this frequency range into \( l \) intervals, where each interval has a width of \( \Delta \omega = (\omega_{\text{max}} - \omega_{\text{min}}) / l \), and the frequencies are given by \( \omega_k = \omega_{\text{min}} + k \Delta \omega, k = 0, \ldots, l - 1 \).

We run the following steps by scanning these frequency points of the probe qubit: first we prepare the initial state of the circuit as \( |1\rangle |\psi\rangle \), such that \( H_R^{(1)} |1\rangle |\psi\rangle = \varepsilon_0 |1\rangle |\psi\rangle \); then set the transition frequency of the probe qubit \( \omega = \omega_k \) and evolve the circuit with the Hamiltonian \( H^{(1)} \) for time \( t \) by implementing the time evolution operator \( U^{(1)} = \exp (-iH^{(1)}t) \); after that, perform a measurement on the probe qubit in its computational basis. Repeat these steps for a number of times to obtain the decay probability of the probe qubit until run over all the frequency points.

After obtaining the ground state eigenvalue \( \sigma^2_{N+1} \) of the matrix \( D \), we encode this value in the Hamiltonian of the algorithm by setting \( \varepsilon_0 \) and \( \omega \) such that \( \sigma^2_{N+1} - \varepsilon_0 = \omega = 1 \), which is the condition for the resonant transition to occur. Then run the algorithm again, once the probe qubit is observed to decay to its ground state \( |0\rangle \), it indicates that the \( n \)-qubit register collapse to the ground state \( |v_{N+1}\rangle \).

In this algorithm, the operator \( F \) acts on the state \( |\psi\rangle \) and can be spanned by the complete set of eigenstates of the matrix \( D \) as \( F|\psi\rangle = \sum_{i=1}^{N+1} g_i |v_i\rangle \), where \( g_i = \langle v_i |F|\psi\rangle \). In basis \( \{|1\rangle, |0\rangle\} \), \( i = 1, 2, \ldots, N + 1 \), with the condition \( \sigma^2_{N+1} - \varepsilon_0 = \omega = 1 \), the resonant transition between states \( |1\rangle \) and \( |0\rangle |v_{N+1}\rangle \) is induced since \( H^{(1)}_{00} = H^{(1)}_{N+1,N+1} \). The system evolves from the initial state to the state \( |0\rangle |v_{N+1}\rangle \) reaches its maximal probability at time \( t \sim \pi / (2c |v_{N+1}|F|\psi|) \), provided that \( \sigma^2_N - \sigma^2_{N+1} \gg c \). Ignoring the off-resonant transitions, the decay probability of the probe qubit can be approximated as \( \sin^2 \left( \frac{Q t}{2} \right) \), where \( Q = 2c |v_{N+1}|F|\psi| \).

If \( |v_{N+1}|F|\psi| \) is finite, the system can be evolved to the state \( |v_{N+1}\rangle \) in finite time.

### B. Algorithm II

We can also obtain the ground state of the matrix \( D \) through projection from an initial guess state and purify it using an iterative procedure based on a resonance mechanism. The Hamiltonian of the second algorithm is constructed as

\[
H^{(2)} = -\frac{1}{2} \omega \sigma_z \otimes I + H_R^{(2)} + c \sigma_x \otimes I, \quad (8)
\]

where

\[
H_R^{(2)} = \varepsilon_0 |1\rangle \langle 1| \otimes I + |0\rangle \langle 0| \otimes D. \quad (9)
\]

In this algorithm, we first make a guess on the state \( |v_{N+1}\rangle \) as \( |\varphi^{(0)}\rangle \). As in algorithm I, we need to obtain the ground state eigenvalue of the matrix \( D \) first, then find the ground state \( |v_{N+1}\rangle \).

By preparing the initial state of the circuit as \( |1\rangle |\varphi^{(0)}\rangle \) and the time evolution operator \( U^{(2)} = \exp (-iH^{(2)}t) \) with \( \tau = \pi / (2c) \), the ground state eigenvalue of the matrix \( D \) can be obtained using the same procedures as in algorithm I. Then we can encode the ground state eigenvalue \( \sigma^2_{N+1} \) in the Hamiltonian of the algorithm by setting \( \varepsilon_0 \) and \( \omega \) such that \( \sigma^2_{N+1} - \varepsilon_0 = \omega = 1 \). Then we can run the following procedures to obtain the state \( |v_{N+1}\rangle \):

1. First, prepare the circuit in state \( |1\rangle |\varphi^{(0)}\rangle \);
2. then implement the time evolution operator \( U^{(2)} \); next perform a measurement on the probe qubit in its computational basis. A measurement is defined as “successful measurement” only if the measurement result on the probe qubit is in its ground state \( |0\rangle \). If a successful measurement is performed, then set the probe qubit in state \( |1\rangle \) and implement the time evolution operator \( U^{(2)} \) again, and perform a measurement on the probe qubit. Repeat these steps until \( j \) continuous successful measurements are achieved. The state \( |\varphi^{(j)}\rangle \) obtained on the last \( n \) qubits of the circuit is close to the ground state \( |v_{N+1}\rangle \) of \( D \).

The state \( |\varphi^{(0)}\rangle \) can be spanned by the eigenstates of the matrix \( D \) as \( |\varphi^{(0)}\rangle = \sum_{i=1}^{N+1} d_i |v_i\rangle \), where \( d_i = \langle \varphi^{(0)} |v_i\rangle \) and \( \sum_{i=1}^{N+1} |d_i| = 2 \). In basis \( \{|1\rangle, |0\rangle\} \), \( i = 1, 2, \ldots, N + 1 \), with the condition \( \sigma^2_{N+1} - \varepsilon_0 = \omega = 1 \), resonant transition between states \( |1\rangle \) and \( |0\rangle |v_{N+1}\rangle \) is induced. As analyzed in Ref. [17], the success probability of achieving \( j \) continuous successful measurements on the probe qubit is proportional to \( |\langle \varphi^{(0)} |v_{N+1}\rangle|^2 \). As long as \( |\langle \varphi^{(0)} |v_{N+1}\rangle|^2 \) is finite, and the gap \( \sigma^2_N - \sigma^2_{N+1} \) between the ground state and the first excited state of \( D \) is not exponentially small and \( \gg c \), the system converges quickly to the state \( |v_{N+1}\rangle \).

The system is evolved to its ground state in polynomial time with polynomial large success probability.

### C. Application of the algorithms for TLS fitting

We have to provide a good initial guess on the ground state of the matrix \( D \) in order to run the algorithms efficiently. In TLS fitting, the errors introduced in the measurement matrix \( A \) are independent and identically distributed random variables. It is reasonable to assume that the effects of these noises are small and can be treated perturbatively. Thus the LS solution of the fitting problem should be a good initial guess to that of the TLS solution. Mathematically, comparing the TLS solution shown in Eq. (4) with the LS solution \( x_{LS} = (A^T A)^{-1} A^T b \) of a fitting problem, we can see that in the TLS solution, the contribution from the smallest singular value of the augmented matrix \( C \) is taken into account. When the singular value \( \sigma_{N+1} \) is sufficiently small, it is reasonable to assume that the LS solution provides a good approximation to the TLS solution of the fitting problem. This can also be derived as follows. From Eq. (4), assuming that \( A \) is of full column rank, we
have
\[ x_{\text{TLS}} = (A^d A - \sigma_{N+1}^2 t)^{-1} A^d b \]
\[ = \left[ I - \sigma_{N+1}^2 (A^d A)^{-1} \right]^{-1} A^d b \]
\[ = \left[ I - \sigma_{N+1}^2 (A^d A)^{-1} \right]^{-1} x_{\text{LS}}. \] (10)

Thus
\[ x_{\text{TLS}} - x_{\text{LS}} = \sigma_{N+1}^2 (A^d A)^{-1} x_{\text{TLS}}. \] (11)

Then we get
\[ \frac{\|x_{\text{TLS}} - x_{\text{LS}}\|_2}{\|x_{\text{TLS}}\|_2} \leq \sigma_{N+1}^2 \left\| (A^d A)^{-1} \right\|_2 = \left( \frac{\sigma_{N+1}}{\sigma_N} \right)^2. \] (12)

We can see that \( x_{\text{LS}} \) is a good approximation to \( x_{\text{TLS}} \) when \( \sigma_{N+1} \ll \sigma_N \).

To resolve the TLS solution of a fitting problem, in algorithm I, we set the initial state of the system as \( |b\rangle \), and implement the Moore-Penrose pseudoinverse of the extended matrix. The evolution time of the algorithm scales as \( O(1/\epsilon^2) \) where \( \epsilon \) denotes error of the ground state eigenvalue of the matrix \( D \). The second part depends on the evolution time of the algorithm and the computational cost for simulating the algorithm Hamiltonians as shown in Eqs. (6) and (8), i.e., implementing the time evolution operator \( e^{-iH^{(1)}t} \) and \( e^{-iH^{(2)}t} \). The evolution time of the algorithm scales as \( \pi/(2c|\langle b|F|\psi\rangle|) \) in algorithm I, and it will be finite as long as \( |\langle b|F|\psi\rangle| \) is finite. In algorithm II, the TLS solution is projected out with a probability proportional to \( |\langle b|F|\psi\rangle|^2 \). As long as the overlap \( |\langle b|F|\psi\rangle|^2 \) is polynomially large, the cost of the algorithm will be polynomial. In general, the LS solution can serve as a good initial guess for the corresponding TLS solution of the fitting problem, therefore the evolution time of the algorithms is finite. The time evolution operators of the algorithms can be implemented through the Trotter formula [18]. There are also other algorithms for Hamiltonian simulation such as Taylor series approach [19] and quantum signal processing [20]. For sparse matrices, they can be simulated in linear time that grows nearly linearly with its sparsity [21, 22]. For dense matrices, it was shown in [23] that given black-box access to the matrix elements, Hamiltonian simulation with an error \( \delta_h \) can be performed in time \( O(N^{2/3} \text{poly} \log N / \delta_h^{1/3}) \). In Ref. [24], instead of assuming black-box access to the matrix elements, they propose to use a memory model where the entries of the matrices are stored in a data structure in a quantum random access memory (qRAM) [25]. The algorithm achieves sparsity-independent runtime scaling of \( O(\kappa^2 N \text{poly} \log (N) / \epsilon) \), where \( \kappa \) is the condition number and \( \epsilon \) is the precision to which the solution is approximated. The Hamiltonians of our algorithm can be calculated directly and simulated using these algorithms. Based on the above analysis, compare with the classical TLS fitting algorithms, our algorithms can achieve at least polynomial speedup in general.

In our algorithm, we obtain the quantum state \( |x_{\text{TLS}}\rangle \), which contains the solution to the TLS problem but different from the classical one, since one has to measure the state to learn the solution. For some problems in machine learning, such as big data classification, the quantum state \( |x_{\text{TLS}}\rangle \) can be used directly. In many cases, the output involves dimensionality reduction or compression, and we extract useful global information, rather than directly accessing each component of the state [26]. For example, in quantum classifier, the TLS solution can be encoded in a quantum state \( |x_{\text{TLS}}\rangle \). Given a query state, we classify it as +1 or -1 (output) by performing a SWAP test with the quantum state \( |x_{\text{TLS}}\rangle \) and measuring the success probability [27].

We can learn the TLS solution of the problem from the quantum state \( |x_{\text{TLS}}\rangle \) using the method in Ref. [12] when it is necessary. We can find the concise representation of fit functions that approximates the vector \( b \) within a certain error by using quantum state tomography and statistical sampling. In fact, one can choose the most important \( M' \) fit functions, where \( M' \) scales as \( \text{poly} (\log N) \), and prepare the state \( |x_{\text{TLS}}\rangle \) using compressed sensing. The fitting parameters for the \( M' \) fit functions in the state \( |x_{\text{TLS}}\rangle \) can be evaluated using SWAP test. We can also estimate the fit quality of the parameters \( |x_{\text{TLS}}\rangle \) efficiently by estimating the quantity \( |\langle b|I(A)|x_{\text{TLS}}\rangle|^2 \), where \( I(A) = \begin{pmatrix} 0 & A \\ A^d & 0 \end{pmatrix} \), as in Ref. [12]. The SWAP test
is used to determine the accuracy by performing a SWAP operation on the two quantum states $|b\rangle$ and $|I(A)x_{TLS}\rangle$ controlled by an auxiliary qubit. There exist the overheads of extracting such useful classical information. If compressed sensing technique is used to reconstruct the state within error $O(\varepsilon)$, we need $O(M^2 \log M^2/\varepsilon^2)$ measurements. The SWAP test for quality estimate needs $O(T_H/\delta^2)$, where $T_H$ is the cost for Hamiltonian simulation and $\delta$ is the accuracy of estimation [12].

IV. NUMERICAL SIMULATION OF THE ALGORITHMS

In the following, we simulate the algorithms through a numerical example in linear prediction (LP). We consider the time series expressed by $p$ sinusoids in the form $s(t) = \sum_{j=1}^{p} c_j e^{\lambda_j t}$, where the $\lambda_j$'s and $c_j$'s are to be determined. The $\lambda_j$'s are fundamental constants representing the natural decay of electromagnetic, acoustic and mechanical systems, while the $c_j$’s depend upon the excitation, sensor location, and time origin, etc. Let $z_j = \exp (\lambda_j T)$, $j = 1, \ldots, p$, where $T$ is a constant of the sample rate. Then we have the approximation of complex valued data $\{s_k\}$ in the form $s_k = \sum_{j=1}^{p} c_j z_j^k$. Such linear sum of damped complex exponentials with uniformly samples is widely used in Prony analysis, and it is essentially a nonlinear fitting problem for the amplitudes and frequencies.

We consider an LP model $\hat{s}_k = \sum_{j=0}^{N-1} a_j s_{k-j}$, where $s_{k-j}$ ($j = 1, \ldots, N$; $k \geq j$) are previous observed values, and $\hat{s}_k$ the predicted signal value. That is, a linear function of previous samples are used to estimate the future values. Let $A_N = [a_1, \ldots, a_N]$, $b_N = -a_{N+1}$, where $a_j = [s_{j-1}, \ldots, s_{j+M-2}]^T$. The linear prediction (LP) equation is formed with the unknown predictor coefficient vector $x = (a_0, a_1, \ldots, a_{N-1})^T$, which is achieved by solving the linear system

$$A_N x = b_N. \quad (13)$$

We can check that $A_N$ is a Hankel matrix and $\text{rank}(A_N) = \min\{N, p\}$. If $N \geq p$, then the linear system (13) is compatible. For any solution, we construct the characteristic equation

$$p_N(t) = a_0 + a_1 t + \cdots + a_{N-1} t^{N-1} + t^N.$$  

We know that $p_N(t)$ always contains $z_1, \ldots, z_p$ as its zeros when $N \geq p$, and hence the frequency can be derived from the roots of the characteristic equation. Then the amplitudes can be solved from the set of observed samples that are linear in amplitudes.

Here we only focus on the linear system (13) and its TLS solution. For the set of LP equations, both the coefficient matrix and the vector are contaminated by noises. It is natural to use the TLS solver, which is a promising method in signal processing. For example, Rahman and Yu [28] presented a method for frequency and amplitude estimations by using TLS to solve the LP equations. We choose $c_j$ and $\lambda_j$ as in Table I, where $p = 12$. The parameters $T = 0.2$, $N = 11$ and $M = 2^5$ are used. This test problem is taken from [7, 29, 30], which is regarded as a benchmark for TLS fitting.

We simulate the algorithm I for solving this TLS fitting problem by setting $\varepsilon_0 = -1.0$, $c = 0.0005$, and the evolution time $t = 30000$. The initial state of the system is set as $|b\rangle$, which is the normalized vector of $b$, and the operator $F$ is set as $F = (A^\dagger A)^{-1} A^\dagger$. By varying the transition frequency $\omega$ of the probe qubit and running the algorithm, we obtain the transition frequency spectrum between the reference state and the ground state of the matrix $D$ as shown in Fig. 1. The ground state eigenvalue of the matrix $D$ was obtained as 0.0046. At $\omega = 1.0046$, we obtain a state whose fidelity deviate only in order of $10^{-13}$ from the ground state of the matrix $D$. In simulating algorithm II, we set $c = 0.0001$ and $\tau = \pi/(2c) = 15708$. The initial state of the system is set as $|\chi_{LS}\rangle$, which is the normalized LS solution $x_{LS}$ of the fitting problem. The transition frequency spectrum of the ground state of the matrix $D$ with respect to the reference state are obtained as shown in Fig. 2. After running the algorithm again for one iteration by setting $\omega = 1.0046$, the state we obtained has fidelity that deviates from the TLS solution of the problem only in order

### Table I. The parameters in LP equation.

| $\lambda_j$ | $c_j$ | $\lambda_j$ | $c_j$ |
|-------------|-------|-------------|-------|
| -0.082 ± 0.926i | 1 | -0.220 ± 6.800i | 1 |
| -0.147 ± 2.874i | 1 | -0.247 ± 8.767i | 1 |
| -0.188 ± 4.835i | 1 | -0.270 ± 10.733i | 1 |

**FIG. 1.** (Color online) Transition frequency spectrum between the reference state $|b\rangle$ and the ground state of the matrix $D$ by simulating algorithm I. The blue solid curve represents the decay probability of the probe qubit at different frequencies with the coupling coefficient $c = 0.0005$ and the evolution time $t = 30000$, the reference parameter is set as $\varepsilon_0 = -1.0$. The red dotted vertical lines represent the known transition frequencies between the reference state and the eigenstates of the matrix $D$.**
of $10^{-12}$. In this example, the overlap between the LS and TLS solutions of the fitting problem, thus the success probability of the algorithm at $\omega = 1.0046$ is about 0.998. The LS solution is very close to the TLS solution of the fitting problem. This can also be predicted from the eigenvalue spectrum of the matrix $D$, the ground state eigenvalue of $D$ is 0.0046, while the eigenvalue of the first excited state is about 0.908, which is much larger than the ground state eigenvalue. In this case, we can see that it is reasonable to use LS solution as an initial guess for TLS problem. From the numerical simulation, we can see that by introducing a resonance mechanism, our algorithm can evolve the initial state quickly to the TLS solution with very high accuracy.

V. DISCUSSION

The TLS fitting method takes into account the errors introduced in the measurement matrix together with those in the observation vector. In the areas such as signal processing, and geophysics, etc., the TLS method is more practical than the LS method, since the measurement matrix $A$ and observation vector $b$ are both contaminated by noises. In the generic case, the TLS method yields a unique solution, which is given in analytic form in terms of the singular value decomposition of the augmented data matrix $C = [A, b]$. Precisely speaking, the TLS solution is expressed by the right singular vector associated with the smallest singular value of $C$, which corresponds to the eigenvector associated with the smallest eigenvalue of the Hermitian matrix $D = C^\dagger C$. The TLS data-fitting method is then transformed to finding the the ground state of a Hermitian matrix. We presented two algorithms based on the quantum simulation of resonant transitions to solve this problem. In our algorithms, any desired eigenstate of a system can be obtained by inducing proper resonant transitions between a probe qubit and a transition in the system that is simulated on a quantum computer. We show that in general, the LS fitting method can be a good approximation to the TLS solution, and thus can be used as the initial guess state in the algorithms. This work can be further generalized to the truncated TLS solution for inverse problems, and this will be our future work.

Adiabatic quantum evolution (AQE) \cite{31} algorithms and the PEA can also be applied for the TLS problem, which is transformed to finding the ground state of a Hermitian matrix, and both algorithms can solve this problem. In AQE, starting from an initial Hamiltonian and its ground state, the system is evolved adiabatically to the target Hamiltonian and its ground state. The runtime depends on the minimum energy gap between the ground and the first excited states of the time-dependent adiabatic evolution Hamiltonian. In our algorithm, the system is evolved to the ground state of the problem Hamiltonian matrix directly through quantum simulation of resonant transitions. It requires only information about the spectrum of the Hamiltonian matrix, without implementing the time-dependent adiabatic evolution Hamiltonian. Besides, whether the system is evolved to its ground state is heralded by the non-invasive measurements on the probe qubit.

The PEA randomly obtains one of the eigenstates of a quantum system from an initial guess state and produces its eigenvalue. The success probability for obtaining a given eigenstate is proportional to the overlap between the the initial guess state and the desired eigenstate. In solving the TLS problem by using the PEA, one can use the quantum state obtained from the LS data-fitting algorithm as an initial guess state, and apply PEA to project out the TLS solution from the LS solution. In algorithm I, the combination $F(\psi)$ plays a somewhat similar role to the initial guess state in the PEA. In our algorithm, once a transition frequency is identified by running the algorithm, the algorithm can be repeated with the parameters set to the resonance condition and the transition to the specific eigenstate occurs deterministically. Future runs of the algorithm can use this information to deterministically induce the transition to prepare the corresponding eigenstate. Also, our algorithm is simpler in that the transitions are heralded by the state of a single qubit obtained through measurements on the probe qubit, this makes the observation easier.

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REFERENCES

[1] S. Van Huffel, and J. Vandewalle, The Total Least Squares Problem: Computational Aspects and Analysis, 1991, SIAM, Philadelphia.
[2] S. Van Huffel, P. Lemmerling (editors), Total Least Squares and Errors-in-Variables Modeling, Analysis, Algorithms and Applications, Springer-Science+Business Media, B.V. 2002.
[3] B. Huang, Detection of abrupt changes of total least squares models and application in fault detection, IEEE Transact on Control Systems Technology, vol. 9, No. 2, 2004, 357-367.
[4] S. Van Huffel, Recent Advances in Total Least Squares Techniques and Errors-in-Variables Modeling, SIAM, Philadelphia, 1997. (Proceedings of the 2nd International Workshop on Total Least Squares and Errors-in-Variables Modeling held in Leuven, August 21–24, 1996).
[5] Petros Drineas, Michael W. Mahoney, S. Muthukrishnan, Sampling algorithms for l2 regression and applications, SODA '06 Proceedings of the seventeenth annual ACM-SIAM symposium on Discrete algorithm, Pages 1127-1136.
[6] G. H. Golub, and C. F. Van Loan, Matrix Computations, 4th Edition, The John Hopkins University Press, Baltimore, MD, 2013.
[7] P. Xie, H. Xiang, and Y. Wei, Randomized algorithms for total least squares problems, Numer. Linear Algebra Appl., e2219 (2018).
[8] P. Shor, Proc. 35th Ann. Symp. on Found. of Comp. Sci., 124–134 (IEEE Comp. Soc. Press, Los Alamitos, CA, 1994).
[9] L. K. Grover, Phys. Rev. Lett. 79, 325-328 (1997).
[10] A. M. Childs and W. van Dam, Rev. Mod. Phys. 82(1), 1-52 (2010).
[11] I. Buluta and F. Nori, Science, 326, 108 (2009).
[12] N. Wiebe, D. Braun, and S. Lloyd, Phys. Rev. Lett. 109, 050505 (2012).
[13] M. Schuermans, I. Markovsky, Peter D. Wentzell, S. Van Huffel, On the equivalence between total least squares and maximum likelihood PCA, Analytica Chimica Acta, 544 (2005), 254-267.
[14] G. H. Golub, and C. F. van Loan, An analysis of the total least squares problem, SIAM J. Numer. Anal., 17 (1980), pp. 883–893.
[15] A. W. Harrow, A. Hassidim, and S. Lloyd, Phys. Rev. Lett. 103, 150502 (2009).
[16] H. Wang, Phys. Rev. A 93, 052334 (2016).
[17] H. Wang, Scientific Reports, 7, 16342 (2017).
[18] M. A. Nielsen, and I. L. Chuang, Quantum Computation and Quantum Information. (Cambridge Univ. Press, Cambridge, England, 2000).
[19] D. W. Berry, A. M. Childs, R. Cleve, R. Kothari & R. D. Somma, Phys. Rev. Lett. 114, 090502 (2015).
[20] G. H. Low and I. L. Chuang, Phys. Rev. Lett. 118, 010501 (2017).
[21] D. Aharonov, and A. Ta-Shma, in Proceedings of the Thirty-fifth Annual ACM Symposium on Theory of Computing, STOC ‘03, edited by L. L. Larmore and M. X. Goemans (ACM, New York, 2003), pp. 20–29.
[22] D. W. Berry, G. Ahokas, R. Cleve, and B. C. Sanders, Commun. Math. Phys. 270, 359 (2007).
[23] D. W. Berry and A. M. Childs, Quantum Inf. Comput. 12, 29 (2012).
[24] L. Wossnig, Z. Zhao, and A. Prakash, Phys. Rev. Lett. 120, 050502 (2018).
[25] V. Giovannetti, S. Lloyd and L. Maccone, Phys. Rev. Lett. 100, 160501 (2008).
[26] P. Rebentrost, T. R. Bromley, C. Weedbrook, S. Lloyd, Quantum hopfield neural network, Phys. Rev. A 98, 042308 (2018).
[27] P. Rebentrost, M. Mohseni, and S. Lloyd, Quantum support vector machine for big data classification, Phys. Rev. Lett. 113, 130503 (2014).
[28] M.D. A. Rahman, K.-B. Yu, Total least squares approach for frequency estimation using linear prediction. IEEE Transactions on Acoustics, Speech and Signal Processing, ASSP-35(10): 1440–1454 (1987).
[29] M. L. Van Blaricum, R. Mittra, Problems and solutions associated with Prony’s method for processing transient data, IEEE Trans. Antennas and Propagation, AP-26, 174–182 (1978).
[30] M. Wei, The analysis for the total least squares problem with more than one solution, SIAM J. Matrix Anal. Appl., 13, 746–763 (1992).
[31] T. Albash and D. A. Lidar, Adiabatic quantum computation, Rev. Mod. Phys. 90, 015002 (2018).