Quantum Information and Computation, Vol. 2, No. 3 (2002) 192–197

QUANTUM ALGORITHM FOR MEASURING THE EIGENVALUES OF $U \otimes U^{-1}$ FOR A BLACK-BOX UNITARY TRANSFORMATION U

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Received September 25, 2001
Revised March 14, 2002

Estimating the eigenvalues of a unitary transformation U by standard phase estimation requires the implementation of controlled-U-gates which are not available if U is only given as a black box. We show that a simple trick allows to measure eigenvalues of $U \otimes U^{\dagger}$ even in this case. Running the algorithm several times allows therefore to estimate the autocorrelation function of the density of eigenstates of U. This can be applied to find periodicities in the energy spectrum of a quantum system with unknown Hamiltonian if it can be coupled to a quantum computer.

Keywords: measurements, energy gaps, quantum phase estimation, spectral gaps, autocorrelation
Communicated by: R Jozsa & C Fuchs

1. Standard phase estimation and its weakness

Finding the eigenvalues of unitary transformations or self-adjoint operators is a central task in quantum mechanics. The spectrum of a Hamiltonian and the corresponding unitary transformations are important to understand the thermodynamic and dynamical properties of a quantum system. Furthermore the estimation of eigenvalues is an important tool in quantum computation [3]. For that reason the algorithm for *phase estimation* has been developed [1, 2, 3, 4]. We rephrase it as follows. We have a Hilbert space $\mathcal{R}_a \otimes \mathcal{H}$ where $\mathcal{H}$ is the *target* register where the considered unitary U acts on and an ancilla register $\mathcal{R}_a$ consisting of k qubits if an accuracy of the eigenvalues of U of the order 2^{-k} is desired. Assume the target register to be in an eigenstate $|\psi_{\mathcal{H}}\rangle$ of U with eigenvalue $\exp(i\phi)$. Initialize the ancilla register in an equal superposition of all its logical states, i.e.,

$$|\psi_{\mathcal{R}}\rangle := (\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle))^{\otimes n} = \frac{1}{\sqrt{2^k}} \sum_{l<2^k} |l\rangle,$$

where l is the binary number corresponding to the k ancilla qubits $j = 0, \ldots, k-1$. On the joint Hilbert space $\mathcal{R}_a \otimes \mathcal{H}$ apply for all $j = 0, \ldots, k-1$ the transformations

$$V_j := |1_j\rangle\langle 1_j| \otimes U^{2^j} + |0_j\rangle\langle 0_j| \otimes 1, \tag{1}$$

where $|1_j\rangle\langle 1_j|$ and $|0_j\rangle\langle 0_j|$ are the projectors onto the $|0\rangle$ and $|1\rangle$ state of the ancilla qubit j, respectively. The operation U^{2^j} is the 2^j-fold iteration of U.

If $\mathcal{H}$ is in the state $|\psi_{\mathcal{H}}\rangle$ then $|\psi_{\mathcal{R}}\rangle$ is converted into the state

$$\frac{1}{\sqrt{2^k}} \sum_l e^{i\phi l} |l\rangle$$

by the 'kick-back-effect' [2]. After Fourier transformation on $\mathcal{R}_a$ we obtain

$$\frac{t}{2^k} \sum_{l,m} e^{-2\pi i l m/(2^k)} e^{i\phi l} |m\rangle,$$

i.e., the probability distribution is peaked around $m = \phi 2^k/(2\pi)$. If $|\psi_{\mathcal{H}}\rangle$ is not an eigenstate of U, than the algorithm will project approximatively (in the limit of large k) onto any of the eigenstates [4]. If the initial state on $\mathcal{H}$ is a density matrix that is diagonal in the basis of U, one will obtain any of the eigenvalues of U with the corresponding probability.

At first sight, quantum phase estimation seems to be applicable for finding energy values and eigenstates of an unknown Hamiltonian of an arbitrary quantum system simply by setting $U := \exp(-iHt)$. This would be interesting for the investigation of complex physical systems. To measure eigenvalues of interaction Hamiltonians in many-spin systems, as molecules or solid states, for instance, would be rather useful.

But there is a severe problem which is essentially that quantum phase estimation does *not* use the implementation of U as a *black box* subroutine. It uses the *conditional* transformations V_j (see eq. (1)) as black boxes and one should emphasize that no canonical conversion procedure building V_j from U is known if U is a black box. Sometimes this fact is hidden by using a language too classical if one explains the action of V_j by claiming that it implements U (or its iterations) if the corresponding ancilla qubit is in the logical state $|1\rangle$. This hides the fact that a superposition state of the ancilla has to lead to a superposition of the two actions 'implementation of U' and 'no implementation'. However, in [5] we have shown that the Hamiltonian evolution according to a Hamiltonian H can in principle be conjugated by other unitary transformations in such a way that the net effect is the evolution according to a 'controlled-H'. But the algorithm presented there is restricted to n-qubit pair-interaction Hamiltonians. Furthermore the black-box query used there is not a specific unitary transformation $U := \exp(iHt)$ but the whole semi-group $(\exp(iHt))_{t>0}$.

Here we address the question how to use quantum phase estimation for obtaining information about the spectrum of U if we have no prior information about U at all. We show that it is at least possible to get the autocorrelation function of the spectrum of U, or, speaking more explicitly, the spectrum of $U \otimes U^\dagger$, provided that the following assumptions are true:

1. The operation U is implementable on a system $\mathcal{H}$ that can be brought into interaction with another register $\mathcal{R}_1$ of equal Hilbert space dimension in such a way that complete exchange of quantum information between $\mathcal{H}$ and $\mathcal{R}_1$ is possible. Explicitly, this means the following. Let ϕ and ψ be states of $\mathcal{H}$ and $\mathcal{R}_1$, respectively. Then the unitary transformation S defined by $S|\phi\rangle \otimes |\psi\rangle := |\psi\rangle \otimes |\phi\rangle$.

   If $U = \exp(-iHt)$ for an appropriate $t > 0$ and H is the real Hamiltonian of the system $\mathcal{H}$ we assume that this exchange of information can either be done on a small time scale compared to the evolution according to H or the natural evolution can be switched off during the implementation of this information exchange.

2. There is another quantum register $\mathcal{R}_2$ with the same dimension as $\mathcal{H}$ and $\mathcal{R}_1$ and an ancilla register $\mathcal{R}_a$ consisting of k bits if the desired accuracy for the eigenvalues is 2^k.

3. On the system $\mathcal{R}_1 \otimes \mathcal{R}_2 \otimes \mathcal{R}_a$ we have a set of quantum transformations available which is universal for quantum computation.

Of course the assumption that the unknown Hamiltonian H can be switched off is problematic, but if additional prior information about the structure of H is available, standard decoupling techniques [6, 7, 8] can be used. Note that assumption 1 is considerably weaker than the assumption that H can be switched on and off by the quantum state of an ancilla qubit.*

2. Implementing a conditional transformation

The essential part of our algorithm is rather simple in contrast to [5] for the cost that we obtain eigenvectors and eigenvalues of $U \otimes U^{-1}$ instead of those of U. It consists of a conjugation of U by known unitary transformations in such a way that the net effect is the conditional transformation

$$V_j' := |1_j\rangle\langle 1_j| \otimes U^{2^j} \otimes 1 + |0_j\rangle\langle 0_j| \otimes 1 \otimes U^{2^j},$$

where $|0_j\rangle$ and $|1_j\rangle$ are states of the ancilla qubit j. One can see easily that the effect on the ancilla's states is the same if the unconditional unitary U^{-2^j} is implemented on $\mathcal{R}_2$ after each implementation of V_j'. This implements the conditional transformation

$$V_j'' := |1_j\rangle\langle 1_j| \otimes U^{2^j} \otimes U^{-2^j} + |0_j\rangle\langle 0_j| \otimes 1 \otimes 1\,.$$

Using standard phase estimation we can use V_j'' for obtaining eigenvalues of $U \otimes U^{\dagger}$.
The procedure for implementing V_j' consists of the following steps for $j = 0, \ldots, k-1$.

1. Implement state exchange of the registers $\mathcal{H}$ and $\mathcal{R}_1$, i.e., the unitary W with $W(|\alpha\rangle \otimes |\beta\rangle) := |\beta\rangle \otimes |\alpha\rangle$.

2. Implement U^{2^j} on $\mathcal{H}$. If $U = \exp(-iHt)$, i.e., if U is the unitary evolution according to the system Hamiltonian H, then one has to wait for a period of time $2^j t$.

3. Implement state exchange of $\mathcal{H}$ and $\mathcal{R}_1$ again. Steps 1-3 implement the transformation $\exp(-iHt)$ on the register $\mathcal{R}_1$.

4. Implement a *conditional* exchange of the states of $\mathcal{R}_1$ and $\mathcal{R}_2$ depending on the state of qubit j in the ancilla state, i.e. we implement

$$|1_j\rangle\langle 1_j| \otimes W + |0_j\rangle\langle 0_j| \otimes 1$$

on $\mathcal{R}_a \otimes \mathcal{R}_1 \otimes \mathcal{R}_2$.

*This is discussed in more detail in [5]

The essential part of the algorithm can be seen in Fig. 1. Note that the algorithm can actually be simplified by substituting $\mathcal{R}_1$ by $\mathcal{H}$ and dropping $\mathcal{R}_1$ completely. Our motivation for formulating the algorithm as we did is that $\mathcal{H}$ may be any physical system that can be made to interact with $\mathcal{R}_1$ in an appropriate way. In the case that $\mathcal{H}$ is not part of the quantum computer's register it is clearly a weaker assumption that an *unconditional* swap can be implemented than assuming that a *conditional* swap can be implemented.

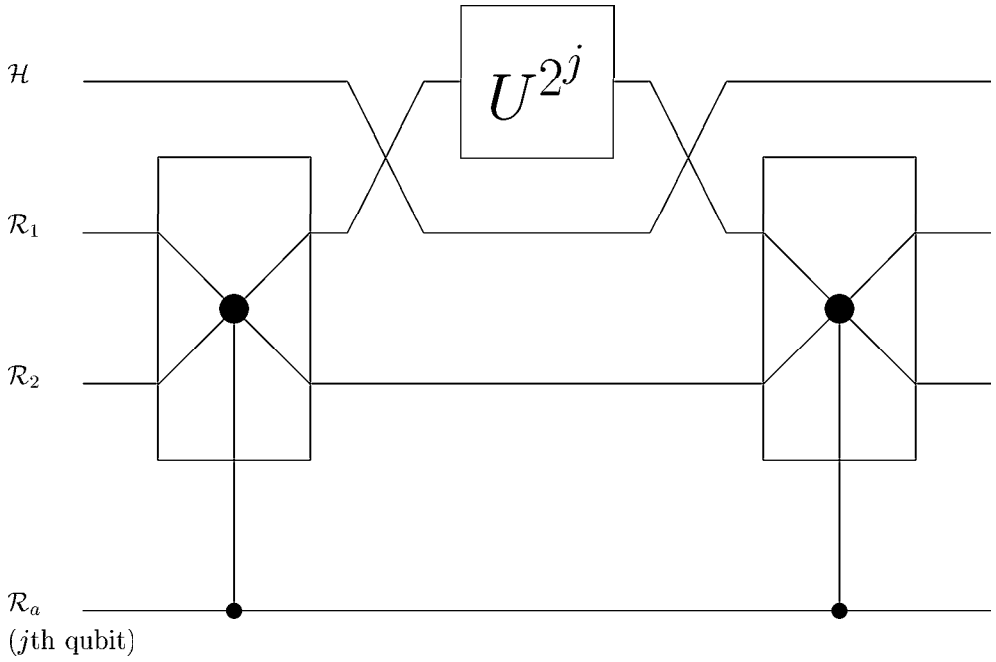

Fig.1: Circuit describing the algorithm. Here only one ancilla qubit is shown.

The conditional exchange between $\mathcal{R}_1$ and $\mathcal{R}_2$ can easily be implemented, if the registers $\mathcal{R}_1$ and $\mathcal{R}_2$ consist of qubits. In this case the conditioned permutation of two corresponding qubits is a usual Fredkin-gate [3]. The Fredkin gate acts on three qubits. They are part of the registers $\mathcal{R}_1, \mathcal{R}_2$, and $\mathcal{R}_a$ and the first two qubits are permuted if and only if the third is in the state $|1\rangle$.

Our algorithm may have applications for investigating the spectrum of a many-particle Hamiltonian in solid-state physics. This is interesting since the spectrum and its gaps determines dynamical and thermo-dynamical behavior of the system [9] and information on the spectrum of many-particle systems is difficult to obtain by classical methods. Of course for many-particle systems it is not possible to find the complete set of eigenvalues of $\exp(-iHt) \otimes \exp(iHt)$ since the dimension of $\mathcal{H}$ grows exponentially. But periodicities in the spectrum of H could be found. We sketch this idea. First we assume that t is chosen in such

a way that $t\Delta \leq \pi$, where Δ is an upper bound on the difference between the largest and smallest eigenvalue of H given by prior knowledge. Prepare both registers in the maximally mixed state. This can easily be done by preparing randomly one of the eigenstates of the computational basis. For every complex number z with $|z| = 1$ we define $M(z)$ as the multiplicity of the eigenvalue z if such an eigenvalue exists and 0 otherwise. Set $m(z) := M(z)/N$

(For systems with large dimensions where many energy levels get close together it is common to substitute the function m by an appropriate piecewise continuous function, the so-called density of states [9].).

The distribution of eigenvalues of $U \otimes U^{-1}$ is given by

$$p(z) := \sum_x m(xz)m(x)$$

Let $\mathcal{R}_1$ and $\mathcal{R}_2$ be in eigenstates of H corresponding to the eigenvalues λ_1 and λ_2, respectively. Then the outcome of the algorithm will be $z = \exp(it(\lambda_1 - \lambda_2))$. Since $(\lambda_1 - \lambda_2)t < 2\pi$ each possible outcome z corresponds uniquely to such an energy difference. The probability for the value $z = \exp(i\phi)$ is given by the autocorrelation function

$$\tilde{p}(\phi) := \sum_\alpha \tilde{m}(\alpha + \phi)\tilde{m}(\alpha)$$

with $\phi \in (-\pi, \pi)$ and where $\tilde{m}$ describes the relative multiplicities of the eigenvalues of tH. The function $\tilde{p}$ describes the relative multiplicities of $H \otimes 1 - 1 \otimes H$. In the many-particle approximation $\tilde{p}$ is the autocorrelation function of the density of states. If the spectrum of H contains periodic gaps this is mirrored in the function $\tilde{p}$. Assume for instance the eigenvalues of H to be $0, 1, 2, \ldots$ (like quasi-particle excitations) then one finds clearly spectral gaps of $H \otimes 1 - 1 \otimes H$. In general the function $\tilde{p}$ contains information on the periodicities in the spectrum of H.

Now we examine the number of runs that will be necessary in order to get reliable estimation on spectral gaps of $U \otimes U^{-1}$.

For every interval $I \subset (-\pi, \pi)$ set $\tilde{p}(I) := \sum_{\phi \in I} \tilde{p}(\phi)$. It is the probability for obtaining an outcome in the interval I. Assume that several runs of the eigenvalue estimation gave no result in I. Then it is straightforward to conclude that $\tilde{p}(I)$ is small. Unfortunately, the reliability of this conclusion cannot be estimated without referring to prior probabilities of the statement "$\tilde{p}(I)$ smaller than ϵ" for an appropriate value $\epsilon > 0$. However, statistical learning theory [11] provides us with the following bound (see [5] for details): Assume we say that the algorithm with k runs of the eigenvalue estimation has succeeded up to the accuracy ϵ if and only if there is at least one outcome in I for every I with $\tilde{p}(I) > \epsilon$. Then the risk that the algorithm fails is less than

$$4\epsilon^2 k^2 \exp(-\epsilon^2 k/4)) .$$

The risk is exponentially decreasing with the number of runs.

As long as the energy gaps that should be detected are not exponentially decreasing with the number of particles the algorithm can be used for finding periodic energy gaps in any many-particle system efficiently.

Acknowledgments

Thanks to P. Wocjan for useful remarks. Part of this work has been supported by the European project Q-ACTA and the DFG-project 'verlustarme Informationsverarbeitung'.

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