Quantum algorithm for finding periodicities in the spectrum of a black-box Hamiltonian or unitary transformation

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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.

I. STANDARD PHASE ESTIMATION AND ITS WEAKNESS

Finding the eigenvalues of unitary transformations or self-adjoint operators is a central task in quantum mechanics. The thermodynamic and dynamical properties of a quantum system are determined by the spectrum of a Hamiltonian and the corresponding unitary transformations. Furthermore the estimation of eigenvalues is an important tool in quantum computation (see [2]). For that reason the algorithm for phase estimation has been developed (see [3] and references therein). We rephrase it as follows. We have a Hilbert space $R_a \otimes H$ where $H$ is the target register where the considered unitary $U$ acts on and an ancilla register $R_a$ 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 $|\psi_H\rangle$ of $U$ with eigenvalue $\exp(i\phi)$. Initialize the ancilla register in an equal superposition of all its logical states, i.e.,

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

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

$$V_j := |1_j\rangle\langle 1_j| \otimes U^2 + |0_j\rangle\langle 0_j| \otimes 1,$$  \hspace{1cm} (1)

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

If $H$ is in the state $|\psi_H\rangle$ then $|\psi_R\rangle$ is converted into the state

$$\frac{1}{\sqrt{2^k}} \sum_{l} e^{i2\pi \phi_m} |l\rangle,$$

by the ‘kick-back-effect’ [3]. After Fourier transformation on $R_a$ we obtain

$$\frac{1}{\sqrt{2^k}} \sum_{l,m} \left\{ \frac{1}{\sqrt{2^k}} \sum_{l,m} e^{-2\pi i \phi m} e^{i\phi_m} |m\rangle \right\},$$

i.e., the probability distribution is peaked around $m = \phi2^k/\pi$. If $|\psi_H\rangle$ 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 $H$ is a density matrix which 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’. Imagine that the black box implementing $U$ contains a memory storing the information whether $U$ is implemented or not. Then such a superposition of implementation is destroyed by the memory. However, in [4] we have shown that the unitary evolution $U$ can in principle be conjugated by other unitary transformations in such a way that the net effect is a ‘controlled-$U$’.

But the class of unitary transformations $U$ considered there is only the evolutions according to $n$-qubit pair-interaction Hamiltonians. Here we address the question.

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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 $\mathcal{H}$ which 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. 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 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.

II. IMPLEMENTING A CONDITIONAL TRANSFORMATION

The essential part of our algorithm is rather simple in contrast to 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

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

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 $U^{-2j}$ is implemented on $\mathcal{R}_2$ after each implementation of $V_j$. This implements the conditional transformation $V_j'' := |1_j\rangle\langle 1_j| \otimes U^{2j} \otimes U^{-2j} + |0_j\rangle\langle 0_j| \otimes 1 \otimes 1$.

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 $U^{2j}$ 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 the time $2lt$.

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

The conditional exchange 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.

Our algorithm might have applications for investigating the spectrum of a many-particle Hamiltonian in solid-state physics, since the spectrum and its gaps determines dynamical and thermo-dynamical behavior of the system. 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 $t \Delta < \pi$, where $\Delta$ is an upper bound on the difference between the largest and smallest eigenvalue of $H$ given by prior knowledge. Assume that $\mathcal{R}_1$ and $\mathcal{R}_2$ are prepared in the same initial density matrix $\rho$. The state $\rho$ defines a probability measure on $\mathbb{R}$ by setting $p(\lambda) = 0$ if $\lambda$ is no eigenvalue of $u$ and $p(\lambda) := \langle \lambda | \rho | \lambda \rangle$ else. If $\rho$ is the maximally mixed state and the dimension of $\mathcal{H}$ is large such that the probability measure can approximatively described by a probability density, this measure is known as the density of states. Running the algorithm several times allows to estimate the density of eigenstates of $H \otimes 1 - 1 \otimes H$ which is the autocorrelation function of the density of eigenstates of $H$. If this density contains periodicities, for instance when

\footnote{This is discussed in more detail in}

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there are spectral gaps with equal distances, they can be
detected by using our algorithm. Note that in solid-state
physics, for instance, energy gaps occur which do not de-
pend on $n$. Hence the size of the required ancilla register
does not necessarily grow with $n$ for detecting interesting
gaps.

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