Quantum algorithm for measuring the energy of $n$ qubits with unknown pair-interactions

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The well-known algorithm for quantum phase estimation requires that the considered unitary is available as a conditional transformation depending on the quantum state of an ancilla register. We present an algorithm converting an unknown $n$-qubit pair-interaction Hamiltonian into a conditional one such that standard phase estimation can be applied to measure the energy. Our essential assumption is that the considered system can be brought into interaction with a quantum computer. For large $n$ the algorithm could still be applicable for estimating the density of energy states and might therefore be useful for finding energy gaps in solid states.

1. INTRODUCTION

Finding the energy spectrum of a given Hamiltonian is an important task in physics since it determines the dynamical and thermodynamical behavior of a quantum system. In solid-states physics, for instance, the spectrum, in particular its gaps, are relevant for the transport properties and in the famous BCS-theory the energy gap between the ground state and the first excited state is decisive for understanding super-conductivity.

Therefore a lot of efforts has been done on calculating the spectrum of many-particle Hamiltonians. Some models are known, where the Hamiltonian can explicitly be diagonalized and advanced mathematical tools like non-commutative geometry could be shown to be useful for finding energy gaps in perfect crystals or those with defects and quasi-periodicity. Nevertheless, the diagonalization of generic many-particle Hamiltonians is computationally hard and even restricted information about its spectrum is difficult to obtain, since the dimension of the Hilbert space grows exponentially with the number of particles. Here we discuss how to obtain information about the spectrum of a Hamiltonian by a quantum computer. Apart from the fact that the algorithm is able to find energy gaps in many-particle systems efficiently, it has a property which is impossible in principle without processing quantum information: we can gain information about the spectrum of a physical system with an unknown Hamiltonian provided that there is an interface between the quantum register and the considered system for exchanging quantum information. If such an interface does not exist the algorithm can be used if the Hamiltonian is known and the quantum computer is able to simulate the corresponding unitary evolution, i.e., if efficient implementations of $\exp(-iHt)$ for each $t > 0$ exist. Then the algorithm can use those implementations as black-box subroutines.

We restrict our attention to an unknown Hamiltonian $H$ of the following form. Let $H$ act on the Hilbert space $\mathcal{H} := (\mathbb{C}^2)^\otimes n$, which we shall refer to as the target register. We assume $H$ to consist of 1-qubit terms and pair-interactions between the $n$ two-level systems, i.e.,

$$H := \sum_{j \leq n, \alpha} r_j^\alpha \sigma^\alpha_j + \sum_{k<l \leq n, \alpha, \beta} J_{k,l,\alpha,\beta} \sigma^\alpha_k \sigma^\beta_l, \quad (1)$$

where $\alpha = x, y, z$ and $\sigma^\alpha_k$ is the Pauli matrix $\sigma_\alpha$ acting on qubit $k$. The $3n \times 3n$-matrix $J$ and the $3n$-vector $r$ specify the interaction uniquely.

First we should discuss why the problem can not be solved by a simple application of the well-known quantum algorithm for phase estimation. The reason is that the algorithm for estimating eigenvalues of a unitary $u$ does not work with black-box queries of $u$, it relies on the quantum transformation

$$\hat{u} := u \otimes |1\rangle\langle1| + 1 \otimes |0\rangle\langle0|$$

implementing $u$ if and only if an ancilla qubit is in the state $|1\rangle$, i.e., the ancilla qubit controls the implementation of $u$. This causes severe problems if $u := \exp(-iHt)$ is the natural time evolution, since phase estimation would require a system with Hamiltonian

$$H \otimes |1\rangle\langle1|,$$

i.e., the time evolution should be switched on and off by the ancilla’s state. First of all it is not clear how to ‘switch off’ the natural dynamics of a system, for example the interaction between nuclear spins in a real molecule. However, this problem can be solved if certain approximations are allowed as it is the case in standard decoupling techniques in Nuclear Magnetic Resonance. Assume that local transformations of the form

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2Of course information about the spectrum of a system’s Hamiltonian can be obtained by sophisticated experiments in principle without using our algorithm. But performing sophisticated quantum measurements is quantum information processing.

3The problem of simulating pair-interaction Hamiltonians by a given one has recently been discussed in [3–8].
can be applied arbitrarily fast (‘fast control limit’). If \( v \) is applied before the system evolves according to its Hamiltonian \( H \) and \( v^d \) is applied afterwards, then the system evolves as if it was subjected to the conjugated Hamiltonian \( vHv^d \). Concatenations of such ‘conjugated evolutions’ for small time intervals make the system approximately evolving as if it was subjected to the ‘average Hamiltonian’ which is given by the convex combination of the different conjugated Hamiltonians \( \tilde{H} \). This technique can be applied for ‘switching off’ Hamiltonians \( \tilde{H} \). At first sight it might seem as if this technique could be applied to control \( H \) by the ancilla’s state. But this would require to substitute the sequence of decoupling local transformations by conditional transformations of the form

\[
\tilde{v} := v \otimes |0\rangle\langle 0| + 1 \otimes |1\rangle\langle 1|.
\]

with \( v \) as eq. (2). The assumption that \( \tilde{v} \) could be implemented arbitrarily fast is much less justified than the usual fast control limit, since such a transformation refers to an interaction between ancilla and the target qubits and we have no reason to assume that this interaction is considerably stronger than the interaction which we want to switch off.

In other words, there is no obvious way to convert \( H \) into \( H \otimes |1\rangle\langle 1| \). Below we present a scheme converting \( H \) into \( H \otimes \sigma_z \), which has essentially the same effect. Our assumptions are the following.

1. The target register \( H \) can be brought into interaction with a quantum computer’s register \( R \). This interaction acts on the same time scale as \( H \). The interaction between \( H \) and \( R \) can be switched off without disturbing \( H \).

2. During that time period where \( H \) interacts with \( R \) the Hamiltonian evolution \( H \) can be switched off. This decoupling is controlled by classical signals and not by a state of a quantum register.

In order to illustrate these assumptions we consider a molecule with \( k := n + m \) nuclear spins. Assume that the interactions between the spin pairs \((j, l)\) for \( j, l \leq n \) are unknown and the interactions between all the other pairs are known. Given an arbitrary subset \( M \subseteq \{1, 2, \ldots, n + m\} \), the following procedure can be applied for switching off all those terms in the Hamiltonians concerning qubits in the set \( M \). For each qubit in \( M \) choose vectors \( x_1, \ldots, x_l \) of equal dimension \( d \) with the following property: The entries are \( 1, x, y, z \) and for each pair \( x_i, x_j \) of vectors each pair \((\alpha, \beta)\) with \( \alpha, \beta = 1, x, y, z \) appear equally often in the list \((x_i^\alpha, x_j^\beta)_{r \leq d}\) if \( x_i^r \) is the \( r^{th} \) entry of the vector \( x_i \). The vectors \( x_1, \ldots, x_l \) are said to form an orthogonal array. If \( x_j^\alpha = \sigma_j \) than the time evolution of spin \( j \) is conjugated by the unitary transformation \( \sigma_j \) during the \( r^{th} \) time period, where we have used the convention that \( \sigma_1 \) is the identity map. If the time periods are small, the resulting time evolution is approximately the identity for all the spins in \( M \) and those terms of \( H \) which do not involve spins in \( M \) are unchanged.

Then we consider the first \( n \) spins as the target register with the unknown Hamiltonian \( H \) and the other spins form the quantum computer’s register \( R \). The total Hamiltonian will be of the same form as eq. (4) characterized by a \( 3(n + m) \)-vector \( r \) and a \( 3(n + m) \times 3(n + m) \) matrix \( J \).

In order to switch off the interaction between \( H \) and \( R \) we choose \( M \) := \{1, 2, \ldots, n + m\}. Then the unknown Hamiltonian \( H \) on the spins 1, 2, \ldots, \( n \) is remaining.

If the Hamiltonian on the target register should be switched off in such a way that the interaction between one specific qubit \( j \leq n \) in the target register and one specific qubit \( n + l \) in the ancilla register remains, one has to take \( M \) as the complement of the set \( \{j, n + l\} \). Note that this does not remove the 1-qubit terms \( \sigma_i^{n+l} \) and \( \sigma_i^{n+l} \). This is important since \( \sigma_i^{n+l} \) is unknown and is therefore disturbing if we want to implement a definite 2-qubit transformation on the qubit pair \((j, n + l)\). Therefore we have to switch it off. This can be done as follow.

The interaction between \( j \) and \( n + l \) is given as

\[
\sum_{\alpha, \beta} g_{\alpha, \beta} \sigma_j^{\alpha} \sigma_j^{\beta}.
\]

Choose a specific pair \( \alpha, \beta \) such that \( g_{\alpha, \beta} \neq 0 \). Cancel all the terms \( \sigma_i^{\alpha} \sigma_i^{\beta} \) with \((\alpha, \beta) \neq (\alpha, \beta) \) by conjugation of the evolution with the 4 unitaries \( 1, \sigma_j^{\alpha}, \sigma_j^{\beta}, \sigma_j^{\alpha} \sigma_j^{\beta} \) on 4 time periods of equal length. The result is that the term

\[
r_j \sigma_j^{\alpha} + r_j \sigma_j^{\beta} + \sigma_j^{\alpha} \sigma_j^{\beta} + g_{\alpha, \beta} \sigma_j^{\alpha} \sigma_j^{\beta}
\]

is remaining. The 1-qubit terms can be cancelled by conjugating the evolution with \( \sigma_j^{\alpha} \sigma_j^{\beta} \) for half of the time period with \( \alpha' \neq \alpha \) and \( \beta' \neq \beta \). Since this changes the sign of the operators \( \sigma_j^{\alpha} \) (by the anti-commutation property of the Pauli-matrices) and \( \sigma_j^{\alpha} \), the bilinear term \( \sigma_j^{\alpha} \sigma_j^{\beta} \) is unchanged.

This shows that the assumptions 1. and 2. above are justified. Note that it is not relevant which interaction between ancilla qubits and register is available. If the true physical interaction is

\[
\sum_{\alpha, \beta} g_{\alpha, \beta} \sigma_i^{\alpha} \sigma_i^{\beta}
\]

then it can be converted into each other Hamiltonian with coefficients \( g_{\alpha, \beta} \) (see [4]) in the sense of the ‘average Hamiltonian’ method. Hence, if we write ‘switch on the interaction \( \sigma_x \otimes \sigma_z \)’ we do not assume the real physical Hamiltonian to be of this form, we assume only that the true Hamiltonian of the system can be used for simulating the required term. This is the continuous analogue of
the usual way of describing algorithms by basic gates as ‘controlled not’ operations: it does not matter whether the quantum computer really has the ‘controlled not’ as a basic operation but it should be capable of ‘simulating’ it by those transformations which are really available. Our way of describing the algorithm by ‘switching on and off interactions’ should therefore only be considered as a convenient language for continuous quantum algorithms.

II. THE ALGORITHM

First we consider only one ancilla qubit and describe how to convert the Hamiltonian \( H \otimes 1 \) into the conditional Hamiltonian \( H \otimes \sigma_z \) controlled by the ancilla’s state.

We can switch off all the coupling except of those on one specific qubit pair \((j, k)\) by so-called selective decoupling [5]. Furthermore we can select those terms in the remaining Hamiltonian which contain only \( \sigma^x \) and \( \sigma^y \) for specific \( \alpha \) and \( \beta \). The remaining term is given by

\[
H_{j,k,\alpha,\beta} = r_{\alpha}^{j} \sigma_{\alpha}^{j} + r_{\beta}^{k} \sigma_{\beta}^{k} + J_{j,k,\alpha,\beta} \sigma_{\alpha}^{j} \sigma_{\beta}^{k}
\]

First we convert \( H_{j,k,\alpha,\beta} \) into the term

\[
H_{j,k,\alpha,\beta}^\prime := \frac{2}{n-1} (r_{\alpha}^{j} \sigma_{\alpha}^{j} + r_{\beta}^{k} \sigma_{\beta}^{k}) + J_{j,k,\alpha,\beta} \sigma_{\alpha}^{j} \sigma_{\beta}^{k}
\]

This can be done by dividing the considered small time interval \([0, \delta]\) into two intervals \([0, \delta(1/2 - 1/(n-1))]\) and \([\delta(1/2 - 1/(n-1)), \delta]\). During the first interval the evolution according to \( H_{j,k,\alpha,\beta} \) is conjugated by \( \sigma_{\alpha}^{j} \sigma_{\beta}^{k} \). This reverses the sign of the 1-qubit terms whereas the 2-qubit term is unchanged. During the second interval the evolution according to \( H_{j,k,\alpha,\beta} \) is applied.

Now we can describe the conversion into a controlled Hamiltonian. By identifying \( x, y, z \) with the additive group \( F_3 := \{0, 1, 2\} \) it can be explained as follows.

1. Apply the unitary transformation \( u_j \) defined by the equation

\[
u_j \sigma_{\alpha}^{j} u_j^\dagger = \sigma_{\alpha+1}^{j}.
\]

2. Apply time evolution corresponding to \( H_{j,k,\alpha,\beta}^\prime \) for a small time period \( \epsilon \).

3. Switch on the interaction between target and ancilla qubit given by

\[
H_{j} := \sigma_{\alpha+1}^{j} \otimes \sigma_z
\]

for the time \( \epsilon \).

4. Simulate evolution according to \(-H_{j,k,\alpha,\beta}^\prime\) for the time \( \epsilon \). Inverting unknown Hamiltonians is described in [5]. In our case the inversion subroutine can be reduced as follows. Choose a large number \( p \). Divide the time interval \([0, 3\epsilon]\) into \(3p\) intervals of equal length. During the interval \( l \) conjugate the evolution according to \( H_{j,k,\alpha,\beta}^\prime \) by the unitary transformations \( \sigma_{\alpha+1}^{j} \otimes \sigma_{\beta}^{k} \) if \( l \) is 0, 1, or 2 mod 2, respectively. In the limit \( p \to \infty \), we obtain a perfect simulation of the evolution according to \(-H_{j,k,\alpha,\beta} \).

5. Switch on the interaction

\[
-H_{j}
\]

for the time \( \epsilon \).

6. Apply \( u_j^\dagger \).

7. Repeat steps 1 to 6 with qubit \( k \).

Up to an error of order \( \epsilon^3 \) this simulates the time evolution corresponding to

\[
iu_j [H_{j,k,\alpha,\beta}, H_{j}] u_j^\dagger + iu_k [H_{j,k,\alpha,\beta}, H_{j}] u_k^\dagger = 2H_{j,k,\alpha,\beta} \otimes \sigma_z
\]

for the time \( \epsilon^2 \) with the definition

\[
H_{j,k,\alpha,\beta}^\prime := \frac{1}{n-1} (r_{\alpha}^{j} \sigma_{\alpha}^{j} + r_{\beta}^{k} \sigma_{\beta}^{k}) + J_{j,k,\alpha,\beta} \sigma_{\alpha}^{j} \sigma_{\beta}^{k}.
\]

Due to the equation

\[
\sum_{\alpha,k<\alpha,\beta} H_{j,k,\alpha,\beta}^\prime = H
\]

the concatenation of the above procedure for all unordered pairs \((j, k)\) and all \( \alpha, \beta \) simulates time evolution according to

\[
H \otimes \sigma_z.
\]

Note that the time required for obtaining the unitary transformation

\[
\exp(-iH \otimes \sigma_z \delta)
\]

goes to zero for \( \delta \to 0 \) but the time overhead required for this simulation depends on the desired accuracy since the resulting evolution is only of second order a non-trivial one. Note that \( \sigma_{\alpha}^{j} \sigma_{\beta}^{k} \) can also be converted into \( \sigma_{\alpha}^{j} \sigma_{\beta}^{k} \otimes \sigma_z \) by a conjugation of the evolution with an appropriate 2-qubit gate acting on qubit \( k \) and the ancilla qubit, since \( \sigma_{\alpha}^{j} \otimes 1 \) and \( \sigma_{\beta}^{k} \otimes \sigma_z \) have the same spectrum as operators on 2 qubits. But this kind of converting the Hamiltonian into a conditional one does not have the property that an infinitesimal time step of the algorithm requires only infinitesimal time. Whether this is a true disadvantage for the desired accuracies has to be checked by thorough numerics.

Now we can apply usual phase estimation procedure to the conditional Hamiltonian evolution.

Now we initialize the ancilla register by a Hadamard transformation on each qubit. We implement the transformation
\[ \exp(-i(H \otimes \sigma^z_j 2^j \tau)) \]

for each ancilla qubit \( j = 0, \ldots, m - 1 \). The total running time of this implementation is \((2^m - 1)\tau\) times the time overhead for simulating \( H \otimes \sigma_z \) with appropriate accuracy.

We choose \( \tau \) in such a way that \( 2\sqrt{\tau} \Delta = \pi \) if \( \Delta \) is an upper bound for the difference between greatest and smallest eigenvalue of \( H \) given by prior knowledge. For every known systems in many-particle physics, \( \Delta \) is always of the order of \( n \), since energy per particle is a well-defined quantity in the thermodynamic limit \( n \rightarrow \infty \). The size \( m \) of the ancilla register has to be chosen in such a way that \( 2^{-m}\tau \) is smaller than the desired accuracy of the energy measurement. It is convenient to consider the ancilla qubit \( j \) as the \( j \)th number of a binary digit. Then the initial state of \( \mathcal{R} \) can be written as

\[ \frac{1}{\sqrt{2^m}} \sum_{l < 2^m} |l\rangle, \]

If the target register is in an eigenstate of \( H \) with eigenvalue \( E \) we obtain (up to an irrelevant global phase) the ancilla state

\[ \frac{1}{\sqrt{2^m}} \sum_l e^{-i2E\tau} |l\rangle, \]

since \( \exp(-i\sigma_z \tau) \) produces a relative phase difference \( \exp(-2i\tau) \) between the ancilla states \( |0\rangle \) and \( |1\rangle \).

By inverse Fourier transformation, one obtains the state

\[ \frac{1}{2^m} \sum_{k,l} e^{-i2\pi kl/(2^m)} e^{i2E\tau} |k\rangle. \]

Measuring the ancilla register in the standard basis provides good estimations for \( E \) since the probability that the measured result \( k \) differs more than \( e \) from \( 2^m E \tau / \pi \) is less than \( 1/(2e - 2) \) \([8]\). If \( 2^{-m}/\tau \) is much smaller than the energy gaps of \( H \), the algorithm projects onto the eigenstates of \( H \) \([9] \). For large \( n \), we cannot expect this to be achievable since the gaps decrease exponentially with \( n \) in the generic case. However, in this case the algorithm can be used for estimating the density of energy states, since the measured results will mostly be around those energy values where the density is high, provided that the target register has been initialized in the maximally mixed state. Estimating the density of states is an important task in solid-state physics \([12]\) and spectral gaps can be detected by this method. Most interesting energy gaps in solid states physics do not depend on the number of particles \([13,14]\). They could be detected without increasing the size of the ancilla register. But one should emphasize that only those gaps can be detected which are localized around typical energy values according to the initial density matrix. Therefore it might be more useful to start with thermodynamic equilibrium states in the target register in order to find gaps around values which are typical for the desired temperature \[10\].

We should mention a difficulty which appears for large \( n \) and how it could be overcome. We assumed that each qubit in the target register can be brought into interaction with each qubit of the ancilla register. Keeping in mind the example with nuclear spins in a molecule, one should take into account that the strength of the interactions is strongly decreasing with the distance between the spins. Accordingly, the interaction time between ancilla and target spin has to be increased for large distances and the resulting running time might become unacceptable. Therefore we emphasize that the algorithm can be rewritten in such a way, that it is not necessary to have an interaction between each qubit in \( H \) and each qubit in \( \mathcal{R} \). Instead, one can transfer the information qubit by qubit into a quantum register. To speak more precisely, one can realize the algorithm within the following setting instead of assumptions 1) and 2) above:

1. Apart from \( \mathcal{R} \), there is a quantum register \( \mathcal{H}' \) with \( n \) qubits such that the ‘information exchange’

\[ w : |\phi \rangle \otimes |\psi \rangle \leftrightarrow |\psi \rangle \otimes |\phi \rangle \]

can be implemented at definite times in such a way that \( \exp(-iHt) \) can be implemented on \( \mathcal{H}' \) by the following subroutine:

- implement \( w \).
- wait the time \( t \).
- implement \( w \).

2. The system \( \mathcal{H}' \otimes \mathcal{R} \) has full capabilities of quantum computation.

Then \( \mathcal{H} \) can be substituted by \( \mathcal{H}' \) if the instruction ‘wait the time \( t \)’ is substituted by the subroutine above. Due to the quantum computation capabilities on \( \mathcal{H}' \otimes \mathcal{R} \) we can clearly implement any desired transformation of the form \( \exp(-i\sigma_{\alpha} \otimes \sigma_z t) \) for all \( t \in \mathbb{R} \) between any arbitrary qubit pair. This shows once more that instructions of the form ‘switch on the interaction \( \sigma_{\alpha} \otimes \sigma_{\alpha+1} \)’ as above should not be taken literally. Having full capabilities of quantum computation, we can clearly implement unitary evolutions corresponding to the interaction \( \sigma_{\alpha} \otimes \sigma_{\alpha+1} \). The best way of ‘simulating’ this interaction is hardware-dependent.

In order to estimate the running time of the algorithm one should keep in mind that \( n(n-1)/2 \) interaction terms

\[ ^3 \text{Concerning the electrons of solid states, for instance, one is often interested in the energy gaps near the Fermi level } [13]. \]
have to be coupled to the ancilla register (The selection of specific coupling does not produce any time overhead). The time for converting one interaction term into a conditional one seems to be independent of \( n \) at first sight. But here might come in a subtle \( n \)-dependence as well: it is possible that the simulation of one term \( H_{j,k,\alpha,\beta} \otimes \sigma_z \) has to be more exact if one wants to find spectral gaps for large \( n \). Estimating the error in the eigenvalues of the total Hamiltonian resulting from an error in the simulation of each coupling might be a difficult task of perturbation theory. But the error of the total Hamiltonian is only \( n^2 \)-times the error of the single coupling terms. Since we are interested in gaps of the order \( 1 \), it should be possible to reproduce them with polynomial time overhead.

The algorithm shows a nice application of ‘simulations of Hamiltonians’: The algorithm can used to find eigenvalues of Hamiltonians by simulating the corresponding unitary evolution on a quantum computer. Apart from its possible application in many-particle physics, the algorithm shows a new aspect for understanding the double-role of self-adjoint operators as observables and generators of transformations, since we have constructed a measurement procedure for \( H \) by using the evolutions \( \exp(-iHt) \) as black-box procedures.

This gives a new scheme for measuring non-trivial joint observables.

The reader might get confused about one little paradox: we claimed to measure the actual energy value of the system despite the fact that only energy differences have physical relevance (as long as general relativity is not involved). This paradox is resolved by specifying more precisely what the algorithm does. We assumed the Hamiltonian \( H \) to be traceless. In case we start with a non-traceless one, only the traceless part will survive the conversion procedure \( H \otimes 1 \mapsto H \otimes \sigma_z \). Hence the algorithm measures the difference between the actual energy and the trace of \( H \), i.e., the average of the energy values over all the states. This seems again to be paradox: in case the system is in a definite eigenstate, why can the ancilla register ‘feel’ the average energy over all the other states despite the fact that the system never deviates from its actual eigenstate? This paradox is only pretended by the ‘infinitesimal language’. Of course the system does deviate a little bit from the actual eigenstate during the algorithm. Note that the procedure simulating \( H \otimes \sigma_z \) consists of a long sequence of transformations (close to the identity) which do not leave the eigenstates of \( H \) invariant.

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\[^4\]In an other setting, this has already been noted in [13].
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