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Simulating quantum systems on a quantum computer

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We show that the time evolution of the wave function of a quantum-mechanical many-particle system can be simulated precisely and efficiently on a quantum computer. The time needed for such a simulation is comparable to the time of a conventional simulation of the corresponding classical system, a performance which can't be expected from any classical simulation of a quantum system. We then show how quantities of interest, like the energy spectrum of a system, can be obtained. We also indicate that ultimately the simulation of quantum field theory might be possible on large quantum computers.

Keywords: quantum computers; simulated decay; fermionic field theories; one-dimensional particle; energy spectrum

1. Quantum computers

Quantum computers are still imaginary devices, but it is hoped that eventually the technical problems involved in their realization can be overcome (Lloyd 1993; Gershenfeld & Chuang 1993; Cirac & Zoller 1995; Monroe *et al.* 1995; Pellizzari *et al.* 1995; Haroche & Raimond 1996; Chuang & Yamamoto 1995; Unruh 1995; Ekert & Jozsa 1996). Quantum computers could solve some problems much faster than conventional computers. Most prominently, Peter Shor (1994) has given a 'quantum algorithm' for factoring large integers in polynomial time.

An l-bit quantum computer may be thought of consisting of l quantum mechanical two-state systems. Computations would be carried out by inducing unitary transformations of a few at a time of these quantum-bits (qubits). This may be done by exterior fields controlled from the outside. Upon observation at the end of the 'unitary part' of the computation the state of the quantum computer collapses into a 'classical' state where each qubit is either a zero or a one. A 'quantum algorithm' has to be designed such that it is possible to extract useful information from a few such computations.

The main technical problem in realizing quantum computers is to prevent unwanted interactions with the environment during the calculation. Such interactions can cause decoherence, such that the quantum computer is no longer in a pure quantum state. Another problem is the accumulation of errors due to inaccuracies in the induced unitary transformations. It has been shown (Knill *et al.* 1996; Aharonov & Ben-Or 1996; Zalka 1996*a*, *b*) that with fault tolerant quantum error correcting codes (Shor 1995) these problems can be suppressed very efficiently once the hardware reaches a certain quality (noise threshold). Actually the error probability can be made exponentially small. It is thus not unrealistic to imagine that we have an ideal quantum computer when we want to investigate what in principle can be done

with quantum computers. This is the point of view adopted in this paper. For a review of quantum computation see, for example, Ekert & Jozsa (1996).

2. Simulating quantum systems

Proposals about using specific quantum systems to simulate other quantum systems have been published, by Feynman (1982, 1986) and Lloyd (1996). Contrary to me, they think of simulating local quantum systems by closely imitating the local interactions of the original system. Lloyd also thinks of putting to use the imperfections of a real quantum computer (while I assume an ideal one). (See also Lloyd's recent preprint (Lloyd 1996) about simulating fermionic many-body systems on a quantum computer.) My implementation is not limited to local quantum systems and allows in particular the efficient simulation of non-relativistic quantum systems. Also I think that the use of quantum error correction is important in simulating quantum systems if we want to obtain precise results.

I present here an implementation of the simulation of quantum mechanical many-particle systems on a general purpose quantum computer. The discretized wave function of the quantum system is stored as the (exponentially many) amplitudes of the 'classical' basis states of the quantum computer and the operations to time-evolve this wave function are carried out in 'quantum-parallelism'. This should make clear that a classical computer trying to do the same would have to have an exponentially larger memory and would use exponentially more time.

Candidate quantum systems which can't easily be simulated on a classical computer include the following: molecules; hadrons seen as QCD bound states; nuclei seen as quantum mechanical bound states of nucleons; non-perturbative field theories in general; symmetry breaking in superstring theories (and the like).

(*a*) *Quantum mechanical particle in one dimension*

Let's first consider the simple case described by the following Schrödinger equation (throughout the paper I set $\hbar = 1$):

$$\mathrm{i}\partial_t \psi(x) = \left(\frac{1}{2m} \hat{P}^2 + V(\hat{X}) \right) \psi(x). \tag{2.1}$$

First we discretize the wave function and impose periodic boundary conditions, choosing the period N large enough so as not to produce unwanted artifacts:

$$a_n = \psi(n\Delta x), \quad a_{n+N} = a_n. \tag{2.2}$$

After proper normalization we store these amplitudes in an l-bit quantum register (later I will show how this could be done):

$$|\psi\rangle = \sum_{n=0}^{N-1} a_n |n\rangle, \quad N = 2^l, \tag{2.3}$$

where $|n\rangle$ is the basis state corresponding to the binary representation of the number n. Note that by choosing the quantum register large enough, we can represent the wave function with exponentially good spatial resolution.

The question now arises how to efficiently implement the time evolution by Δt of this. Independently, and at practically the same time, Wiesner (1996) and I (Zalka 1996*a*, *b*) have made public preprints with closely related ideas on how to do this. I adopt here Wiesner's method, as it allows a more direct way to improve its precision.

Wiesner's idea is as follows: the time evolution operator is given by

$$\hat{U}(\Delta t) = \mathrm{e}^{-\mathrm{i}\Delta t\hat{H}} = \mathrm{e}^{-\mathrm{i}\Delta t((1/2m)\hat{P}^2 + V(\hat{X}))}.$$

This can approximately be written as

$$\hat{U}(\Delta t) = \mathrm{e}^{-\mathrm{i}\Delta t(1/2m)\hat{P}^2}\mathrm{e}^{-\mathrm{i}\Delta t V(\hat{X})} + O(\Delta t^2). \tag{2.4}$$

The second factor corresponds to a diagonal unitary transformation (rephasing) of the quantum computer state $|\psi\rangle$ which I show below how to carry out. The first factor can be applied in the same way after we have gone to momentum-space by Fourier transforming $|\psi\rangle$. The fast Fourier transformation algorithm (FFT) is straight forward to implement on a quantum computer with only about $\frac{1}{2}l^2$ computational steps (l = number of qubits) (Shor 1994; Coppersmith 1994; Ekert & Jozsa 1996).

Diagonal unitary transformations of the type

$$|n\rangle \to \mathrm{e}^{\mathrm{i}cF(n)}|n\rangle, \tag{2.5}$$

where $F(n)$ is some function of n, can be done with the following succession of steps:

$$|n,0\rangle \to |n,F(n)\rangle, \quad |F(n)\rangle \to \mathrm{e}^{\mathrm{i}cF(n)}|F(n)\rangle, \quad |n,F(n)\rangle \to |n,0\rangle. \tag{2.6}$$

In the first and last step the vectors represent two quantum registers. The first step corresponds to parallel classical calculations. It can be carried out on a quantum computer in 'quantum parallelism' with only a somewhat higher cost than just one such calculation on a conventional computer (see, for example, Shor 1994). As all transformations are unitary they can just as well be inverted, so that the last step is also possible. The second step is really a transformation of the form

$$|n\rangle \to \mathrm{e}^{\mathrm{i}cn}|n\rangle, \tag{2.7}$$

which can be carried out in a straightforward manner in l steps by transforming each qubit separately by an appropriate transformation.

The maximal allowable size of the simulation time steps is determined by the requirement that the approximation in equation (2.4) should be sufficiently good. This is true if the exponents are small, thus we get the condition $\Delta t \ll 1/E$, where E is a typical energy of the system. This shows us the great advantage of being able to simulate quantum systems in the non-relativistic approximation, as otherwise E would also have to include the rest mass energies of the particles.

(*b*) *Improved precision (splitting formulae)*

Above we have used

$$\mathrm{e}^{t(\hat{A}+\hat{B})} = \mathrm{e}^{t\hat{A}}\mathrm{e}^{t\hat{B}} + O(t^2). \tag{2.8}$$

This can be improved to arbitrary order $O(t^n)$ by using roughly $2n$ exponential factors, e.g. from the well-known formula

$$\mathrm{e}^{t(\hat{A}+\hat{B})} = \mathrm{e}^{t\hat{A}}\mathrm{e}^{t\hat{B}}\mathrm{e}^{-\frac{1}{2}t^2[\hat{A},\hat{B}]} + O(t^3), \tag{2.9}$$

we get

$$\mathrm{e}^{t(\hat{A}+\hat{B})} = \mathrm{e}^{(t/2)\hat{A}}\mathrm{e}^{t\hat{B}}\mathrm{e}^{(t/2)\hat{A}} + O(t^3). \tag{2.10}$$

Still higher-order splitting formulae can be derived from the general Baker–Campbell–Hausdorff formula (Dragt 1995).

In the case of an exterior magnetic field we may not be able to write the

Hamilton operator as a sum $f(\hat{P}) + g(\hat{X})$, as there may be terms of the form $\hat{P} \cdot A(\hat{X}) + A(\hat{X}) \cdot \hat{P}$. But this is equal to $[\hat{P}^2, \tilde{A}(\hat{X})]$ where $\tilde{A}(x) = \int^x A(x')\,\mathrm{d}x'$. Similar techniques as for the splitting formulae can then be used to write the exponential of a commutator as a product of exponentials of the individual operators, e.g. from equation (2.9) we get the lowest-order formula

$$\mathrm{e}^{t^2[\hat{A},\hat{B}]} = \mathrm{e}^{t\hat{A}}\mathrm{e}^{t\hat{B}}\mathrm{e}^{-t\hat{A}}\mathrm{e}^{-t\hat{B}} + O(t^3). \tag{2.11}$$

As with any higher-order simulation technique, care must be taken as the higher-order terms may get out of control. As is usual with classical simulations of differential equations, it may be advisable not to go beyond second or third order.

Note that also with splitting formulae, Δt has to be safely smaller than a typical energy of the simulated system. This is a major limitation of my proposal.

(*c*) *Many particles and field theory*

The generalization to many particles is straightforward. For n particles in three dimensions we need $3n$ quantum registers. If the potential $V(\hat{\boldsymbol{X}}_1, \hat{\boldsymbol{X}}_2, \ldots)$ couples different degrees of freedom, we will need to carry out diagonal unitary transformations acting on several registers, e.g.

$$|n, n', n''\rangle \to \mathrm{e}^{\mathrm{i}cF(n,n',n'')}|n, n', n''\rangle. \tag{2.12}$$

Such a transformation can be carried out analogously to equation (2.6). For identical particles the initial state of the quantum computer has to be chosen symmetric resp. antisymmetric.

Also quantum field theory could be simulated, e.g. by spatial discretization. A discretized bosonic quantum field corresponds to one quantum mechanical particle for each lattice point.

Classical computations of non-perturbative field theoretic problems are notoriously hard, still give only results of limited precision (e.g. 10%) and are furthermore controversial due to the many simplifying assumptions necessary to make the computation possible. For an account of lattice QCD results see, for example, Weingarten (1996).

(*d*) *Fermionic field theories*

Fermionic quantum fields pose some problems, as their functional formulation (path integrals, wave functionals, etc.) involves anticommuting Grassmann numbers. There is no wave functional in terms of the usual complex numbers, so we have to look for a representation of the fermionic field operator-algebra on some other Hilbert space. One possibility is the Fock space, where we have for the n-particle sector a totally antisymmetric wave function of n variables. Another possibility is to give the occupation number for each particle species at each lattice point. For fermions this can only be zero or one and thus requires only one qubit.

I expect that further difficulties which arise with quantum fields, like 'fermion doubling' can be dealt with along the same lines as it is done in lattice QCD (Montvay & Münster 1994).

3. Other manipulations

(*a*) *Simulating a decay to obtain the ground state*

Often one is interested in the ground state of a quantum system, be this the ground state of a molecule, the vacuum of a field theory or a hadron stable under the strong

interaction. I propose here to obtain the ground state essentially in the same way as nature does it, namely by letting some initial state decay. Decays happen because the unstable particle is coupled to some other quantum system, like the electromagnetic field in its vacuum state. The model I have in mind for the decay is given by the following Hamilton operator:

$$\hat{H} = \underbrace{\hat{H}_1 + \hat{H}_2}_{\hat{H}_0} + \underbrace{\hat{H}_{1I} \otimes \hat{H}_{2I}}_{\hat{H}_I}. \tag{3.1}$$

Here the subscript 1 denotes operators acting on the system of interest, whereas 2 refers to an auxiliary system with continuous energy spectrum $E = 0 \ldots E_{\max}$, where $E_{\max}$ should be chosen larger than the energy of any sizeable contribution to the original state of the system. For simplicity I have chosen the interaction term to be of a simple tensor product form and I set $\hat{H}_{2I}$ to be:

$$\hat{H}_{2I} = |0\rangle \int \langle E| \, \mathrm{d}E + \int |E\rangle \, \mathrm{d}E \langle 0|. \tag{3.2}$$

The operator $\hat{H}_{1I}$ should be chosen in an intelligent manner depending on the given Hamilton operator $\hat{H}_1$. Its matrix elements between $\hat{H}_1$ eigenstates will determine which transitions are possible and how fast they will occur.

The principle of the decay is now as follows. We initialize the auxiliary system to its ground state $|0\rangle$. If $\hat{H}_I$ is sufficiently small, the expectation value $\langle \hat{H}_0 \rangle$ will remain approximately constant during the decay, so because $\langle \hat{H}_2 \rangle$ will become positive, $\langle \hat{H}_1 \rangle$ has to decrease. To see how fast the decay proceeds, I use the interaction picture and first-order time-dependent perturbation theory (see any standard quantum theory textbook). For simplicity I assume that we start in the $\hat{H}_1$ eigenstate $|n\rangle$. We then get for the amplitude of the state $|m, E\rangle$:

$$\langle m, E|\mathrm{e}^{-\mathrm{i}t\hat{H}}|n, 0\rangle = \mathrm{e}^{\mathrm{i}\ldots} \frac{\sin(\frac{1}{2}t(E_m + E - E_n))}{\frac{1}{2}(E_m + E - E_n)} \langle m|\hat{H}_{1I}|n\rangle \langle E|\hat{H}_{2I}|0\rangle.$$

The transition probability is then obtained as usual by integrating the absolute value squared of these amplitudes over E. To do this I use the fact that $\langle E|\hat{H}_{2I}|0\rangle$ is actually independent of E:

$$p(n \to m) = \int_0^{E_{\max}} |\langle m, E|\mathrm{e}^{-\mathrm{i}t\hat{H}}|n, 0\rangle|^2 \, \mathrm{d}E \approx 2\pi t |\langle m|\hat{H}_{1I}|n\rangle|^2 |\langle E|\hat{H}_{2I}|0\rangle|^2,$$

where we have essentially assumed that $E_m < E_n$ and that $t \gg 1/E_{\max}$. This means that we are in the regime where $p \sim t$ and thus where the exponential decay law becomes valid.

Let us further abstract from physical reality. Say we apply alternatingly $\mathrm{e}^{-\mathrm{i}\Delta t\hat{H}_0}$ and $\mathrm{e}^{-\mathrm{i}\Delta t\hat{H}_I}$ to the composite system. How can we understand that $\langle \hat{H}_0 \rangle \approx$ const.? Of course I assume that $\Delta t\hat{H}_0 \ll 1$ for all eigenvalues and also $\hat{H}_I \ll \hat{H}_0$ in an appropriate sense. Imagine also for simplicity that we begin with an $\hat{H}_0$ eigenstate. Consider now the successive contributions to some other $\hat{H}_0$ eigenstate by the applications of $\mathrm{e}^{-\mathrm{i}\Delta t\hat{H}_I} \approx 1 - \mathrm{i}\Delta t\hat{H}_I$. The phase of these contributions will advance from step to step unless we consider an $\hat{H}_0$ eigenstate with the same eigenvalue as the original state. Thus for all other eigenvalues the advancing phase will effectively make the contributions cancel each other out.

Of course eventually we have to discretize the energy spectrum of $\hat{H}_2$. For the

energy eigenstates we choose simply the 'classical' states $|n\rangle$ of some register. For $\hat{H}_{2I}$ I chose

$$\hat{H}_{2I} = |0\rangle \frac{1}{\sqrt{2^{l-1}}} \sum_{n \text{ odd}} \langle n| + \text{h.c.}, \tag{3.3}$$

as this is easy to diagonalize. In the above expressions we then have to replace the integral over the $\hat{H}_2$ eigenvalues by a sum. The sum can then be approximated by the integral provided that $t \ll 1/(\Delta E)$, where ΔE is the constant spacing of the $\hat{H}_2$ eigenvalues. We then get for the transition probabilities

$$p(n \to m) \approx 2\pi t \frac{1}{E_{\max}} |\langle m|\hat{H}_{1I}|n\rangle|^2,$$

provided that $t \gg 1/E_{\max}$, as before. We may want to reset the auxiliary system once in a while to its ground state to make sure that the exponential decay law continues to be valid for large times. Resetting quantum theoretically also means observing, thus by resetting the auxiliary system we collapse the quantum computer state somewhat. The system of interest will be in a state close to an $\hat{H}_1$-eigenstate according to the decay probabilities. Note that the overall probabilistic treatment remains correct. By resetting every few simulation steps we may actually allow the auxiliary register to be small, as in practice the above relations '$\gg$' and '$\ll$' do not have to be fulfilled very well. Also the time step Δt may be chosen of the same order of magnitude as $1/E_{\max}$. Thus the decay probabilities per time step are of the order

$$p(n \to m) \lesssim \frac{1}{E_{\max}^2} |\langle m|\hat{H}_{1I}|n\rangle|^2.$$

For the actual speed of the decay, much will depend on an appropriate choice for $\hat{H}_{1I}$ (which we also must be able to simulate, possibly using splitting formulae). As a simple (and rather unrealistic) model imagine that $\hat{H}_{1I}$ would only have non-zero matrix elements for m and n both being smaller than some N, and that these matrix elements would all be of the same size. The again somewhat relaxed condition $\hat{H}_I \ll \hat{H}_0$ leads then to

$$p(n \to m) \lesssim 1/N.$$

This means that to end up in a state with a sizeable contribution of the ground state, we have to compute of the order of N simulation steps. This result could be substantially improved if we knew beforehand the ground-state energy, resp. the eigenvalue of any other $\hat{H}_1$ eigenstate which we wanted to obtain. First we could obtain some $\hat{H}_1$ eigenstate at random by the measurement procedure described below. Then we would use a two-state auxiliary system with just the energy difference of the intended transition. In this case the amplitude deposited in the wanted state will increase linearly with the number of simulation steps, thus the transition probability would be $p \sim t^2$. Thus it would be unwise to observe and reset the auxiliary system before $p \approx 1$. The number of steps necessary for this is of order $\sqrt{N}$. This is the same order as for Grover's quantum search algorithm (Grover 1996), but the constant in front of the $\sqrt{N}$ is worse (larger) than for Grover's algorithm. Actually I think it should also be possible to get a $\sqrt{N}$ performance if we do not know the lowest eigenvalue, e.g. by guessing that the eigenvalue lies in some band and narrowing down this band through successive computations.

Note that it is enough to simulate the decay until the few lowest-lying states (which

are of interest) have a large amplitude. Then one can follow the measuring procedure of § 4 *b* to obtain one of the energy eigenstates.

It may be that simulating the decay of a quantum system with many degrees of freedom in the way described above will take too long. For this case it is reassuring to know that Lloyd has shown (Lloyd 1996) that any quantum system can be simulated on a quantum computer in something roughly proportional to real time. Thus, any decay that does not take too long to happen in nature could in principle also be simulated in not too much time on a quantum computer. Note also that for our purposes the decay simulation does not have to be very accurate.

(*b*) *Putting a wave function on a quantum computer*

I expect that for most applications it will not be necessary to initialize the quantum computer with a specific state. Rather, the methods of decay simulation and measurement (described below) allow to obtain specific states from a largely arbitrary initial state of the quantum computer. Nevertheless I describe here a method of initializing the quantum computer with a given wave function. This method is efficient provided that certain integrals over the absolute value squared of the function can be calculated efficiently. This method may also be of interest for other quantum computer applications. I demonstrate the method for the case of a scalar quantum mechanical particle in one dimension. The generalization to multi-dimensional wave functions is then rather straightforward. Here I show only how the absolute value of the wave function can be stored in a quantum register. The correct complex phase can then be introduced in a second step with a diagonal unitary transformation, as shown above.

So we want to carry out the following transformation on an l-bit quantum register which initially is in the state $|0\rangle$:

$$|0\rangle \to k \sum_{n=0}^{2^l-1} \left|\psi\left(n\frac{L}{2^l}\right)\right| |n\rangle, \quad \text{where } \psi(x+L)=\psi(x), \tag{3.4}$$

and k is an appropriate normalization constant. The idea now is to split the norm squared of the initial state (which is one, of course) successively l times such that in the end we get the correct 2^l contributions for the single basis states $|n\rangle$. This corresponds to a binary tree with l levels and 2^l leaves (end points). For this to work out correctly each split has to yield the right ratio. For this we must have a (classical) algorithm which can compute with reasonable efficiency the following integrals over 'binary intervals' of the absolute value squared of the wave function:

$$I_{i,k} = \int_{k2^i(L/2^l)}^{(k+1)2^i(L/2^l)} |\psi(x)|^2 \,\mathrm{d}x, \quad \text{for } k=0,\ldots,2^{l-i}-1 \quad \text{and} \quad i=0,\ldots,l-1. \tag{3.5}$$

The first split is realized by a real $O(2)$ rotation acting on the most significant qubit (qubit no. $l-1$) of the quantum register:

$$|0,\ldots\rangle \to \sqrt{I_{l-1,0}}|0,\ldots\rangle + \sqrt{I_{l-1,1}}|1,\ldots\rangle. \tag{3.6}$$

The rotation angle of this $O(2)$ rotation is given by

$$\tan(\varphi_{l-1}) = \sqrt{I_{l-1,1}}/\sqrt{I_{l-1,0}}. \tag{3.7}$$

The rotation angle of qubit number i (with $i < l-1$) will depend on the values of

the more significant bits:

$$\tan(\varphi_{i,b_{l-1},\ldots,b_{i+1}}) = \frac{\sqrt{I_{i,2k+1}}}{\sqrt{I_{i,2k}}}, \quad \text{where } k = b_{i+1} + 2b_{i+2} + \cdots + 2^{l-i-2}b_{l-1}. \quad (3.8)$$

These calculations and the subsequent rotation of qubit number i are then carried out in quantum parallelism conditional on the values of the more significant bits.

4. Obtaining results of interest

(*a*) *'Simple' measurements*

Of course one can simply observe the quantum computer to obtain statistical information about the absolute value of the wave function, corresponding to a position measurement in quantum mechanics. This will of course take many identical simulations on the quantum computer. To sample the momentum distribution the same can be done after Fourier transforming the wave function.

In practice we will want to be more sophisticated. By applying an appropriate unitary transformation before observing the quantum computer we can 'measure' observables which we may not know how to measure in a real experiment. This would, for example, allow us to directly access the s- and p-wave contributions of the final state of a scattering experiment by 'measuring' the angular momentum observable. In the next paragraph I describe how such measurements could be done in an elegant manner.

Eventually still more efficient ways may be used to extract the information of interest from a few simulations.

(*b*) *Measuring arbitrary observables*

To study the measurement problem in quantum theory, J. von Neumann has proposed an idealized simple interaction (von Neumann 1955; DeWitt 1970) between the quantum system and the part of the measuring apparatus that directly interacts with the system. For convenience this part of the apparatus can be chosen to be equivalent to a quantum mechanical particle in one dimension. That is to say its Hilbert space is spanned by the basis vectors

$$|x\rangle \quad x \text{ real} \quad \text{and} \quad \hat{X}|x\rangle = x|x\rangle. \quad (4.1)$$

The time evolution during the measurement of an observable $\hat{A}$ shall then be given by

$$\hat{U}(t)|\Psi_a\rangle|x\rangle = |\Psi_a\rangle|x + k \cdot a \cdot t\rangle, \quad \text{with } \hat{A}|\Psi_a\rangle = a|\Psi_a\rangle, \quad (4.2)$$

where $|\Psi_a\rangle$ is the state of the system. One easily verifies that the Hamilton operator $\hat{H} = k\hat{P}\hat{A}$ leads to this time evolution. Here $\hat{P}$ is the usual momentum operator for the imaginary quantum mechanical particle, thus $[\hat{X}, \hat{P}] = \mathrm{i}\hbar$.

Now we simply have to implement this time evolution on the quantum computer. This can be done efficiently, at least for any Hermitian operator $\hat{A}$ which is amendable to some splitting formula decomposition, thus $\hat{A}$ could, for example, represent the energy, momentum, angular momentum, etc., of the quantum system.

Then, after simulating this 'first stage von Neumann measuring process', we can observe the auxiliary quantum register and should find a number proportional to an eigenvalue of $\hat{A}$. By repeating this, we get the spectrum of $\hat{A}$ and the weight of the various $\hat{A}$-eigenstates in the original system state. Also after each observation the

system will be in an eigenstate of $\hat{A}$. Thus this is a way of obtaining, for example, the energy eigenstates.

An analysis shows that the relative accuracy of the obtained eigenvalues will be somewhat less than the number of simulation steps.

Note the connection to the work by Kitaev (1995) who describes how to approximately obtain the eigenvalues of a given unitary transformation using a quantum computer.

5. Conclusion

I have demonstrated that quantum computers are well suited for precise and efficient simulations of quantum systems, which allows us to compute interesting results which may be out of reach of classical computers. Quantum mechanical simulations may, for example, be useful in chemistry (reaction dynamics, protein folding, etc.).

I think that for high-energy physics, the possibility to simulate quantum fields could become of importance in the future. This subject may need further and more detailed investigation. For example, it is not clear how severe are the restrictions due to the need for field discretization, as the size of the hardware is proportional to the number of lattice points. Also the question of how fast the ground state could be obtained for a specific system will have to be investigated in more detail. Nevertheless it may well be that quantum computers will one day be indispensable for investigations of fundamental theories (grand unified theories, superstrings, etc.), which of course is a major objective of theoretical physics.

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