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Quantum computer inverting time arrow for macroscopic systems

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Abstract. Since Boltzmann developed the statistical theory for macroscopic thermodynamics the question has relentlessly been put forward of how time-reversibility at microscopic level is compatible with macroscopic irreversibility. Here we show that a quantum computer can efficiently simulate a macroscopic thermodynamic process with chaotic microscopic dynamics and invert the time arrow even in presence of quantum errors. In contrast, small errors in classical computer simulation of this dynamics grow exponentially with time and rapidly destroy time-reversibility.

PACS. 03.67.Lx Quantum computation – 05.45.Ac Low-dimensional chaos – 05.45.Mt Semiclassical chaos ("quantum chaos")

A legend tells [1] that once Loschmidt asked Boltzmann on what happens to his statistical theory if one inverts the velocities of all particles, so that, due to the reversibility of Newton's equations, they return from the equilibrium to a nonequilibrium initial state. Boltzmann only replied "then go and invert them". This problem of the relationship between the microscopic and macroscopic descriptions of the physical world and time-reversibility has been hotly debated from the XIXth century up to nowadays [2–9]. At present, no modern computer is able to perform Boltzmann's demand for a macroscopic number of particles. In addition, dynamical chaos [10–13] implies exponential growth of any imprecision in the inversion that leads to practical irreversibility. Here we show that a quantum computer [14–18] composed of a few tens of qubits, and operating even with moderate precision, can perform Boltzmann's demand for a macroscopic number of classical particles. Thus, even in the regime of dynamical chaos, a realistic quantum computer allows to rebuild a specific initial distribution from a macroscopic state given by thermodynamic laws.

To study the relations between microscopic deterministic classical dynamics, macroscopic thermodynamic laws and quantum computation, we choose a simple area − preserving map:

$$\bar{y} = y + x \ (\mathrm{mod\ L}), \quad \bar{x} = x + \bar{y} \ (\mathrm{mod\ 1}). \qquad (1)$$

Here the first equation can be seen as a kick which changes the momentum y of a particle, while the second one corresponds to a free phase rotation in the interval $-0.5 \leq x < 0.5$; bars mark the new values of the variables. The map dynamics takes place on a torus of integer length L in the y direction. For $L = 1$ this map reduces to the well-known Arnold cat map [10], which describes a fully chaotic dynamics with positive Kolmogorov-Sinai entropy $h \approx 0.96$. As a result, the dynamics is characterized by exponential divergence of nearby trajectories, so that any small error ϵ (for example round-off error) grows exponentially with time, and reversibility of a trajectory is lost after $t_{\mathrm{E}} \approx |\ln \epsilon|/h$ map iterations. For $\epsilon \sim 10^{-8}$ comparable to ordinary precision of the Pentium III, this time scale is rather short ($t_{\mathrm{E}} \approx 20$). For $L \gg 1$ chaos leads to the diffusive spreading of particles in momentum, which is well described by the Fokker-Planck equation:

$$\partial w(y,t)/\partial t = (D/2)\partial^2 w(y,t)/\partial^2 y, \qquad (2)$$

where the diffusion coefficient $D \approx \langle x^2 \rangle = 1/12$. Thus after a time $t \gg 1/h$ an initial distribution of particles in (1) evolves towards a Gaussian statistical distribution $w(y,t) = w_{\mathrm{g}}(y,t) = \exp(-(y-y_0)^2/(2Dt))/\sqrt{2D\pi t}$ with $\langle y^2 \rangle = Dt + y_0^2$, where $y_0 = \langle y \rangle$ at $t = 0$. On a finite torus this diffusive process relaxes to a homogeneous distribution in y after a time $t_{\mathrm{D}} \approx L^2/D$.

For the case $L = 1$ it was shown that a quantum computer can simulate a discretized version of this map with exponential efficiency [19]. Here we show that for $L \gg 1$ a similar quantum algorithm enables to simulate the evolution of a macroscopic number of classical particles which is governed by the thermodynamic diffusion law. To perform this evolution on a lattice of size LN^2 (with $N = 2^{n_q}$ and $L = 2^{n_{q'} - n_q}$) this algorithm uses three quantum registers. The first one with n_q qubits holds the values of the coordinate x ($x_i = -0.5 + i/N, i = 0, ..., N-1$), the second one with $n_{q'}$ qubits holds the y coordinates ($y_j = -L/2 + j/N, j = 0, ..., LN-1$) and the last one with $n_{q'} - 1$ qubits is used as a workspace. The first two registers describe the discretized classical phase space with L cells

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and N^2 points per cell. In this way, the initial positions of $N_{\rm d} \sim N^2$ particles can be represented by one quantum state $\sum_{i,j} a_{ij}|x_i\rangle|y_j\rangle|0\rangle$, where $a_{i,j} = 0$ or $1/\sqrt{N_{\rm d}}$. The quantum algorithm is based on modular additions performed in a way similar to the one described in [20], through Toffoli and controlled-not gates (CNOT). It requires $10n_q + 6n_{q'} - 17$ gate operations per map iteration, in contrast to $O(2^{2n_q})$ operations for the classical algorithm. The time inversion is also realized by $8n_q + 4n_{q'} - 13$ gate operations which effectively change y into $-y$ halfway between kicks [19,21]. In this way, the quantum computer acts in a way similar to Maxwell's demon [22,23] who reverses the velocity of each individual particle. Thus the time inversion for exponentially many classical particles is done in polynomial number of operations of a quantum computer.

A perfect quantum computer simulates exactly the discretized map (1). This discrete classical map is perfectly time-reversible, as well as the continuous one, since the symplectic structure of the dynamics is preserved by the discretization. In the field of classical chaos, such a symplectic discretization, which can always be done, is broadly used for the investigation of chaotic dynamics of area-preserving maps [24]. This is related to the fact that a universal classical computing machine can be made reversible (see *e.g.* [17]). The optimal discretization is not necessarily the one automatically made by a computer with finite precision (round-off errors), which can break reversibility (*e.g.* [25] for the standard map). For investigation of the origin of irreversibility it is important to understand if the time reversibility is preserved/stable in the presence of small errors done at the moment of time-inversion $t_{\rm r}$. Indeed, such errors naturally appear in realistic physical systems which always have some imperfections. For a classical computer, *e.g.* Pentium III iterating map (1), random errors of amplitude ϵ in the values of the classical variables done at $t_{\rm r}$ destroy the time-reversibility of the map dynamics after $t_{\rm E}$ iterations. This fact is illustrated in Figure 1 where it is assumed that the demon inverts the velocities of all trajectories after $t_{\rm r} = 35$ iterations with a precision ϵ. After that, the macroscopic distribution starts to return back but after $t_{\rm E} \approx |\ln \epsilon|/h$ iterations the errors become too large and the diffusion process restarts again. In contrast to that, a quantum computer can simulate enormous number of orbits going on very fine scales in the phase space. However, a quantum computer has its own natural errors which can be viewed as imprecisions of amplitude ϵ in the gate operations. The comparison of the two types of errors natural for classical and quantum computers is displayed in Figure 1. It shows that the quantum computation with precision $\epsilon = 0.01$ in each gate at each map iteration is able to reverse effectively the diffusion process up to the initial state. That is in striking contrast with the irreversibility of the classical computation with errors of amplitude $\epsilon = 10^{-8}$ made only once at $t = t_{\rm r}$ when the demon acts. We note that a similar behaviour takes place also for higher moments of distribution. In this way, the quantum computer succeeds to reverse the thermodynamic diffusive process with enormous number

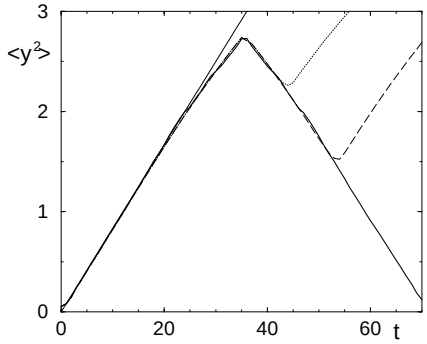

Fig. 1. Diffusive growth of the second moment $\langle y^2 \rangle$ of the distribution $w(y,t)$ generated by the map (1) with $L = 8$, simulated on a classical (Pentium III) and quantum ("Quantium I") computers. At $t = t_{\rm r} = 35$ one inverts all velocities. For Pentium III inversion is done with precision $\epsilon = 10^{-4}$ (dotted line) and $\epsilon = 10^{-8}$ (dashed line); 10^6 orbits are simulated, initially distributed inside the demon image (see Fig. 3). For Quantium I, the computation is done with 26 qubits ($n_q = 7, n_{q'} = 10$) (thick full line); each quantum gate operates with imperfections of amplitude $\epsilon = 0.01$ (unitary rotation on a random angle of this amplitude). The straight line shows the theoretical macroscopic diffusion with $D = 1/12$.

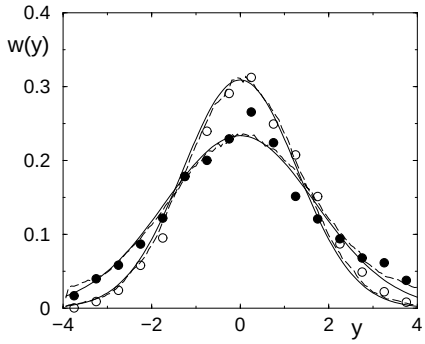

Fig. 2. Distribution of particles in y for map (1) simulated by Pentium III (dashed lines) and Quantium I (circles) for the case of Figure 1, at $t = 20$ (dashed lines and open circles) and $t = t_{\rm r} = 35$ (dashed lines and filled circles). Full lines show the theoretical solution of the Fokker-Planck equation (2).

of particles. Indeed, at the moment of inversion $t_{\rm r}$, the distribution of particles is a Gaussian of width $\sigma = \sqrt{2Dt_{\rm r}}$ in agreement with the solution of (2), as is shown in Figure 2.

Figure 3 shows explicitly the distribution in phase space at different moments of time. The initial distribution mimics a demon, which at $t = t_{\rm r}$ is transformed to a statistical homogeneous distribution in the x-direction, with a smooth variation in y described by (2). The quantum computer operating with 1% accuracy is able to recover the initial image with good precision, whereas the classical computer with round-off errors 10^{-8} completely fails to reproduce it. The striking difference between the two final distributions at $t = t_{2\rm r}$ generated by the two computers can be easily detected from a polynomial number of measurements. For example, the Fourier harmonics of

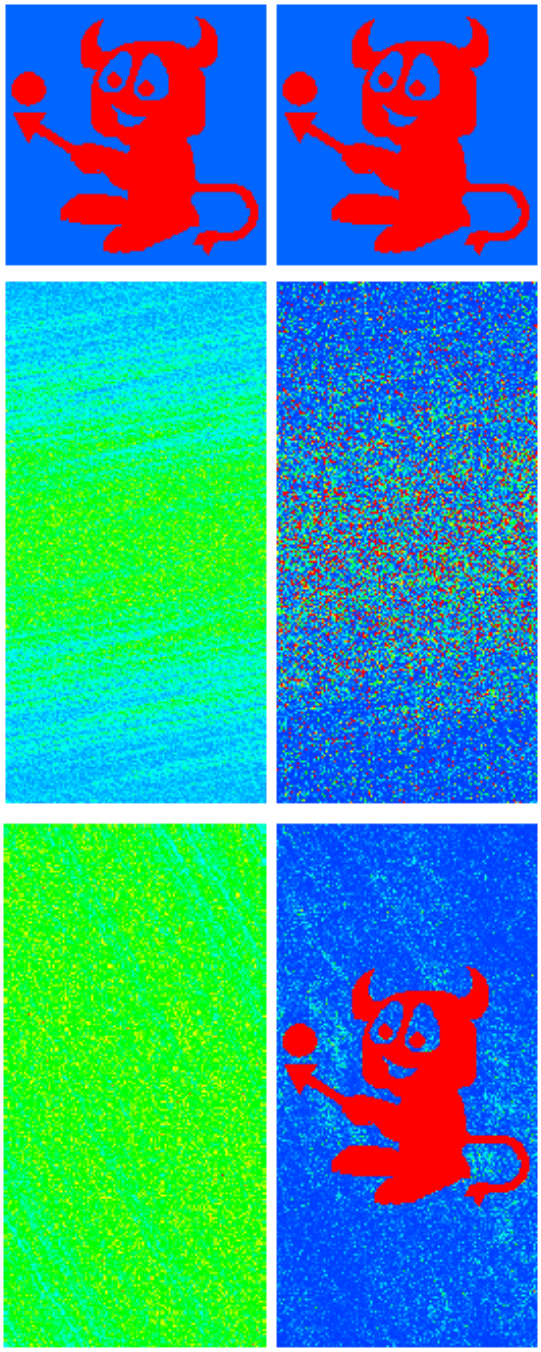

Fig. 3. Evolution of a demon image through map (1). Left column shows the simulation on Pentium III, right column on Quantium I. Top: initial distribution in the central cell ($-0.5 \leq x, y < 0.5$). Middle: distribution at $t = t_r = 35$ in the whole phase space ($-0.5 \leq x < 0.5, -4 \leq y < 4$). Bottom: distribution at $t = 2t_r = 70$ in the two central cells ($-0.5 \leq x < 0.5, -1 \leq y < 1$). The time-inversion is made at $t_r = 35$, with accuracy $\epsilon = 10^{-8}$ for Pentium III (error is done only at t_r), and with accuracy $\epsilon = 0.01$ for Quantium I (error is done at each gate operation). Color marks the density of particles/probability, from blue (minimal) to red (maximal value). Here as in Figure 1 $n_q = 7, n_{q'} = 10$, with in total 26 qubits used for Quantium I; for Pentium III, 10^6 orbits are simulated.

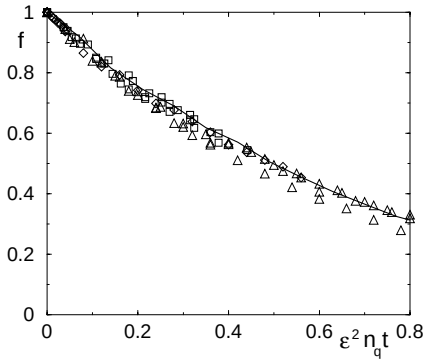

Fig. 4. Fidelity f as a function of $\epsilon^2 n_q t$ for the quantum simulation of the map (1) on Quantium I for $L = 8$. Symbols show data for $n_q = 4, 5, 6, 7$ for $\epsilon = 10^{-2}$ (diamonds), $\epsilon = 3 \times 10^{-2}$ (squares) and $\epsilon = 0.1$ (triangles up). Full line shows $n_q = 7$, $\epsilon = 0.1$.

the final Liouville density distribution can be efficiently obtained with the help of the quantum Fourier transform, as it was discussed in [19,26]. In the régime of chaos more and more weight is transfered to high harmonics (with large wave vectors $k \sim \exp(ht)$) [13,27]. They involve very small scales in phase space and therefore exponentially many orbits are required to obtain them on a classical computer. A measurement procedure in the phase space (x, y), discussed in [28], is based on the polynomial number of measurements of only few initial qubits and gives a coarse-grained image directly in (x, y). However, as shown in [28], the information about the Liouville density distribution in (x, y) space can be obtained by classical Monte Carlo simulations with a comparable efficiency. On the contrary, in the Fourier space a polynomial number of measurements of the first n_f qubits ($n_f < n_q$) gives a coarse-grained image of probability distribution in the Fourier space, including very high harmonics, which are unaccessible to classical computations. In total $O(n_q^2)$ operations are required to extract this coarse-grained image from quantum computation while any known classical algorithm will require $O(2^{2n_q})$ operations. In the quantum case the precision improves polynomially with the number of measurements.

The previous results are supported by the data for the fidelity $f(t)$ defined as the projection of the quantum state in presence of gate imperfections on the exact state without imperfections. For $f = 1$ both states coincide, whereas for $f \ll 1$ both distributions are completely different. The results in Figure 4 show that $f(t)$ smoothly decreases with number of iterations t even if classical dynamics is exponentially unstable. The probability of transition from the exact state to other states induced by imperfections can be estimated as of the order of ϵ^2. Hence, since imperfections in each gate are assumed to be uncorrelated, $f(t)$ should drop by $n_q \epsilon^2$ at each map iteration (for $n_q \sim n_{q'}$). This determines a time scale

$$t_f \approx C/(n_q \epsilon^2) \tag{3}$$

on which the fidelity of quantum computation for the algorithm is reasonable ($f(t_f) = 0.5$)), even in absence of error

correction. This scaling is in agreement with the data in Figure 4 (see also [19]) which give the numerical factor $C \approx 0.5$. This is in sharp contrast with classical errors for which computation of trajectories remains correct only up to a time scale $t_{\rm E} \approx |\ln \epsilon|/h$. It is interesting to note that the situation is similar to the time evolution of a physical system in the regime of quantum chaos, which is stable against small quantum errors even though the underlying classical dynamics is chaotic [25]. We note that the application of quantum error-correcting codes (see *e.g.* [17]) can give further improvement of computation accuracy.

For simplicity, in the above studies we considered a relatively simple map (1) but it should be stressed that other area-preserving chaotic maps can be also efficiently simulated on a quantum computer (*e.g.* the Chirikov standard map [29] or the perturbed cat map [26]). The stability of quantum computation of dynamical chaos should apply for such maps as well.

The relation (3) implies that a quantum computer operating with realistic accuracy can invert velocities of all particles at a given moment of time, so that a specific initial state is reliably reproduced from a statistical distribution described by a diffusive process. Such a simulation for a macroscopic number of particles $N_{\rm d}$ can be performed with few tens of qubits. For example, for $N_{\rm d} = 6.022 \times 10^{23}$ (Avogadro's number) the simulation with $L = 8$ requires only 125 qubits. Moreover, according to (3), the accurate simulation of such an enormously large number of particles remains reliable ($f(t) > 0.5$) up to a time $t \approx 150$ with a modest gate accuracy $\epsilon = 0.01$. This time can be increased with the help of quantum error correcting codes (see *e.g.* [17] and references therein) although it will require larger number of qubits. Such a computation is far out of reach of any modern supercomputer, and clearly shows the power of quantum computers. This shows that this power can be used not only for simulation of quantum evolution, as envisioned by Feynman [14], but also for classical dynamics. It also opens interesting perspectives for cryptography since an initial image can be coded in a thermodynamic distribution with very large entropy and then reliably recovered. Thus quantum computers open new possibilities for the investigation of the relations between microscopic deterministic dynamics and macroscopic thermodynamic laws.

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$T(TCT)^{n_q-1}T^{n_{q'}-n_q-1}(CT)^{n_{q'}-n_q-1}CTCT$
$(CCTCT)^{n_q-2}CCTCRCC(TC)^{n_{q'}-n_q-1}$
$T^{n_{q'}-n_q-1}CT(TCT)^{n_q-2}\ (CCTCT)^{n_q-2}CCTC$
and for the time inversion: $R^{n_{q'}}CT^{n_{q'}-2}(CT)^{n_{q'}-2}$
$CCRT(TCT)^{n_q-2}(CCTCT)^{n_q-2}CCTC$
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