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HOW TO SOLVE THE CLASSICAL PROBLEMS ON QUANTUM COMPUTERS

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1. Introduction

If we can solve the quantum problems with the quantum computers [1], we can probably solve the classical problems, too. With this paper we start the investigation of computational hard problems of classical physics such as the turbulent phase of hydrodynamics, with the methods of Quantum Computing (QC).

In Sec.2 of this paper we consider time-reversible classical dynamical systems and corresponding quantum extensions.

Sec.3 describes an algorithm of solution of the quantum problems with QC.

Sec.4 deals with a (re)formulation of the classical dynamics in the form of quantum dynamics and gives an algorithm of solution of classical problems with QC.

In Sec.5, we present our conclusions and show some perspectives.

Some technical details and illustrations are considered in Appendixes.

2. Time-reversible classical discrete dynamical systems (computers) and corresponding (quantum) extraparts

The contemporary digital computer and its logical elements can be considered as a spatial type of discrete dynamical systems described by the following motion equation:

$$s_n(k+1) = \phi_n(s(k)), \tag{1}$$

where $s_n(k)$, $1 \leq n \leq N(k)$, is the state vector of the system at the discrete time step k. Note that with time steps, k can change not only value, but also the dimension, $N(k)$ of the state vector, $s(k)$.

Definition. We assume that the system (1) is time-reversible if we can define the reverse dynamical system

$$s_n(k) = \phi_n^{-1}(s(k+1)). \tag{2}$$

In this case the following matrix

$$M_{nm} = \frac{\partial \phi_n(s(k))}{\partial s_m(k)} \tag{3}$$

is regular, i.e. has an inverse.

If the matrix is not regular, this is the case, for example, when $N(k+1) \neq N(k)$, we have an irreversible dynamical system (usual digital computers and/or corresponding irreversible gates).

Let us consider an extension of the dynamical system (1) given by following action functional:

$$A = \sum_{kn} l_n(k)(s_n(k+1) - \phi_n(s(k))) \tag{4}$$

and corresponding motion equations

$$\begin{aligned} s_n(k+1) &= \phi_n(s(k)), \\ l_n(k-1) &= l_m(k)\frac{\partial \phi_m(s(k))}{\partial s_n(k)} = l_m(k)M_{mn}(s(k)). \end{aligned} \tag{5}$$

In the regular case, we put this system in an explicit form

$$\begin{aligned} s_n(k+1) &= \phi_n(s(k)), \\ l_n(k+1) &= l_m(k)M^{-1}_{mn}(s(k+1)). \end{aligned} \tag{6}$$

From this system it is obvious that, when the initial value $l_n(k_0)$ is given, the evolution of vector $l(k)$ is defined by evolution of the state vector $s(k)$. So we have the following

Theorem. The regular dynamical system (1) and the extended system (6) are equivalent.

Note that the corresponding statement from [2] concerning to the continual time dynamical systems is not as transparent as our statement for discrete time dynamical systems.

In the continual time approximation, the discrete system (6) reduces to the corresponding continual one, [3]:

$$\begin{aligned} \dot{x}_n(t) &= v_n(x), \\ \dot{p}_n(t) &= -\frac{\partial v_m}{\partial x_n}p_m. \end{aligned} \tag{7}$$

Indeed. Let us change the dependent variables as follows:

$$\begin{aligned} s_n(k) &= x_n(t_k), \\ l_n(k) &= p_n(t_k), \quad t_k = k\Delta t, \quad \Delta t << 1. \end{aligned} \tag{8}$$

Then the action functional (4) can be transformed as follows:

$$\begin{aligned} A &= \sum_{kn} p_n(t_k)(x_n(t_k+\Delta t) - \phi_n(x(t_k))) \\ &= \sum_{kn} \Delta t p_n(t_k)(\dot{x}_n(t_k) - v_n(x(t_k))) \\ &\Rightarrow \int dt p_n(t)(\dot{x}_n - v_n(x)), \end{aligned} \tag{9}$$

where

$$\phi_n(x(t_k)) - x_n(t_k) = \Delta t v_n(t_k), \tag{10}$$

and the corresponding motion equations are presented by the system (7).

The equation of motion for $l_n(k)$ is linear and has an important property that a linear superpositions of the solutions are also solutions.

Statement. Any time-reversible dynamical system (e.g. a time-reversible computer) can be extended by a corresponding linear dynamical system (quantum processor) which is controlled by the dynamical system and which, due to the superposition and entanglement properties, has a huge computational power.

3. Solution of the Quantum problems with the Methods of the Quantum Computing

The standard classical computing - the technology of storing and transforming information, is based on the classical physical theory and can be universally divided (factored) on the hardware (body)-memory and processor of computers, and software (soul)- algorithms and programs of users, parts, [4].

Under the Quantum computing, we mean an extension of the classical computing by hardware which is described by the (corresponding formulation of the) quantum theory - quantum registers and quantum logical units and corresponding software, [5].

A quantum system can be described by corresponding Schrödinger equation, [6]

$$i\hbar\frac{d}{dt}|\psi>=\hat{H}|\psi>, \tag{11}$$

where $|\psi>=|\psi(t)>$ is the state vector from the state Hilbert space and $\hat{H}=H(\hat{p},\hat{x})$ is operator-Hamiltonian. In the case of one nonrelativistic particle the operator is

$$\hat{H}=\hat{T}+\hat{V}=\frac{\hat{p}^2}{2m}+V(\hat{x}). \tag{12}$$

The fundamental bracket is

$$[\hat{x},\hat{p}]=\hat{x}\hat{p}-\hat{p}\hat{x}=i\hbar. \tag{13}$$

The configuration space form of the equation (11) is

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=\hat{H}\psi(x,t), \tag{14}$$

where $\psi(x,t)=<x|\psi(t)>$ and Hamiltonian is

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x). \tag{15}$$

In the momentum space form, we have

$$i\hbar\frac{\partial\psi(p,t)}{\partial t}=\hat{H}\psi(p,t), \tag{16}$$

where $\psi(p,t) =< p|\psi(t) >$ and Hamiltonian is

$$\hat{H} = \frac{p^2}{2m} + V(i\frac{d}{dp}). \qquad (17)$$

With proper normalization,

$$1 = \int dx\psi^*(x,t)\psi(x,t) =< \psi(t)| \int dx|x >< x|\psi(t) >=< \psi(t)|\psi(t) >= 1, \qquad (18)$$

$\rho(x,t) = \psi^*(x,t)\psi(x,t)$ is the probability density of finding the particle at the point x.

The formal solution of the equation (11) is

$$|\psi(t) >= U(t)|\psi_0 >, \qquad (19)$$

where

$$U(t) = exp(-\frac{i}{\hbar}t\hat{H}). \qquad (20)$$

The main steps maid in QC is the following:

$$U(t) = (U^{1/N})^N = (U_T U_V)^N + O(1/N), \qquad (21)$$

where

$$\begin{aligned} U^{1/N} &= exp(-\theta\hat{H}) = exp(-\theta\hat{T})exp(-\theta\hat{V}) + O(1/N^2) \\ &= U_T U_V + O(1/N^2), \quad \theta = \frac{i}{\hbar}\tau, \quad \tau = \frac{t}{N}. \end{aligned} \qquad (22)$$

Then, for corresponding matrix element we have (see Appendix 1)

$$< x_{n+1}|U^{1/N}|x_n >\sim exp(\theta(\frac{m}{2}(\frac{x_{n+1}-x_n}{\tau})^2 - V(x_n))) + O(1/N^2) \qquad (23)$$

and

$$\begin{aligned} < x_{out}|U(t)|x_{in} > &\sim \int dx_1 dx_2 ... dx_N exp(\frac{i}{\hbar}\tau\sum_{n=0}^{N}(\frac{m}{2}(\frac{x_{n+1}-x_n}{\tau})^2 - V(x_n))) \\ &+ O(1/N), \quad |x_0 >= |x_{in} >, \quad < x_{N+1}| =< x_{out}|. \end{aligned} \qquad (24)$$

This finite dimensional integral representation of the matrix element is in the ground of the functional (continual) integral formulation of the quantum theory [7].

We can discretize the wave function in (14) and impose the periodic boundary condition [8]

$$a_n(t) = \psi(x_n,t), \quad a_{n+N} = a_n, \quad x_n = n\Delta x. \qquad (25)$$

We store these amplitudes in a k-bit quantum register

$$|\psi(t)>=\sum_{n=1}^{N} a_n|n>, \quad N=2^k, \tag{26}$$

where $|n>$ is the basis state corresponding to the binary representation of the number n.

The second factor in (22) in a coordinate representation corresponds to a diagonal unitary transformation of the quantum computer state $\psi(x,t)$. After Fourier transforming $\psi(x,t)$ into momentum-space representation, $\psi(p,t)$ the first factor in (22) can be applied in the same way.

Diagonal unitary transformations of the type

$$|n>\rightarrow e^{iF(n)}|n>, \tag{27}$$

where $F(n)$ is some function of n, can be done [8] with the following succession of steps

$$\begin{aligned} |n> &\rightarrow |n,0>\rightarrow |n,F(n)>\rightarrow e^{iF(n)}|n,F(n)>\rightarrow e^{iF(n)}|n,0> \\ &\rightarrow e^{iF(n)}|n>. \end{aligned} \tag{28}$$

For n particles in d dimensions we need nd quantum registers. If the potential $V(\hat{x}_1,\hat{x}_2,...)$ couples different degrees of freedom, we need the diagonal unitary transformations acting on several registers, e.g.

$$|n_1,n_2>\rightarrow e^{iF(n_1,n_2)}|n_1,n_2>. \tag{29}$$

The discretized bosonic quantum fields correspond to one scalar particle for each lattice point, one vector particle for each lattice link, one tensor particle for each lattice placket, and so on (see e.g. [10]). Note that in Kähler's formulation of the Dirac's equation [9]

$$(\delta+d-m)\psi=0$$

we cannot associate the fermion field to a geometric object like site, link, placket, and so on. This is an indication about the extended (composed, coherent, non-fundamental) nature of the fermion particles, from the viewpoint of the discrete models of space.

4. Solution of the Classical problems with the Methods of the Quantum Computing

Operational and functional formulations of classical theories (see e.g. [11]) with the QC methods might help to investigate some interesting phenomena, e.g. that of fully developed turbulence (see e.g. [12]), which are difficult for other methods.

We usually formulate the classical problems as a Hamiltonian system of motion equations [13]

$$\dot{q}_n = \frac{\partial H}{\partial p_n},$$
$$\dot{p}_n = -\frac{\partial H}{\partial q_n}, \quad 1 \leq n \leq N, \tag{30}$$

where q_n are coordinates for the configuration space of the system and p_n are corresponding momentum, $H = H(q,p)$ is a Hamiltonian function(al). The system (30) belongs to the more general class of the dynamical systems defined by the following system of motion equations

$$\dot{x}_n = v_n(x), \quad 1 \leq n \leq N, \tag{31}$$

when N is an even integer and

$$v_n(x) = \varepsilon_{nm} \frac{\partial H(x)}{\partial x_m} = \{x_n, H\},$$

where the fundamental canonical bracket is

$$\{x_n, x_m\} = \delta_{nm}.$$

Note that any dynamical system (31) can be extended to the following Hamiltonian form, (see, e.g. [3] and section 2 of this paper)

$$\dot{x}_n = v_n(x) = \{x_n, H\},$$
$$\dot{p}_n = -\frac{\partial v_m}{\partial x_n} p_m = \{p_n, H\}, \tag{32}$$

where Hamiltonian is

$$H(x,p) = v_n(x) p_n \tag{33}$$

and the fundamental canonical bracket is

$$\{x_n, p_m\} = \delta_{nm}. \tag{34}$$

For any observable $\psi(x)$ of a Hamiltonian dynamical system, we have the following motion equation:

$$\begin{aligned} \dot{\psi}(x) \quad &= \{\psi, H_1\} = \varepsilon_{nm} \frac{\partial \psi}{\partial x_n} \frac{\partial H_1}{\partial x_m} = -\hat{L}\psi \\ &= [\psi, H_2], \end{aligned} \tag{35}$$

where

$$
\begin{aligned}
\hat{L} &= v_n(x)\frac{\partial}{\partial x_n} = \frac{i}{\hbar}v_n(x)\hat{p}_n \\
&= \frac{i}{\hbar}\hat{H}_2.
\end{aligned} \tag{36}
$$

H_1 is the classical Hamiltonian function and $\hat{H}_2$ is the quantum Hamiltonian operator. Now we can consider Eq.(35) as a classical Hamiltonian one with Hamiltonian H_1 or as a quantum Schrödinger equation with the Hamiltonian operator $\hat{H}_2$. For the second point of view we can apply the QC methods developed in the previous section.

Note that the operator $\hat{H}_2$ is a self-adjoint operator, $\hat{H}_2^+ = \hat{H}_2$, when $divv = 0$ and we can put it in the second-order form with respect to the momentum operator,

$$
\begin{aligned}
\hat{H}_2 &= v_k\hat{p}_k = \frac{1}{2}(\hat{p}_k v_k + v_k\hat{p}_k) \\
&= \frac{i}{\hbar}[\hat{p}_k^2, u_k],
\end{aligned} \tag{37}
$$

where

$$
u_k = \frac{1}{2}\int^{x_k} dx_k v_k, \quad 1 \le k \le d, \quad d \ge 2. \tag{38}
$$

As an example, we consider the harmonic oscillator in Appendix 2.

Now the formal solution (19) is

$$
|\psi(t)> = U(t)|\psi_0> = exp(-\frac{i}{\hbar}t\hat{H}_2)|\psi_0> = exp(-\frac{t}{\hbar^2}[\hat{u},\hat{p}^2])|\psi_0>
$$

and for factorized form (21) we have

$$
U^{1/N} = exp(-\tau^2[\hat{u},\hat{p}^2]) = \prod_{k=1}^{d} e^{i\tau\hat{u}_k}e^{i\tau\hat{p}_k^2}e^{-i\tau\hat{u}_k}e^{-i\tau\hat{p}_k^2} + O(\tau^3), \tag{39}
$$

where

$$
\tau = \pm(\frac{t}{\hbar^2 N})^{1/2}.
$$

Now we are ready to apply the formalism of the QC considered in Sec.3 to the classical problems.

5. Conclusions and perspectives

In this paper we constructed the algorithm of solving the computational hard problems of classical physics on quantum computers. In the future publications we will consider some applications to the three-body problem of classical mechanics, the Hamiltonian dynamics of heavy particle accelerators, the

Hamiltonian dynamics of the incompressible fluid and propose algorithms of solution and estimate the corresponding resources of QC.
Note that before we will get a real quantum computer, we can simulate it on classical computers [14].

We are free to take $l_n(k)$ in (4) and p_n in (9) as grassmann valued, than the corresponding Hamiltonian $H_1 = v_n p_n$, (33) will be nilpotent, $H_1^2 = 0$ and corresponding bracket (34) will be odd, [3].

It is interesting to investigate the functional integral formulation of the classical theory based on the discrete representation (39).

Then, Dirac's equation for electron

$$\begin{aligned} i\hbar\partial_t\psi(t,x) &= (\alpha_n\hat{p}_n + \beta m)\psi(t,x) \\ &= (\frac{i}{\hbar}[\hat{p}_n^2, u_n] + \beta m)\psi, \end{aligned} \tag{40}$$

where

$$u_n = \frac{1}{2}\int dx_n\alpha_n = \alpha_n x_n/2, \tag{41}$$

for $m = 0$, has the form similar to the classical equation (35), where α_n is velocity matrices and the Planck's constant $\hbar$ can be cancelled. This is an inverse to the consideration made when we try to find quantum (photon) nature of the (classical) Maxwell's equations and put them in the "Dirac's form", (see e.g. [15]). It is possible to formulate similar equations for high spin massless fields . It is interesting to find a corresponding classical interpretation of these equations and make observable predictions, [16]. The effects of two of them (the photon's and graviton's) are obvious in everyday life. What about the effects of other massless particles?

After the development of the classical theory of the Cherenkov's radiation [17], the question arises if there exist any differences between radiation of (massive) particles with different spins and corresponding corrections due to spin degrees of freedom where calculated. It was found that these correction are small with respect to the spin independent classical contribution. The point is that at the threshold of the Cherenkov's radiation the classical contribution is zero and remains just quantum corrections [18].

Then, in a discrete form, Dirac's equation has problems, (see e.g.[19]), with a chiral invariance or a spectrum multiplication or it is nonlocal. In the second-order form, we hope to solve these problems.

Appendix 1

In the main text of this paper we used the following relation,

$$e^{\varepsilon A}e^{\varepsilon B}e^{-\varepsilon A}e^{-\varepsilon B} = e^{\varepsilon^2[A,B]} + O(\varepsilon^3). \tag{42}$$

The following relation may also be useful:

$$(1+\varepsilon A)(1+\varepsilon B)(1+\varepsilon A)^{-1}(1+\varepsilon B)^{-1} = (1+\varepsilon^2[A,B]) + O(\varepsilon^3). \tag{43}$$

Now we calculate the following matrix element

$$\begin{aligned} < x_{n+1}|exp(-a\hat{p}^2)|x_n > &= \int d^D p < x_{n+1}|p >< p|x_n > exp(-ap^2) \\ &= \int \frac{d^D p}{(2\pi\hbar)^D} exp(i\frac{p(x_{n+1}-x_n)}{\hbar} - ap^2) \\ &= \frac{A^D}{(2\pi\hbar)^D} exp(-\frac{(x_{n+1}-x_n)^2}{4a\hbar^2}), \end{aligned} \tag{44}$$

where in the case of the quantum mechanics of the particle, (22)

$$a = i\frac{t}{2m\hbar N} \tag{45}$$

and in the case of classical mechanics, (39)

$$a = i(\frac{t}{\hbar^2 N})^{1/2}, \tag{46}$$

$$A = \int dp exp(-ap^2) = \sqrt{\frac{\pi}{a}}. \tag{47}$$

Coordinate and momentum state vectors are correspondingly $|x>$ and $|p>$,

$$\begin{aligned} &\hat{x}|x>= x|x>, \quad \hat{p}|p>= p|p>, \\ &< p|x >= \psi_x(p) = \frac{1}{\sqrt{2\pi\hbar}} exp(-\frac{i}{\hbar}px), \\ &\hat{x}\psi_x(p) = i\hbar\frac{\partial}{\partial p}\psi_x(p) = x\psi_x(p), \\ &< x|y >= \int dp < x|p >< p|y >= \int \frac{dp}{2\pi\hbar} exp(\frac{i}{\hbar}p(x-y)) \\ &= \delta(x-y). \end{aligned} \tag{48}$$

Appendix 2

As an example, we consider the harmonic oscillator. The Hamiltonian in this case is

$$H = \frac{p^2}{2m} + \frac{kq^2}{2} = \frac{1}{2}x_n k_{nm} x_m. \tag{49}$$

Corresponding Hamiltonian equations of motion are

$$\dot{x}_1 = \frac{x_2}{m} = v_1 = k_{22}x_2,$$
$$\dot{x}_2 = -kx_1 = v_2 = -k_{11}x_1. \tag{50}$$

For any observable $\psi(x)$,

$$\dot{\psi} = \{\psi, H\} = \varepsilon_{nm}\frac{\partial\psi}{\partial x_n}\frac{\partial H}{\partial x_m} = \varepsilon_{nm}k_{ml}x_l\frac{\partial}{\partial x_n}\psi = v_n\frac{\partial}{\partial x_n}\psi, \tag{51}$$

$$u_n = \int dx_n v_n, \quad u_1 = k_{22}x_1x_2, \quad u_2 = -k_{11}x_1x_2. \tag{52}$$

References

[1] A. Ecert and R. Jozsa, *Rev. Mod. Phys.* **68** 115 (1996).

[2] G.D. Birkhoff, *Dynamical Systems*, Amer. Math. Soc., Providance, R.I., 1927.

[3] N. Makhaldiani, O. Voskresenskaya, *Communications of the JINR*, Dubna **E2-97-418** 1997.

[4] *Dictionary of Computing,* Market House Books Ltd., 1986.

[5] N. Makhaldiani, *Quantum Computing,* in preparation.

[6] F. Berezin, M. Shubin, *Schrödinger equation,* Kluwer, Dordrecht, 1991.

[7] R.P. Feynman and A.R. Hibbs, *Quantum Mechanics and Path Integrals,* McGraw-Hill, New York, 1965.

[8] C. Zalka, *Proc.Roy.Soc.Lond.* **A454** 313 (1998).

[9] P. Becher, H. Joos, *Z. Phys.* **C 15** 343 (1982).

[10] N.V. Makhaldiani, *Computational Quantum Field Theory, Communications of the JINR*, Dubna **P2-86-849** 1986.

[11] E. Gozzi, *Progr. Theor. Phys. Suppl.* **111** 115 (1992).

[12] L.Ts. Adzhemyan, N.V. Antonov, A.N. Vasiliev, *Field Theoretic Renormalization Group in Fully Developed Turbulence*, Gordon and Breach Science Publishers, 1998.

[13] L.D. Faddeev and L.A. Takhtajan, *Hamiltonian methods in the theory of solitons*, Springer, Berlin, 1987.

[14] Hans De Raedt et al. *Comp. Phys. Com.* **132** 1 (2001).

[15] James D. Bjorken, Sidney D. Drell, *Relativistic Quantum Mechanics*, McGraw-Hill, New York, 1965.

[16] N. Makhaldiani, work in progress.

[17] I.M. Frank and I.E. Tamm, *Dokl. Akad. Nauk, SSSR* **14** (3) 109 (1937).

[18] N. Makhaldiani, in preparation.

[19] N.B. Nielsen and M. Ninomiya, *Phys. Lett.* **B105** 219 (1981).

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Махалдиани Н. E2-2001-137
Как будет решать квантовый компьютер классические задачи

Найдено расширение любой заданной динамической системы с помощью соответствующей линейной (квантовой) системы. Рассмотрены функциональная и операторная формы формальных решений соответствующих уравнений движения. Построен алгоритм расчета классических задач на квантовых компьютерах.

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Makhaldiani N. E2-2001-137
How to Solve the Classical Problems on Quantum Computers

An extension of a time-reversible dynamical system by corresponding linear (quantum) system is given. Functional and operational forms of the formal solutions to the corresponding motion equations are considered. An algorithm of solution to the motion equations of the classical dynamical systems on the quantum computers is constructed.

The investigation has been performed at the Laboratory of Information Technologies, JINR.

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