Quantum Information Science and Nanotechnology

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Abstract

In this note is touched upon an application of quantum information science (QIS) in nanotechnology area. The laws of quantum mechanics may be very important for nano-scale objects. A problem with simulating of quantum systems is well known and quantum computer was initially suggested by R. Feynman just as the way to overcome such difficulties. Mathematical methods developed in QIS also may be applied for description of nano-devices. Few illustrative examples are mentioned and they may be related with so-called fourth generation of nanotechnology products.

1 Brief history

The beginning of era of nanotechnology is often associated with two works: the lecture of R. Feynman [1] at Caltech in 1959 and book of E. Drexler [2] devoted to nanotechnology and published in 1986. Both works mentioned examples from (molecular) biology as an inspiration.

Later, the “pure technical” approach was criticized sometimes and an example is the debate of Drexler and R. Smalley [3]. Often nanotechnology is considered [4, 5] using both “top-down” approach with application of more or less traditional “macroscopic”
technological processes for creation and modification of nanostructures and “bottom-up” one with “shaping things atom by atom”.

It may be reasonable to consider impact of chaotic motion described by thermodynamic laws and additional indeterminacy due to principles of quantum mechanics. If the size of few nanometers would be really an obstacle for creation of difficult devices, how do biological molecular “machines” [6] work? On the other hand, if it possible to compare bacteria or virus with “nanobot”, i.e., nanomechanical device with processor, memory, and different mechanisms for motion and interaction with environment?

An accurate consideration let us avoid some illusory contradictions. The thermodynamic problem due to miniaturization were investigated in the works of R. Landauer, C. Bennett [7], et al quite long time ago and should be discussed elsewhere. It is enough to mention, that heating may be reduced to zero for some kind of computing devices [7].

An application of quantum mechanics for description of molecular technologies also has certain history. For example, Yu. I. Manin wrote about “genetic automata” in introduction to brochure [8] published in 1980: “Perhaps, for better understanding of this phenomenon, we need a mathematical theory of quantum automata”. In classical theory of algorithms it is common to use a Turing machine, i.e., an automaton with a tape for program and data. A modification of such a model for quantum systems was developed by P. Benioff [9] on conference PhysComp (Physics and Computations) in 1981. On the same conference R. Feynman made talk [10] affecting problems with modeling of quantum systems.

There is specific problem with modeling of nano-systems, because description of the system as collection of properties of separate atoms already too complicated, but statistical methods may be absolutely inappropriate due to certain reasons. Modern computers might model evolution of billions elementary classical systems. In quantum mechanics the situation is quite different due to exponential complication of system description with respect to number of elements, and it was noted both in work of Yu. I. Manin cited earlier [8] and talk of R. Feynman mentioned above [10]. So, even system with three decades of particles may require few gigabytes of memory for accurate modeling.
Feynman [10] suggested creation special simulating device as a method to overcome the problem with modeling of the quantum systems. Such a device should be universal enough to model as many different quantum systems as possible. Feynman introduced term “quantum computer” as a synonym of “universal quantum simulator” and it sometimes causes rather limited interpretation of such approach, because the work of such device should not necessary be associated with any computations.

The Feynman’s quantum simulator could be compared with acceleration card attached to computer for modeling of quantum systems. D. Deutsch [11] in 1985 developed further the model of Feynman and proved possibility to simulate very extensive class of systems with fixed set of elementary operations. The physical motivation of considered operations also was emphasized in this work and term “algorithm” might be interpreted not only as computation or computer program, but rather as realization of broad class of different actions or even as arbitrary physical process.

The book “Engines of Creation” by Drexler [2] was published in 1986 and, so, theory of cybernetic devices with atomic scale already existed at this time. Drexler had mentioned in his book model of Feynman’s quantum computers, but nanotechnological applications of the quantum information science and technology (QIS&T) is still at early stage of development.

2 Applications

Let’s consider four generations of nanotechnology products, cf [5]

- **First Generation.** Passive nanostructures: nano-particles, nano-wires, nano-tubes and nano-layers, etc.

- **Second Generation.** Active nanostructures and nanodevices: transistors, amplifiers, sensors, actuators, adaptive nanostructures, targeted drugs and chemicals, etc.

- **Third Generation.** Integrated nanosystems: 3D nanosystems, multiscale synthesis and assembly techniques, bioassembly, hierarchical structures, etc.
Fourth Generation. Heterogeneous multifunctional nanosystems: apparatuses with nanoscale components, where each aggregate of atoms has a particular structure and implements its own function within the assemblies (“fifth state of matter”). Radically improved capabilities of this generation may be compared with some properties of simple natural biosystems still not accessible by modern technologies.

QIS&T is included in “nanosupplement” to PACS 2008 (03.67) and may be associated with all generations of nanotechnologies, e.g., quantum dots belong already to 1′st-2′nd generations [5] and nowadays are widely used almost in any area of QIS&T [12, 13].

It may be useful to consider application of methods related with QIS&T to basic problem, discussed in Drexler-Smalley debate [3] and related in such a classification with fourth generation of nanotechnologies (and beyond) or with second-generation nanomachines in Drexler terminology [2].

Drexler emphasized possibility of creation of so-called assemblers, viz, the “engines of creation” [2] associated with bottom-up approach to “maneuvering things atom by atom” [1]. Drexler considered that as the basic purpose of nanotechnology, but Smalley (who won the Nobel Prize in Chemistry for discovery of fullerenes) did not include conception of the assemblers in nanotechnology and even denied possibility of creation of such nano-devices.

Smalley considered idea of some nano-scale manipulator for construction of things from separate atoms, as too primitive one, because instead of motion in usual space for description of molecular interactions it is necessary to use a formal “many-dimensional hyperspace” [3]. Indeed, in QIS&T construction of Hamiltonians, providing necessary evolution of a system, may be described using geometric algebras for some hyperspaces (Clifford algebras) [14].

It was already mentioned, the idea of universality in QIS&T [11] is concerned not only with possibility of realization of any algorithm, but also may be applied to research of possibilities and limitation for “constructing” of different quantum states. Results about universality obtained by Feynman, Deutsch, and other researchers ensure preparation of practically arbitrary state using fixed set of simple operations. In 1997 Benioff considered mathematical model
of quantum robot \[15\] and simplified analogue, the “qubot” (cf
“nanobot”), was suggested by author of this note at “Think-tank
on Computer Science Aspects” in 2000 \[16\].

The idea of “quantum processor” \[17\] is also quite useful and
may be defined as an autonomous system, acting according to in-
ternal program. It is not necessary some kind of calculations. Say,
the qubot may use a program for control of motion and interaction
with environment. Similar methods were used in \[18\] for bypass-
ing “no-go” results like limitations to self-reproducing automata
due to laws of quantum mechanics formulated by E. P. Wigner \[19\]
in 1961 and “quantum no-cloning theorem” by W. K. Wootters and
W. H. Zurek \[20\] in 1982. It may have direct relation with the
question about possibility of Drexler’s assemblers.

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