Stairway Quantum Computer

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Abstract

In the paper is considered stairway-like design of quantum computer, *i.e.,* array of double quantum dots or wells. The model is quite general to include wide variety of physical systems from coupled quantum dots in experiments with solid state qubits, to very complex one, like DNA molecule. At the same time it is concrete enough, to describe main physical principles for implementation of universal set of quantum gates, initialization, measurement, decoherence, *etc.*

Introduction

"Perhaps, for better understanding of this phenomenon [DNA replication], we need a mathematical theory of quantum automata. Such a theory would provide us with mathematical models of deterministic processes with quite unusual properties. One reason for this is that the quantum state space has far greater capacity than the classical one . . . "

Yuri I. Manin (1980)

In modern theory of quantum computation is used wide range of different models. There is class of formal mathematical models with abstract qubits. Attempts to understand set of processes relevant to description of a real physical system need for other class of models with high level of complexity and details sometime inaccessible for present level of experimental techniques.

The *stairway model* of quantum computation and control uses a compromise between such opposite classes. From the one hand it is quite concrete model with array of double quantum wells, on the other one, the theoretical methods and mathematical equations discussed here are still quite general and valid for wide variety of different physical systems.

The model itself is introduced in Sec. 2. Description is general enough and often only basic knowledge of quantum mechanics is assumed. In Sec. 1 is discussed more special theme about universal set of quantum gates convenient for considered model. It is set of one- and two-qubits gates Eq. (19). Formally it uses theory of Clifford algebras and Spin groups, but applications may be explained with simpler methods and relevant also with some other models in theory of quantum computing.

1 Universality and Clifford algebras

1.1 Universal sets of quantum gates

A set of quantum gates is universal, if it is possible to represent any operation as composition of elements from the set. Basic theory of quantum gates and networks may be found in [1, 2]. It is possible to use different universal sets of quantum gates. Here it is convenient to consider a special one, based on theory of Spin groups, Clifford and Lie algebras [3, 4]. Let us recall it briefly.

For fixed Hamiltonian, *i.e.,* Hermitian matrix $\mathbf{H}$, evolution of system is described by unitary matrix

$$\mathbf{U} = \mathbf{U}(\tau) = \exp(i\mathbf{H}\tau), \tag{1}$$

where τ is time of action. It is possible to describe universality using the Hamiltonians Eq. (1) instead of quantum gates itself. It is necessary to have some set $\mathbf{H}_k$ with property: arbitrary Hamiltonian may be expressed as linear combinations of $\mathbf{H}_k$ and arbitrary number of commutators $\mathbf{H}_{k,l} = i[\mathbf{H}_k, \mathbf{H}_l] = i(\mathbf{H}_k\mathbf{H}_l - \mathbf{H}_l\mathbf{H}_k)$, $\mathbf{H}_{k,l,m} = i[\mathbf{H}_{k,l}, \mathbf{H}_m] = -\big[[\mathbf{H}_k, \mathbf{H}_l], \mathbf{H}_m\big]$, *etc.*

Usual proof of the property uses theory of Lie algebras and groups [5, 6] and formulae

$$\mathbf{U}_1\mathbf{U}_2 = e^{i\mathbf{H}_1\delta}e^{i\mathbf{H}_2\delta} \cong e^{i(\mathbf{H}_1+\mathbf{H}_2)\delta} + O(\delta^2) \tag{2}$$

$$\mathbf{U}_1\mathbf{U}_2\mathbf{U}_1^{-1}\mathbf{U}_2^{-1} = e^{i\mathbf{H}_1\delta}e^{i\mathbf{H}_2\delta}e^{-i\mathbf{H}_1\delta}e^{-i\mathbf{H}_2\delta} \cong e^{i(i[\mathbf{H}_1,\mathbf{H}_2])\delta^2} + O(\delta^3) \tag{3}$$

where $O(\delta^k)$ denotes order of error.

There is some problem with practical application of expression Eq. (3). The term with commutator has multiplier δ^2 and so it is necessary to take $\tau = \sqrt{\delta}$ in exponents with $\mathbf{U}_1$, $\mathbf{U}_2$ for construction $\mathbf{U}_{1,2} = \exp(i\mathbf{H}_{1,2}\tau)$ Eq. (3). The final expression has error $O(\tau^{1.5})$. It was considered only first commutator, for k consequent commutators it is necessary to take $\tau = \sqrt[k]{\delta}$, $\delta = \tau^k$.

It is not very convenient, because formulae use τ as small parameter, say for some expression with 10 commutators and error about 1% we should use $\delta = 10^{-10}$. It resembles "car parking" [7] with almost mutually cancelling actions and miserable result. The construction of commutator Eq. (3) may be more convenient for abstract proof of universality, than for concrete algorithms.

1.2 Faster construction of commutators

It is useful to look for some other methods of construction of "higher order" gates. One such method based on theory of Clifford algebras, has first order term δ instead of δ^2 and *zero error* [4]. Let us consider special choise of Hamiltonians, when for any two of them is true formulae

$$\mathbf{H}_k\mathbf{H}_j = \pm\mathbf{H}_j\mathbf{H}_k, \quad \mathbf{H}_k^2 = \mathbf{1}. \tag{4}$$

where $\mathbf{1}$ is unit matrix. The case $\mathbf{H}_k\mathbf{H}_j = \mathbf{H}_j\mathbf{H}_k$ is trivial (commutator simply is zero) and for $\mathbf{H}_k\mathbf{H}_j = -\mathbf{H}_j\mathbf{H}_k$ instead of Eq. (3) it is possible to use

$$e^{i\tau\, i[\mathbf{H}_k,\mathbf{H}_j]/2} = e^{-\tau\mathbf{H}_k\mathbf{H}_j} = e^{i\frac{\pi}{4}\mathbf{H}_k}e^{i\tau\mathbf{H}_j}e^{-i\frac{\pi}{4}\mathbf{H}_k}. \tag{5}$$

Really,

$$e^{i\frac{\pi}{4}\mathbf{H}_k}e^{i\tau\mathbf{H}_j}e^{-i\frac{\pi}{4}\mathbf{H}_k} = \exp\big(e^{i\frac{\pi}{4}\mathbf{H}_k}i\tau\mathbf{H}_j e^{-i\frac{\pi}{4}\mathbf{H}_k}\big),$$

but for any operator with property $\mathbf{H}^2 = \mathbf{1}$ it can be written

$$e^{i\phi\mathbf{H}} = \cos(\phi)\mathbf{1} + i\sin(\phi)\mathbf{H}, \quad \text{and so,} \quad e^{\pm i\frac{\pi}{4}\mathbf{H}_k} = \tfrac{\sqrt{2}}{2}(\mathbf{1} \pm i\mathbf{H}_k),$$

finally,

$$\tfrac{\sqrt{2}}{2}(\mathbf{1} + i\mathbf{H}_k)\mathbf{H}_j\tfrac{\sqrt{2}}{2}(\mathbf{1} - i\mathbf{H}_k) = \tfrac{1}{2}(\mathbf{1} + i\mathbf{H}_k)(\mathbf{1} + i\mathbf{H}_k)\mathbf{H}_j = i\mathbf{H}_k\mathbf{H}_j.$$

1.3 Universality, Pauli matrices, and Spin groups

For quantum computation with n two-dimensional systems (qubits) a simple set of Hamiltonians satisfying Eq. (4) may be expressed as tensor products of Pauli matrices

$$\boldsymbol{\sigma}_{i_1} \otimes \boldsymbol{\sigma}_{i_2} \otimes \cdots \otimes \boldsymbol{\sigma}_{i_n}, \tag{6}$$

there $\boldsymbol{\sigma}_{i_k}$ are either one $\boldsymbol{\sigma}_0 = \mathbf{1} = \left(\begin{smallmatrix}1 & 0\\ 0 & 1\end{smallmatrix}\right)$ or Pauli matrices

$$\boldsymbol{\sigma}_1 = \boldsymbol{\sigma}_x = \left(\begin{smallmatrix}0 & 1\\ 1 & 0\end{smallmatrix}\right), \quad \boldsymbol{\sigma}_2 = \boldsymbol{\sigma}_y = \left(\begin{smallmatrix}0 & -i\\ i & 0\end{smallmatrix}\right), \quad \boldsymbol{\sigma}_3 = \boldsymbol{\sigma}_z = \left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right) \tag{7}$$

More abstract example is *Clifford algebra* with generators $\boldsymbol{e}_k$ satisfying relations

$$\{\boldsymbol{e}_k, \boldsymbol{e}_j\} = \boldsymbol{e}_k\boldsymbol{e}_j + \boldsymbol{e}_j\boldsymbol{e}_k = 2\delta_{kj}. \tag{8}$$

Both cases are close related and for Clifford algebra with $2n$ generators there is well known representation [3] using products like Eq. (6)

$$\begin{aligned} \boldsymbol{e}_{2k} &= \underbrace{\boldsymbol{\sigma}_z \otimes \cdots \otimes \boldsymbol{\sigma}_z}_{k} \otimes \boldsymbol{\sigma}_x \otimes \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{n-k-1}, \\ \boldsymbol{e}_{2k+1} &= \underbrace{\boldsymbol{\sigma}_z \otimes \cdots \otimes \boldsymbol{\sigma}_z}_{k} \otimes \boldsymbol{\sigma}_y \otimes \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{n-k-1}. \end{aligned} \tag{9}$$

System with n qubits is described by 2^n-dimensional Hilbert space, group of unitary operators acting on such space is $\mathrm{U}(2^n)$. Dimension of the group is 4^n. The same dimension has linear space of all possible Hamiltonians, *i.e.,* Hermitian $2^n \times 2^n$ matrices and as basis of the space may be used 4^n different *tensor products* of four matrices $\boldsymbol{\sigma}_k$ Eq. (6).

Any such Hamiltonian may be also expressed as *product* of $2n$ elements Eq. (9), but in condition of universality are used *commutators*. Let us recall some facts [4] about the set Eq. (9). The set is not universal, such Hamiltonians generate only some subgroup of $\mathrm{SU}(2^n)$. The subgroup is isomorphic with $\mathrm{Spin}(2n+1)$ and so only $(2n+1)n$-dimensional[1] [4].

On the other hand, it is enough to annex only one Hamiltonian, say

$$\boldsymbol{g}_2 = \boldsymbol{e}_0\boldsymbol{e}_1\boldsymbol{e}_2 = \boldsymbol{\sigma}_x^{(2)} = \mathbf{1} \otimes \boldsymbol{\sigma}_x \otimes \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{n-2}, \tag{10}$$

to produce universal set.

It is also convenient instead of $\boldsymbol{e}_k$ Eq. (9) to use products $\boldsymbol{d}_k \equiv i\boldsymbol{e}_k\boldsymbol{e}_{k+1}$ together with $\boldsymbol{e}_0$, because they correspond to one- and two-qubits gates

$$\boldsymbol{e}_0 = \boldsymbol{\sigma}_x^{(1)} = \boldsymbol{\sigma}_x \otimes \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{n-1}, \tag{11}$$

$$\boldsymbol{d}_{2k} = \boldsymbol{\sigma}_z^{(k+1)} = \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{k} \otimes \boldsymbol{\sigma}_z \otimes \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{n-k-1}, \tag{12}$$

$$\boldsymbol{d}_{2k+1} = \boldsymbol{\sigma}_x^{(k+1)} \otimes \boldsymbol{\sigma}_x^{(k+2)} = \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{k} \otimes \boldsymbol{\sigma}_x \otimes \boldsymbol{\sigma}_x \otimes \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{n-k-2}. \tag{13}$$

So we have $2n+1$ Hamiltonians described by equations Eqs. (10–13) and they are universal, *i.e.,* may generate whole 4^n-dimensional space of all possible operations for system with n qubits.

The set of gates may be divided on two parts: first one is n one-qubit gates Eq. (12) together with $n-1$ two-qubit gates Eq. (13), they generate subgroup isomorphic to $\mathrm{Spin}(2n)$. Second part, the two extra gates Eq. (11) and Eq. (10) makes the set universal.

1.4 Model with spin-1/2 systems

An universal quantum computer based on such set of gates is depicted on Fig. 1. This model with spin-1/2 particles is rather abstract, but convenient as an understanding scheme. For example $\boldsymbol{\sigma}_z$ and $\boldsymbol{\sigma}_x$ may be represented as rotation of "spin direction" (Bloch vector) around z and x axis respectively Fig. 2.

The visual models like Fig. 2 are widely used for spin-1/2 system in NMR quantum information processing [8] and really have universal application for any two-states quantum system (qubit).

[1] $\mathrm{Spin}(k)$ group is 2-1 cover of group $\mathrm{SO}(k)$ of rotations in k-dimensional space and has the same dimension $k(k-1)/2$.

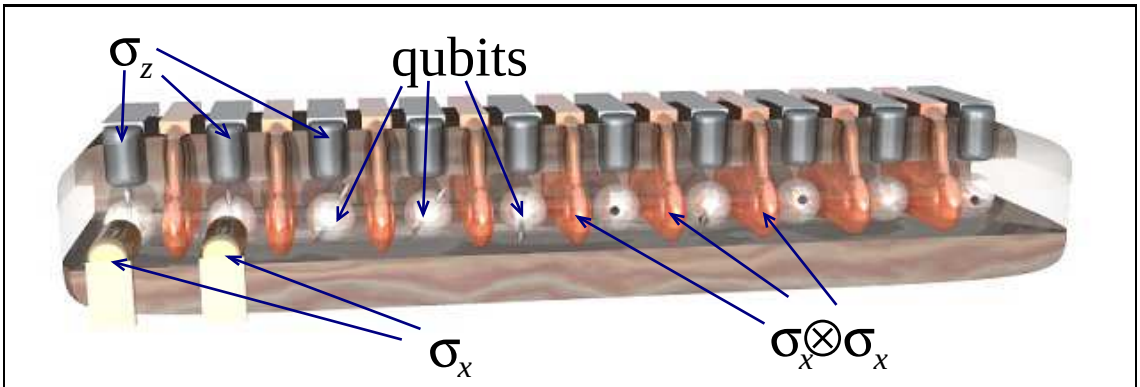

Figure 1: Schematic model of quantum computer with spin-1/2 particles. Where $\boldsymbol{\sigma}_z$, $\boldsymbol{\sigma}_x \otimes \boldsymbol{\sigma}_x$, and $\boldsymbol{\sigma}_x$ denote Hamiltonians ($\mathbf{H}$) of gates. The gates itself are unitary operations $\exp(i\mathbf{H}\tau)$ with one or two "nearest" qubits.

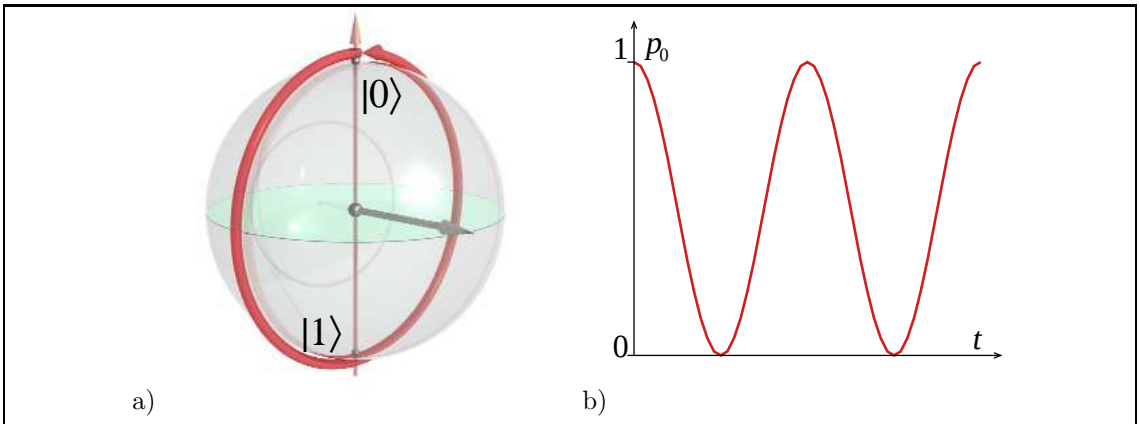

Figure 2: Rotation around x axis used for representation of Hamiltonian $\boldsymbol{\sigma}_x$.

Any Hamiltonian for such system is 2×2 Hemitian matrix and may be represented in form

$$\mathbf{H} = h_0\mathbf{1} + h_1\boldsymbol{\sigma}_x + h_2\boldsymbol{\sigma}_y + h_3\boldsymbol{\sigma}_z \tag{14}$$

where h_k are real numbers. The density matrix of such system also may be presented in similar form

$$\boldsymbol{\rho} = (\mathbf{1} + r_x\boldsymbol{\sigma}_x + r_y\boldsymbol{\sigma}_y + r_z\boldsymbol{\sigma}_z)/2, \tag{15}$$

where r_ν again are real numbers. For pure state the vector r has unit length

$$\boldsymbol{\rho} = |\psi\rangle\langle\psi|, \quad \boldsymbol{\rho}^2 = \boldsymbol{\rho}, \quad r_x^2 + r_y^2 + r_z^2 = 1. \tag{16}$$

Action of Hamiltonian is

$$|\psi(t)\rangle = e^{-it\mathbf{H}}|\psi\rangle, \quad \boldsymbol{\rho}(t) = e^{-i\mathbf{H}t}\boldsymbol{\rho}e^{i\mathbf{H}t}, \tag{17}$$

but Eq. (17) rewritten with h_k Eq. (14) and r_ν Eq. (15) corresponds to rotation of vector (r_x, r_y, r_z) around axis (h_1, h_2, h_3) in some abstract 3D space due to usual properties of Pauli matrices[2].

[2]Three matrices $i\sigma_\nu$ coincide with definition of *quaternions* and so it is representation of 3D rotations by quaternions well known in mathematics since Hamilton.

For given density matrix $\boldsymbol{\rho}$ usual formula for probabilities associated with states $|0\rangle$ and $|1\rangle$ may be also expressed using Eq. (15)

$$p_0 = \langle 0|\boldsymbol{\rho}|0\rangle = \frac{1+r_z}{2}, \quad p_1 = \langle 1|\boldsymbol{\rho}|1\rangle = \frac{1-r_z}{2}, \tag{18}$$

where r_z is coordinate on Bloch sphere. Well known oscillatory behavior of such probability for Hamiltonian $\boldsymbol{\sigma}_x$ is shown on Fig. 2b.

Implementation of two-qubit gates is less obvious, say Hamiltonian $\boldsymbol{\sigma}_x \otimes \boldsymbol{\sigma}_x$ corresponds to Heisenberg-like interaction (anisotropic along x axis).

Rest part of the work uses model with quantum wells instead of spin-half systems. It is more convenient also to exchange $\boldsymbol{\sigma}_x$ and $\boldsymbol{\sigma}_z$ in all definitions above and use set of gates

$$\boldsymbol{e}'_0 = \boldsymbol{\sigma}_z^{(1)}, \quad \boldsymbol{g}'_2 = \boldsymbol{\sigma}_z^{(2)}, \quad \boldsymbol{d}'_{2k} = \boldsymbol{\sigma}_x^{(k+1)}, \quad \boldsymbol{d}'_{2k+1} = \boldsymbol{\sigma}_z^{(k+1)} \otimes \boldsymbol{\sigma}_z^{(k+2)} \tag{19}$$

2 Stairway-like model of quantum gates array

2.1 Double quantum wells (dots) model

Despite of using theory of Spin groups, set of gates described above has wider area of applications, than spin-1/2 quantum systems. Here is discussed design with quantum wells, where all gates may be described using elementary methods. It is used modified set of gates Eq. (19). The model with array of quantum wells (sometime also called double quantum dots) is depicted on Fig. 3.

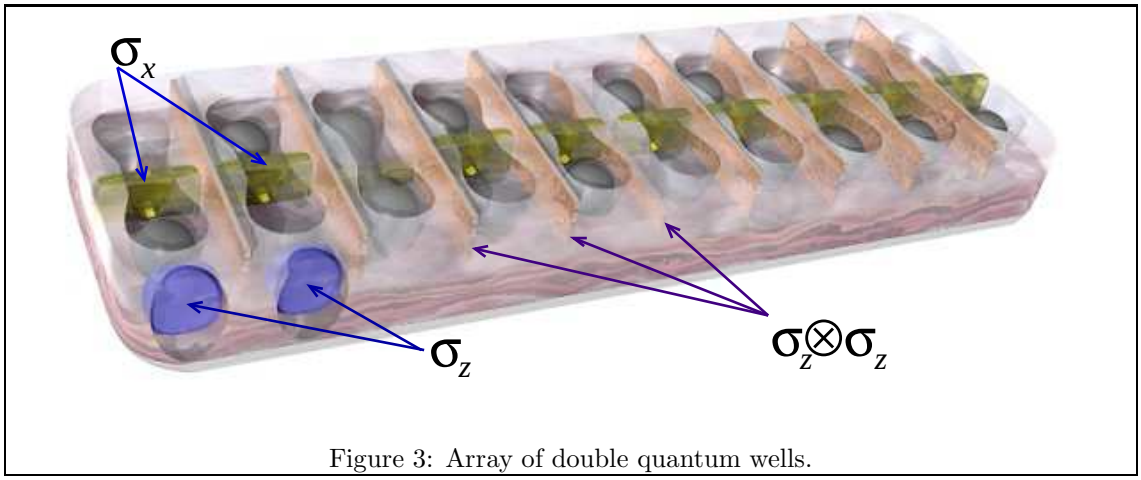

Figure 3: Array of double quantum wells.

Diagrams of such quantum wells for different potentials are shown on Fig. 4 and Fig. 5.

For second case, Fig. 5, it is possible to talk practically about two different wells with exponentially small amplitude of tunelling and denote state of system in first or second one as $|0\rangle$ and $|1\rangle$ respectively.

Let us wrote a Hamiltonian in the computational basis as

$$\mathbf{H} = \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix}, \quad H_{01} = \bar{H}_{10}. \tag{20}$$

Two eigenvalues, *i.e.,* energies of stationary states may be expressed as [9]

$$E_\pm = \frac{H_{00}+H_{11}}{2} \pm \sqrt{\Big(\frac{H_{00}-H_{11}}{2}\Big)^2 + H_{01}H_{10}}. \tag{21}$$

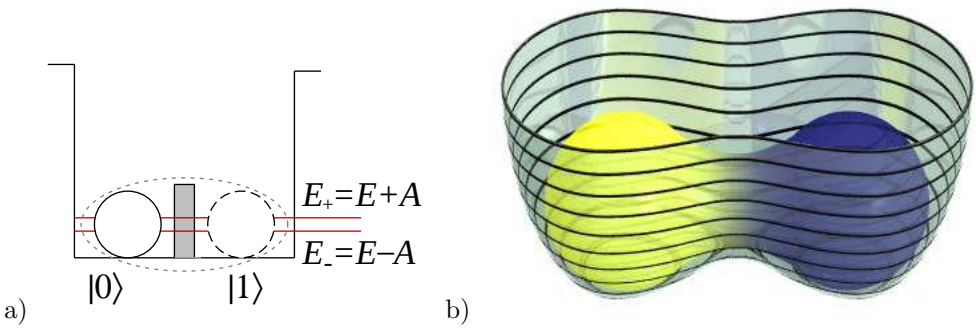

Figure 4: Double quantum well. As "computational" basis $|0\rangle$, $|1\rangle$ are used two states localized in first and second part of well respectively (formally such description more instructive for case depicted on Fig. 5 with bigger potential barrier and small amplitude of transition). Eigenstates may be expressed as $|\pm\rangle = |1\rangle \pm |0\rangle)/\sqrt{2}$. a) Scheme with rectangular partitions. b) 3D diagram of potential and state $|-\rangle = (|1\rangle - |0\rangle)/\sqrt{2}$.

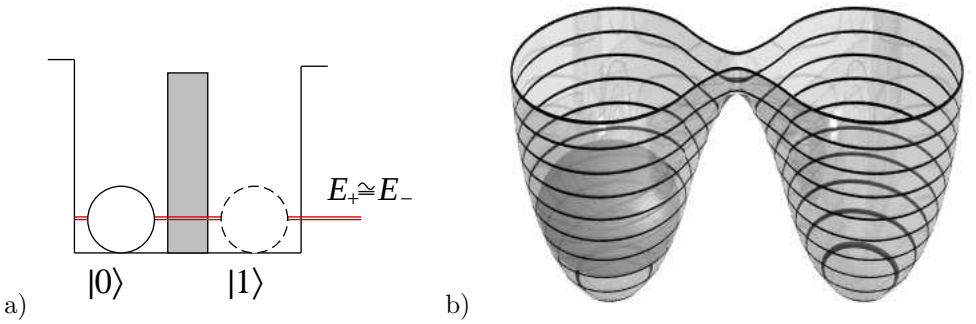

Figure 5: Potential with negligible tunneling amplitude.

In considered case $H_{00} = H_{11} = E$ due to symmetry and using notation $A_T = |H_{01}|$ for transition (tunneling) term, it is possible to rewrite Eq. (21) as [9]

$$E_\pm = E \pm A_T. \tag{22}$$

In such a case corresponding eigenvectors are

$$|+\rangle = \frac{\sqrt{2}}{2}(|1\rangle + |0\rangle), \quad |-\rangle = \frac{\sqrt{2}}{2}(|1\rangle - |0\rangle). \tag{23}$$

The value A_T may be arbitrary small if two positions of the system on Fig. 5 are separated enough and so we may have almost degenerate system $E_+ \cong E_- \cong E$ convenient for safe keeping state of such qubit.

If $H_{00} \neq H_{11}$ eigenvectors may be described as [9]

$$|\pm\rangle = c_0^\pm|0\rangle + c_1^\pm|1\rangle, \quad c_0^\pm = \frac{H_{01}}{D_\pm}, \quad c_1^\pm = \frac{E_\pm - H_{00}}{D_\pm}, \quad D_\pm = e^{i\phi}\sqrt{(E_\pm - H_{00})^2 + H_{01}H_{10}}. \tag{24}$$

Finally, wave function of arbitrary state (nonstationary solution) is

$$|\psi\rangle = |+\rangle e^{-itE_+/\hbar} + |-\rangle e^{-itE_-/\hbar} = |+\rangle e^{-i\omega_+ t} + |-\rangle e^{-i\omega_- t}, \tag{25}$$

so if we initially have well-separated parts Fig. 5 and system in state $|0\rangle$, then the change of coupling parameter A_T to some nonzero value Fig. 4 is producing oscillations between $|0\rangle$ and $|1\rangle$.

Really, $|0\rangle = (|+\rangle - |-\rangle)/\sqrt{2}$, but terms of the expression Eq. (25) have different frequencies $\omega_\pm$ and so after time $T_{1/2}$, where $(\omega_+ - \omega_-)T_{1/2} = \pi/2$, the system has state $|1\rangle = (|+\rangle + |-\rangle)/\sqrt{2}$. Such operation with different durations τ generates quantum gates corresponding to Hamiltonian $\boldsymbol{\sigma}_x$.

Distortion of potential Fig. 6 $H_{00} \neq H_{11}$ let us implement $\boldsymbol{\sigma}_z$.

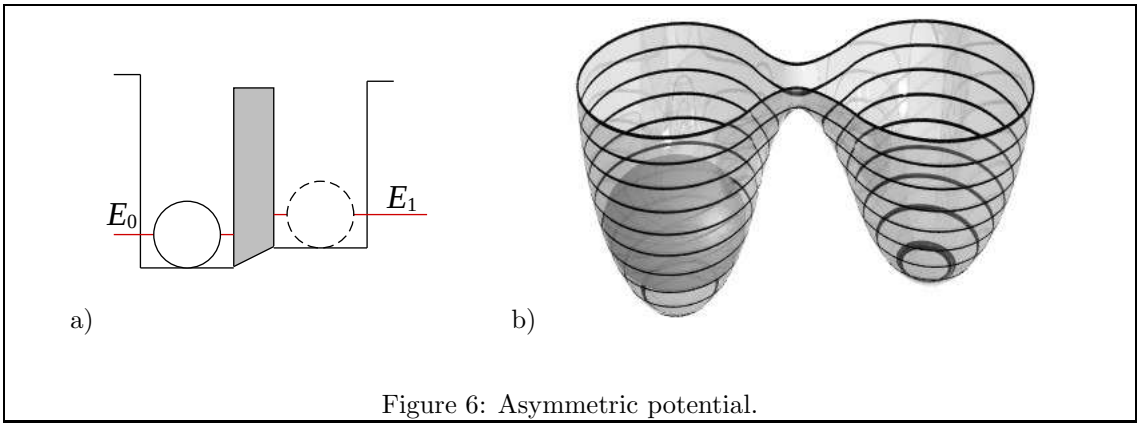

Figure 6: Asymmetric potential.

It is possible directly describe all the one-qubit gates using decomposition of Hamiltonian on Pauli matrices $\mathbf{H} = \sum_k h_k \boldsymbol{\sigma}_k$ Eq. (14) with coefficients

$$h_0 = \frac{H_{00} + H_{11}}{2}, \quad h_1 = \frac{H_{01} + H_{10}}{2}, \quad h_2 = \frac{H_{01} - H_{10}}{2i}, \quad h_3 = \frac{H_{00} - H_{11}}{2}, \tag{26}$$

where h_1 and h_2 are real and complex part of transition amplitude. It is also convenient to write Eq. (14) in normalized form

$$\mathbf{H} = h_0\mathbf{1} + h_r(h_x\boldsymbol{\sigma}_x + h_y\boldsymbol{\sigma}_y + h_z\boldsymbol{\sigma}_z) \quad h_r = \sqrt{h_1^2 + h_2^2 + h_3^2},\ h_x = \frac{h_1}{h_r},\ h_y = \frac{h_2}{h_r},\ h_z = \frac{h_3}{h_r}, \tag{27}$$

and in such a case

$$e^{i\mathbf{H}t} = e^{ih_0t}\big(\cos(h_rt)\mathbf{1} + i\sin(h_rt)(h_x\boldsymbol{\sigma}_x + h_y\boldsymbol{\sigma}_y + h_z\boldsymbol{\sigma}_z)\big), \quad (h_x^2 + h_y^2 + h_z^2) = 1. \tag{28}$$

Formally for complex H_{01} instead of $\boldsymbol{\sigma}_x$ we are applying some combination of $\boldsymbol{\sigma}_x$ and $\boldsymbol{\sigma}_y$, but it does not matter, because all expressions used above in discussion about universality may be rewritten for substitutions like $\boldsymbol{\sigma}_x \to h_x\boldsymbol{\sigma}_x + h_y\boldsymbol{\sigma}_y$, $\boldsymbol{\sigma}_y \to h_x\boldsymbol{\sigma}_y - h_y\boldsymbol{\sigma}_x$ and similar property was already used ($\boldsymbol{\sigma}_x \leftrightarrow \boldsymbol{\sigma}_z$) in Eq. (19). So it is possible to consider Hamiltonians with real H_{01} without lost of generality.

It was already discussed that understanding model with Bloch sphere may be used for any two-states quantum system due to representation of density matrix in form Eq. (15). Application of $\boldsymbol{\sigma}_x$ Hamiltonian was depicted on Fig. 2 above (page 4).

The Hamiltonian proportional to $\boldsymbol{\sigma}_z$ was implemented by changing depth of one well Fig. 6 if amplitude of transition is negligible. On the other hand, the potential should be symmetric for application of $\boldsymbol{\sigma}_x$ described above. Undesirable combination of tunneling and asymmetry is demonstrated on Fig. 7

The picture Fig. 7 shows, that for system in initial state $|0\rangle$ and for triple (h_x, h_y, h_z) corresponding to asymmetric potential $h_z \neq 0$, oscillations do not have complete sweep (unlike $h_z = 0$, Fig. 2b) and such system never reach state $|1\rangle$.

It was described only one-qubit gates, but for universality it is necessary to use two-qubit gates also. In universal set Eq. (19) such gates are generated by Hamiltonian $\boldsymbol{\sigma}_z \otimes \boldsymbol{\sigma}_z$ applied to adjacent

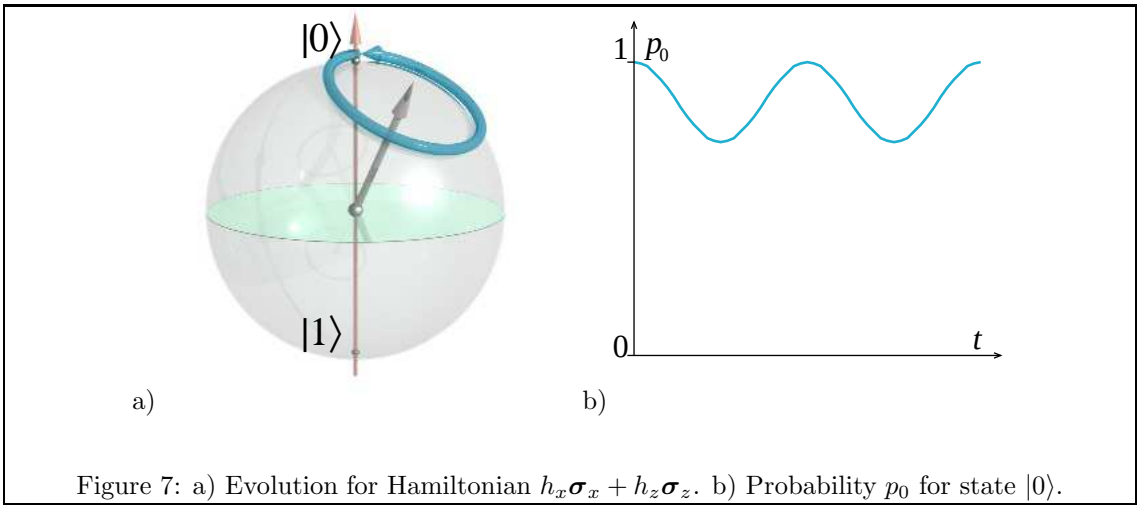

Figure 7: a) Evolution for Hamiltonian $h_x\boldsymbol{\sigma}_x + h_z\boldsymbol{\sigma}_z$. b) Probability p_0 for state $|0\rangle$.

qubits. It is convenient, that such Hamiltonian is diagonal in computation basis. It is enough to consider interaction, then energy of two systems in same states $|00\rangle$ and $|11\rangle$ is not equal to energy in states $|01\rangle$ and $|10\rangle$, *i.e.,* in basis $|00\rangle$,$|01\rangle$,$|10\rangle$,$|11\rangle$ the Hamiltonian of interaction has diagonal form

$$\mathbf{H}_{int} = \begin{pmatrix} E_1 & 0 & 0 & 0 \\ 0 & E_2 & 0 & 0 \\ 0 & 0 & E_2 & 0 \\ 0 & 0 & 0 & E_1 \end{pmatrix}, \tag{29}$$

Simple example is Coulomb interaction between two particles, where in Eq. (29) $H_{00} = H_{33} = E_1$, and $H_{11} = H_{22} = E_2$ due to symmetry and $E_1 \neq E_2$ because distances between particles in such states are different Fig. 8.

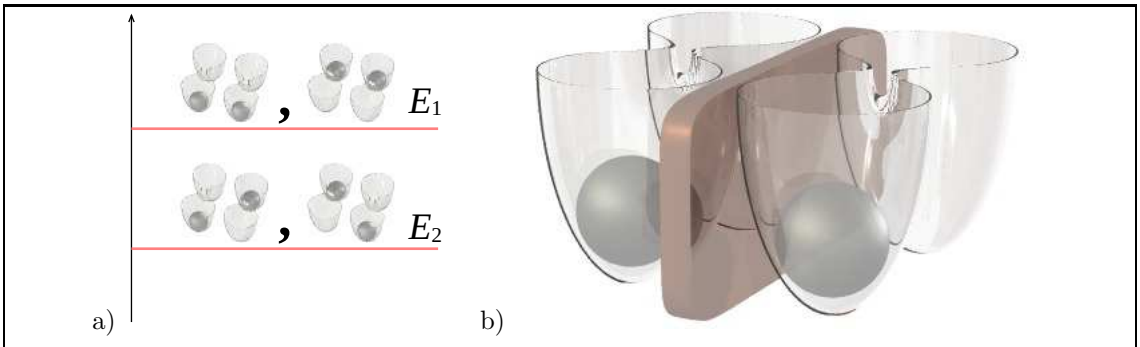

Figure 8: a) Energy levels for simple interaction of two double wells: E_1 for states $|00\rangle, |11\rangle$ and E_2 for $|01\rangle, |10\rangle$. b) The quantum wells with screening separator (state $|00\rangle$).

More general form of Coulomb interaction with symmetrical potentials also could have off-diagonal term $c_e(\boldsymbol{\sigma}_x \otimes \boldsymbol{\sigma}_x + \boldsymbol{\sigma}_y \otimes \boldsymbol{\sigma}_y)$ corresponding to exchange $|01\rangle \leftrightarrow |10\rangle$, but it is small for wells with big potential barrier, because in such a case any off-diagonal process with change of state is suppressed.

The exchange would have analogue with Föster process in exitonic quantum dots [10, 11]. On the other hand the off-diagonal term often was discussed for construction of different entangled states, but considered set of quantum gates Eq. (19) let us prepare any state using only simpler diagonal two-qubit gate with Hamiltonian Eq. (29).

More difficult problem is impossibility to "turn-off" the Coulomb interaction, so on Fig. 3 and Fig. 8b the two-qubit gates are depicted schematically as some kind of variable "screening" shields.

There are proposals to use design with all-optical control of exitonic quantum dots [10, 11, 12], but it is possible to discuss simpler scheme, where tuning of interaction between two dots performed by change of distance.

2.2 Polymer model with double chain.

On Fig. 9 is depicted scheme of such implementation of quantum gates with a double polymer chain. As computational basis is used two states of system in a "stair," it is again a potential well with two minima. It is rather abstract scheme may be applied to different kinds of physical systems, and it should be mentioned, that different proposals with one-dimensional arrays and polymer chains are widely discussed since first papers about practical implementation of quantum computer [13, 14], till more recent times [15, 16, 17].

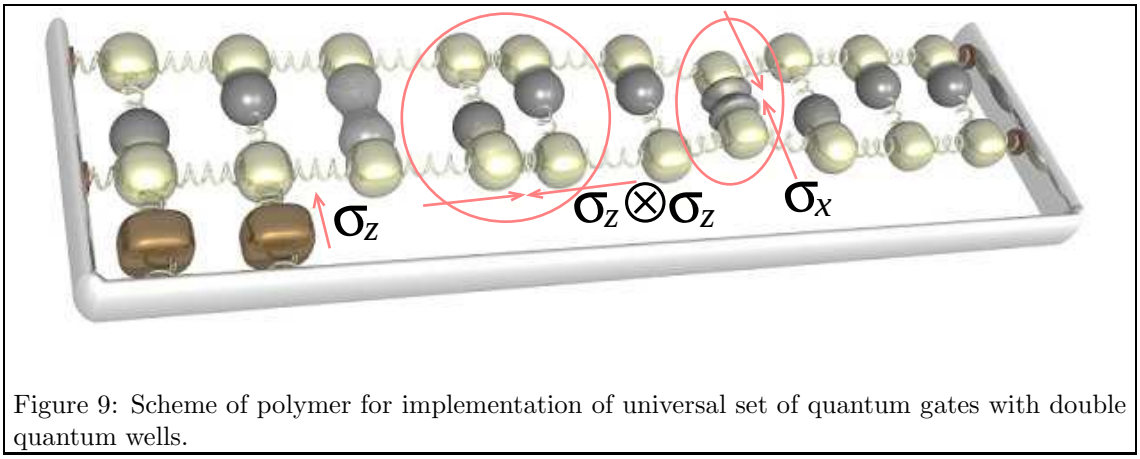

Figure 9: Scheme of polymer for implementation of universal set of quantum gates with double quantum wells.

On Fig. 9 denoted implementation of all three necessary kinds of gates from universal set Eq. (19). The gates with Hamiltonian $\boldsymbol{\sigma}_x^{(k)}$ may be implemented by deformation of polymer double chain with shortening of k-th "stair." In such a case potential with small tunneling amplitude Fig. 5 is transformed to potential like Fig. 4.

The only necessary two-qubit gates with Hamiltonian $\boldsymbol{\sigma}_z^{(k)} \otimes \boldsymbol{\sigma}_z^{(k+1)}$ may be implemented by other kind of deformation (see Fig. 9) with approaching of two "stairs." Here is suggested, that tunnelling of particles between two stairs even in such nearer positions is still impossible for such process and only result is change of energy level Fig. 8, because two systems with same state, *i.e.,* $|00\rangle, |11\rangle$ are closer and interact stronger, than with opposite one $|01\rangle, |10\rangle$, see Fig. 8 and Fig. 9.

It was mentioned earlier, that such set with $2n-1$ gates is still not universal. It is interesting, that for given model the set of gates has simple meaning as transverse and longitudinal deformations of the double chain. The deformations save symmetry of system with respect to reflection, but two additional gates with Hamiltonian $\boldsymbol{\sigma}_z$ are necessary for universality and do not have such property.

In given model such gates are considered as asymmetric deformation of potential due to additional "handles" from one side of "stair." The set of quantum gates Eq. (19) is convenient, because it is necessary to apply such operation only to last two systems in array.

Maybe such polymer system is not too fine for precise implementation of quantum gates, but convenient for metrological and complexity research. For example due to excitation of transverse and longitudinal vibrations of polymer may be generated set of gates with only quadratic complexity, additional asymmetric interaction with first system still does not change the situation and only special

actions on *two* first "stairs" of chain produce universal set and exponential complexity. The example with non-universality shows, that the exponential complexity is not an omnipresent elementary property of arbitrary quantum evolution and may be related with rather fine tuning.

2.3 Control of chain without access to every qubit

The same property of considered universal set of quantum gates also provides useful possibility to control chain only by action on the ends. Really, any combination of quantum gates may be decomposed in consequent actions of pairs: 1) action of gates from subgroup generated by transverse ($\boldsymbol{\sigma}_x^{(k)}$) and longitudinal ($\boldsymbol{\sigma}_z^{(j)} \otimes \boldsymbol{\sigma}_z^{(j+1)}$) deformations of chain, 2) asymmetric action on two first qubits ($\boldsymbol{\sigma}_z^{(1)}$ and $\boldsymbol{\sigma}_z^{(2)}$).

The access to end of chain is quite simple, but deformations of arbitrary segment may be difficult operation. To avoid such a problem, let us consider wave of transverse and longitudinal deformations exited near ends of chain. Let us consider Fig. 9 as demonstration of two waves travelling in opposite directions. The result of such process depends on site, there such waves met.

Full group generated only by such deformations is Spin($2n$), isomorphic with group SO($2n$) of rotations in 2n-dimensions (up to ± 1 multiplier) and so it is possible to associate the excitations of chain with rotations. The whole set of gates produced by such scenario is universal, if subset of symmetric wave excitations discussed above is universal in SO($2n$) group.

Such analysis depends on concrete form of excitations, but the group SO($2n$) is *not* exponential like U(2^n), and so it maybe performed in principle. If we know, how to generate any element of SO($2n$) group, then using combinations of consequent excitations of chain together with asymmetric ($\boldsymbol{\sigma}_z$) actions on last two segments it is possible to generate any element of U(2^n).

It should be mentioned also, that more rigor analysis of the model may demand quantum approach to excitations of chain, *i.e., phonons* and so becomes closer to some ideas discussed in [15] or [17]. The interaction of vibrational modes with quantum transitions in "stairs" (bases) of double helical chain also is important for analysis of mutations in DNA and a quantum model (with different, bosonic model of transitions) may be found for example in [18], but structures (see Fig. 10) and processes are more complex and should be discussed elsewhere.

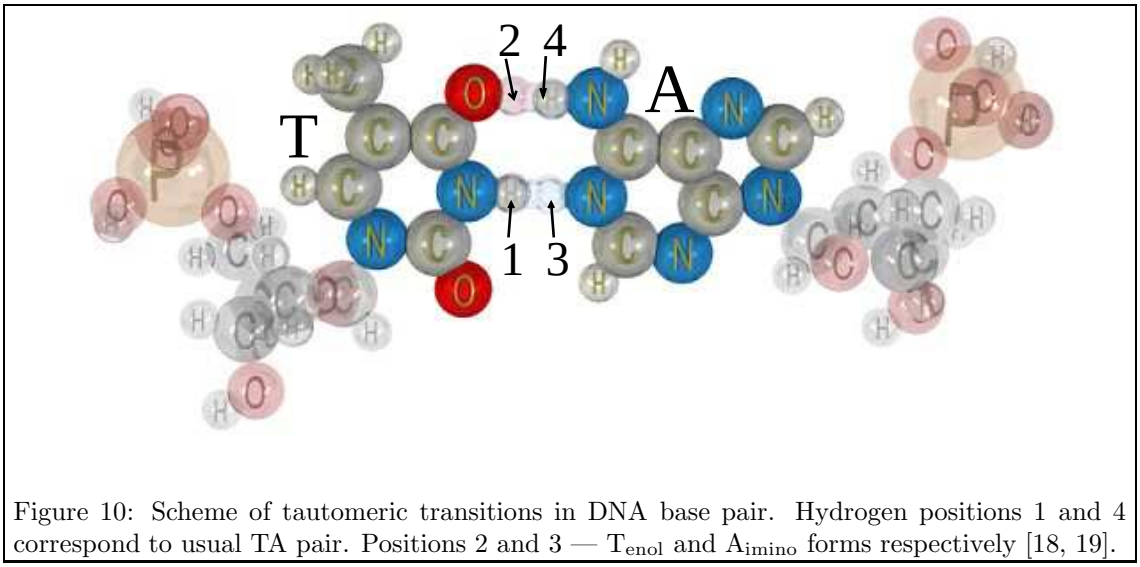

Figure 10: Scheme of tautomeric transitions in DNA base pair. Hydrogen positions 1 and 4 correspond to usual TA pair. Positions 2 and 3 — T_{enol} and A_{imino} forms respectively [18, 19].

2.4 Initialization and measurement

2.4.1 Two alternative approaches

Initialization of a chain in some fixed state is necessary for quantum computations and may be done using different methods. It was discussed above, that for small value of potential barrier Fig. 4 instead of almost degenerate system there are two states $|-\rangle$ and $|+\rangle$ with different energies. So if transition to lower state $|-\rangle$ with emission of photon is allowed it is enough to set chains in closest position and wait some time[3] to initialize system in state $|-\rangle \cdots |-\rangle$ Fig. 11.

Figure 11: Scheme of (radiative) initialization to state $|-\rangle \cdots |-\rangle$.

Schemes of measurement may be similar with used in more traditional double quantum dots design [20], but another approach to initialization and measurement exists also.

The model uses double polymer chain, so it is possible to prepare for initialization two separate chains of different kinds and join them Fig. 12. First chain here contains only empty nodes and second one — only nodes with attached system, so double chain after union has state $|0\rangle \cdots |0\rangle$ Fig. 12.

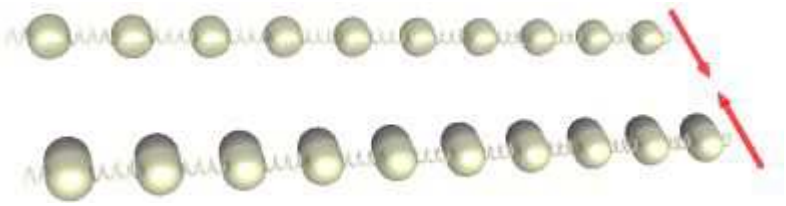

Figure 12: Scheme of initialization with two separate polymer chains.

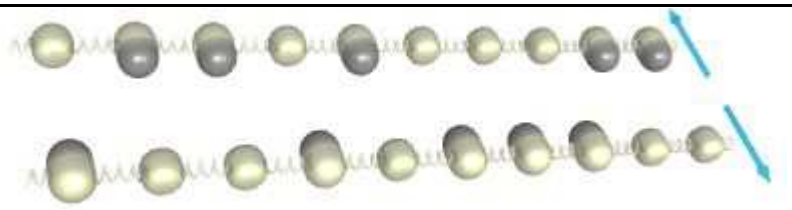

Figure 13: Scheme of separation with two polymer chains (a picture may not represent result of possible superpositions of states from computational basis).

Similar approach is possible to use for measurement of state. It is necessary first to disjoin two chains Fig. 13. Formally it simply corresponds to infinite big value of separation parameter in already used model with quantum gates.

[3]Here formal irreversibility of such process is related with consideration of open system, otherwise emitted photons could always be absorbed with transition to upper level.

The separation alone is not measurement process, but now transitions between chains are not possible, and it is enough to consider task of measurement with single polymer chain containing two kinds of nodes.

Such "destructive" approach may be too rough for some fine quantum algorithms, but again is essential for measures of complexity and other fundamental issues underlying quantum computation and control. Two chains are joining together (initialization, Fig. 12), suffering different kinds of interactions, corresponding to some set of quantum gates described above (quantum control, or "computation") and finally are separating. If the system really possesses "universal access" to whole exponentially big Hilbert space of quantum states? If the separated chains display desired kind of quantum correlations?

The question about universality was already discussed above. For analysis of quantum correlations and different measurement problems the considered scheme with separated chains Fig. 13 may be also convenient due to closer resemblance with standard design in most experiments with quantum correlations, communications *etc.*

2.4.2 Digression to quantum communications area

For more generality it is convenient to consider slighly different design of double quantum well array with two kinds of systems Fig. 14. We have two systems A and B and two states of quantum well $|0\rangle = |AB\rangle$, $|1\rangle = |BA\rangle$.

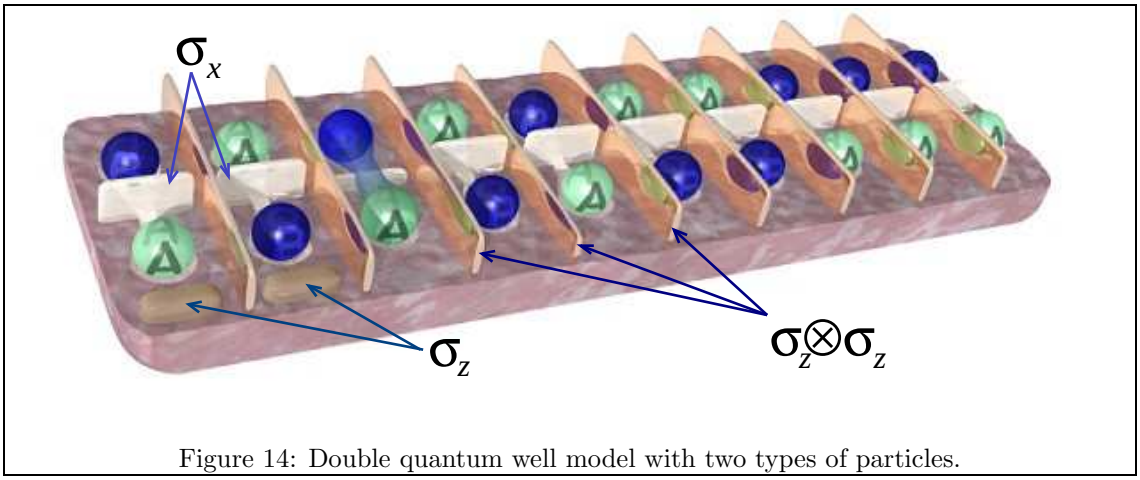

Figure 14: Double quantum well model with two types of particles.

The double chain used above also may be represented in such a way, if to consider empty node as A and node with attached system as B. For similar situations with A and B are two different systems there are two different cases: it is possible to consider quantum superposition of the systems, or it is prohibited by superselection rule (see also [16]). And finally A and B may be simply two different states of the same system, for example two states of photon with different polarizations.

Let us consider now, that the systems in array are separated Fig. 15 and have sent to Alice and to Bob, two usual personages in the area of quantum communications.

If the systems A and B are two different states of photon, then it is similar with standard design for testing Bell inequalities, quantum communications, cryptography *etc.*, [21, 22, 23], but for more difficult processes with many correlated photons.

If the state of system with n double wells was expressed as sum with 2^n terms

$$\sum_{\mathbf{K}} \alpha_{\mathbf{K}} |\mathbf{K}\rangle = \sum_{k_1,\ldots,k_n} \alpha_{k_1,\ldots,k_n} |k_1\rangle \cdots |k_n\rangle, \quad k_j = 0, 1, \quad j = 1, \ldots, n, \tag{30}$$

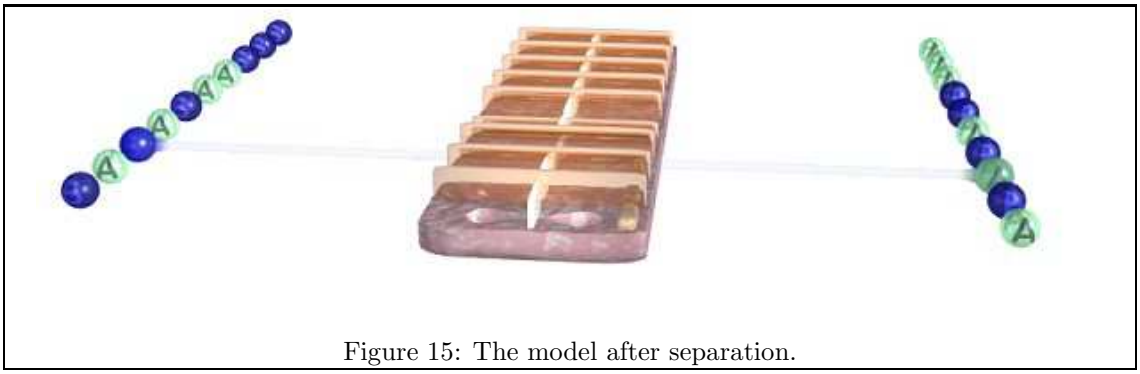

Figure 15: The model after separation.

then result of separation may be expressed as

$$\sum_{\mathbf{K}} \alpha_{\mathbf{K}} |\mathbf{K}_A\rangle |\mathbf{K}_B\rangle = \sum_{\mathbf{K}} \alpha_{\mathbf{K}} |\mathbf{K}_A\rangle |\mathbf{K}_{\neg A}\rangle, \tag{31}$$

where $\neg A$ is bitwise NOT and for any $\mathbf{K}$ state $\mathbf{K}_A$ is produced as $|0\rangle \to |A\rangle$, $|1\rangle \to |B\rangle$, *e.g.,*

$$|\mathbf{K}\rangle = |00101\rangle \quad \Longrightarrow \quad |\mathbf{K}_A\rangle = |AABAB\rangle, \quad |\mathbf{K}_B\rangle = |\mathbf{K}_{\neg A}\rangle = |BBABA\rangle.$$

In a case with n pairs of photons both Alice and Bob would receive n entangled systems and for large amount of such events they could try to look for quantum correlations, like in experiments with Bell's inequalities. On the other hand, the example with states of same system has a problem with undisturbed transmission, due to possible transitions between $|A\rangle$ and $|B\rangle$ already after separation and before measurement.

Let us now consider another case, when A and B are two different systems. From the one hand, such a model may be safer, because only possible error after transmission is *change of relative phases* for coefficients $\alpha_{\mathbf{K}}$ in superposition Eq. (31). For any other transformation of state Eq. (31) it is necessary to perform an operation with both parts of separated system, but change of phase may be caused by difference of energies for particular states of each chain.

On the other hand, for such a system *there is a problem with distinguishing between quantum and classical correlations.* It is enough to consider one pair of particles after separation

$$\psi_{AB} = \alpha |A \wr B\rangle + \beta |B \wr A\rangle. \tag{32}$$

Even if superposition of A and B prohibited by superselection rule, state Eq. (32) is valid, because it is superposition of two states of same system AB, it is simply "limiting case" of double well with almost zero tunneling amplitude.

Unlike testing Bell inequalities with photons such kinds of superposition are still not checked due to enormous difficulty of such experiments. It is not clear even, if it is possible in principle to check directly such superposition — the problem, that for test of quantum correlations each party should have possibility not only measure state $|A\rangle$ and $|B\rangle$, but some superposition of the states $|A\rangle$ and $|B\rangle$ [21, 22].

For example with state of same system it is possible and checked in many experiments with entangled photons [22], but for different systems superposition of states $|A\rangle$ and $|B\rangle$ may be prohibited by superselection rule and usual scheme of testing quantum correlations becomes impossible.

Even if superposition is not prohibited by superselection rules, it may be not allowed by other reasons. Let us consider example, then both, Alice and Bob are trying to measure systems in basis $0.5^{0.5}(|A\rangle \pm |B\rangle)$, but in such a case any joint outcome of such measurement may be represented as superposition $\frac{1}{2}(\pm|AB\rangle \pm |BA\rangle \pm |AA\rangle \pm |BB\rangle)$, but terms $|AA\rangle$ and $|BB\rangle$ of such superposition correspond to physically impossible states, if initially only one system of each kind presents.

Anyway, existence of some superposition states for joint "AB" system like

$$|\underset{AB}{-}\rangle = \frac{\sqrt{2}}{2}\big(|AB\rangle - |BA\rangle\big), \quad |\underset{AB}{+}\rangle = \frac{\sqrt{2}}{2}\big(|AB\rangle + |BA\rangle\big), \tag{33}$$

is rather usual quantum phenomenon. Often it may be checked measuring transitions due to emission or absorption between the energy eigenstates Eq. (33) like in organic dyes [9]. The problem appears during and after separation and may be also explained using ideas of "einselection" theory [24].

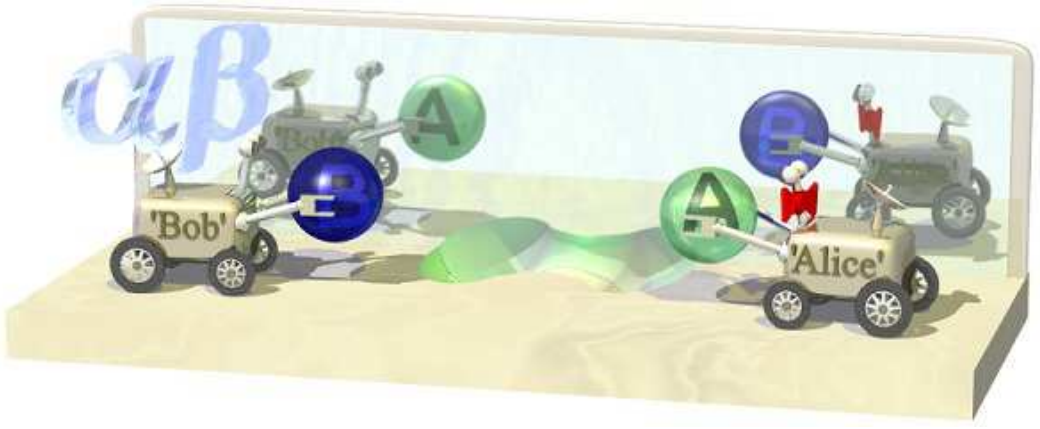

Figure 16: State $\alpha\big|$Alice with A and Bob with $B\big\rangle + \beta\big|$Alice with B and Bob with $A\big\rangle$. Alice and Bob are depicted as unspecified "agents." The "β-branch" is shown "through the looking glass."

The only thing we can expect for series of experiments with separation of states Eq. (33), that with equal probability will be detected two outcomes, Fig. 16: 1) Alice receiving system A and Bob receiving system B, 2) Alice receiving system B and Bob receiving system A. But the same result may be generated by classical experiment, then system is separated with equal chance either in state AB or in state BA. More general case Eq. (32) of superposition with arbitrary α and β corresponds to probabilities $|\alpha|^2$ and $|\beta|^2$.

In principle, measuring of quantum correlations may be still possible with cooperation of Alice and Bob. The simplest example is union of spearate systems and measuring state of AB. It is also possible to perform "conditional exchange" with state transfer to auxiliary system:

$$\big(\alpha|A \wr B\rangle + \beta|B \wr A\rangle\big)|0\rangle \;\longrightarrow\; |A \wr B\rangle\big(\alpha|0\rangle + \beta|1\rangle\big). \tag{34}$$

The operation Eq. (34) is described by action of SWAP gate

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{in basis} \quad \begin{matrix} |A \wr B\rangle|0\rangle \\ |B \wr A\rangle|0\rangle \\ |A \wr B\rangle|1\rangle \\ |B \wr A\rangle|1\rangle \end{matrix} . \tag{35}$$

After such operation each participant receive "proper marble" (A for Alice and B for Bob) and state is stored using auxiliary local system not suffering from superselection limitations.

Here cooperation between Alice and Bob is essential. *E.g.*, in initial model Fig. 13 A is node of chain and B is node with system (or otherwise). It is very close to example with A is a system and B is "nothing", it was simply not convenient in considered model to talk about registration of event like "Bob receives nothing." On the other hand, it corresponds to standard interferometer setup with

two mirrors or two slits experiments. So registration of quantum correlations is possible, but need for cooperation between parties, it corresponds to interference of initially separated beams in the simpler experiment with one system.

The problem, that in more difficult case with two systems we most likely will not be able to measure any correlation. It is the usual problem with environmental superselection. If system had chance to interact with environment, instead of Eq. (34) it is necessary to write

$$\big(\alpha|e_0\rangle|A\wr B\rangle+\beta|e_1\rangle|B\wr A\rangle\big)|0\rangle\ \longrightarrow\ |A\wr B\rangle\big(\alpha|e_0\rangle|0\rangle+\beta|e_1\rangle|1\rangle\big), \tag{36}$$

where $|e_i\rangle$ are states of environment. In Eq. (34) auxiliary system had state $\alpha|0\rangle+\beta|1\rangle$ and it make possible to measure quantum corellations, but it is not so for Eq. (36) and $\alpha|e_0\rangle|0\rangle+\beta|e_1\rangle|1\rangle$.

Such environment induced decoherence process often is explained as supression of off-diagonal elements of reduced density matrix, but may be described using expressions with pure states as well [25, 26]. We still have superposition, considered kind of decoherence is not relevant with *definite outcomes in quantum measurements* [27]. On the other hand, there are different kinds decoherence processes [28].

For "not accurate" separation it may be produced "classical kind" of definite outcomes instead of superposition. Such process is possible, because for asymmetric potential we have two energy levels (see Fig. 6 on page 7) and if emission with transition to level with lower energy is possible, the system becomes localized in one well. Similar kind of "radiative" decoherence processes was already discussed and used above for preparation of initial state (see Fig. 11 on page 11). It should be mentioned also, that after such transition with asymmetric potential, system may stay localized around one minimum even for further coherent evolution (see Fig. 7 on page 8).

After separation decoherence processes may not cancel superposition and only hide and even "lock" it, formally it produces some analogue of isolated "Everett branches" [27, 29]. The possibility of "branching" sometime causes active objections, but except of aesthetical reasons there is still not found any strong evidence against it. Really idea of quantum computer was considered from very beginning as a possible experimental test of Everett's interpretation of quantum mechanics [30].

Anyway such quantum register is not worse for measurements, than some other models, it is rather more convenient for explanation of some standard problems. If we may guarantee, that separation is performed accurate enough, *i.e.,* does not change coefficients $|\alpha|$ and $|\beta|$ in Eq. (34) and if we may prepare quantum register in same state ψ arbitrary number of times, we may use standard methods of quantum tomography to find the state. It is necessary to have possibility not only measure the state ψ, but also perform some set of known quantum gates (say $\boldsymbol{\sigma}_\nu$) before some measurements in the series. The same is true for arbitrary number of qubits [31].

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