Problems of Modern Physics

Lecture 2

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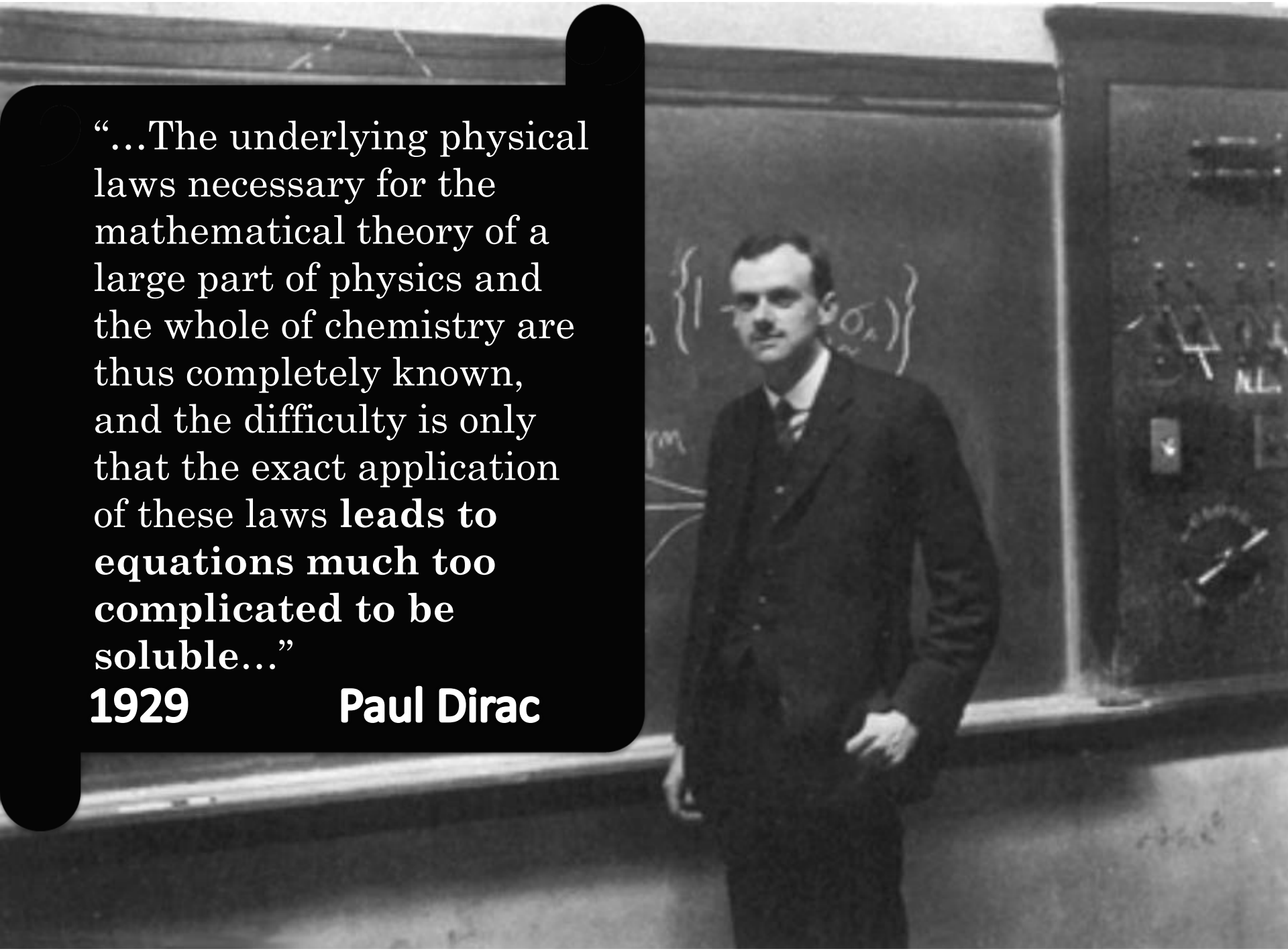
Modeling of quantum systems

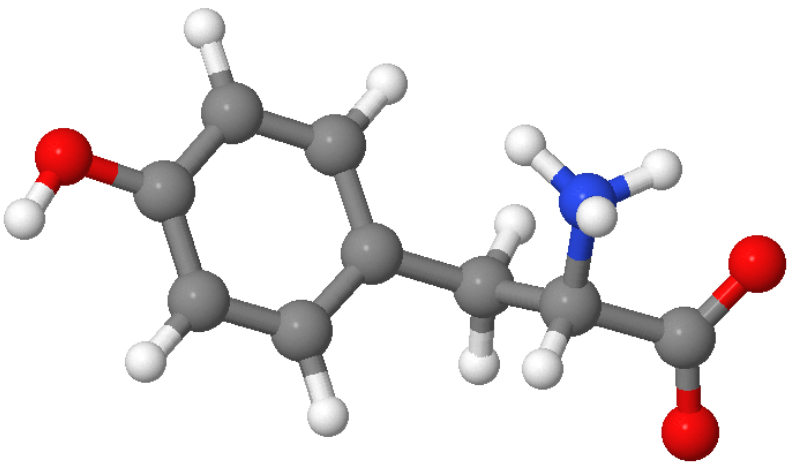


"…The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws **leads to equations much too complicated to be soluble…**"

1929 **Paul Dirac**

Modeling of quantum systems

Tyrosine amino acid



$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$$

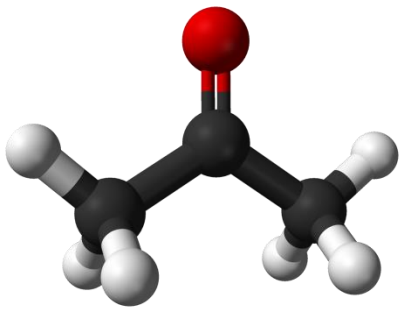
$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

1 particle – n equations:

$$H\Psi = \begin{pmatrix} H_{00} & H_{01} & \dots \\ H_{10} & H_{11} & \dots \\ \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} \Psi_0 \\ \Psi_1 \\ \dots \end{pmatrix}$$

L particles – n^L equations!

Current simulation paradigm



quantum system

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

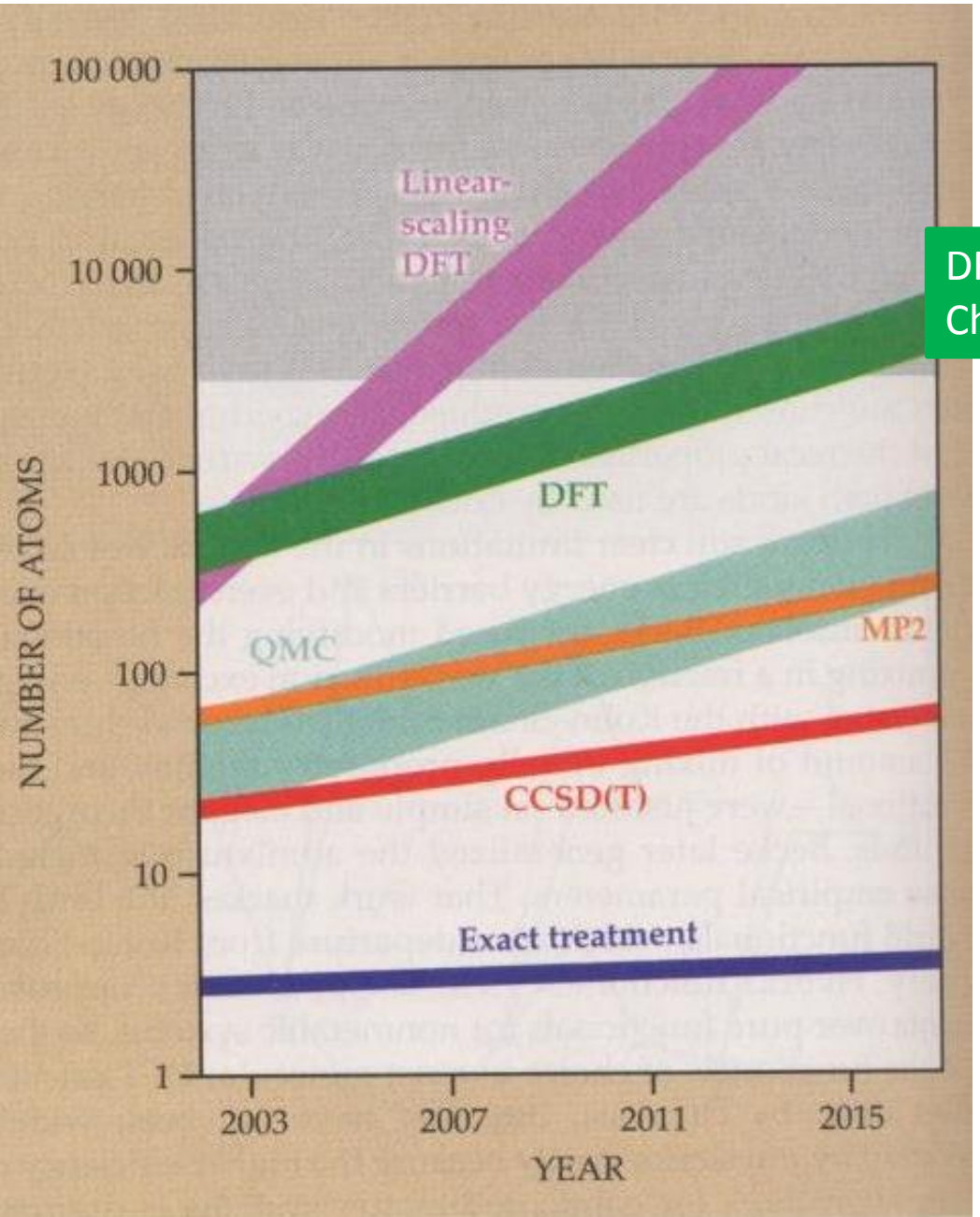
Quantum model
(quantum information)

Classical information
processor

E = -192.0492 Hartree

Classical information

Classical computer algorithms



DFT: Errors in transition states,
Charge transfer excitations, anions,…

DFT = density functional theory
QMC = Quantum Monte Carlo
MP2 = Second order perturbation scheme
CCSD(T) = Coupled cluster scheme

M. Head-Gordon, M. Artacho, ***Physics Today*** 4 (2008)

QC simulations of physical systems

“Возможно, для прогресса в понимании таких явлений нам недостает математической теории квантовых автоматов. Такие объекты могли бы показать нам математические модели детерминированных процессов с совершенно непривычными свойствами...”

Ю. И. Манин, Вычислимое и невычислимое. 1980

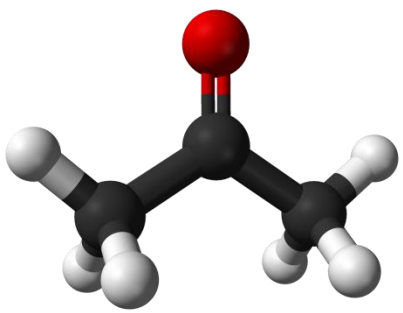
“[...] Nature isn't classical, ..., and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.”

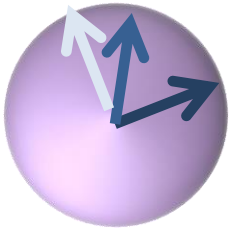
R.P. Feynman – Int. J. Theor. Phys. 21, 467 (1982)

Quantum computer simulation

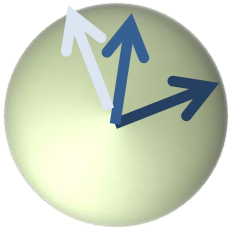
$$|\Psi^{mol}\rangle \quad \rightarrow \quad |\Psi^{QC}\rangle$$

$$\hat{U}^{mol}(t) = e^{-i\hat{H}^{mol}t} \quad \rightarrow \quad \hat{U}^{QC}(t) = e^{-i\hat{H}^{QC}t}$$





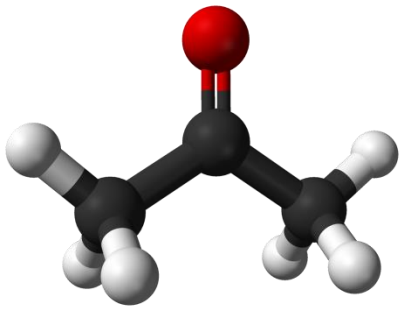
$\rightarrow$



quantum system

quantum system
(quantum information)

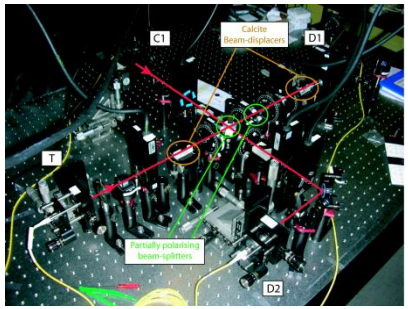
Quantum computing paradigm



quantum system

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

Quantum model
(quantum information)



Quantum information
processor

E = -192.0492 Hartree

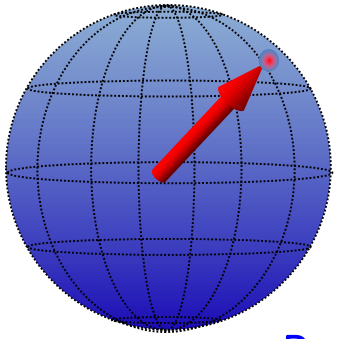
Classical information

Elements of quantum computation

Bits and qubits

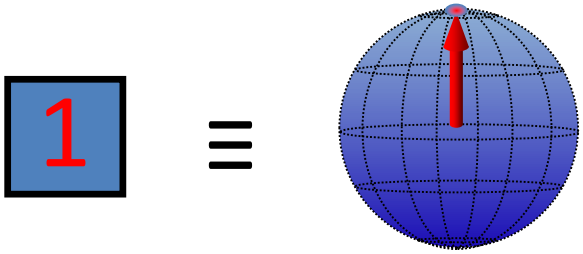
- Two states classical bit

- Two levels quantum system (qubit)

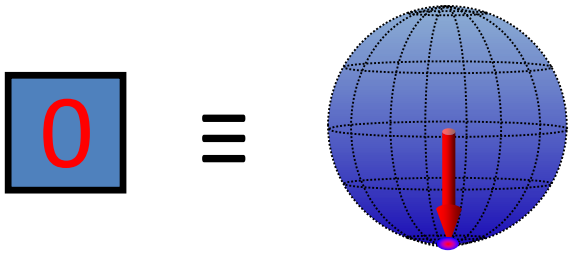


Polarization vector:

S=(**S_φ S_ϑ** S_R=const)



$$\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \Rightarrow |1\rangle$$



$$\rho = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \Rightarrow |0\rangle$$

Density matrix:

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix}$$

Measurement

Physical states as vectors in a <u>complex vector</u> spaces

$$|\uparrow\rangle = |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |\downarrow\rangle = |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Basis states

$$\boxed{\begin{aligned} &|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \\ &|\alpha|^2 + |\beta|^2 = 1 \end{aligned}}$$

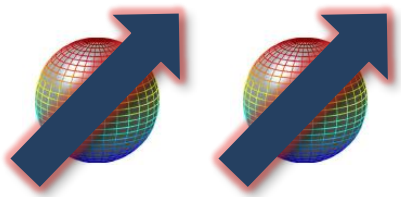
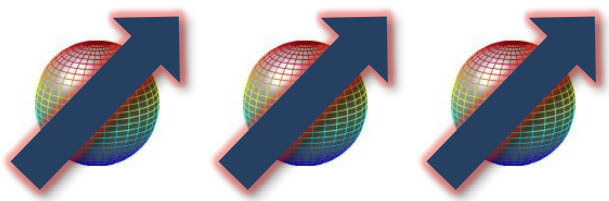
Observables as <u>Hermitian matrices</u>

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \qquad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Result of measurements related to eigenvalues and eigenvectors

$$p_\lambda = |\langle\lambda|\psi\rangle|^2 \qquad p_\uparrow^{(z)} = \left| \begin{bmatrix} 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right|^2 = |\alpha|^2$$

Quantum superposition

qubits	levels (basis states)	general state
	2	$\alpha\|0\rangle + \beta\|1\rangle$
	4	$\alpha\|00\rangle + \beta\|01\rangle + \gamma\|10\rangle + \delta\|11\rangle$
	8	$\alpha\|000\rangle + \beta\|001\rangle + \gamma\|010\rangle + \delta\|011\rangle +$ $\epsilon\|100\rangle + \zeta\|101\rangle + \eta\|110\rangle + \theta\|111\rangle$

Quantum superposition

Composition of multiple quantum systems: tensor product structure

$$\left\{ |0\rangle, |1\rangle \right\} \otimes \left\{ |0\rangle, |1\rangle \right\} \quad \Rightarrow \quad \left\{ |0\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |0\rangle, |1\rangle \otimes |1\rangle \right\}$$

$$|\phi\rangle = \begin{bmatrix} \phi_0 \\ \phi_1 \end{bmatrix}, \quad |\psi\rangle = \begin{bmatrix} \psi_0 \\ \psi_1 \end{bmatrix} \quad \Rightarrow \quad |\phi\rangle \otimes |\psi\rangle = \begin{bmatrix} \phi_0 \, |\psi\rangle \\ \phi_1 \, |\psi\rangle \end{bmatrix} = \begin{bmatrix} \phi_0 \, \psi_0 \\ \phi_0 \, \psi_1 \\ \phi_1 \, \psi_0 \\ \phi_1 \, \psi_1 \end{bmatrix}$$

Separable states vs. entangled states

separable

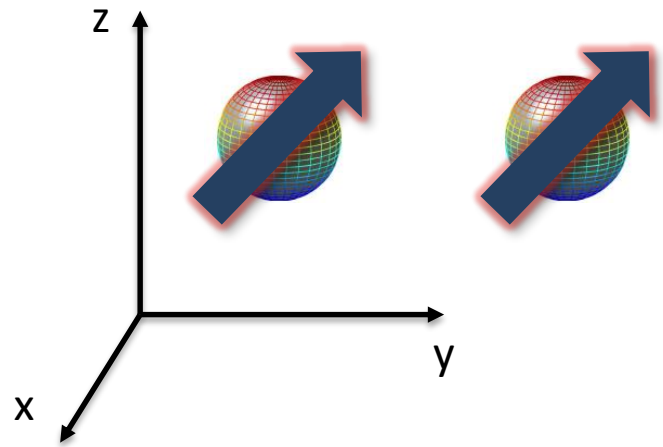
$$|\phi\rangle = \frac{|00\rangle + |01\rangle + |10\rangle + |11\rangle}{2} \quad \Rightarrow \quad |\phi\rangle = \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}} \right) \otimes \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}} \right)$$

$$|\phi\rangle = \frac{|00\rangle + |01\rangle + |10\rangle - |11\rangle}{2} \quad \Rightarrow \quad |\phi\rangle = \frac{|0\rangle}{\sqrt{2}} \otimes \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}} \right) + \frac{|1\rangle}{\sqrt{2}} \otimes \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}} \right)$$

non separable, then entangled

Two-qubits

Basis states



Separable: $|\uparrow\uparrow\rangle \quad |\downarrow\downarrow\rangle \quad |\uparrow\downarrow\rangle \quad |\downarrow\uparrow\rangle$

Entangled:

$$|\Phi_{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle\right)$$

$$|\Psi_{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle\right)$$

EPR Paradox

EPR = Einsten, Podolsky, and Rosen

Let us use a bit different notation:

$$|+z\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |-z\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|-z\rangle \neq -|z\rangle$$

Then

$$|+x\rangle = U_Y(\pi/2)|+z\rangle = \frac{1}{\sqrt{2}}\left(|+z\rangle - |-z\rangle\right)$$

$$|-x\rangle = U_Y(-\pi/2)|+z\rangle = \frac{1}{\sqrt{2}}\left(|+z\rangle + |-z\rangle\right)$$

$$|\Psi_-\rangle = \frac{1}{\sqrt{2}}\left(|+z,-z\rangle - |-z,+z\rangle\right)$$

This is a singlet state, it is isotropic

$$|\Psi_-\rangle = \frac{1}{\sqrt{2}}\left(|+x,-x\rangle - |-x,+x\rangle\right)$$

But

Physical reality

If, without in any way disturbing a system, we can predict with certainty (i.e, with probability equal to unity) the value of physical quantity, then there exists an element of physical reality corresponding to this physical quantity.

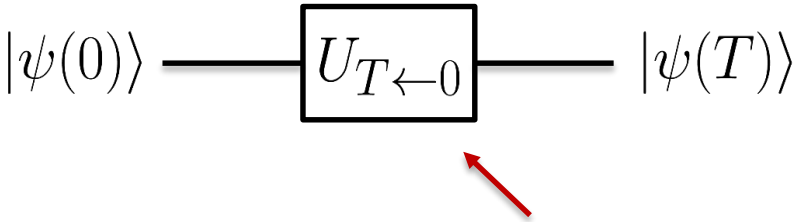
Quantum gates

Dynamics governed by Schrödinger equation

$$\partial_t \left|\psi(t)\right\rangle = -\frac{i}{\hbar} H \left|\psi(t)\right\rangle$$

From continuous-time dynamics to gate operations

$$\begin{aligned}\left|\psi(T)\right\rangle &= \left|\psi(0)\right\rangle + \int_0^T \mathrm{d}t\, \partial_t \left|\psi(t)\right\rangle = e^{-\frac{i}{\hbar} H\, T} \left|\psi(0)\right\rangle \\ &= U_{T\leftarrow 0} \left|\psi(0)\right\rangle\end{aligned}$$



unitary matrix

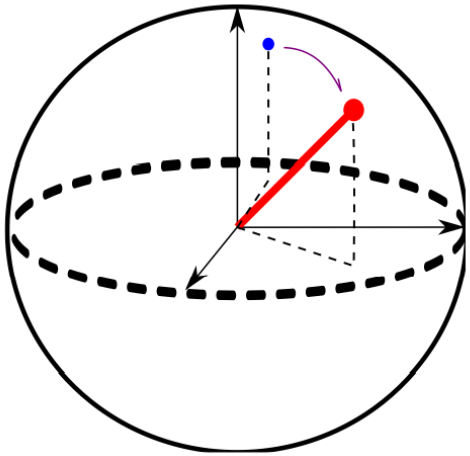
Single qubit operations

Hadamard gate $-\boxed{\mathrm{H}}- = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$

Rotations of Bloch sphere $-\boxed{R_{\hat{n}}}- = \exp[-i(\vec{\sigma}.\hat{n})\theta/2],\ \hat{n}.\hat{n} = 1$

$$\vec{\sigma} \equiv [\sigma_x, \sigma_y, \sigma_z]$$

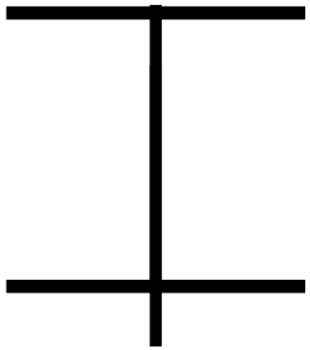
$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$



Two qubits operations

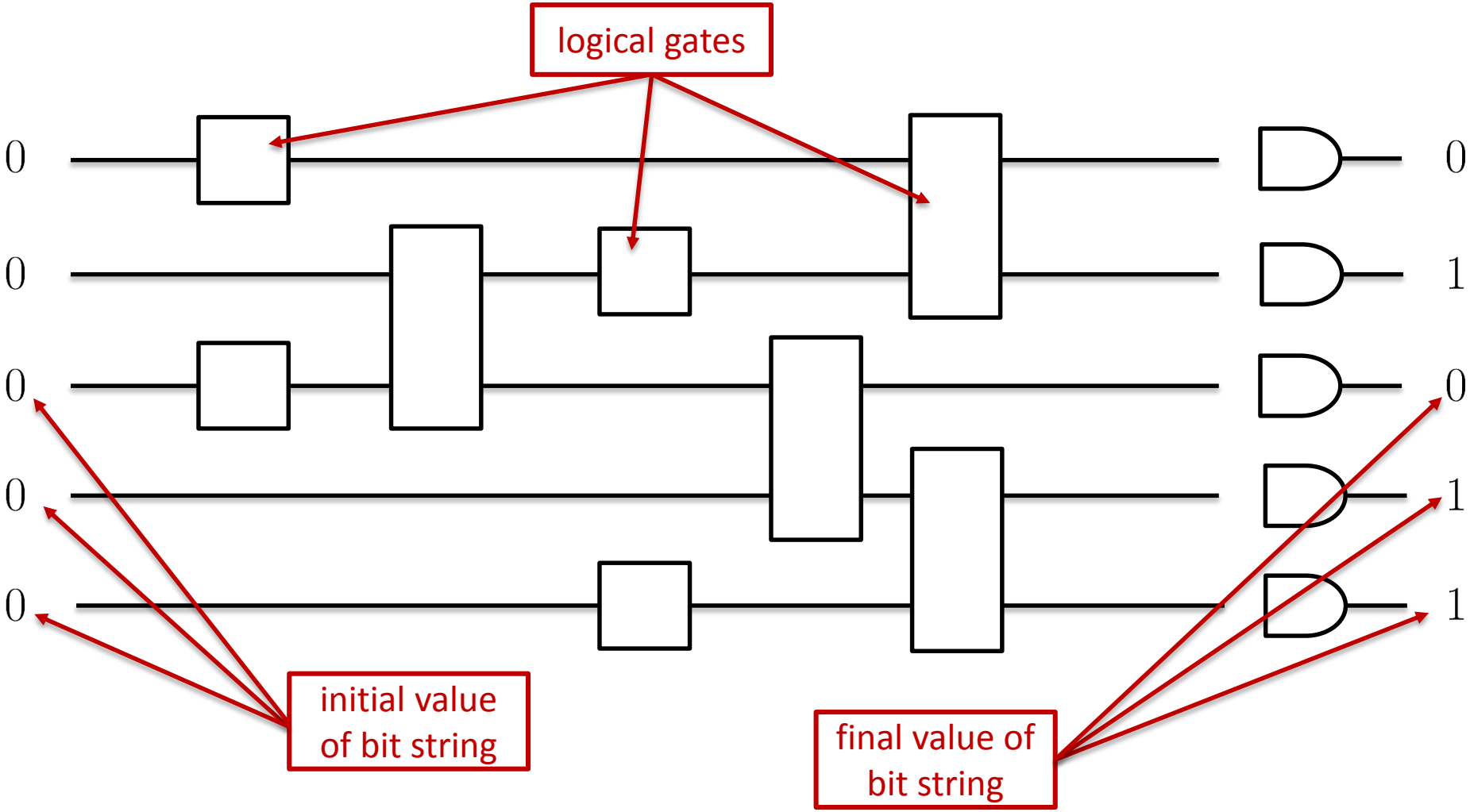
All unitary transformations on n qubits can be described with one-qubit gates and any two-qubit entangling gate

CNOT gate generates entanglement between qubits

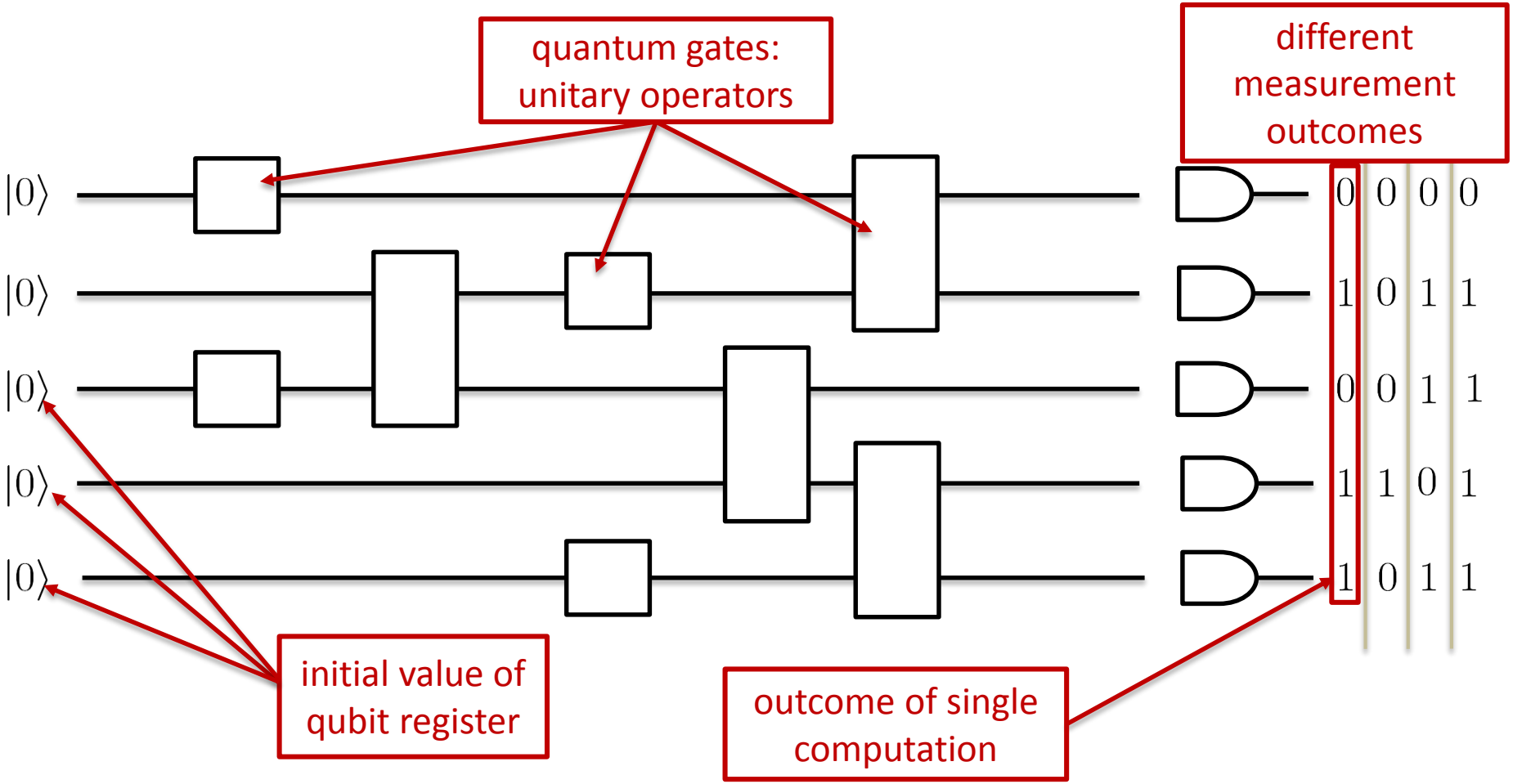


$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{cases} |00\rangle & \rightarrow & |00\rangle \\ |01\rangle & \rightarrow & |01\rangle \\ |10\rangle & \rightarrow & |11\rangle \\ |11\rangle & \rightarrow & |10\rangle \end{cases}$$

Classical computation



Quantum computation



[M.A. Nielsen & I.L. Chuang – "Quantum computation and quantum information" (2010, 2nd ed.)]

Quantum algorithms

Quantum computers hold the promise to drastically reduce the complexity of problems that have a **THEORETICAL AND PRACTICAL RELEVANCE** and no (known) efficient classical solution.

Examples:

- **Deutsch-Jozsa** algorithm has **theoretical** relevance
- **Grover** search algorithm has **practical** relevance (quadratic speed-up)
- **Shor** factoring algorithm has **both** theoretical and practical relevance

[D. Deutsch & R. Jozsa - Proc. Roy. Soc. A 439, 553 (1992)]
[L.K. Grover - Phys. Rev. Lett. 79, 325 (1997)]
[P.W. Shor - SIAM Review 41, 303 (1999)]

Requirements for universal QC

- Large ($>10^3$) collection of bits.
- Initialization (set all qubits to 0) should be possible.
- Single and two-qubits quantum operations.
- Sufficiently low error rate.
- Reliable output of the final result.

D. P. DiVincenzo, G. Burkard, D. Loss, E. V. Sukhorukov, cond-mat/9911245