Problems of Modern Physics

Lecture 1

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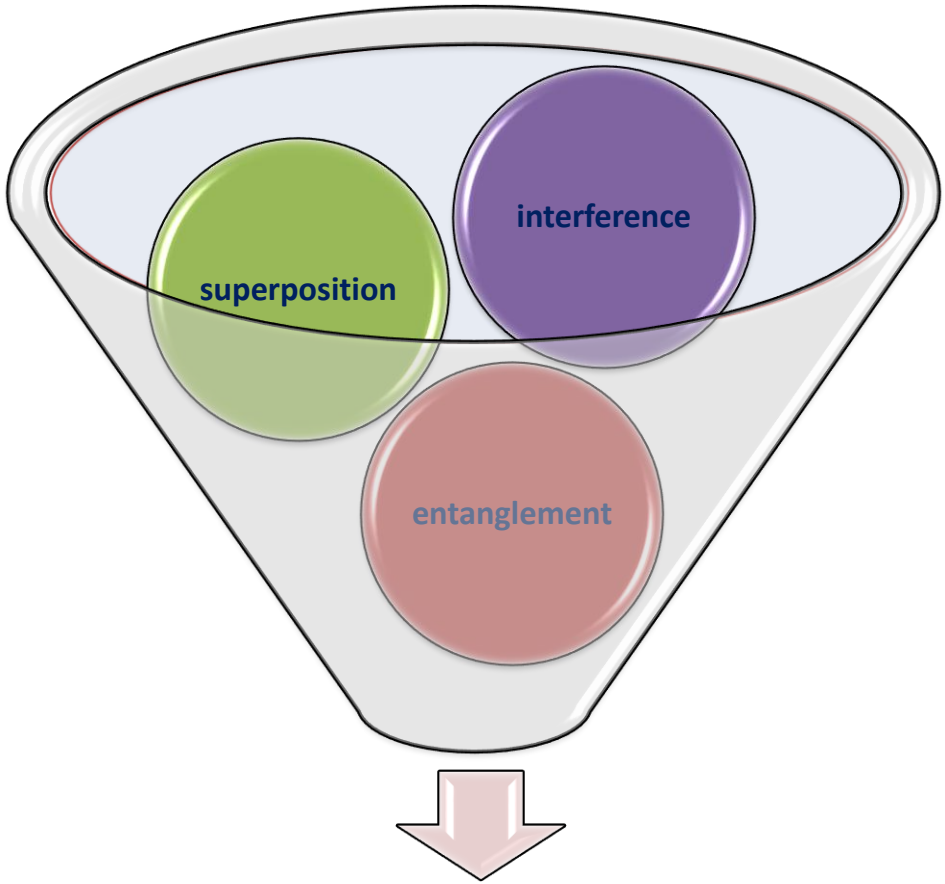
Overview

Overview

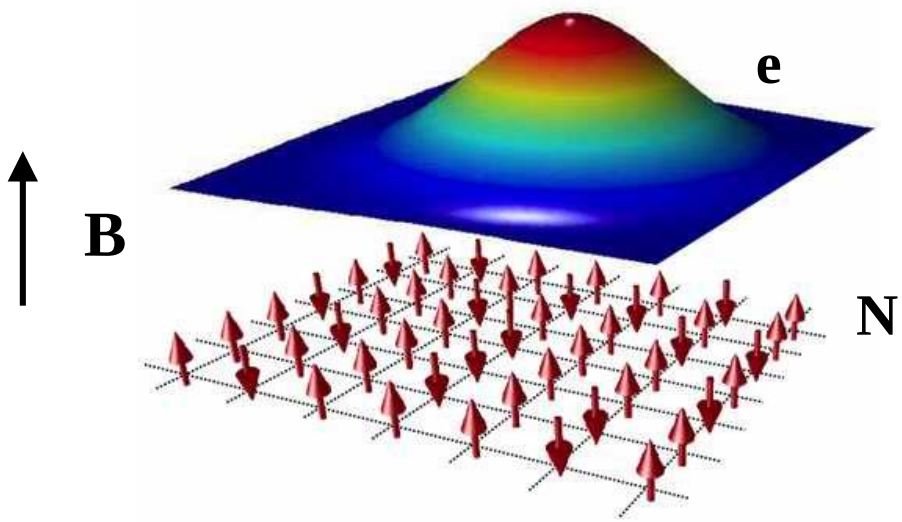
Quantum Computers

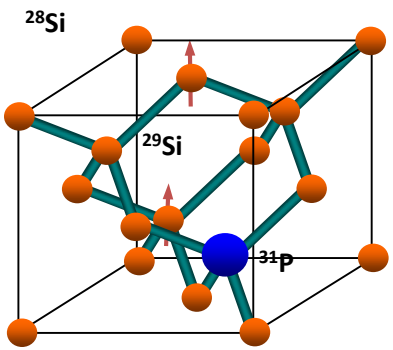


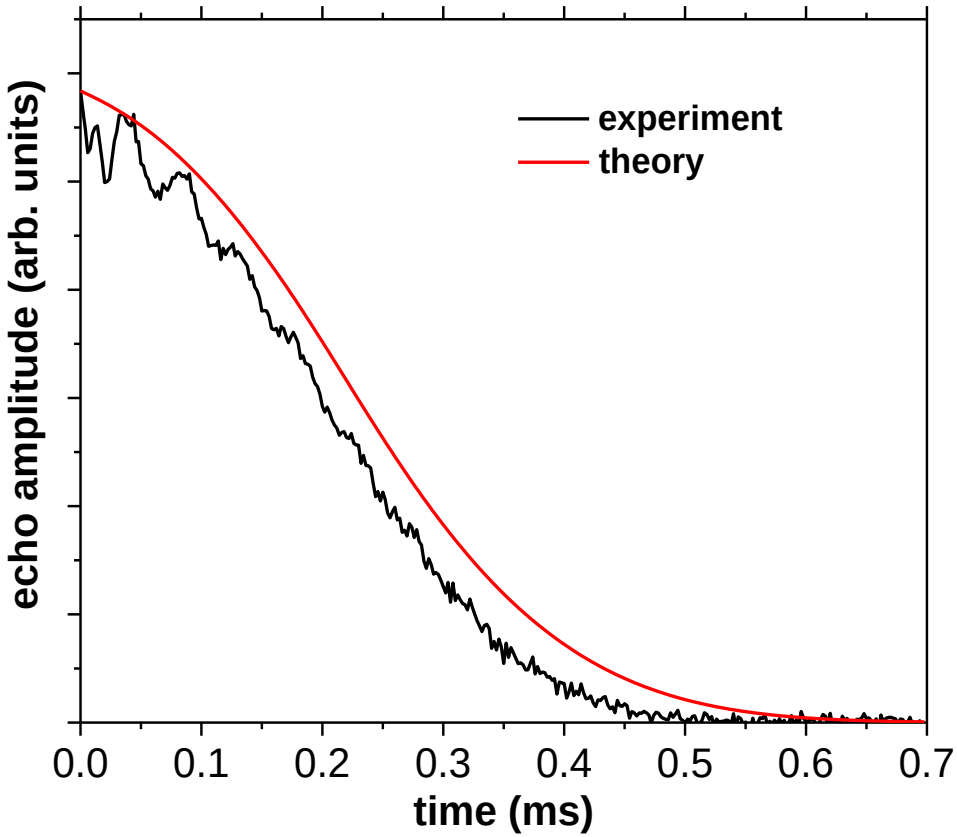
Quantum computing

Overview

Dynamics of open quantum systems



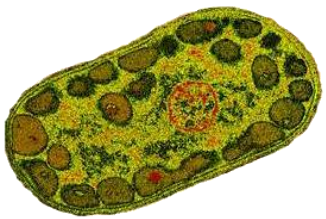




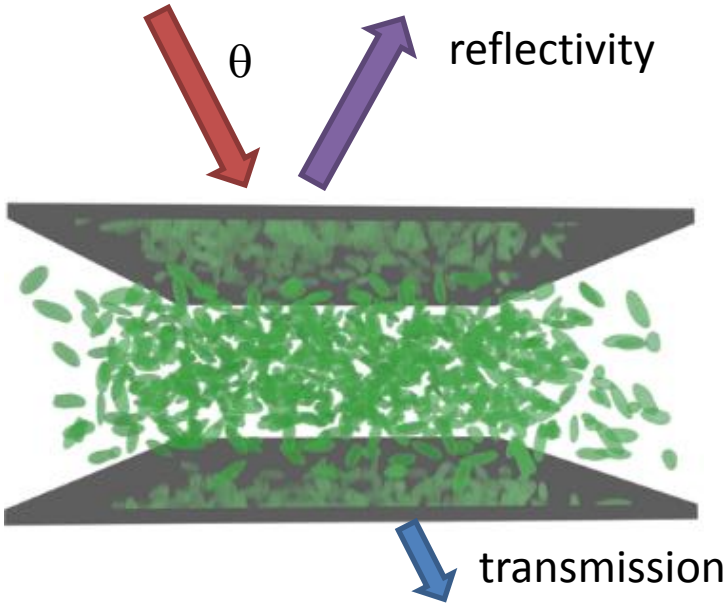
Overview

Excitonics

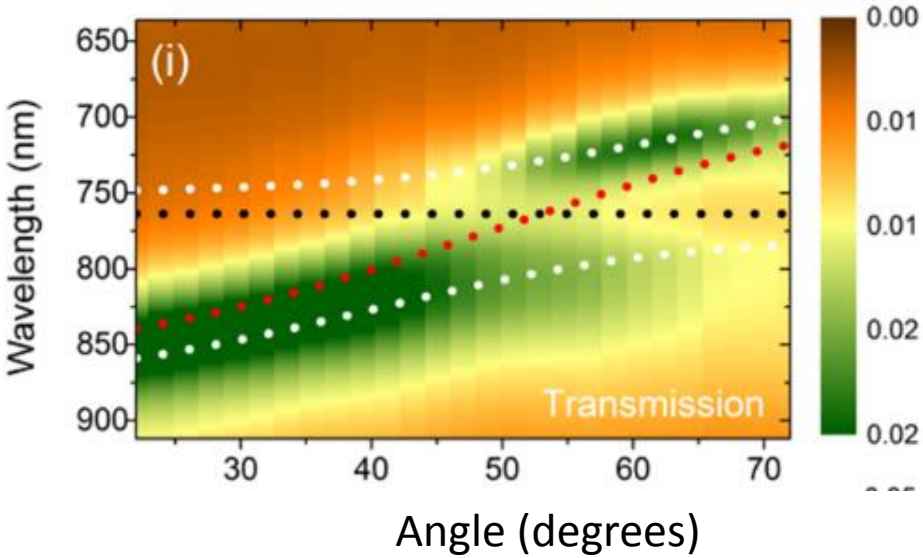
Green sulfur bacteria



Light-harvesting complexes of bacteria in a cavity



Strong coupling



Dynamics of scientific ideas

Idea as a virus

Elements of the epidemic process	Viruses	Ideas
• Agent	• Infectious material	• Idea
• Infective	• Case of disease	• Author of paper
• Susceptible	• Person	• Reader
• Removal	• Death of immunity	• Loss of interest

W. Goffman, V. A. Newill, Generalization of epidemic theory: an application to the transmission of ideas. *Nature* **204**, 225 (1964)

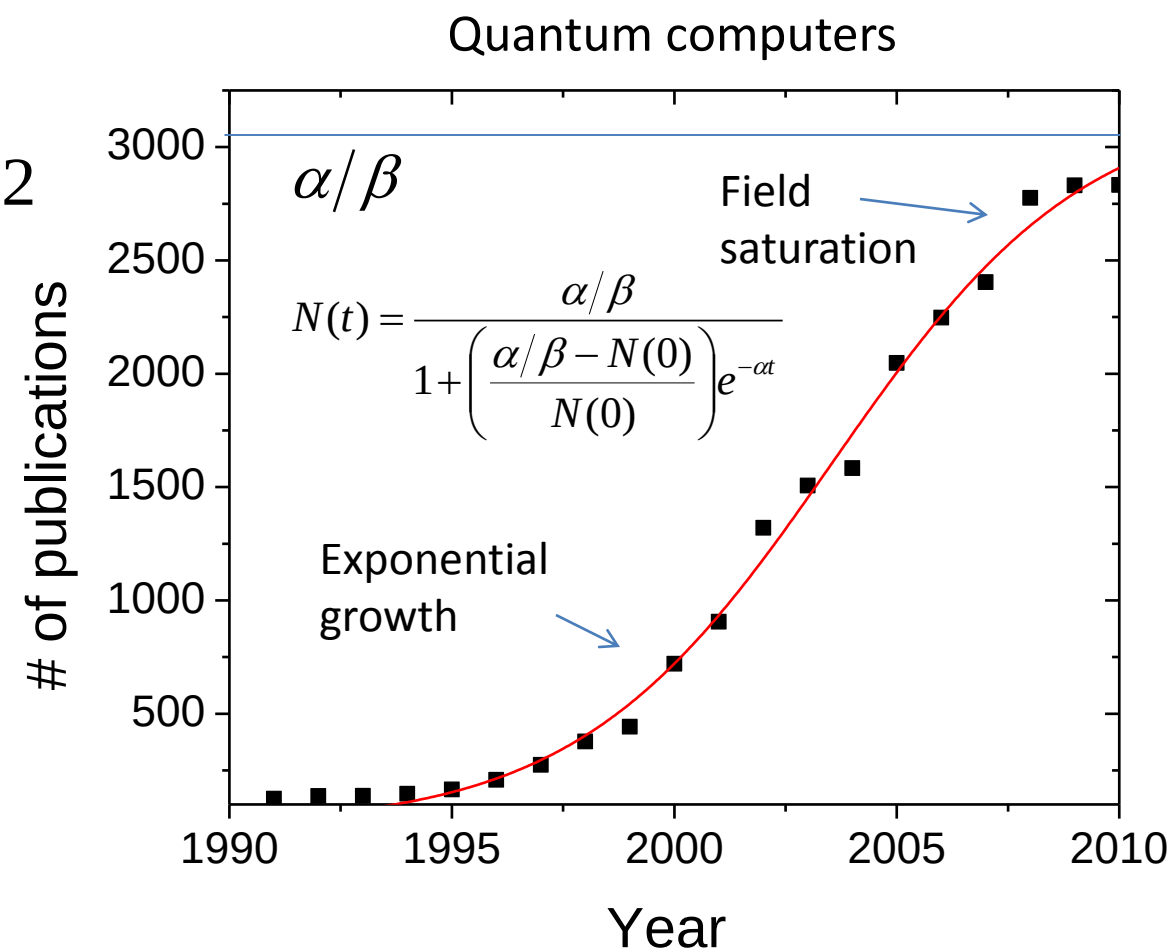
Population dynamics model

Lotka-Volterra equation

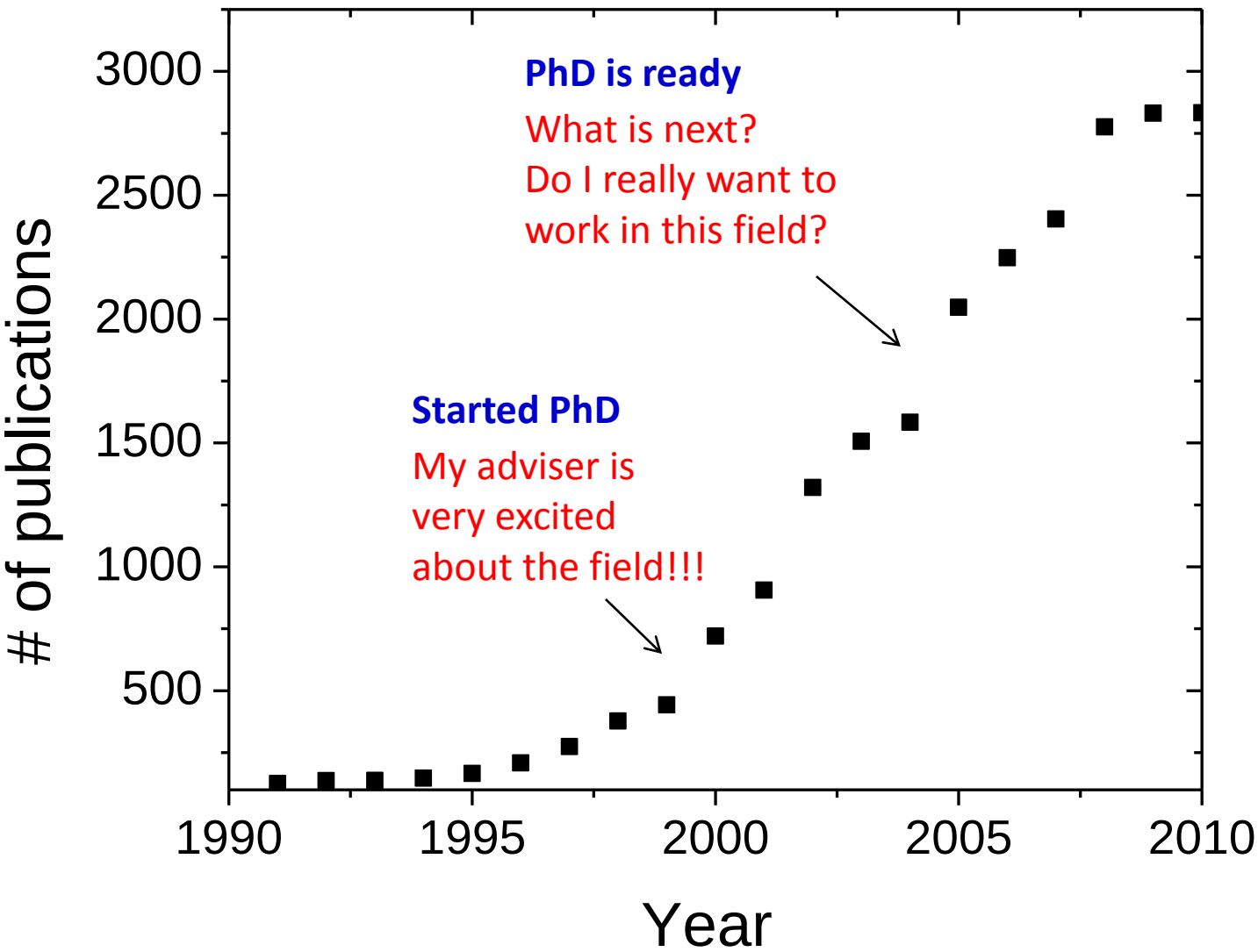
$$\frac{dp}{dt} = \alpha p - \beta p^2$$

Exponential growth

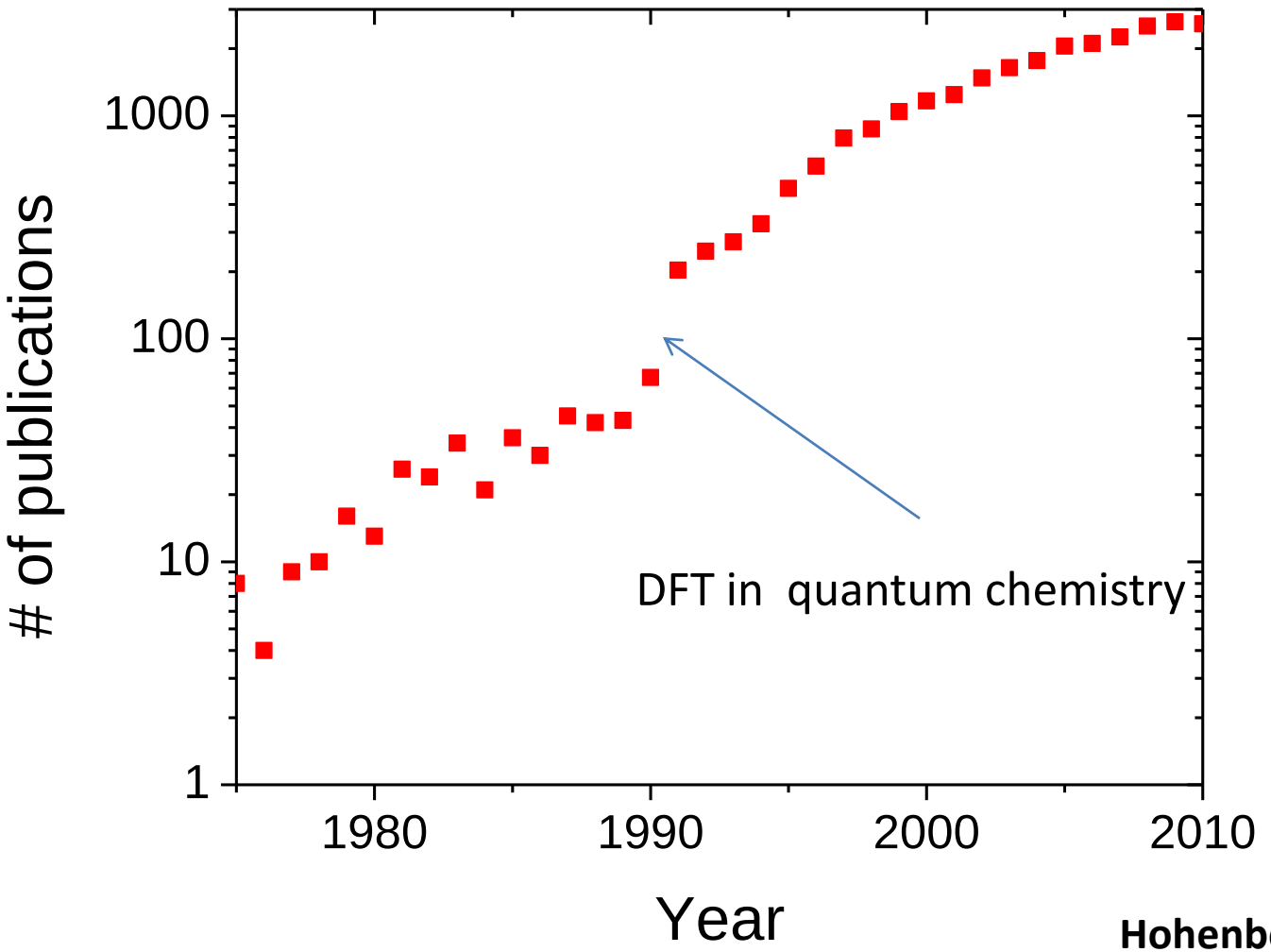
Saturation



What should I do with my PhD work?

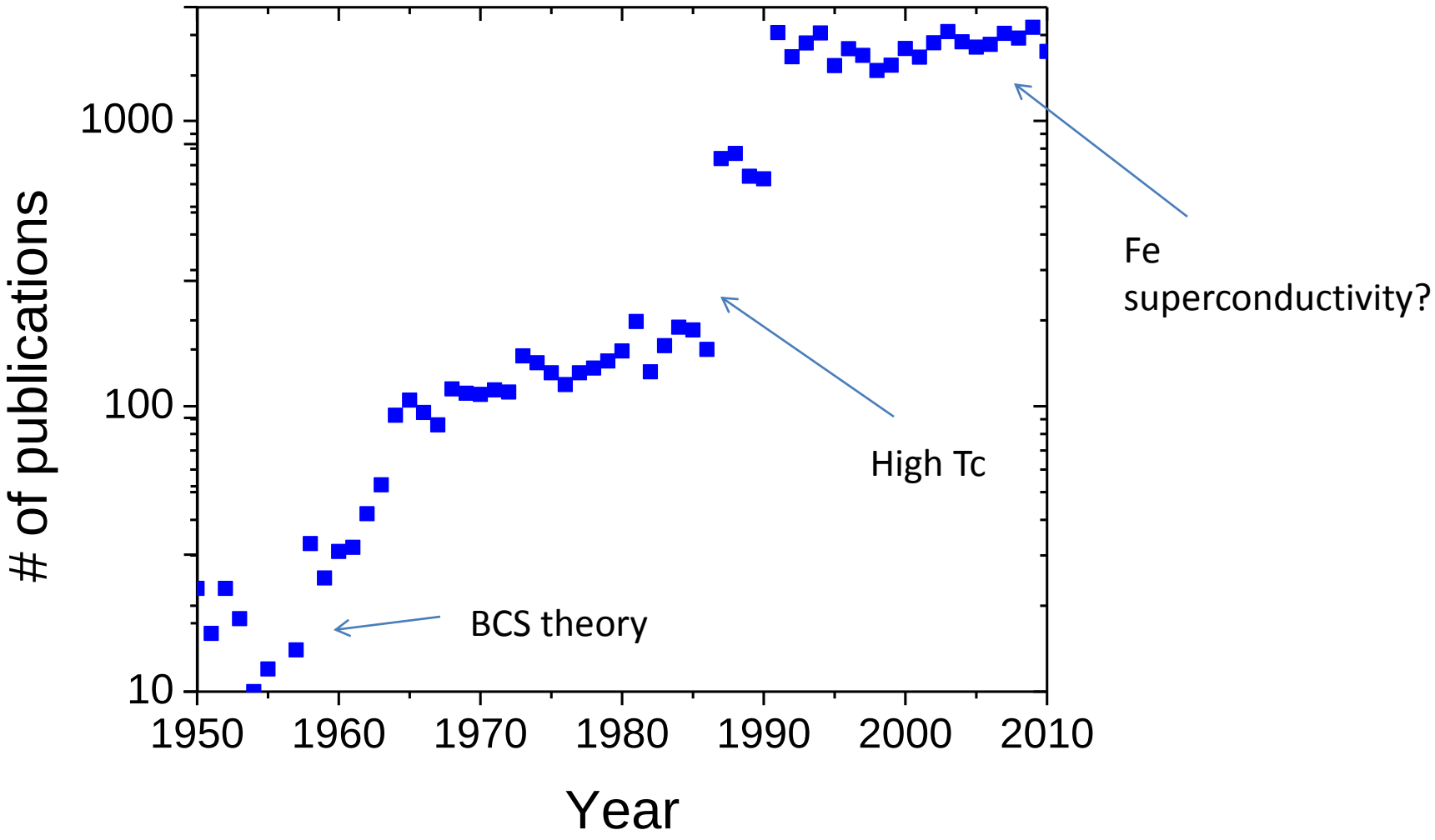


Example 1: Density functional theory



Hohenberg -Kohn theorem 1964
Kohn-Sham theorem 1965

Example 2: Superconductivity



How ideas evolve?

Mutations:

- Inclusion
- Cross mutations

Nonlocal!
Not limited to single fields

Can we predict a breakthrough?

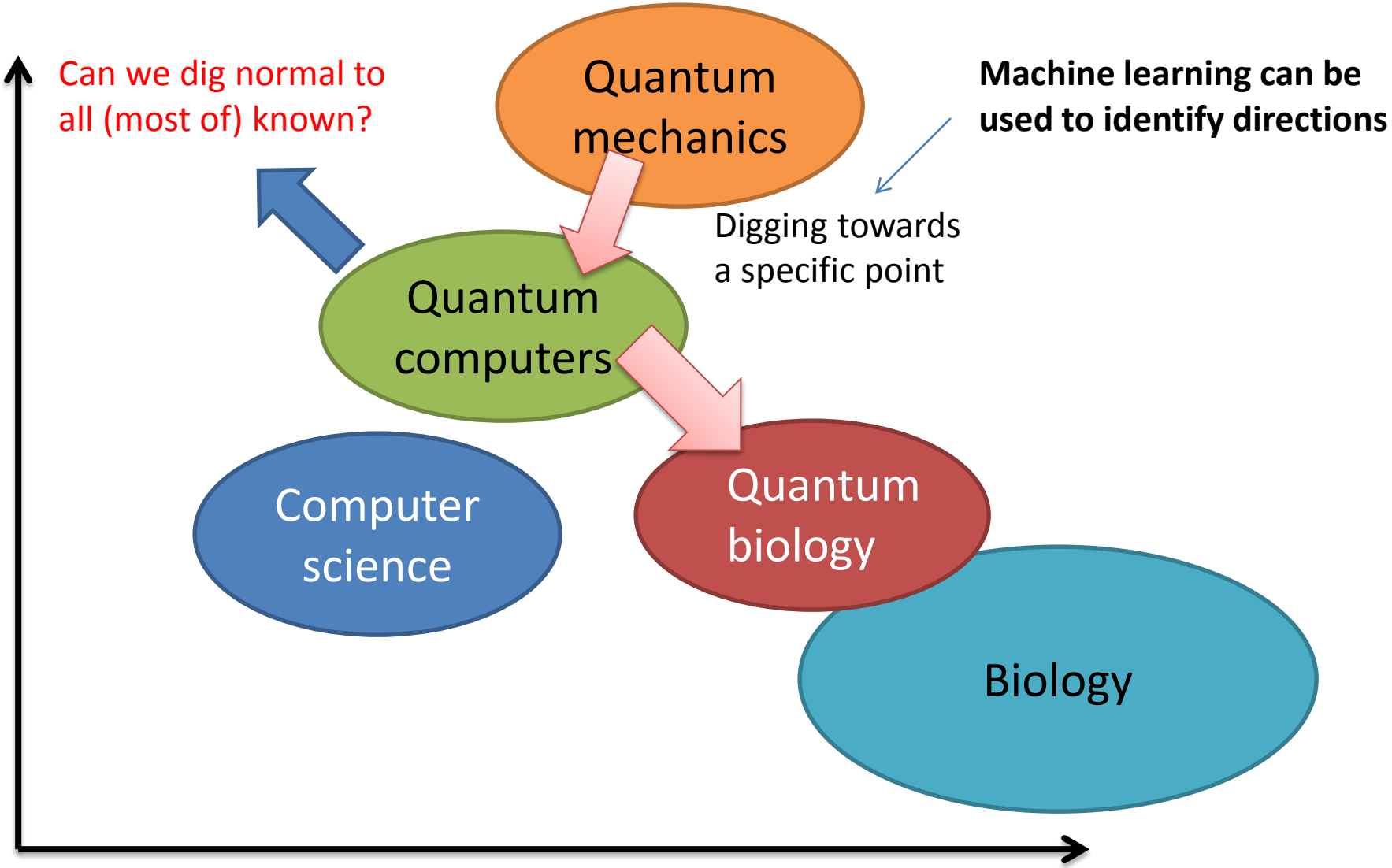
- Automatic learning of classifiers
- Noise analysis

More to read:

1. W. Goffman, G. Harmon , Nature **229**, 103 (1971)
2. M. Schmidt, H. Lipson, Science **324**, 81 (2009)

Diggers model

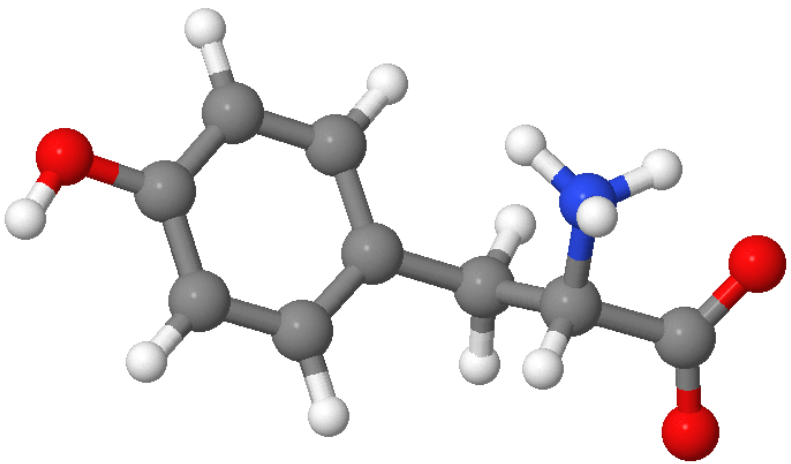
N-dimensional space of ideas (network?)



Quantum computers

Modeling of quantum systems

Tyrosine amino acid



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

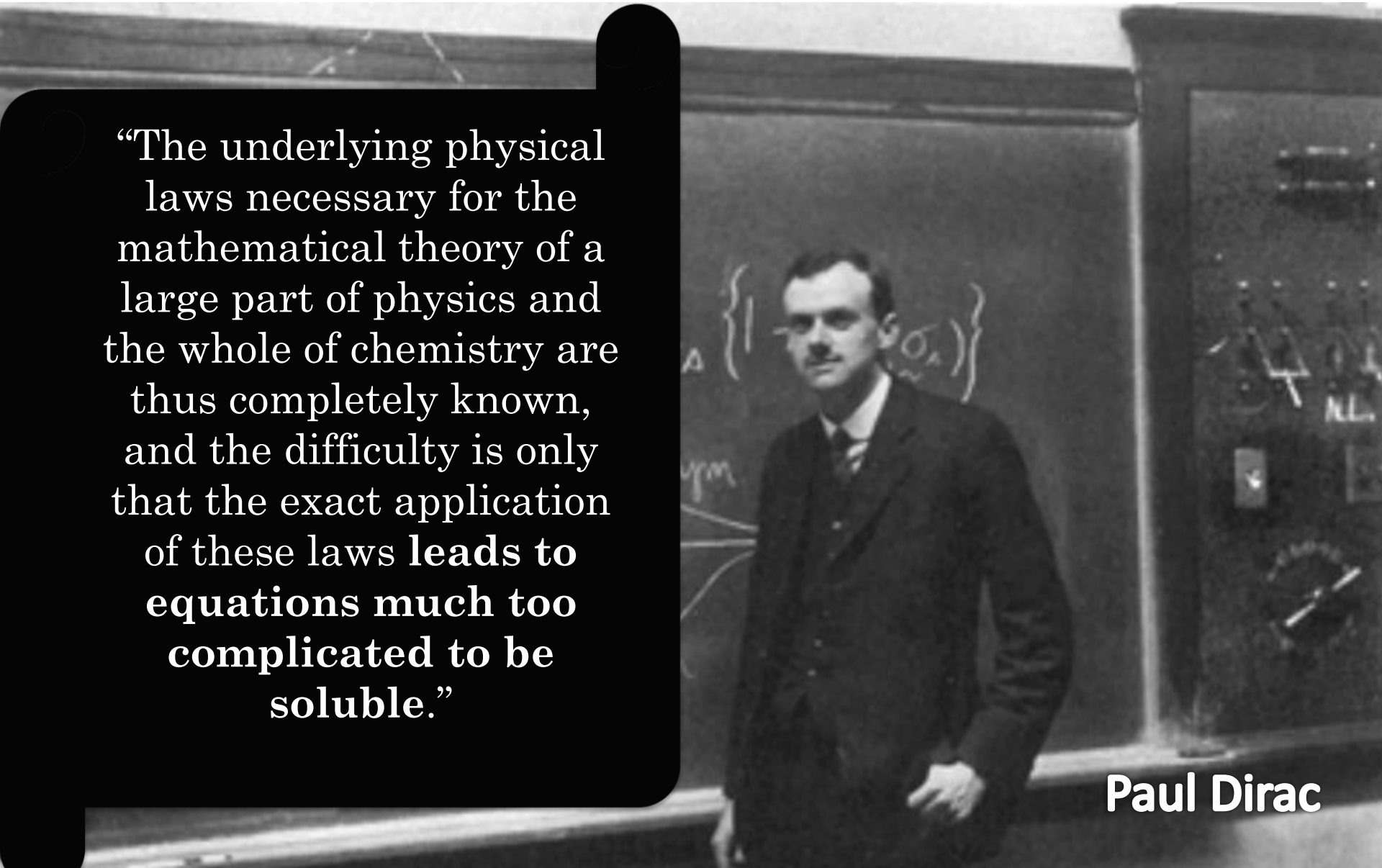
$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

1 particle – n equations:

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

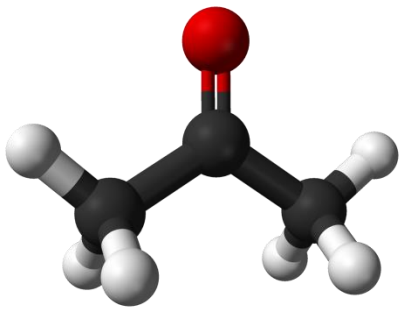
L particles – n^L equations!

Current simulation paradigm



"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.**"

Current simulation paradigm



quantum system

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

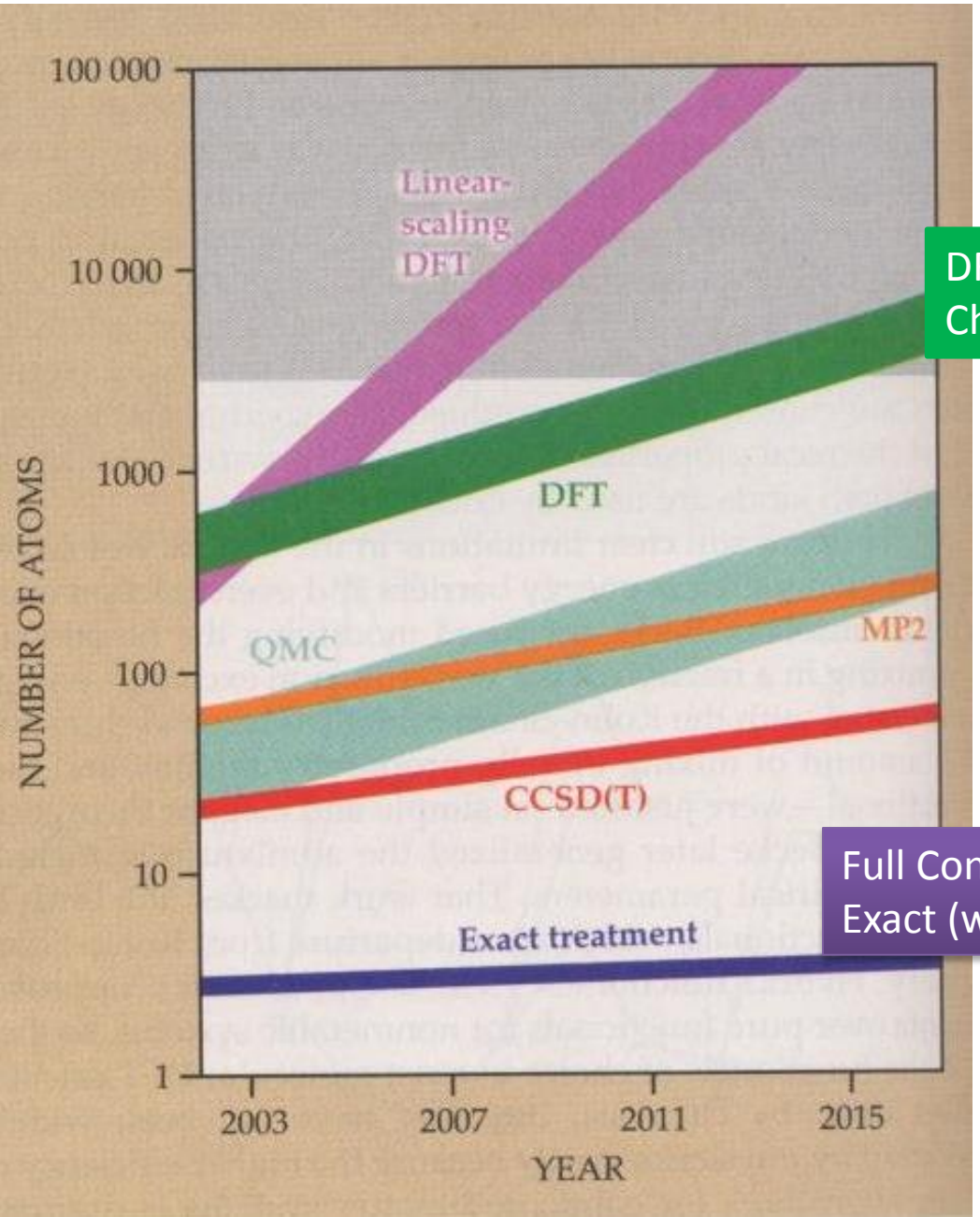
Quantum model
(quantum information)

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

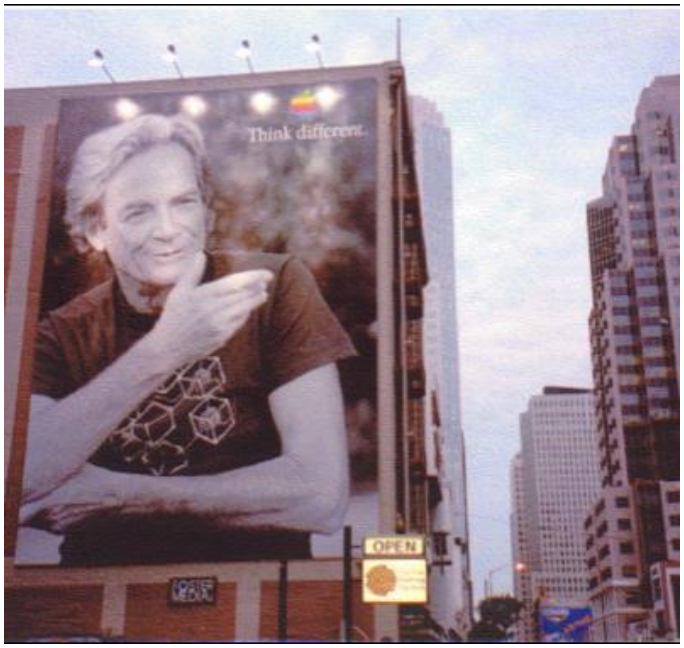
Full Configuration Interaction:
Exact (within a basis)

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

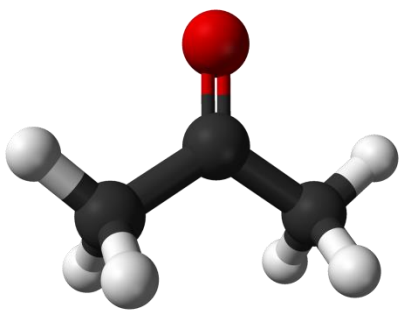


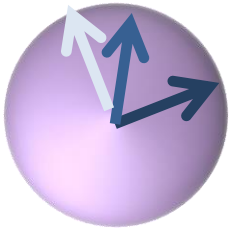
Richard Feynman, 1982

Quantum computer simulation

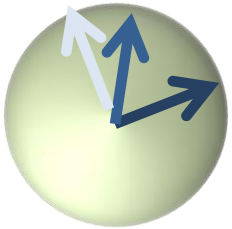
$$|\Psi^{mol}\rangle \quad \rightarrow \quad |\Psi^{QC}\rangle$$

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





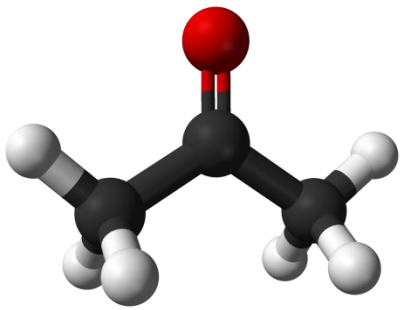
$\rightarrow$



quantum system

quantum system
(quantum information)

Quantum computing paradigm



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Quantum model
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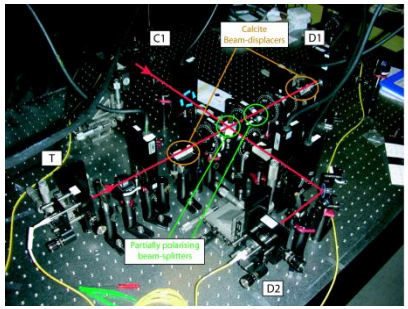
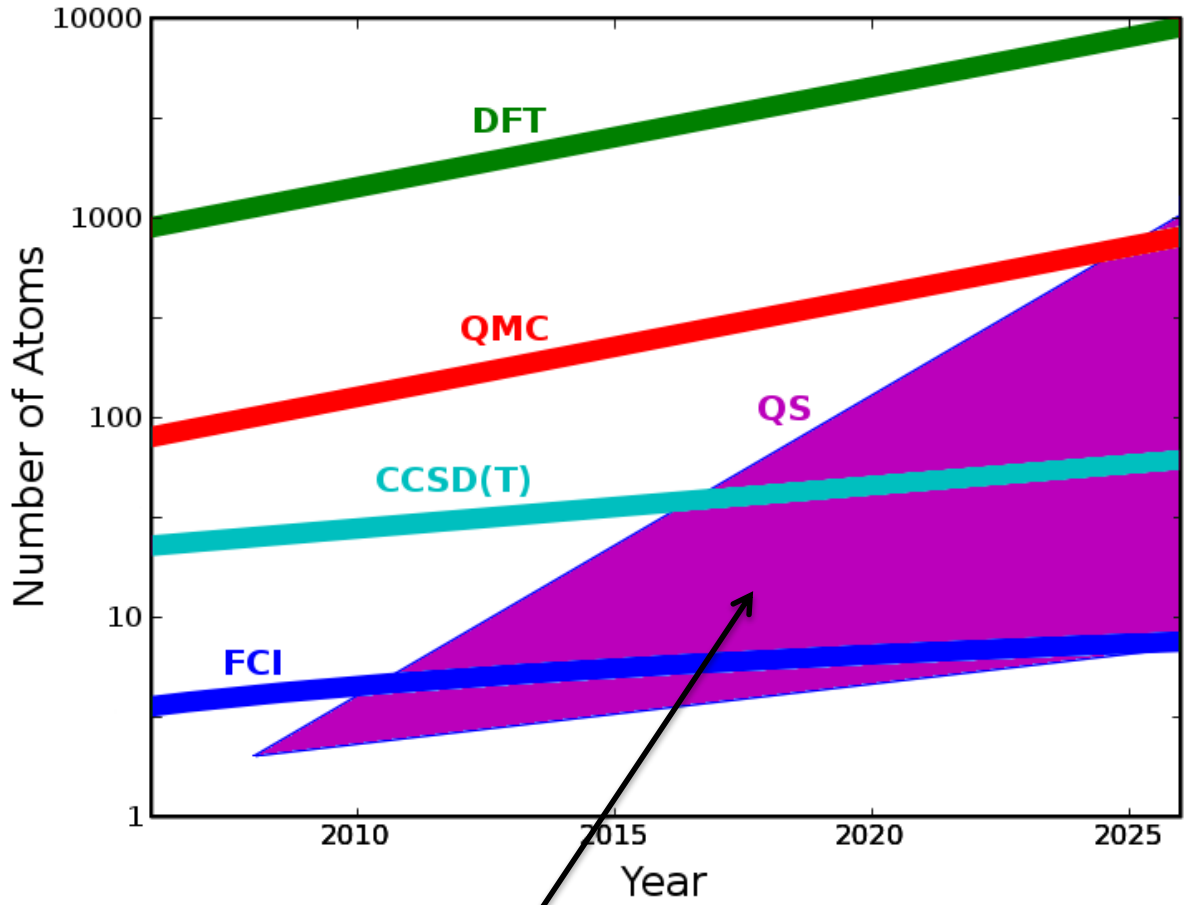


Quantum information
processor

E = -192.0492 Hartree

Classical information

Exponential speedup

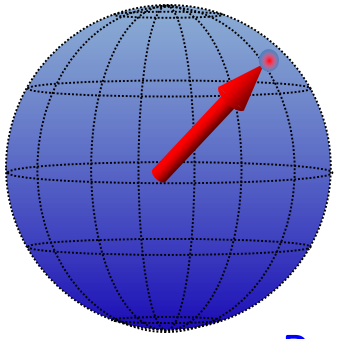


Can we achieve this?

Bits and qubits

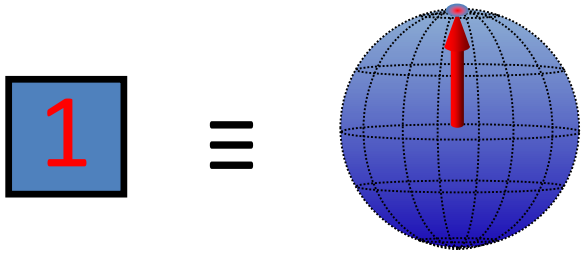
- Two states classical bit

- Two levels quantum system (qubit)

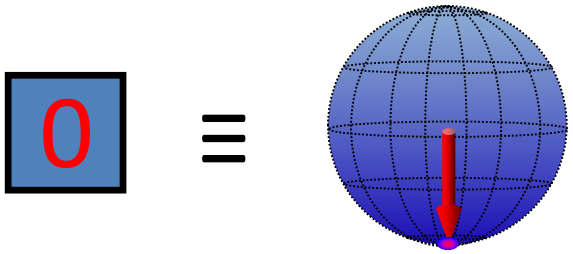


Polarization vector:

S=(S_φ S_ϑ S_R=const)



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

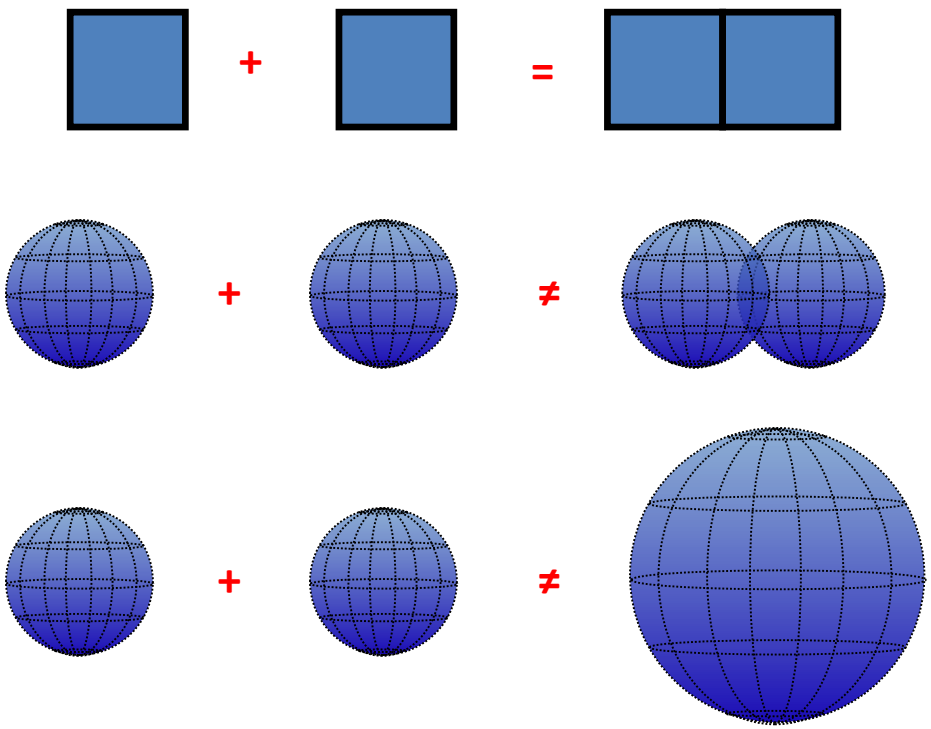


$$\equiv \quad \rho = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \Rightarrow |0\rangle$$

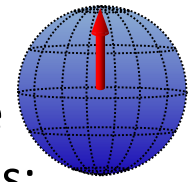
Density matrix:

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

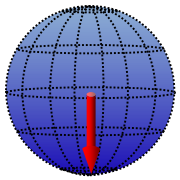
Bits and qubits



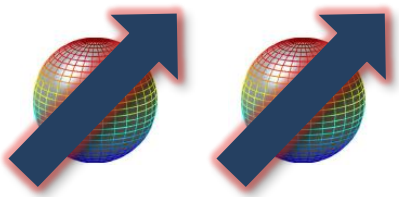
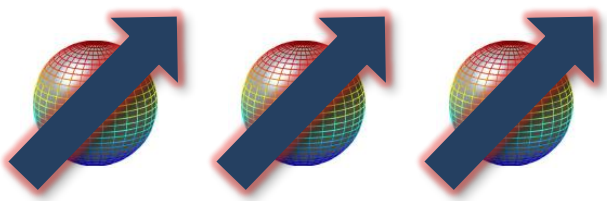
Non-separable quantum states:



$$\frac{1}{\sqrt{2}}\left(\left|0_A 1_B\right\rangle - \left|1_A 0_B\right\rangle\right) \Rightarrow \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$



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	$\alpha\|000\rangle + \beta\|001\rangle + \gamma\|010\rangle + \delta\|011\rangle +$ $\epsilon\|100\rangle + \zeta\|101\rangle + \eta\|110\rangle + \theta\|111\rangle$

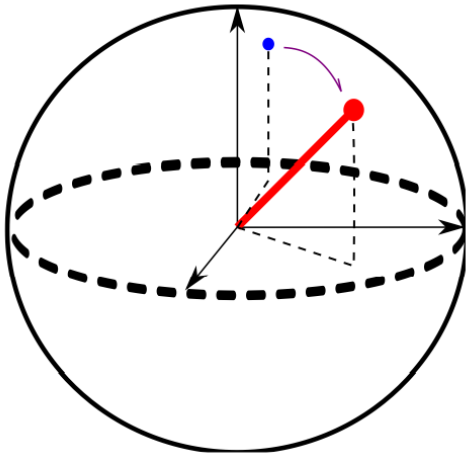
Single qubit operations

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

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

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

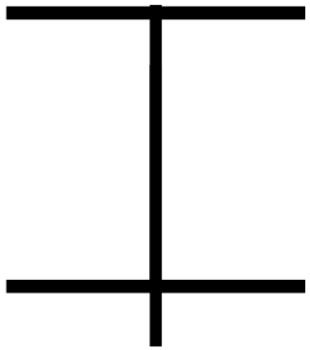
$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$



Two qubits opeations

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



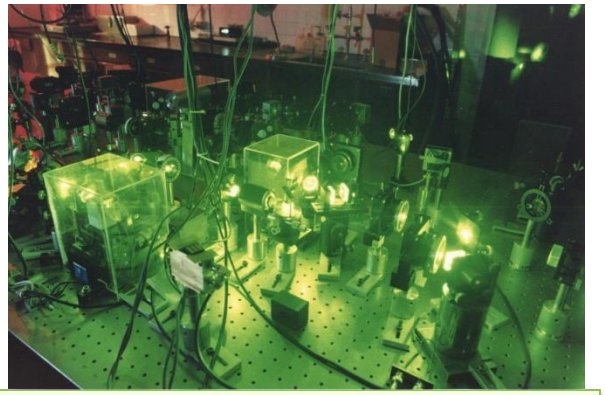
$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{cases} |00\rangle & \rightarrow & |00\rangle \\ |01\rangle & \rightarrow & |01\rangle \\ |10\rangle & \rightarrow & |11\rangle \\ |11\rangle & \rightarrow & |10\rangle \end{cases}$$

Requirements for universal QC

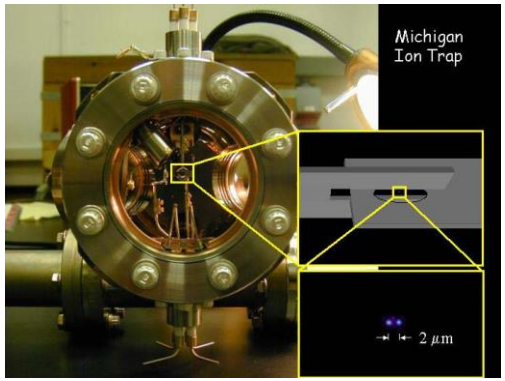
- Large ($>10^3$) collection of bits.
- Initialization (set all qubits to 0) should be possible.
- Single and two-qubits quantum operations.
- Sufficiently low error rate.
- Reliable output of the final result.

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

Hardware

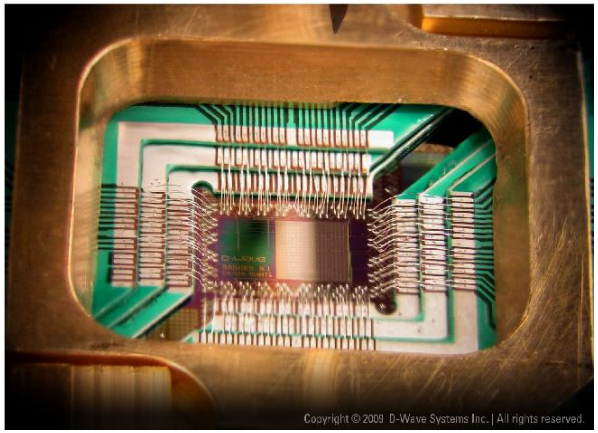


quantum optics

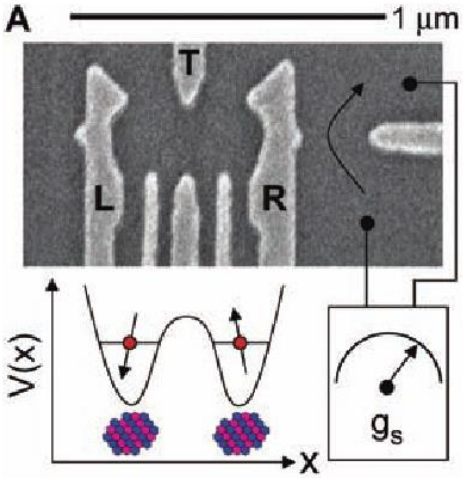


trapped ions

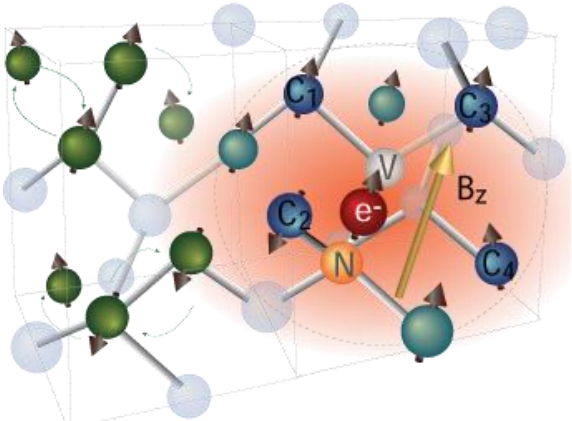
nuclear magnetic resonance



superconducting loops



semiconductor quantum dots



nitrogen vacancies in diamond