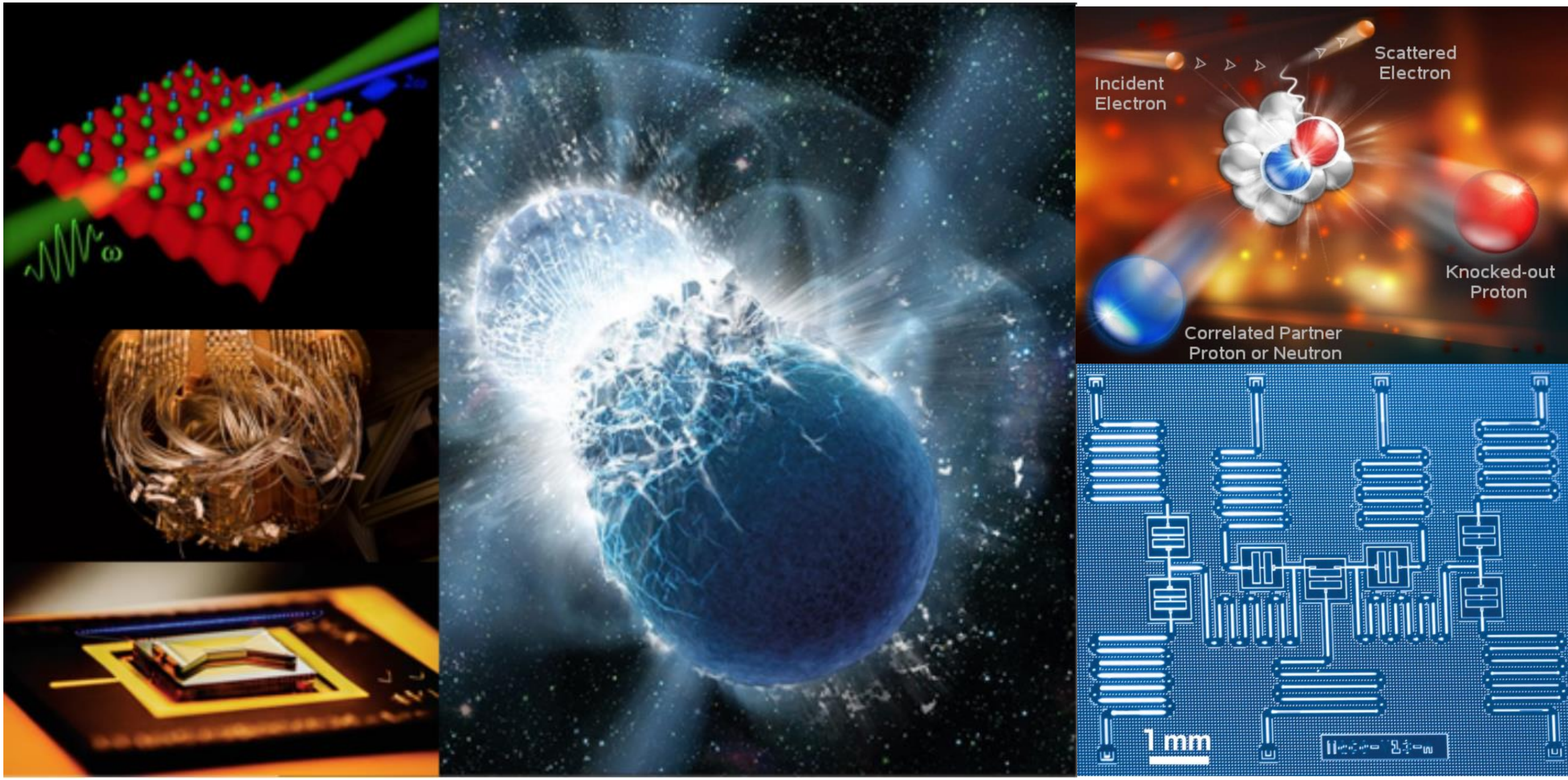


Quantum Simulation of Nuclear Scattering

Weijie Du (杜伟杰)

Iowa State University

Institute of Modern Physics, CAS

2020. 8. 7.

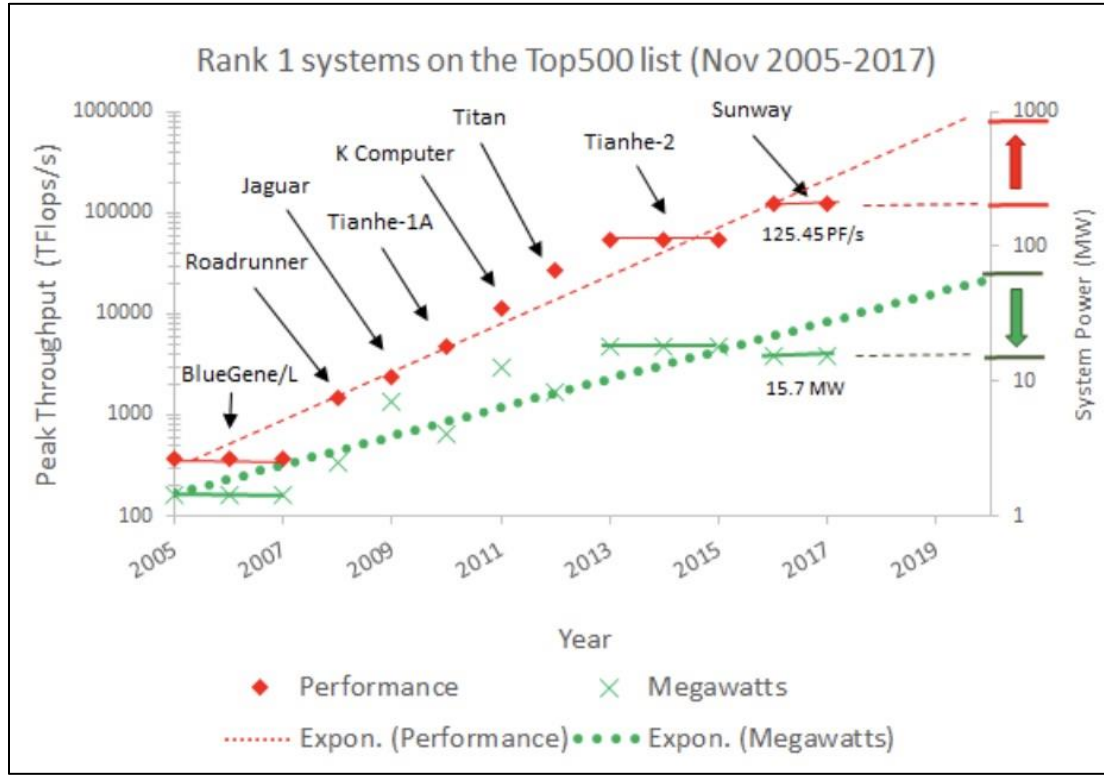
Outline

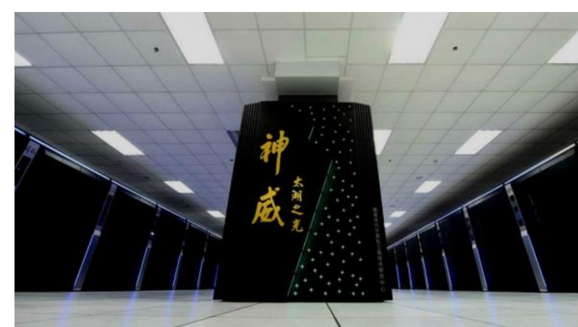
1. Background and basics
2. Time-Dependent Basis Function on Qubits (TBFQ) method
3. Future efforts and summary

Limitations of world leading supercomputing techniques

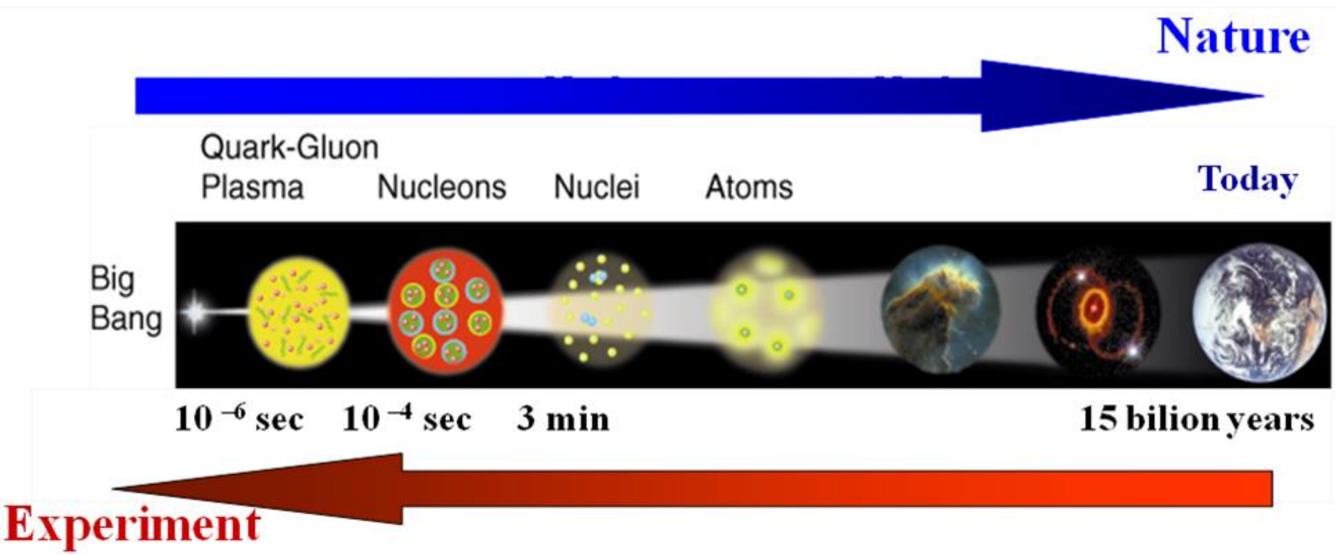
Problems:

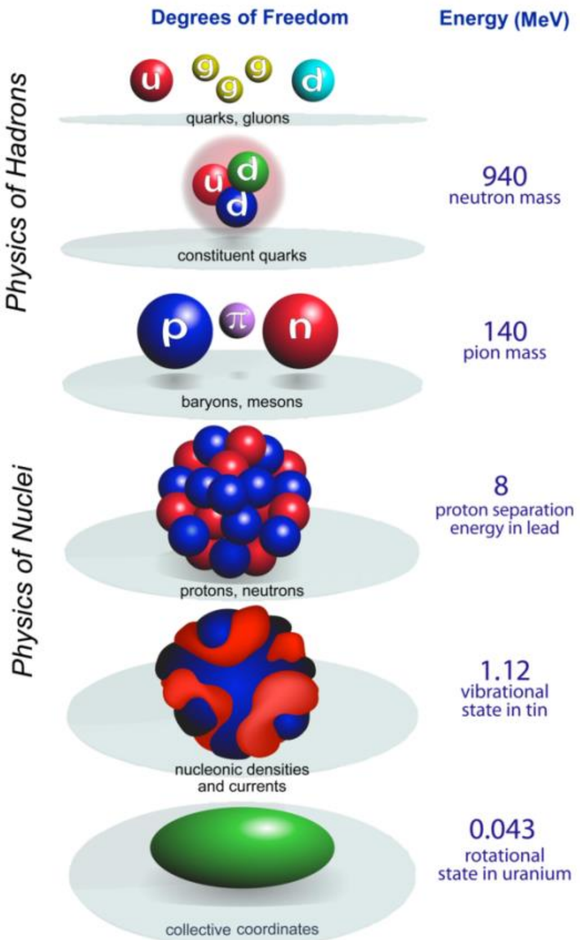
- Exascale supercomputer extremely power consuming
- Complex architecture and algorithms
- Transistor size ($\sim 8 - 10\ nm$) decreases; quantum effects manifest





Computation resources at exascale and beyond





Grand challenge: to describe nuclear physics at all scales based on the most fundamental *d.o.f.*

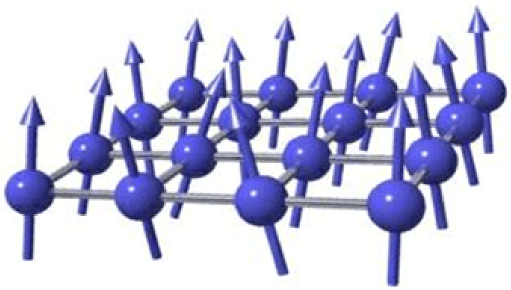
Difficulty: exponential growth in the number of states as particle number increases

A scaling problem for classical computation

Question: what is the dimension of the wave function of a spin system?

Particle number	Basis set	Dimension
1	$\{\vert\uparrow\rangle, \vert\downarrow\rangle\}$	2^1
2	$\{\vert\uparrow\uparrow\rangle, \vert\uparrow\downarrow\rangle, \vert\downarrow\uparrow\rangle, \vert\downarrow\downarrow\rangle\}$	2^2
3	$\{\vert\uparrow\uparrow\uparrow\rangle, \vert\uparrow\uparrow\downarrow\rangle, \vert\uparrow\downarrow\uparrow\rangle, \vert\uparrow\downarrow\downarrow\rangle,$ $\vert\downarrow\uparrow\uparrow\rangle, \vert\downarrow\uparrow\downarrow\rangle, \vert\downarrow\downarrow\uparrow\rangle, \vert\downarrow\downarrow\downarrow\rangle\}$	2^3
⋮	⋮	⋮
N	⋯	2^N

- Laptop: 40-particle system ($\sim 2^{40}$ bytes)
- 100-particle system **beyond** the capability of largest supercomputer nowadays ($< 2^{100}$ bytes) !



Seminal idea: let's make the computation fully quantum mechanical

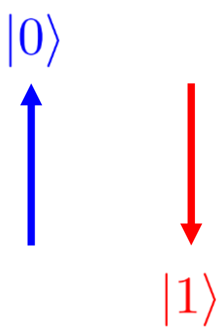
[Int. J. Theor. Phys. Vol. 21, pp. 467-488, (1982)]

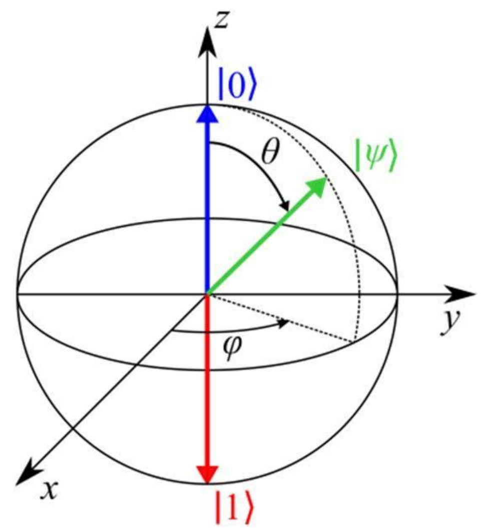
"I'm not happy with all the analyses that go with the classical theory, because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy." --- R. P. Feynman's vision in 1982

From classical to quantum mechanical

Classical bit	Quantum bit (qubit)
$\|0\rangle$ or $\|1\rangle$	$\|\psi\rangle = \alpha\|0\rangle + \beta\|1\rangle$
2 states	infinite number of states

transistor ON or OFF

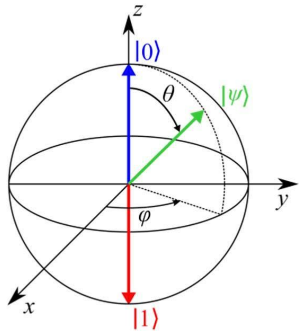




The principles of quantum computing

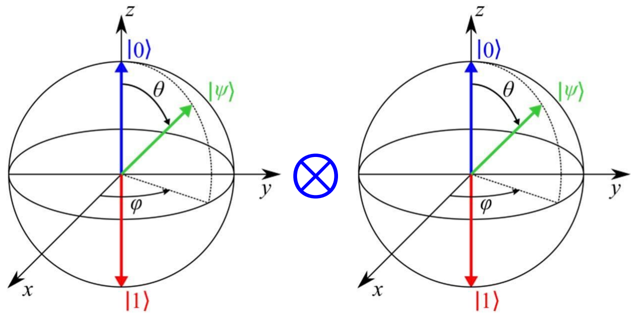
Superposition, e.g.,

$$|\psi\rangle \quad = \quad \alpha|0\rangle + \beta|1\rangle$$



Entanglement, e.g.,

$$|\psi\rangle \quad = \quad \frac{|1\rangle_1|0\rangle_2 + |0\rangle_1|1\rangle_2}{\sqrt{2}}$$

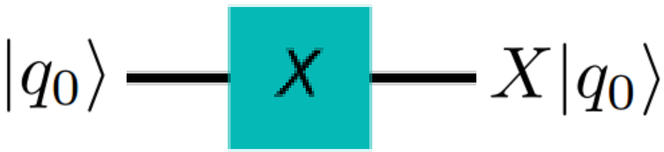


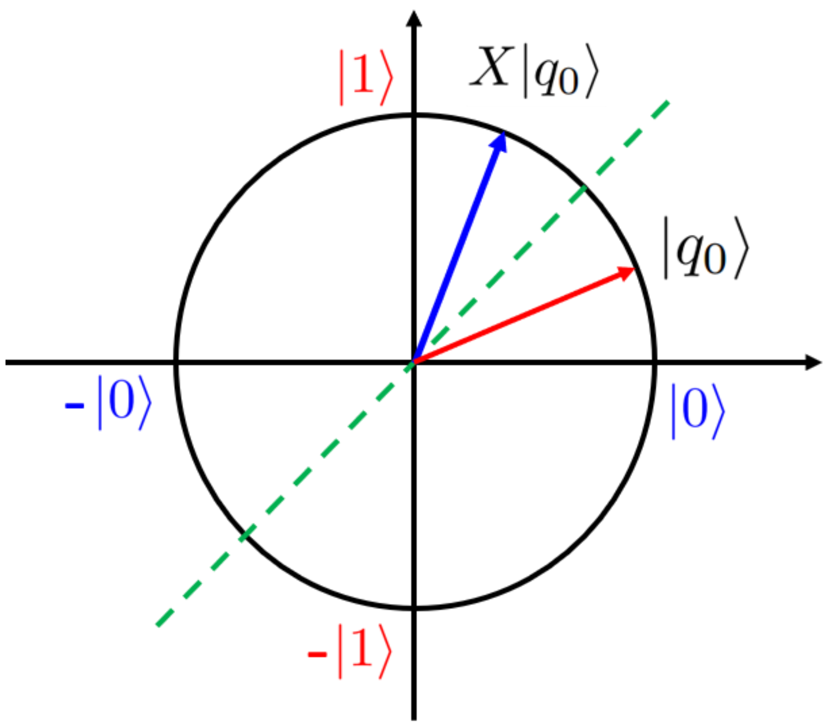
Fundamental change

- computation methodology and algorithm
- information storage and manipulation

Operating a qubit (illustration)

Quantum operation





Matrix interpretation

$$\mathbf{X}\,|0\rangle = |1\rangle\,,\ \mathbf{X}\,|1\rangle = |0\rangle$$

$$\mathbf{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

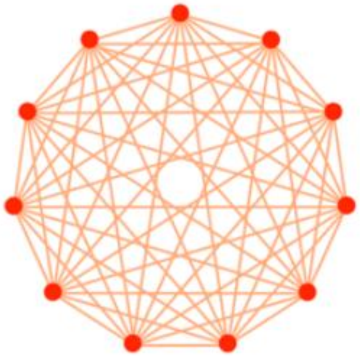
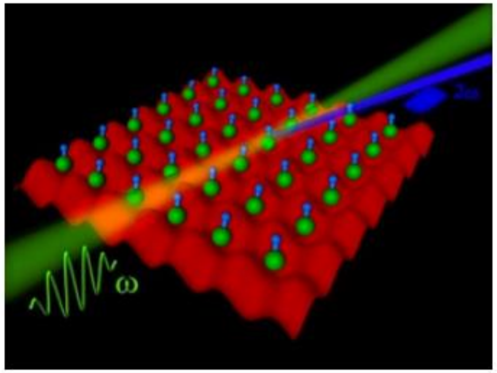
$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \beta \\ \alpha \end{bmatrix}$$

$$|q_0\rangle = \alpha|0\rangle + \beta|1\rangle$$
$$X|q_0\rangle = \alpha|1\rangle + \beta|0\rangle$$

Various other operations, e.g., the phase gate, the Hadamard gate etc.

Quantum computers

- Quantum computers make use of quantum systems to perform calculations
- Such quantum systems need to be well controlled and sufficiently isolated from the environment
- Quantum computers can potentially circumvent the roadblock of exponential cost in computational science

Hemmerling, Cornel, https://www.photonics.com/Article.aspx?AID=64150

Quantum leap in computation power

Factorization into two prime numbers

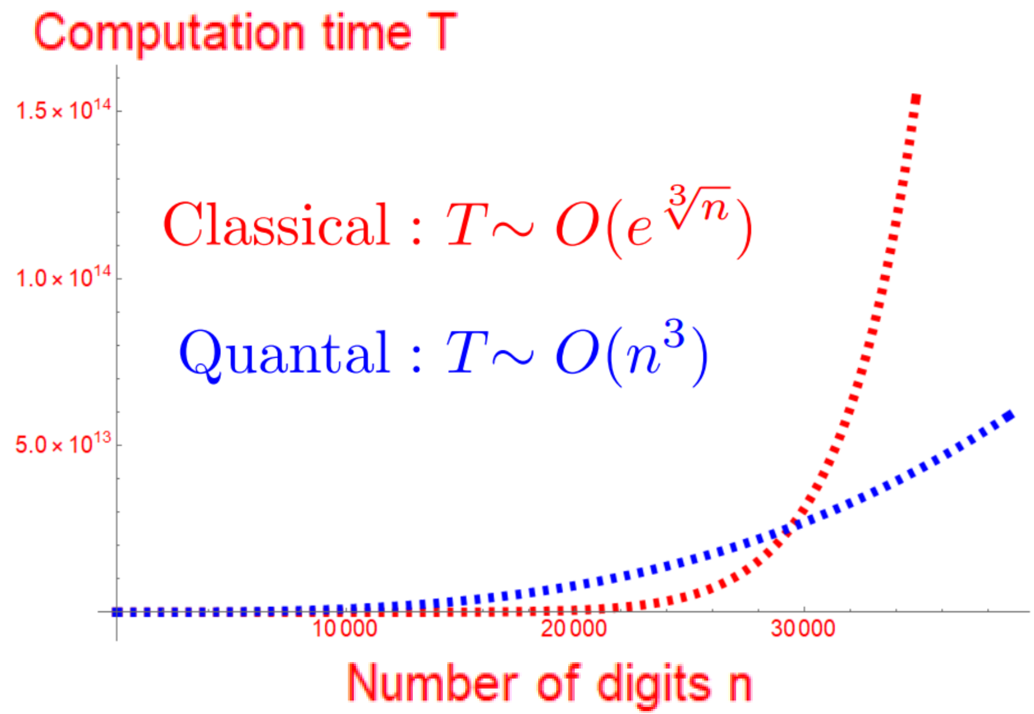
rsa_250=2140324650240744961264423072839333563008614715144755017797754920881418023447140136643345519095804679610992851872470914587687396261921557363047454770520805119056493106687691590019759405693457452230589325976697471681738069364894699871578494975937497937

$= p \times q$

Need 2700 core-years!

p=64135289477071580278790190170577389084825014742943447208116859632024532344630238623598752668347708737661925585694639798853367

q=33372027594978156556226010605355114227940760344767554666784520987023841729210037080257448673296881877565718986258036932062711



[https://lists.gforge.inria.fr/pipermail/cado-nfs-discuss/2020-February/001166.html]

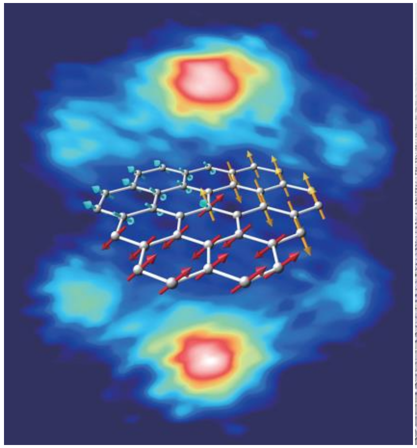
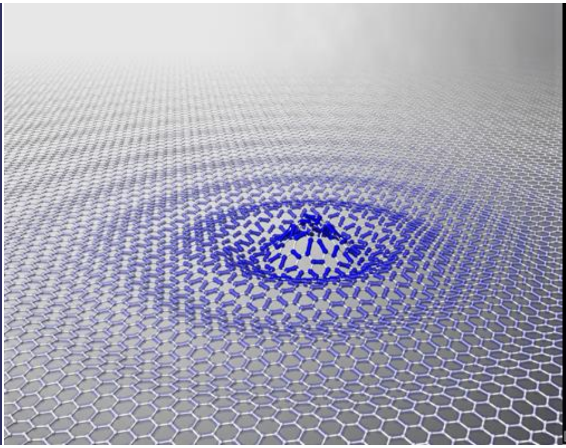
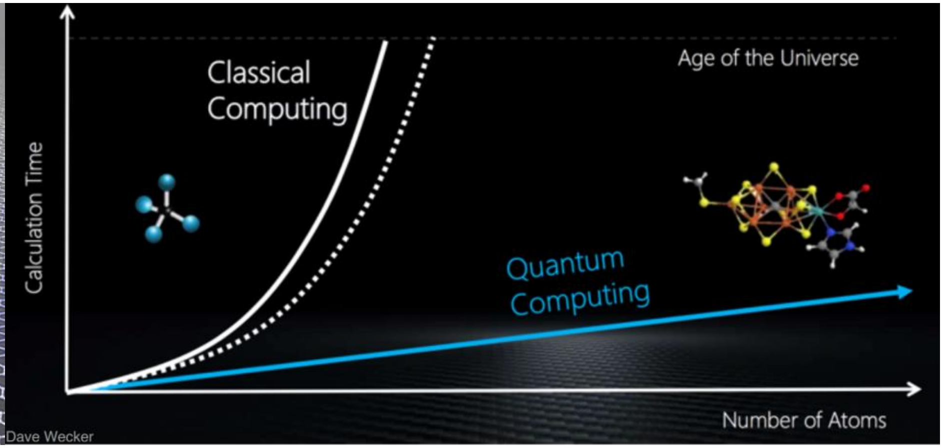
Natural way of processing quantum information

Expressing a quantum state of N-particle system

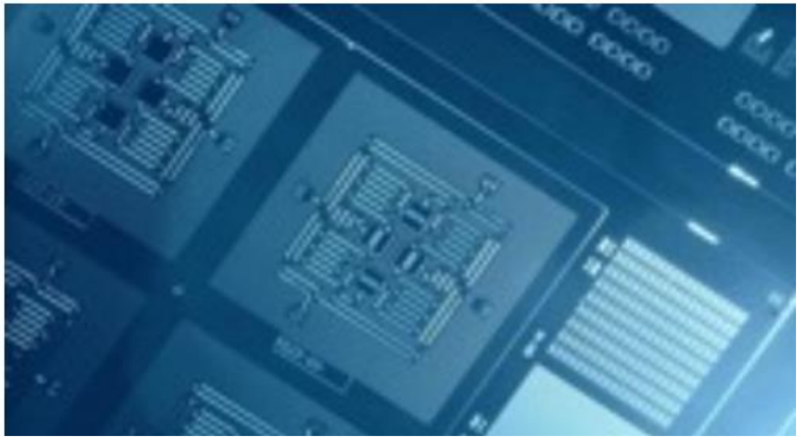
- Classical computer: intractable as N increases (exponential)
- Quantum computer: $\sim N$ qubits

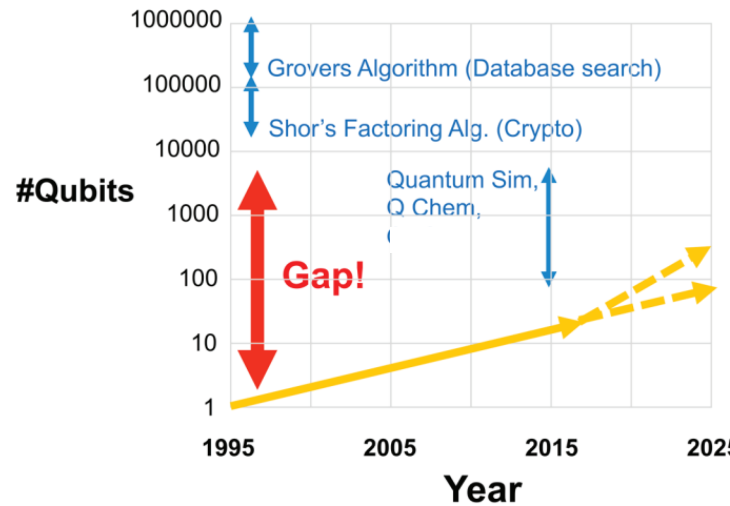
$$|\Psi\rangle = (\alpha_1|\uparrow\rangle_1 + \beta_1|\downarrow\rangle_1) \otimes (\alpha_2|\uparrow\rangle_2 + \beta_2|\downarrow\rangle_2) \cdots \otimes (\alpha_N|\uparrow\rangle_N + \beta_N|\downarrow\rangle_N)$$

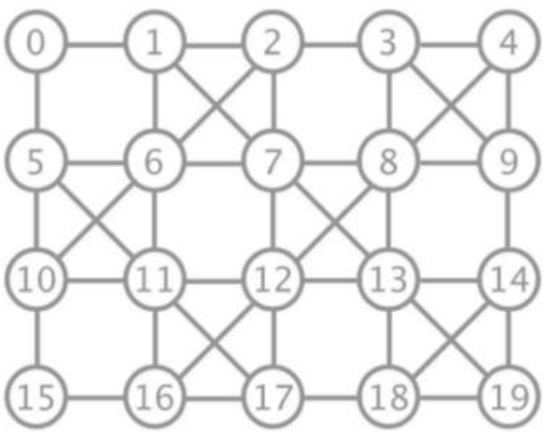
Quantum computer: natural way to express and manipulate quantum states

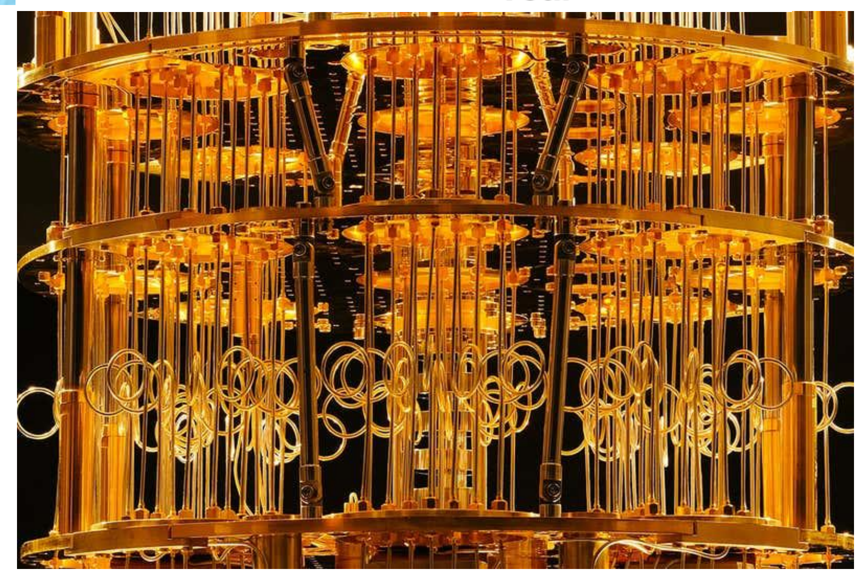




Hardware development









Hardware improvement/innovations

- joint tasks for scientists from many areas

Challenges: decoherence time, precise control/readout, scalability with error corrections

Circuit-based quantum processors [edit]

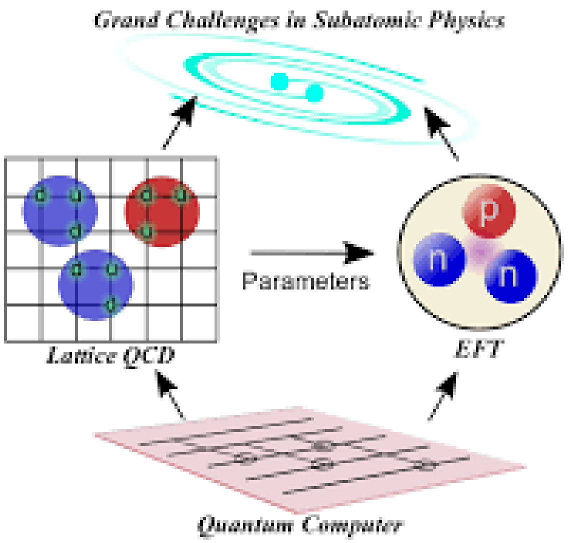
[Wikipedia]

These QPUs are based on the quantum circuit and quantum logic gate-based model of computing.

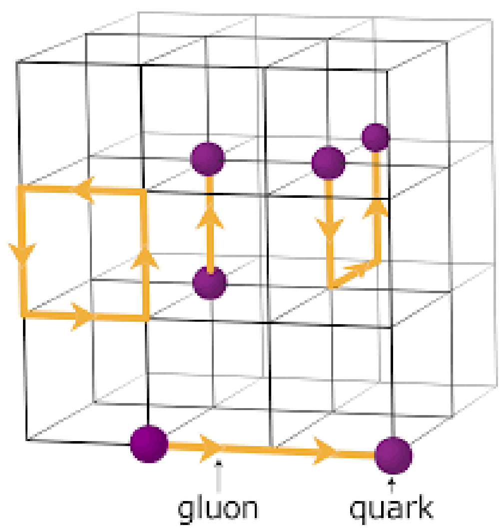
Manufacturer	Name/Codename/Designation	Architecture	Layout	Socket	Fidelity	Qubits	Release date
Google	N/A	Superconducting	N/A	N/A	99.5%[1]	20 qb	2017
Google	N/A	Superconducting	7×7 lattice	N/A	99.7%[1]	49 qb[2]	Q4 2017 (planned)
Google	Bristlecone	Superconducting	6×12 lattice	N/A	99% (readout) 99.9% (1 qubit) 99.4% (2 qubits)	72 qb[3][4]	5 March 2018
Google	Sycamore	Nonlinear superconducting resonator	N/A	N/A	N/A	54 transmon qb 53 qb effective	2019
IBM	IBM Q 5 Tenerife	Superconducting	bow tie	N/A	99.897% (average gate) 98.64% (readout)	5 qb	2016[1]
IBM	IBM Q 5 Yorktown	Superconducting	bow tie	N/A	99.545% (average gate) 94.2% (readout)	5 qb	
IBM	IBM Q 14 Melbourne	Superconducting	N/A	N/A	99.735% (average gate) 97.13% (readout)	14 qb	
IBM	IBM Q 16 Rüschlikon	Superconducting	2×8 lattice	N/A	99.779% (average gate) 94.24% (readout)	16 qb[5]	17 May 2017 (Retired: 26 September 2018)[6]
IBM	IBM Q 17	Superconducting	N/A	N/A	N/A	17 qb[5]	17 May 2017
IBM	IBM Q 20 Tokyo	Superconducting	5x4 lattice	N/A	99.812% (average gate) 93.21% (readout)	20 qb[7]	10 November 2017
IBM	IBM Q 20 Austin	Superconducting	5x4 lattice	N/A	N/A	20 qb	(Retired: 4 July 2018)[6]
IBM	IBM Q 50 prototype	Superconducting	N/A	N/A	N/A	50 qb[7]	
IBM	IBM Q 53	Superconducting	N/A	N/A	N/A	53 qb	October 2019
Intel	17-Qubit Superconducting Test Chip	Superconducting	N/A	40-pin cross gap	N/A	17 qb[8][9]	10 October 2017
Intel	Tangle Lake	Superconducting	N/A	108-pin cross gap	N/A	49 qb [10]	9 January 2018
Rigetti	8Q Agave	Superconducting	N/A	N/A	N/A	8 qb	4 June 2018[11]
Rigetti	16Q Aspen-1	Superconducting	N/A	N/A	N/A	16 qb	30 November 2018[11]
Rigetti	19Q Acorn	Superconducting	N/A	N/A	N/A	19 qb[12]	17 December 2017
IBM	IBM Armonk[13]	Superconducting	Single Qubit	N/A	N/A	1 qb	16 October 2019
IBM	IBM Ourense[13]	Superconducting	T	N/A	N/A	5 qb	03 July 2019
IBM	IBM Vigo[13]	Superconducting	T	N/A	N/A	5 qb	03 July 2019
IBM	IBM London[13]	Superconducting	T	N/A	N/A	5 qb	13 September 2019
IBM	IBM Burlington[13]	Superconducting	T	N/A	N/A	5 qb	13 September 2019
IBM	IBM Essex[13]	Superconducting	T	N/A	N/A	5 qb	13 September 2019

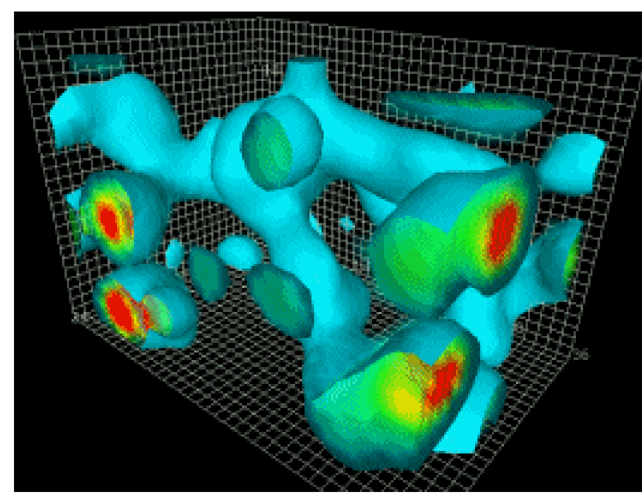
The Noisy Intermediate-Scale Quantum era is arriving!

Requests for quantum algorithms in nuclear physics



Rapidly developing quantum hardware **boosts/requests** inventions/discoveries of new quantum algorithms.



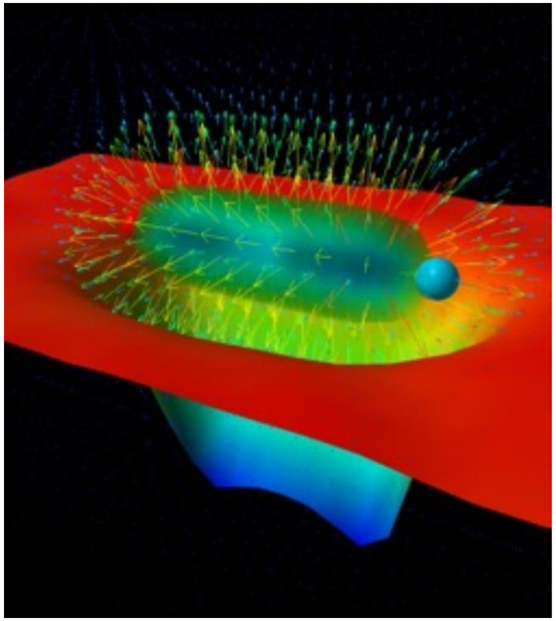


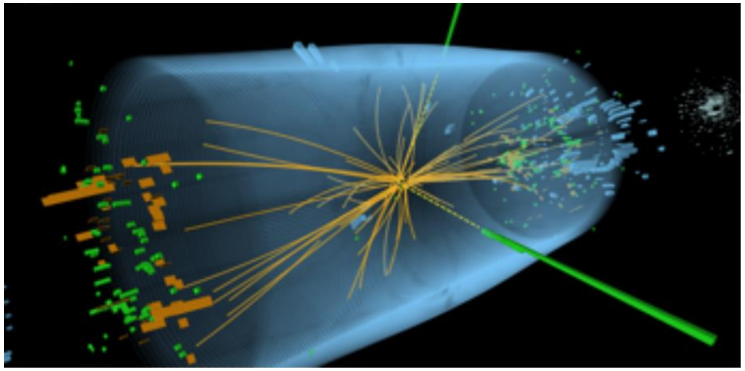
Interesting problem set:

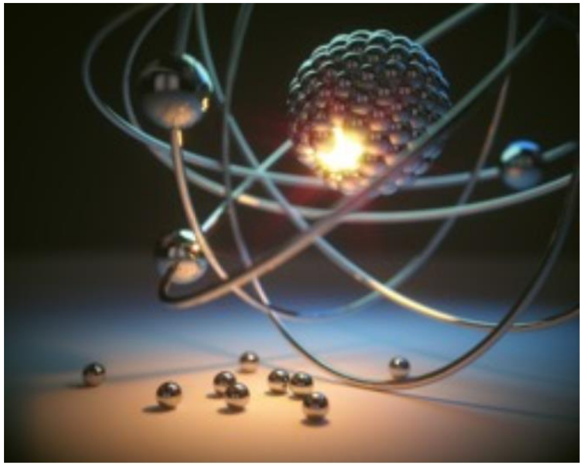
- Many-particle problems
- Strongly coupled systems
- Real-time evolution and dynamics

[J. Preskill, arXiv: 1801.00862]

Potential applications of quantum computing







Quantum Field Theories and Fundamental Symmetries

- indefinite particle number
- gauge symmetries and constraints
- entangled ground states

Real-Time Dynamics

- nuclear reactions
- neutrino-nucleus interactions
- neutrinos in matter
- early universe
- non-equilibrium - heavy-ions
- parton showers fragmentation

Dense Matter

- neutron stars
- gravity waves ?
- heavy nuclei
- chemical potentials

[Adapted from M. J. Savage's talk in NUCLEI - SciDAC, June 2020]

Ground-breaking activities in nuclear physics

RESEARCH ARTICLE

Quantum Algorithms for Quantum Field Theories

Stephen P. Jordan[1,*], Keith S. M. Lee[2], John Preskill[3]

[Science vol. 336, pp. 1130-1133 (2012)]

Quantum computing for neutrino-nucleus scattering

Alessandro Roggero,[1,*] Andy C. Y. Li,[2,†] Joseph Carlson,[3,‡] Rajan Gupta,[3,§] and Gabriel N. Perdue[2,‖]

[PRD 101, 074038 (2020)]

Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu,[1] A. J. McCaskey,[2] G. Hagen,[3,4] G. R. Jansen,[5,3] T. D. Morris,[4,3] T. Papenbrock,[4,3,*] R. C. Pooser,[1,4] D. J. Dean,[3] and P. Lougovski[1,†]

[PRL 120, 210501 (2018)]

Neutrino oscillations in a quantum processor

C. A. Argüelles[1] and B. J. P. Jones[2]

[Phys. Rev. Research 1, 033176 (2019)]

Real-time dynamics of lattice gauge theories with a few-qubit quantum computer

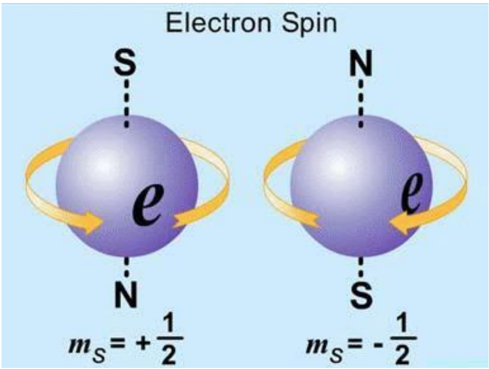
Esteban A. Martinez[1*], Christine A. Muschik[2,3*], Philipp Schindler[1], Daniel Nigg[1], Alexander Erhard[1], Markus Heyl[2,4], Philipp Hauke[2,3], Marcello Dalmonte[2,3], Thomas Monz[1], Peter Zoller[2,3] & Rainer Blatt[1,2]

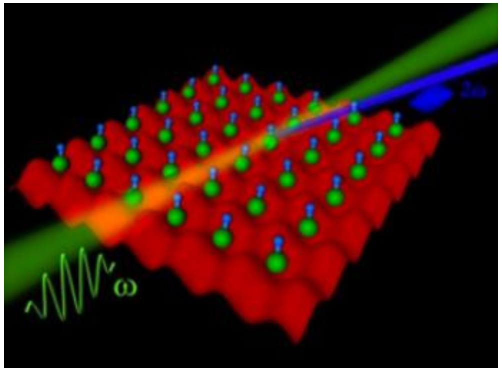
[Nature vol. 538, pp.517 (2016)]

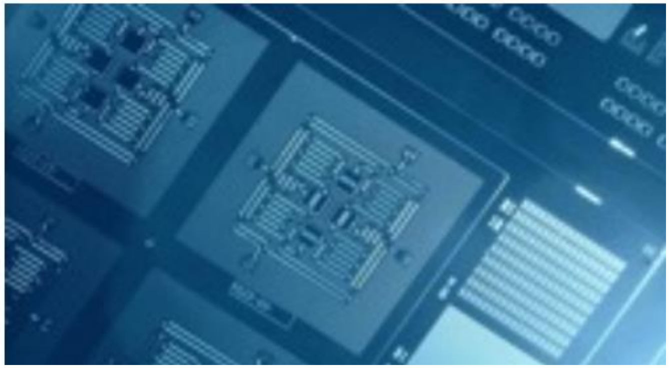
Elements of quantum computing: qubit system

Quantum bit (qubit)

- the basic element in quantum computation
- a two-level quantum system (e.g., spin-$\frac{1}{2}$ system)







Basis states of two-level quantum system

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

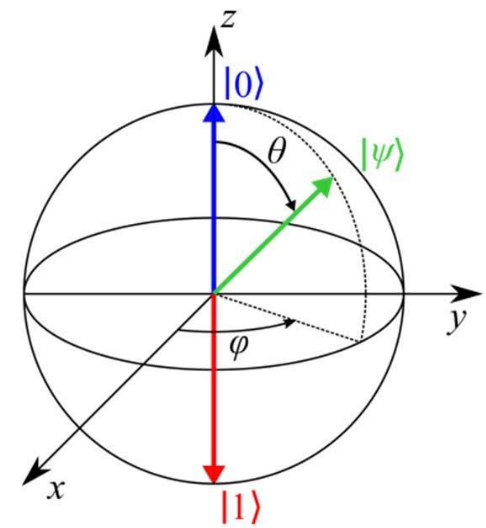
Elements of quantum computing: qubit system

1-qubit case

- a general **superposition** of basis states (infinite state vectors)

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$|\psi\rangle = \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$



Bloch representation of a general state vector

- normalization

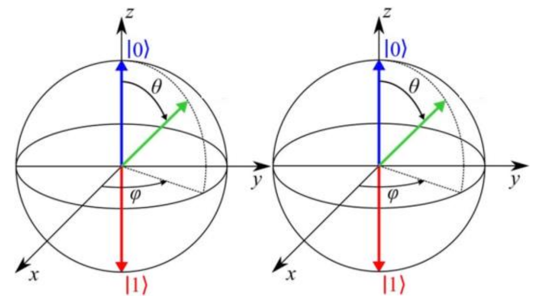
$$|\alpha|^2 + |\beta|^2 = 1$$

Elements of quantum computing: qubit system

2-qubit case

- **Superposition of basis states**

$$|\psi\rangle = \alpha|0\rangle_1|0\rangle_2 + \beta|0\rangle_1|1\rangle_2 + \gamma|1\rangle_1|0\rangle_2 + \delta|1\rangle_1|1\rangle_2$$



- **2^2 basis states**

$$|0\rangle_1|0\rangle_2 \equiv |0\rangle_1 \otimes |0\rangle_2 = \begin{bmatrix}1\\0\end{bmatrix}_1 \otimes \begin{bmatrix}1\\0\end{bmatrix}_2 = \begin{bmatrix}1\\0\\0\\0\end{bmatrix},\ |0\rangle_1|1\rangle_2 = \begin{bmatrix}0\\1\\0\\0\end{bmatrix},\ |1\rangle_1|0\rangle_2 = \begin{bmatrix}0\\0\\1\\0\end{bmatrix},\ |1\rangle_1|1\rangle_2 = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

- **Normalization**

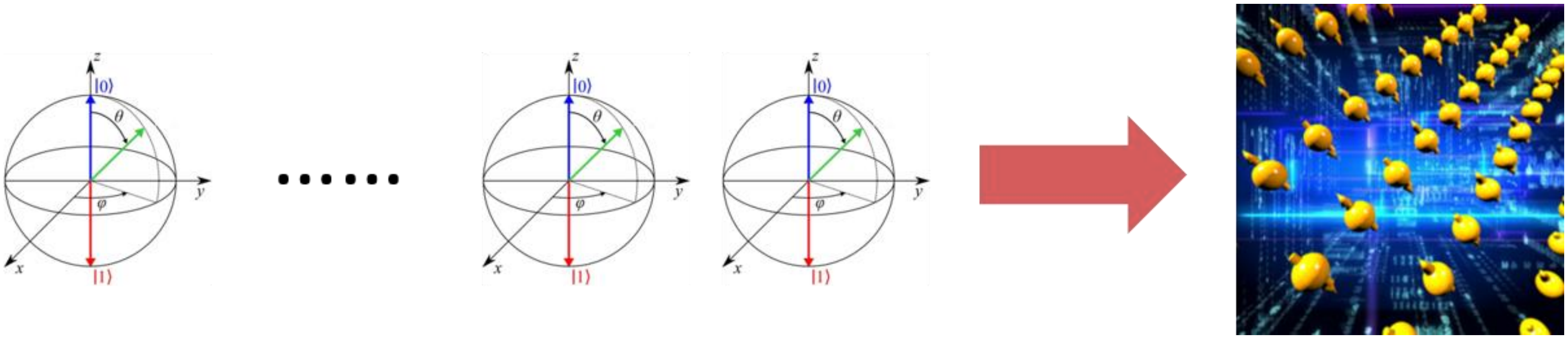
$$|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 \quad = \quad 1$$

Elements of quantum computing: qubit system

N-qubit case

- **Superposition of basis states**

$$|\psi\rangle = \sum_{i_1\in\{0,1\}} \sum_{i_2\in\{0,1\}} \cdots \sum_{i_N\in\{0,1\}} \alpha_{i_1 i_2 \cdots i_N} |i_1\rangle_1 |i_2\rangle_2 \cdots |i_N\rangle_N$$



- **2^N basis states**

$$|0\rangle_1|0\rangle_2\cdots|0\rangle_N,\ |0\rangle_1|0\rangle_2\cdots|1\rangle_N,\ \cdots,\ |1\rangle_1|1\rangle_2\cdots|1\rangle_N$$

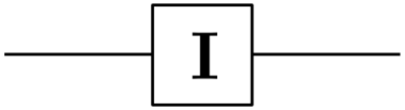
- **Normalization**

$$\sum_{i_1\in\{0,1\}} \sum_{i_2\in\{0,1\}} \cdots \sum_{i_N\in\{0,1\}} |\alpha_{i_1 i_2 \cdots i_N}|^2 = 1$$

Elements of quantum computing: quantum gates

Quantum gates: controlled local **unitary** operations applied on qubit(s)

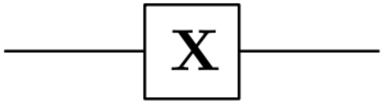
- **Identity gate**



$$\mathbf{I}\,|0\rangle = |0\rangle\,,\ \mathbf{I}\,|1\rangle = |1\rangle$$

$$\mathbf{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

- **X gate (NOT gate)**

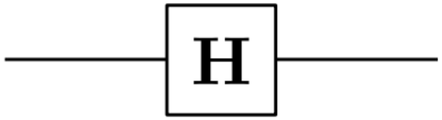


$$\mathbf{X}\,|0\rangle = |1\rangle\,,\ \mathbf{X}\,|1\rangle = |0\rangle$$

$$\mathbf{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \beta \\ \alpha \end{bmatrix}$$

Elements of quantum computing: quantum gates

- **Hadamard gate**



$$\mathbf{H}\left|0\right\rangle = \frac{1}{\sqrt{2}}\left|0\right\rangle + \frac{1}{\sqrt{2}}\left|1\right\rangle, \; \mathbf{H}\left|1\right\rangle = \frac{1}{\sqrt{2}}\left|0\right\rangle - \frac{1}{\sqrt{2}}\left|1\right\rangle$$

$$\mathbf{H} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

- **Phase gate**

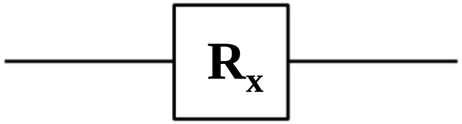
$$\mathbf{R}_\phi\left|0\right\rangle = \left|0\right\rangle, \; \mathbf{R}_\phi\left|1\right\rangle = e^{i\phi}\left|1\right\rangle$$

$$\mathbf{R}_\phi = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}$$

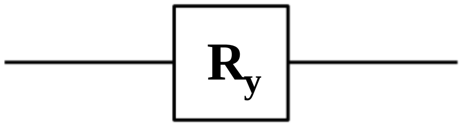
Elements of quantum computing: quantum gates

- **Rotational gates**

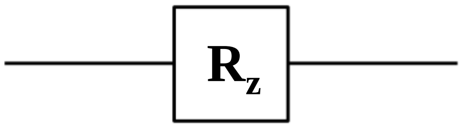
$$R_x(\theta) \equiv e^{-i\theta X/2} = \cos\frac{\theta}{2} I - i\sin\frac{\theta}{2} X = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$



$$R_y(\theta) \equiv e^{-i\theta Y/2} = \cos\frac{\theta}{2} I - i\sin\frac{\theta}{2} Y = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$



$$R_z(\theta) \equiv e^{-i\theta Z/2} = \cos\frac{\theta}{2} I - i\sin\frac{\theta}{2} Z = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}$$

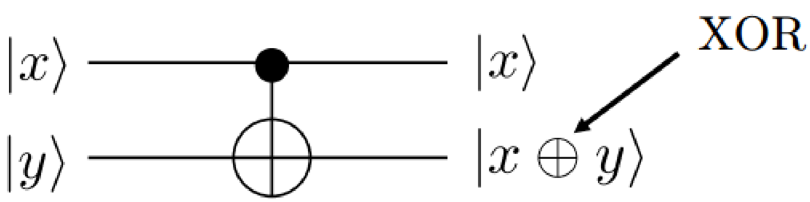


with the Pauli gates

$$X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad Y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad Z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Elements of quantum computing: quantum gates

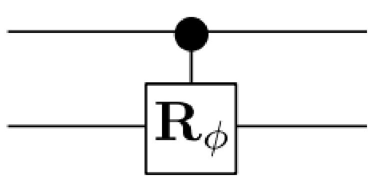
- **Controlled-NOT (CNOT) gate**



$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$|00\rangle \rightarrow |00\rangle \qquad |01\rangle \rightarrow |01\rangle \qquad |10\rangle \rightarrow |11\rangle \qquad |11\rangle \rightarrow |10\rangle$$

- **Controlled phase gate**

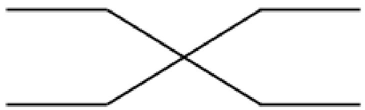


$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{bmatrix}$$

$$|00\rangle \rightarrow |00\rangle \qquad |01\rangle \rightarrow |01\rangle \qquad |10\rangle \rightarrow |10\rangle \qquad |11\rangle \rightarrow e^{i\phi}|11\rangle$$

Elements of quantum computing: quantum gates

- **SWAP gate**



$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$|00\rangle \rightarrow |00\rangle$ $|01\rangle \rightarrow |10\rangle$ $|10\rangle \rightarrow |01\rangle$ $|11\rangle \rightarrow |11\rangle$

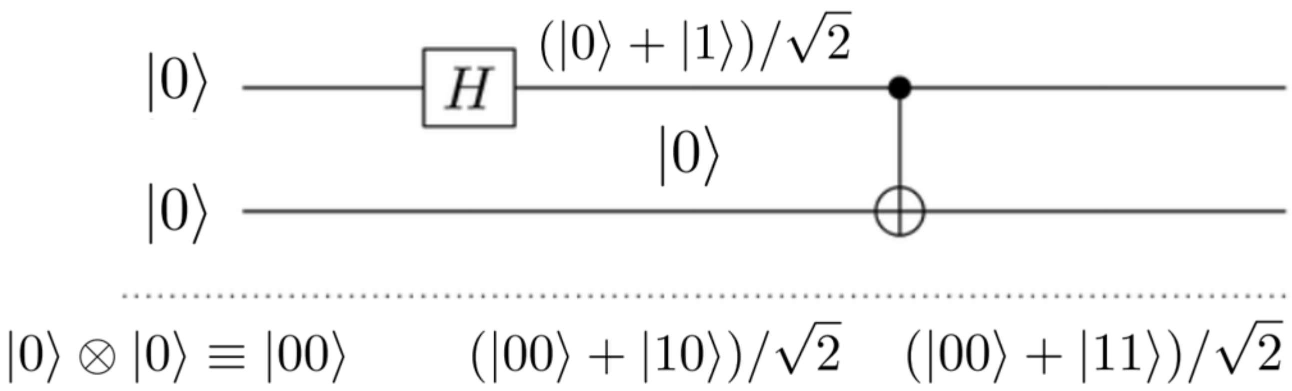
- **More gates**

Available at:
https://qiskit.org/textbook/ch-states/single-qubit-gates.html

Basic concepts of quantum computing

Quantum circuit

- a sequence of quantum gates output the solution to a problem



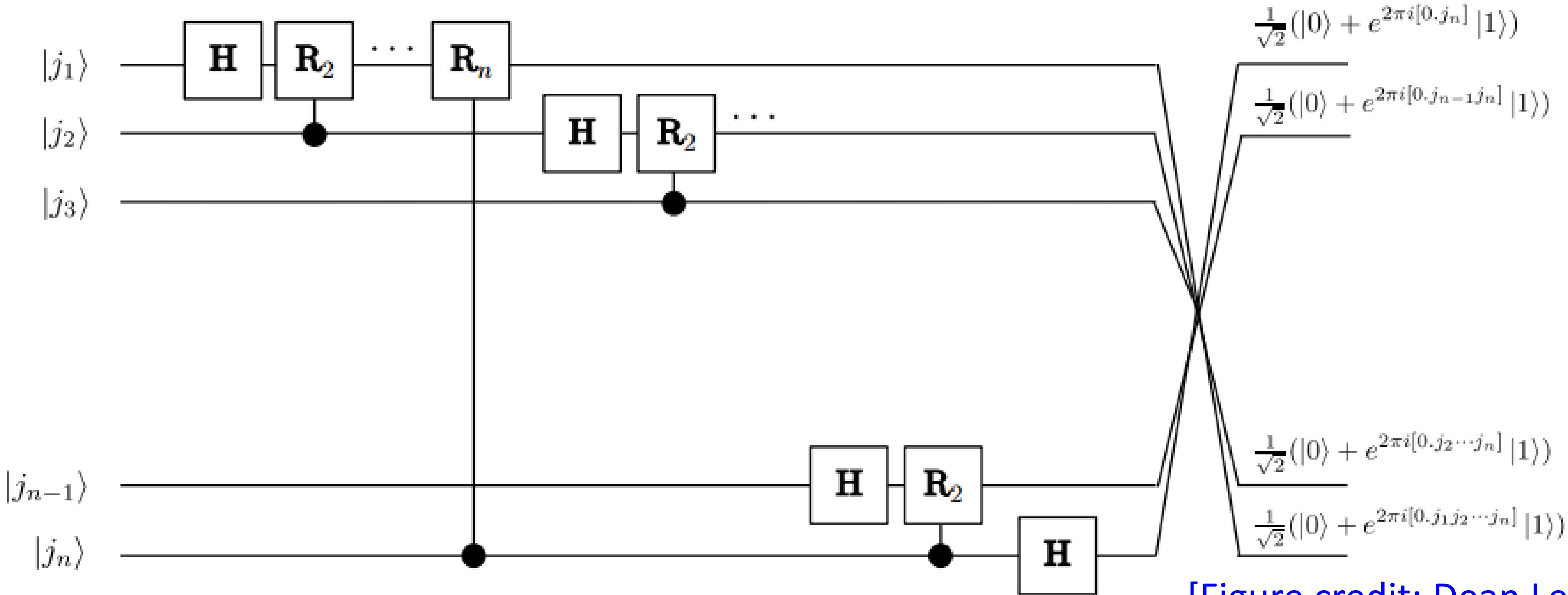
Quantum algorithm

- designing a quantum circuit for a particular problem
- performance of a quantum algorithm characterized by
  - the number of gates
  - the run time as a function of the problem size (dimension)

Algorithm illustration: quantum Fourier transformation

$$|j\rangle \longrightarrow \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i jk/N} |k\rangle$$

$$= \frac{1}{2^{n/2}} \left(|0\rangle + e^{2\pi i 0.j_n}|1\rangle\right)\left(|0\rangle + e^{2\pi i 0.j_{n-1}j_n}|1\rangle\right)\ldots\left(|0\rangle + e^{2\pi i 0.j_1 j_2 \cdots j_n}|1\rangle\right)$$



[Figure credit: Dean Lee]

Exponential speedup

Quantum Fourier transform $\sim O(n^2)$ gates

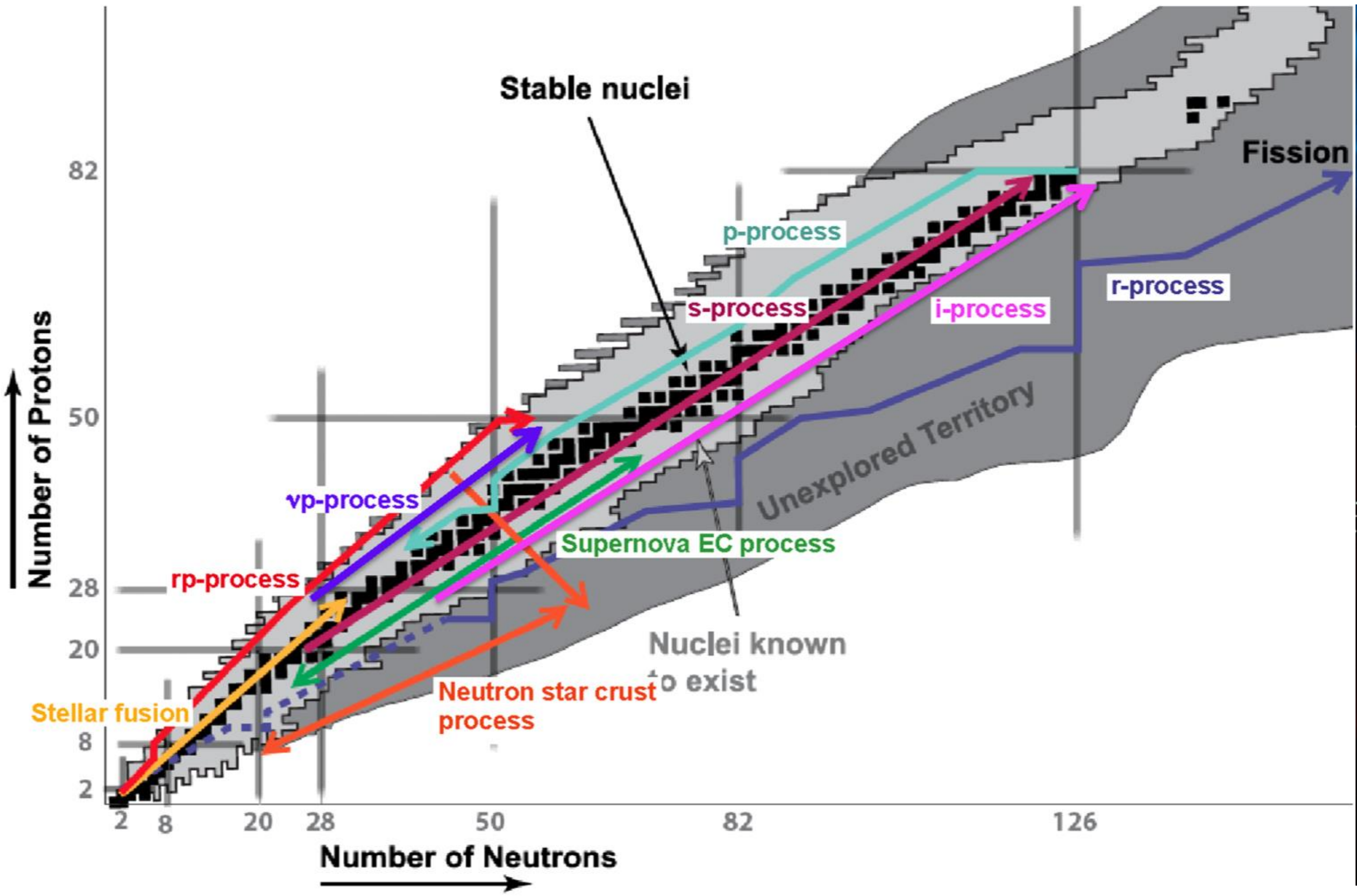
Classical Fourier transform $\sim O(n2^n)$ gates

Outline

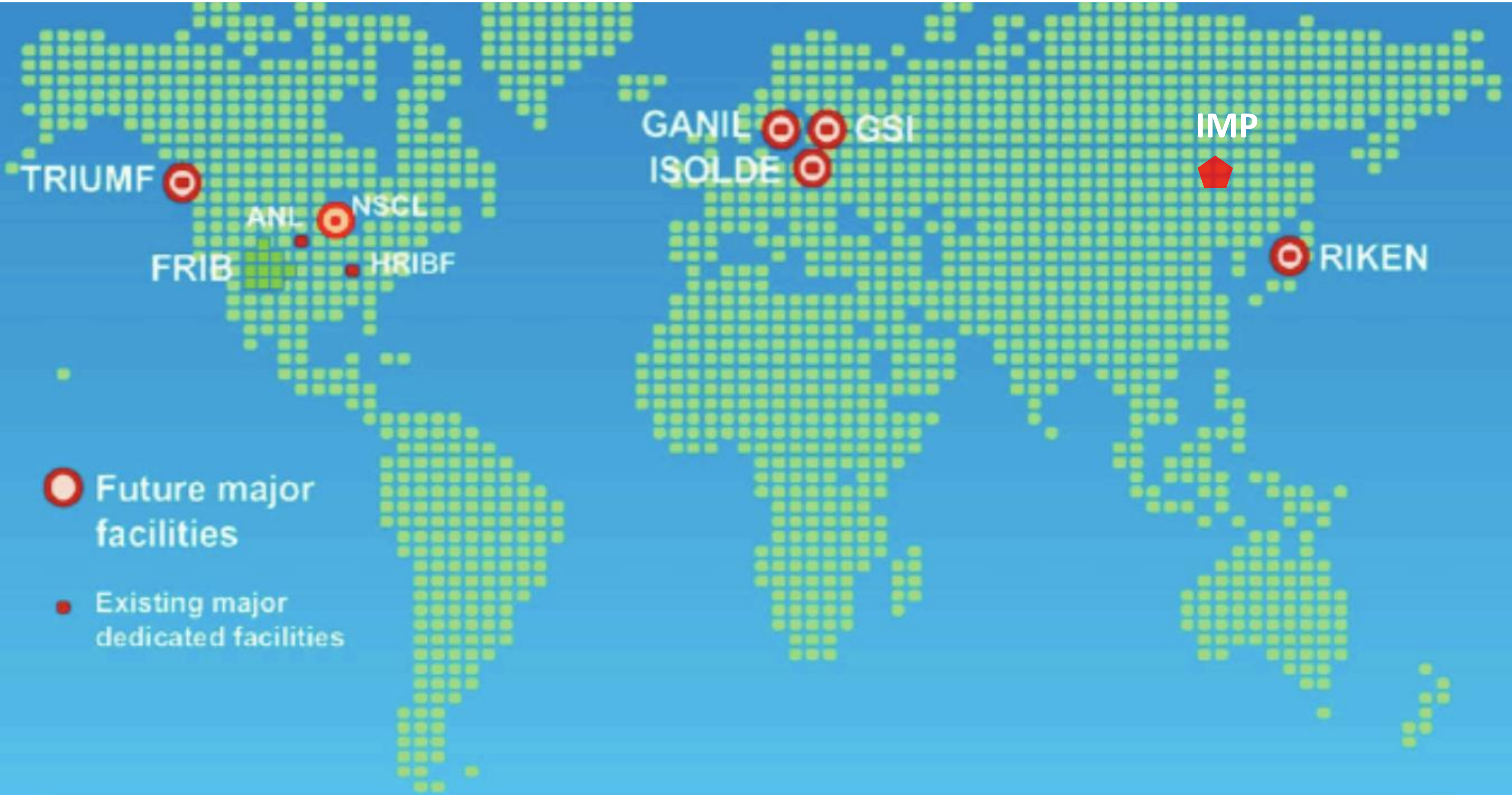
1. Background and basics
2. Time-Dependent Basis Function on Qubits (TBFQ) method
3. Future efforts and summary

Motivations

- Construct a unified *ab initio* theory for nuclear structure and reaction
- Study complex nuclear processes (e.g., rare isotopes)
- Investigate nuclear interaction (both on- and off- shell properties)



Requests for theories with predictive power for nuclear structures and reactions

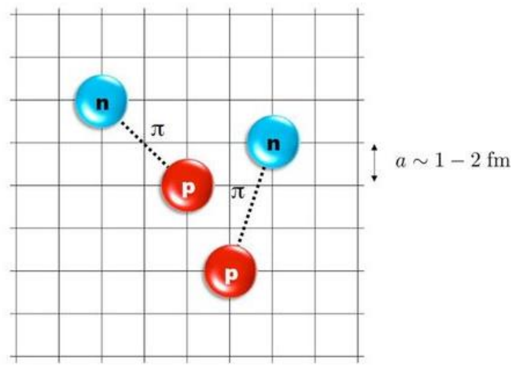


Global investment in RIBs over next decade ~$4B (OECD)

Background

Existing methods, e.g.,

- No-core Shell Model with Continuum
- No-core Shell Model/Resonating Group Method
- Gamow Shell Model
- Harmonic Oscillator Representation of Scattering Equation
- Green's Function Approaches
- Nuclear Lattice Effective Field Theory



Challenges

- Retaining full quantal coherence
- Tracking all potentially possible nuclear processes (rare isotopes)
- Large and complex reaction systems (exponential scaling)

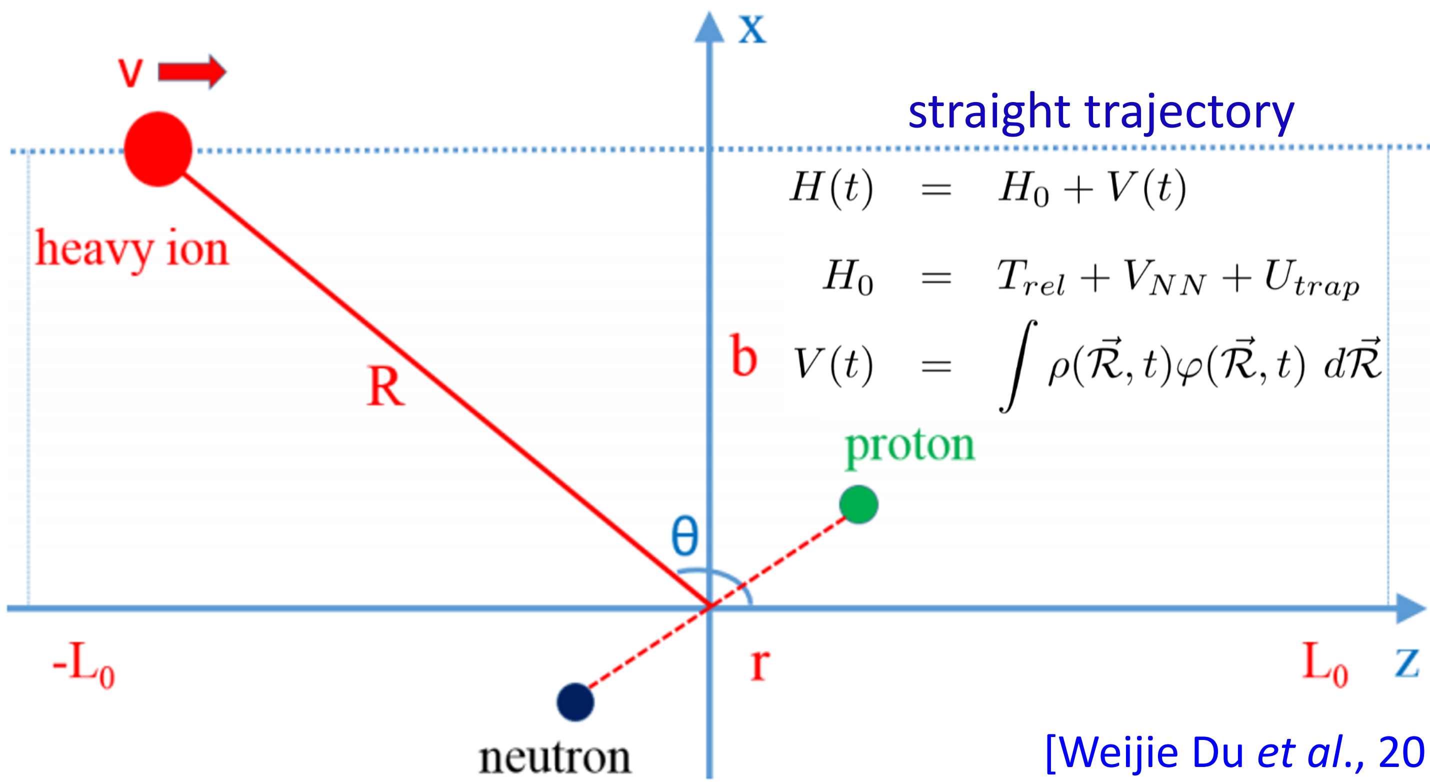
Solutions

- Hamiltonian dynamics
- Real-time evolution; information on the amplitude level
- Quantum computation

Time-dependent Basis Function on Qubits (TBFQ) algorithm (Hamiltonian simulation)

- Unified structure and reaction theory
- Based on successful nuclear structure theory
- *Ab initio* approach
- Non-perturbative method
- Retaining full quantal coherence & entanglement
- Circumventing the exponential cost in computation resource in simulating real-time many-body dynamics

Demonstration problem: Coulomb excitation of deuterium system by peripheral scattering with heavy ion



[Weijie Du *et al.*, 2017]

- H_0: Target (deuteron in trap) Hamiltonian
- φ: Coulomb field from heavy ion (U^{92+}) sensed by target
- ρ: Charge density distribution of target

Elements of TBFQ

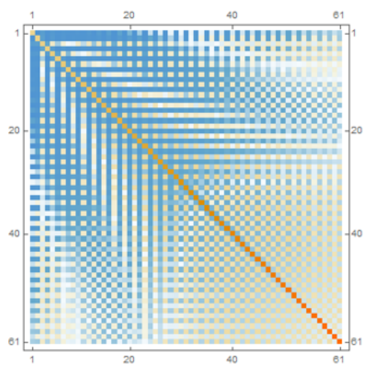
Construct the basis representation from *ab initio* nuclear structure calculation

$$H_0|\beta_i\rangle = E|\beta_i\rangle$$

$$H_0 = T_{rel} + V_{QCD}$$

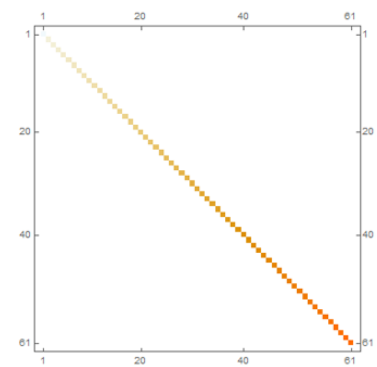
Basis representation

$$\{|\beta_1\rangle, |\beta_2\rangle, \cdots, |\beta_n\rangle\}$$



Free Hamiltonian H_0

Diagonalization



Eigenenergies and eigenbases

Game plan for TBFQ

1. Prepare the initial state – can be entangled state
2. Time-evolve the state – Trotterized evolution operator & qubitization
3. Measurement

The algorithm (Hamiltonian simulation)

State vector evolution

$$|\psi; t\rangle_I = U_I(t; t_0)|\psi; t_0\rangle_I = \hat{T}\left\{ \exp\left[-i \int_{t_0}^{t} V_{\text{int}}^I(t')dt' \right] \right\}|\psi; t_0\rangle_I$$

Time discretization

$$U_I(t; t_0) \approx \hat{T}\left\{ \exp\left[-i\left[V_{\text{int}}^I(t)\delta t + V_{\text{int}}^I(t_{n-1})\delta t + \cdots + V_{\text{int}}^I(t_1)\delta t\right] \right\}$$

Trotterization (1^{st} order)

$$U_I(t; t_0) = \underbrace{e^{-iV_{\text{int}}^I(t)\delta t}}_{U(t;\ t_{n-1})} \cdots \underbrace{e^{-iV_{\text{int}}^I(t_k)\delta t}}_{U(t_k;\ t_{k-1})} \cdots \underbrace{e^{-iV_{\text{int}}^I(t_1)\delta t}}_{U(t_1;\ t_0)} + \mathcal{O}(\delta t^2)$$

Qubitization

$$\{ \underbrace{|\beta_0\rangle}_{|000\cdots\rangle_n} , \underbrace{|\beta_1\rangle}_{|100\cdots\rangle_n} , \cdots , \underbrace{|\beta_N\rangle}_{|111\cdots\rangle_n} \}$$

$\langle\beta_j|U_I(t; t_0)|\beta_i\rangle$ ➡ **Quantum circuit**

$\mathbf{n \sim \lceil \mathit{log}\, N_{basis} \rceil}$

Basis set of the inelastic scattering problem

$(^3S_1, ^3D_1)$	$M = -1$	-0.65289 MeV
$(^3S_1, ^3D_1)$	$M = 0$	-0.65289 MeV
$(^3S_1, ^3D_1)$	$M = +1$	-0.65289 MeV
$^3P_0$	$M = 0$	12.0733 MeV
$^3P_1$	$M = -1$	12.7585 MeV
$^3P_1$	$M = 0$	12.7585 MeV
$^3P_1$	$M = +1$	12.7585 MeV

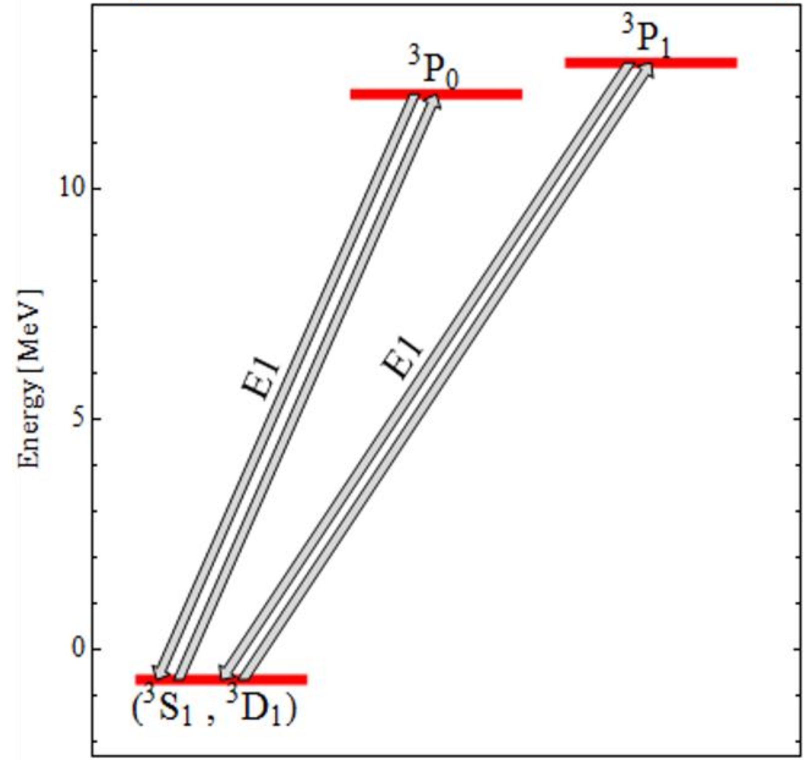
1. 7 basis states of the target solved via *ab initio* structure calculation
2. Initial state set to be antiparallel to z-axis

[Weijie Du et al., 2017]

Basis set of the inelastic scattering problem

$$
\begin{pmatrix}
({}^3S_1,{}^3D_1) & M=-1 & -0.65289\ \mathrm{MeV} \\
({}^3S_1,{}^3D_1) & M=\ \ 0 & -0.65289\ \mathrm{MeV} \\
({}^3S_1,{}^3D_1) & M=+1 & -0.65289\ \mathrm{MeV} \\
{}^3P_0 & M=\ \ 0 & 12.0733\ \mathrm{MeV} \\
{}^3P_1 & M=-1 & 12.7585\ \mathrm{MeV} \\
{}^3P_1 & M=\ \ 0 & 12.7585\ \mathrm{MeV} \\
{}^3P_1 & M=+1 & 12.7585\ \mathrm{MeV}
\end{pmatrix}
$$

E1 radiative transitions



1. 7 basis states of the target solved via *ab initio* structure calculation
2. Initial state set to be antiparallel to z-axis
3. E1 radiative transitions retained in dynamics (time-evolution operator)

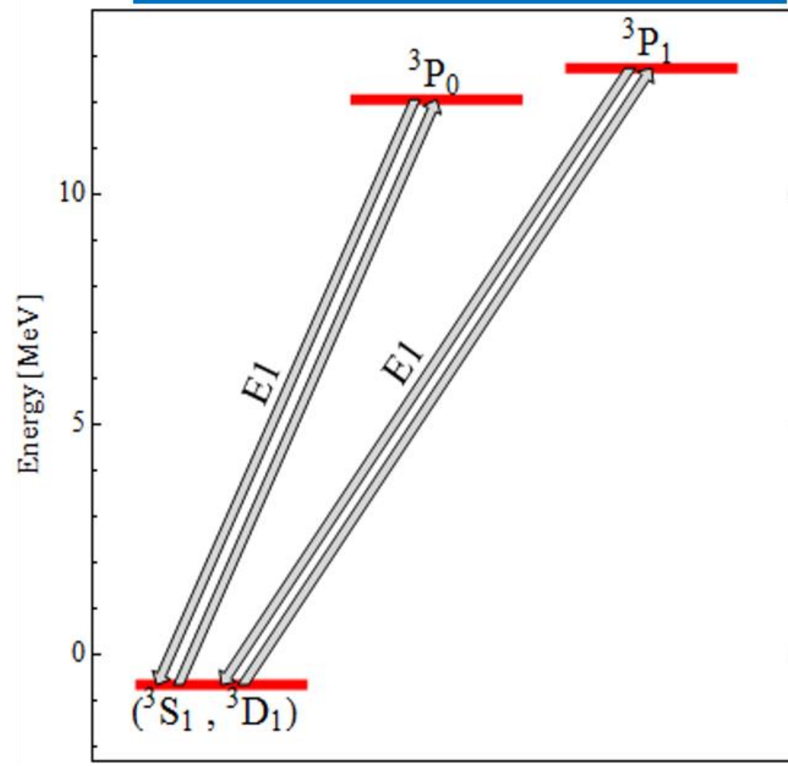
[Weijie Du et al., 2017]

Basis set of the inelastic scattering problem

|000>	$({}^3S_1, {}^3D_1)$	$M = -1$	-0.65289 MeV
|100>	$({}^3S_1, {}^3D_1)$	$M = 0$	-0.65289 MeV
|010>	$({}^3S_1, {}^3D_1)$	$M = +1$	-0.65289 MeV
|110>	${}^3P_0$	$M = 0$	12.0733 MeV
|001>	${}^3P_1$	$M = -1$	12.7585 MeV
|101>	${}^3P_1$	$M = 0$	12.7585 MeV
|011>	${}^3P_1$	$M = +1$	12.7585 MeV

$$n \sim [\log N_{basis}]$$

E1 radiative transitions



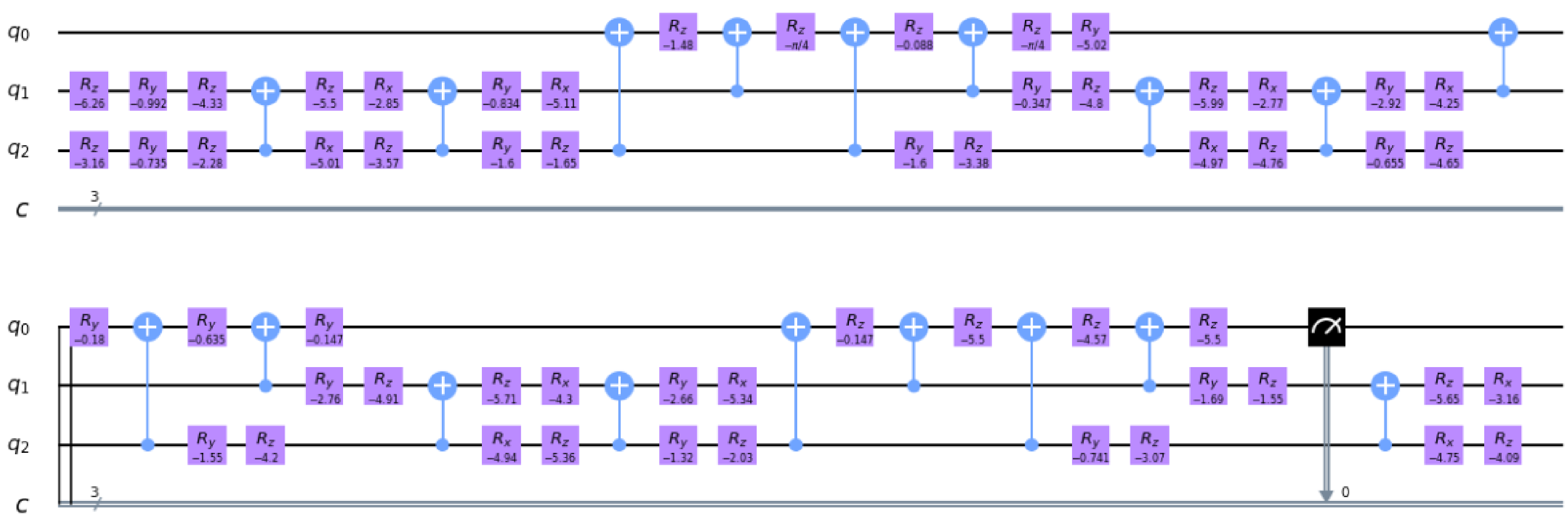
1. 7 basis states of the target solved via *ab initio* structure calculation
2. Initial state set to be antiparallel to z-axis
3. E1 radiative transitions retained in dynamics (time-evolution operator)
4. Trotterization; 7 basis states ***mapped*** to 3 qubits

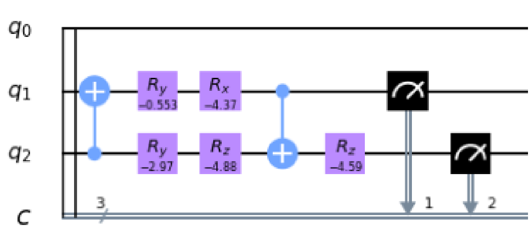
[Weijie Du et al., 2017]

Illustration: what's going on in the Hamiltonian simulation?

- The initial state in the qubit representation is |000>
- The quantum circuit is constructed by Quantum Shannon Decomposition

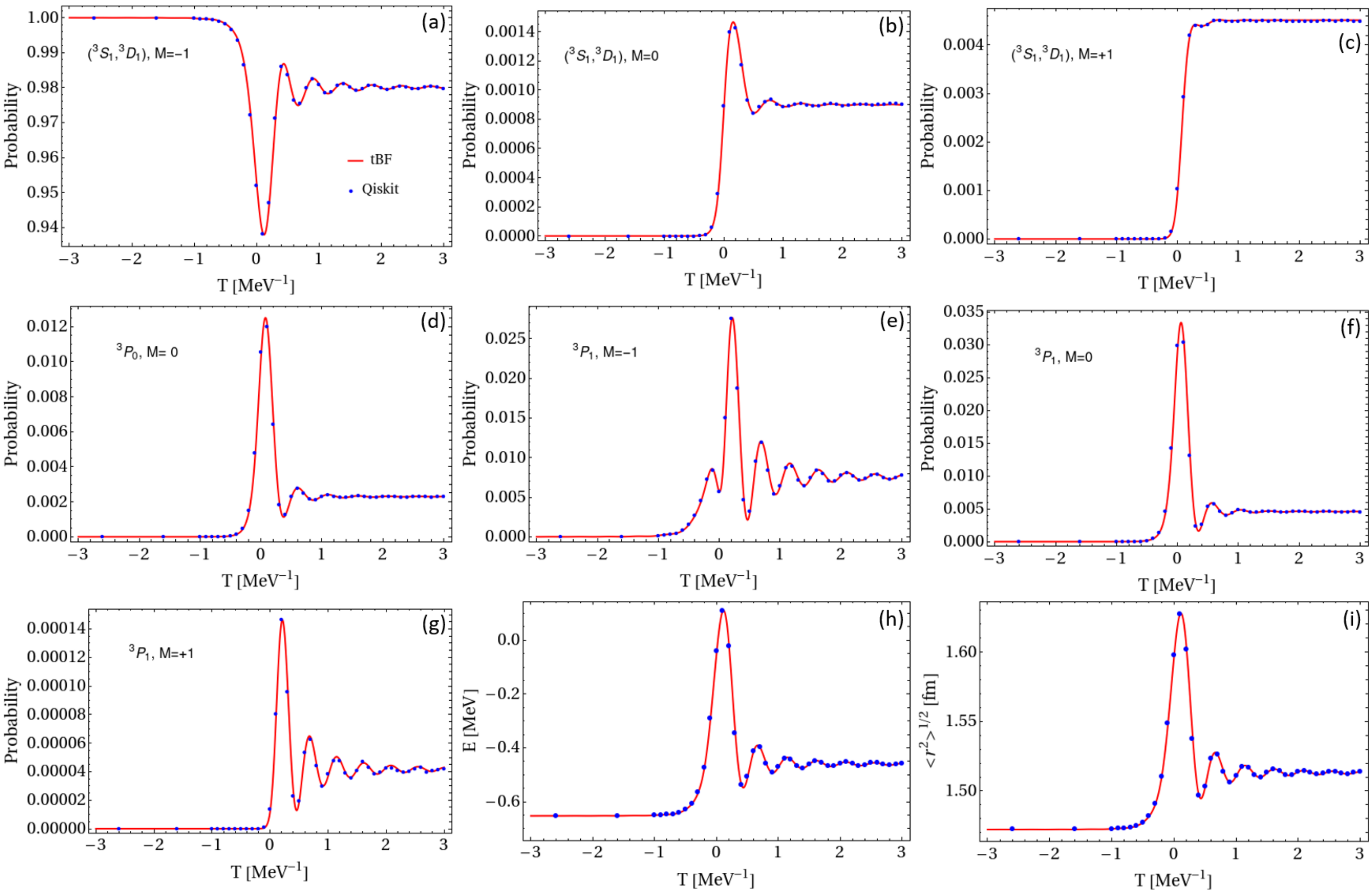
|0> =
|0> =
|0> =





By measurement, we obtain the final state in terms of probability distribution.

Transition probabilities and observables



[Weijie Du et al., arXiv:2006.01369]

Outline

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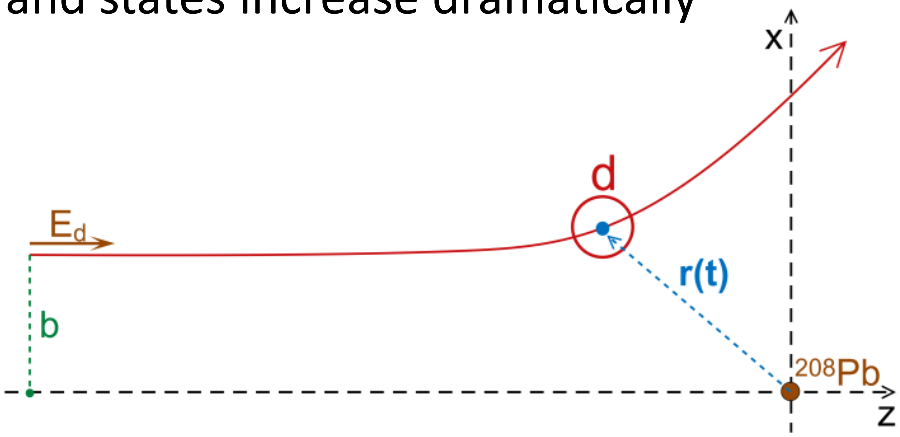
3. Future efforts and summary

Future efforts

Generalization to real scattering

- Channels and states increase dramatically



[P. Yin, WD et al., arXiv: 1910.10586]

Real-time dynamics in gauge fields

- Electron scattering in intense E&M fields (e.g., laser facilities)
- Quark scattering in color field
- Particle production and evolution in the glasma field

[X. Zhao et al., PRD 88 065064 (2013)]
[G. Chen et al., PRD 95 096012 (2017)]
[M. Li et al., PRD 101 076016 (2020)]
[M. Li et al., private communication]

Summary

- Quantum computing techniques make use quantum mechanics principles to outperform classical computers
- The rapid development of quantum computing techniques shed light on many challenging problems in nuclear physics
- We develop the TBFQ algorithm to simulate low-energy nuclear scattering on quantum computers
- This work can be further generalized to study complicated problems in low-energy nuclear, QED and QCD scattering processes
- Stay tuned…

Thanks!