Can we simulate hadrons on a quantum computer?

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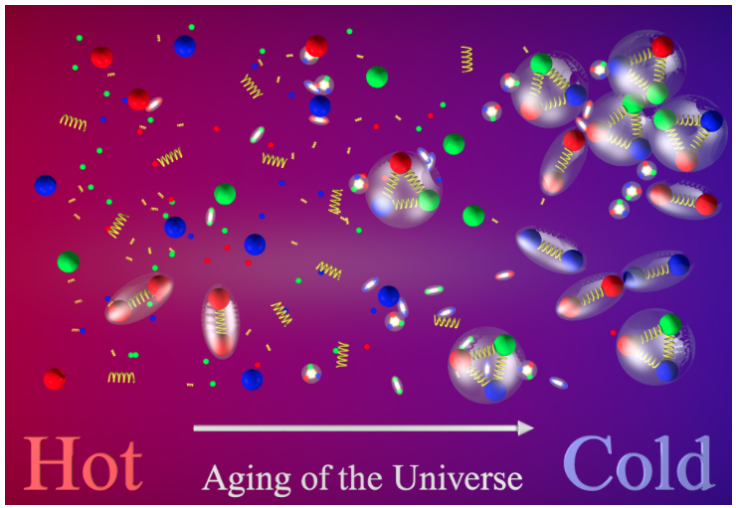
Hadron Physics

- The main goal of Hadron Physics is to provide a quantitative understanding of the strong interaction, especially in the low-energy regime.

  examples:
  – understand how the spectrum and structure of hadrons (bound-states of quarks and gluons) emerge from the forces among their fundamental constituents,
  – find out whether there are new forms of matter $\rightsquigarrow$ exotic states.



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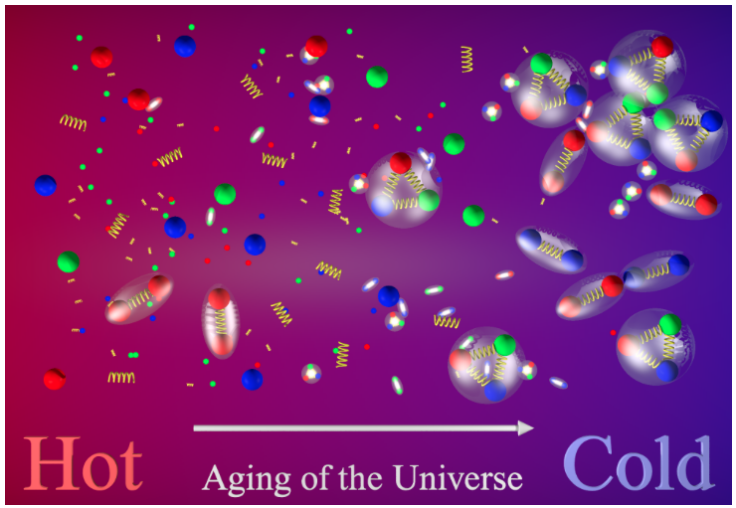
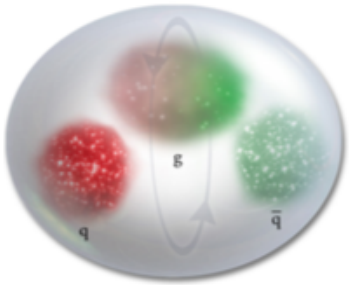
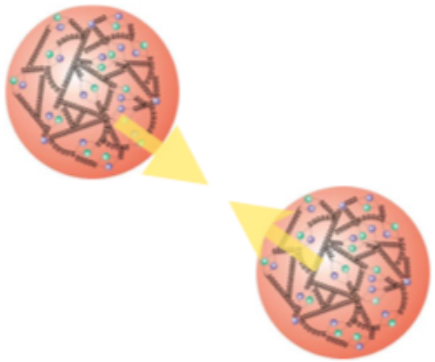


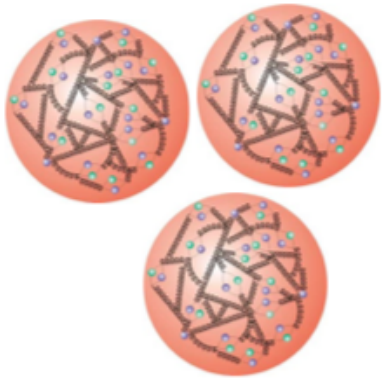
- Big challenge:
  – *Why are single quarks not observed in isolation?* $\rightsquigarrow$ confinement - Millennium prize.

QCD theoretical tools for Hadron Physics

- Understand the origin of visible matter in our Universe $\rightsquigarrow$ unravel the physics of hadrons!







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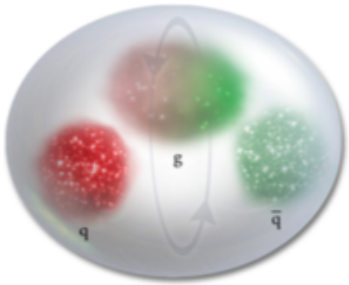
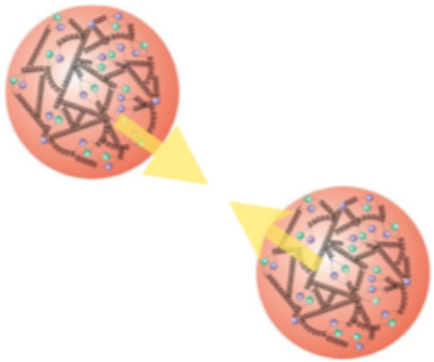
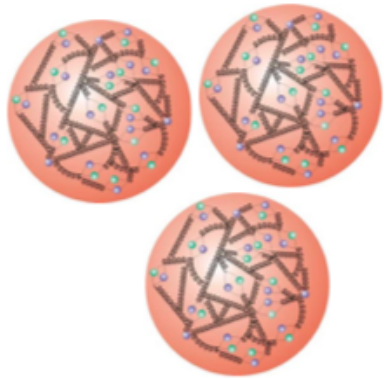




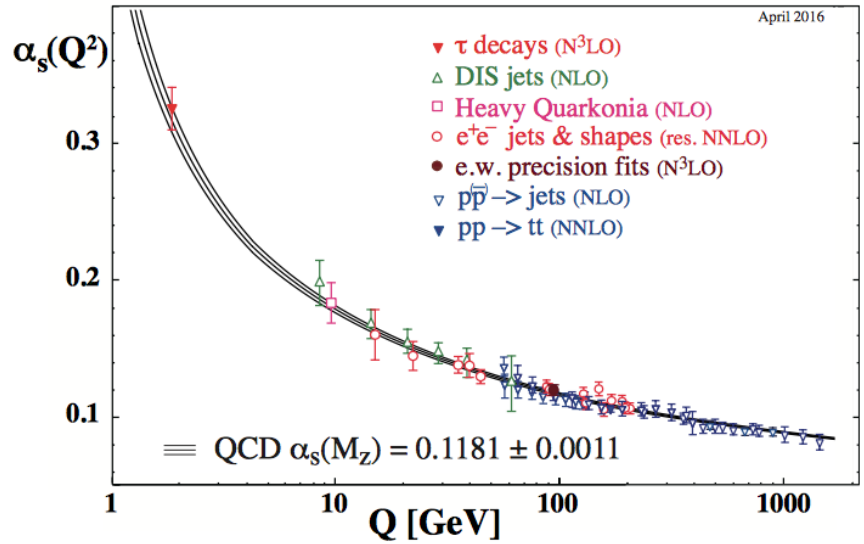


- Knowledge from first principles (QCD) $\rightsquigarrow$ difficult in the nonperturbative regime.

QCD theoretical tools for hadron physics

Lattice QCD EFTs DSEs etc. ...

$\hookrightarrow$ ... *Still*, alternative approaches are needed!



Previous work - Relativistic phenomenology of mesons

- Recently, I have used the Covariant Spectator Theory (CST) to construct

  a **manifestly covariant** theoretical model for **all mesons** interpreted as quark-antiquark bound states, and derived directly in **Minkowski space-time**.

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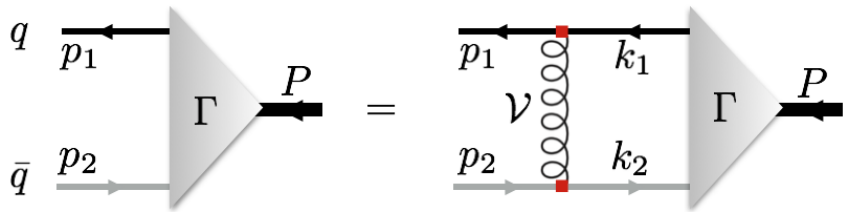

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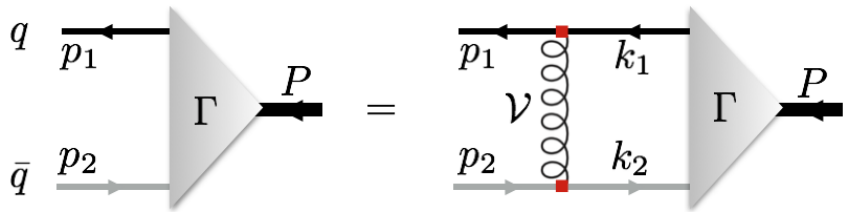
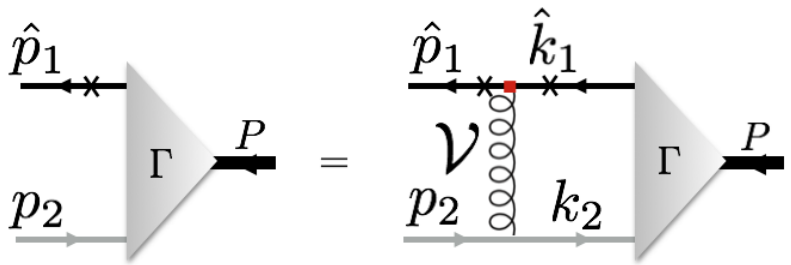


- Integrate over k_0 but keep *only* pole contributions from constituent particle propagators $\rightsquigarrow$ reduction to 3D loop integrations, but covariant!

$$\int_{\mathbf{k}_i} \to \int \frac{d^4k}{(2\pi)^4}\delta_+(m_i^2 - k^2) \to \int \frac{d^3k}{(2\pi)^3}\frac{m_i}{E_{ik}},$$



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- Covariant kernel: $\mathcal{V}(p,k;P) = \underbrace{\frac{3}{4}\mathbf{F}_1\cdot\mathbf{F}_2}_{=1,\ \text{singlets}} \sum_K \underbrace{V^K(p,k;P)}_{\text{momentum dep.}} \underbrace{\Theta_1^{K(\mu)}\otimes\Theta^K_{2(\mu)}}_{\text{Lorentz structure } \mathbf{1}_i,\,\gamma_i^5,\,\gamma_i^\mu}$

  ✓ Confining interaction: Lorentz (scalar + pseudoscalar) mixed with vector
  Coupling strength σ, mixing parameter y:

$$\mathcal{V}_{\rm L}(p,k) = [(1-y)\underbrace{\left(\mathbf{1}_1\otimes\mathbf{1}_2+\gamma_1^5\otimes\gamma_2^5\right)}_{\substack{\text{equal weight}\\ \text{(constraint from chiral symm.)}}} - y\,\gamma_1^\mu\otimes\gamma_{\mu 2}]V_{\rm L}(p,k)$$

  ✓One-gluon exchange with constant coupling strength α_s+ Constant interaction (in r-space) with strength C (Lorentz vector)

$$\mathcal{V}_{\rm OGE}(p,k)+\mathcal{V}_{\rm C}(p,k) = -\gamma_1^\mu\otimes\gamma_{\mu 2}\,[V_{\rm OGE}(p,k)+V_{\rm C}(p,k)]$$

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- Ultimately, test CST by comparing the theoretical predictions with experimental data.

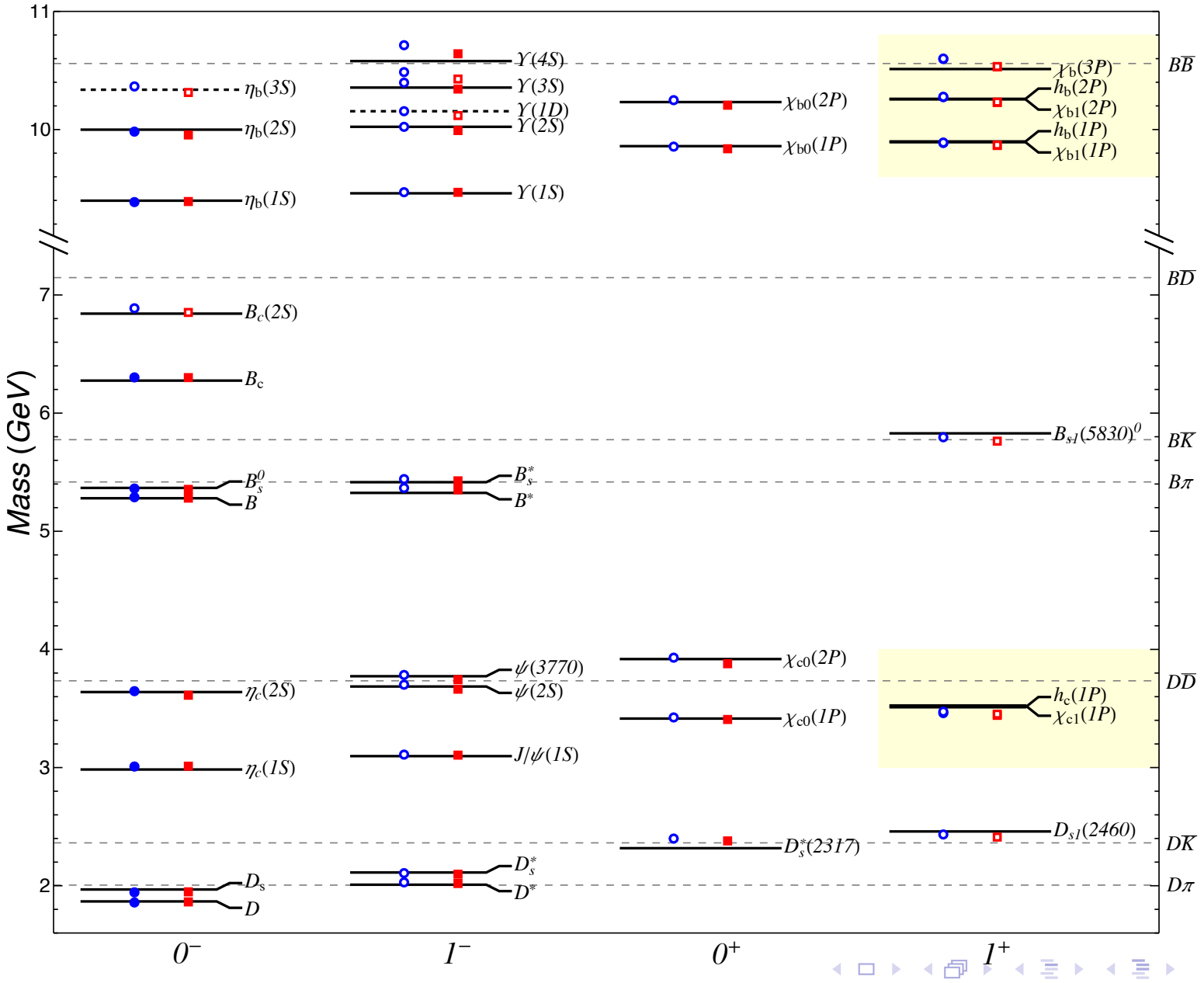
Previous work - Data sets used to fit the spectrum

State	$J^{P(C)}$	Exp. Mass	Data set S1	S2	S3
$\Upsilon(4S)$	1^{--}	10579.4 ± 1.2		•	•
$\chi_{b1}(3P)$	1^{++}	10512.1 ± 2.3			•
$\Upsilon(3S)$	1^{--}	10355.2 ± 0.5		•	•
$\eta_b(3S)$	0^{-+}	10337			
$h_b(2P)$	1^{+-}	10259.8 ± 1.2			•
$\chi_{b1}(2P)$	1^{++}	$10255.46 \pm 0.22 \pm 0.50$			•
$\chi_{b0}(2P)$	0^{++}	$10232.5 \pm 0.4 \pm 0.5$		•	•
$\Upsilon(1D)$	1^{--}	10155			
$\Upsilon(2S)$	1^{--}	10023.26 ± 0.31		•	•
$\eta_b(2S)$	0^{-+}	9999 ± 4	•	•	•
$h_b(1P)$	1^{+-}	9899.3 ± 0.8			•
$\chi_{b1}(1P)$	1^{++}	$9892.78 \pm 0.26 \pm 0.31$			•
$\chi_{b0}(1P)$	0^{++}	$9859.44 \pm 0.42 \pm 0.31$		•	•
$\Upsilon(1S)$	1^{--}	9460.30 ± 0.26		•	•
$\eta_b(1S)$	0^{-+}	9399.0 ± 2.3	•	•	•
$B_c(2S)^{\pm}$	0^{-}	6842 ± 6			•
B_c^{+}	0^{-}	6275.1 ± 1.0	•	•	•
$B_{s1}(5830)$	1^{+}	5828.63 ± 0.27			•
$B_1(5721)^{+,0}$	1^{+}	5725.85 ± 1.3			•
B_s^{*}	1^{-}	5415.8 ± 1.5		•	•
B_s^{0}	0^{-}	5366.82 ± 0.22	•	•	•
B^{*}	1^{-}	5324.65 ± 0.25		•	•
$B^{\pm,0}$	0^{-}	5279.45	•	•	•

State	$J^{P(C)}$	Exp. Mass	Data set S1	S2	S3
$X(3915)$	0^{++}	3918.4 ± 1.9		•	•
$\psi(3770)$	1^{--}	3773.13 ± 0.35		•	•
$\psi(2S)$	1^{--}	3686.097 ± 0.010		•	•
$\eta_c(2S)$	0^{-+}	3639.2 ± 1.2	•	•	•
$h_c(1P)$	1^{+-}	3525.38 ± 0.11			•
$\chi_{c1}(1P)$	1^{++}	3510.66 ± 0.07			•
$\chi_{c0}(1P)$	0^{++}	3414.75 ± 0.31		•	•
$J/\Psi(1S)$	1^{--}	3096.900 ± 0.006		•	•
$\eta_c(1S)$	0^{-+}	2983.4 ± 0.5	•	•	•
$D_{s1}(2536)^{\pm}$	1^{+}	2535.10 ± 0.06			•
$D_{s1}(2460)^{\pm}$	1^{+}	2459.5 ± 0.6			•
$D_1(2420)^{\pm,0}$	1^{+}	2421.4			•
$D_0^{*}(2400)^{0}$	0^{+}	2318 ± 29		•	•
$D_{s0}^{*}(2317)^{\pm}$	0^{+}	2317.7 ± 0.6		•	•
$D_s^{*\pm}$	1^{-}	2112.1 ± 0.4		•	•
$D^{*}(2007)^{0}$	1^{-}	2008.62			•
$D_s^{\pm}$	0^{-}	1968.27 ± 0.10	•	•	•
$D^{\pm,0}$	0^{-}	1867.23	•	•	•

- S1: 9 PS mesons,
- S2: 25 PS+S+V mesons,
- S3: 39 PS+S+V+A mesons.

Previous work - Spectroscopy



Predictive power of the covariant kernels

- Constant constituent quark masses $m_b, m_c, m_s, m_q = m_{u/d}$ held fixed during the fits (values in **bold**).
  - Model P1: fitted to 9 pseudoscalar meson masses only (set S1)
  - Model PSV1: fitted to 25 pseudoscalar+scalar+vector meson masses

Model	σ (GeV^2)	α_s	C (GeV)	y	m_b (GeV)	m_c (GeV)	m_s (GeV)	m_q (GeV)	N_s	$\delta_{\rm rms}$ (GeV)
P1	0.2493	0.3643	0.3491	**0.0000**	**4.892**	**1.600**	**0.4478**	**0.3455**	9	0.036
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- Almost 100% $L = 0, S = 0$ (S-wave, spin singlet)

$$\langle 0^-|\boldsymbol{L}\cdot\boldsymbol{S}|0^-\rangle = 0 \quad \text{Spin-orbit force vanishes}$$

$$\langle 0^-|S_{12}|0^-\rangle = 0 \quad \text{Tensor force vanishes}$$

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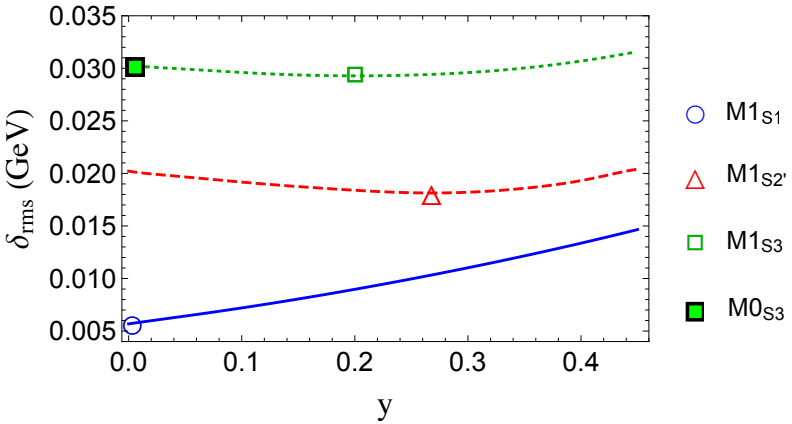
- Good test for a covariant kernel: Pseudoscalar states do not constrain spin-orbit and tensor forces, and cannot separate spin-spin from central force $\rightsquigarrow$ Model P1 indeed predicts spin-dependent forces correctly!

Sensitivity to the parameters

- In a new series of fits we treat quark masses and mixing parameter y as adjustable parameters.

Model	σ (GeV^2)	α_s	C (GeV)	y	m_b (GeV)	m_c (GeV)	m_s (GeV)	m_q (GeV)	N_s	$\delta_{\rm rms}$	$\Delta_{\rm rms}$ (GeV)
(P1)M0$_{S1}$	0.2493	0.3643	0.3491	**0.0000**	**4.892**	**1.600**	**0.4478**	**0.3455**	9	0.017	0.037
M1$_{S1}$	0.2235	0.3941	0.0591	0.0000	4.768	1.398	0.2547	0.1230	9	0.006	0.041
(PSV1)M0$_{S2}$	0.2247	0.3614	0.3377	**0.0000**	**4.892**	**1.600**	**0.4478**	**0.3455**	25	0.028	0.036
M1$_{S2}$	0.1893	0.4126	0.1085	0.2537	4.825	1.470	0.2349	0.1000	25	0.022	0.033
M1$_{S2'}$	0.2017	0.4013	0.1311	0.2677	4.822	1.464	0.2365	0.1000	24	0.018	0.033
(best)M1$_{S3}$	0.2022	0.4129	0.2145	0.2002	4.875	1.553	0.3679	0.2493	39	0.030	0.030
M0$_{S3}$	0.2058	0.4172	0.2821	**0.0000**	4.917	1.624	0.4616	0.3514	39	0.031	0.031

y held fixed, other parrameters refitted



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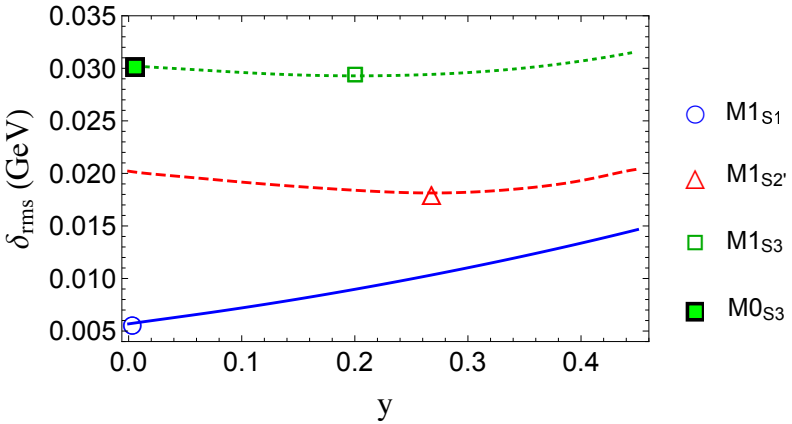

- Quality of fits not much improved.

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M1$_{S2'}$	0.2017	0.4013	0.1311	0.2677	4.822	1.464	0.2365	0.1000	24	0.018	0.033
(best)M1$_{S3}$	0.2022	0.4129	0.2145	0.2002	4.875	1.553	0.3679	0.2493	39	0.030	0.030
M0$_{S3}$	0.2058	0.4172	0.2821	**0.0000**	4.917	1.624	0.4616	0.3514	39	0.031	0.031

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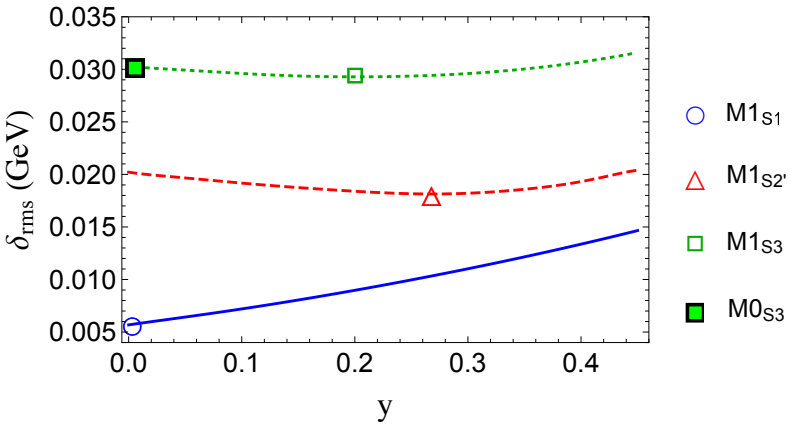

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Sensitivity to the parameters

- In a new series of fits we treat quark masses and mixing parameter y as adjustable parameters.

Model	σ (GeV^2)	α_s	C (GeV)	y	m_b (GeV)	m_c (GeV)	m_s (GeV)	m_q (GeV)	N_s	$\delta_{\rm rms}$	$\Delta_{\rm rms}$ (GeV)
(P1)M0$_{S1}$	0.2493	0.3643	0.3491	**0.0000**	**4.892**	**1.600**	**0.4478**	**0.3455**	9	0.017	0.037
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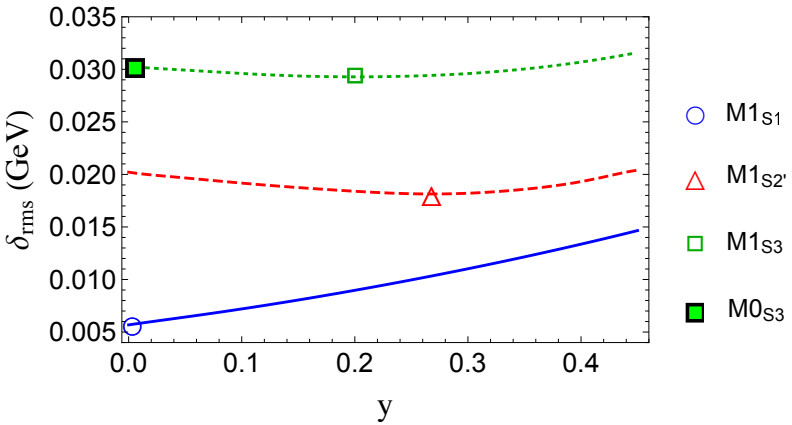

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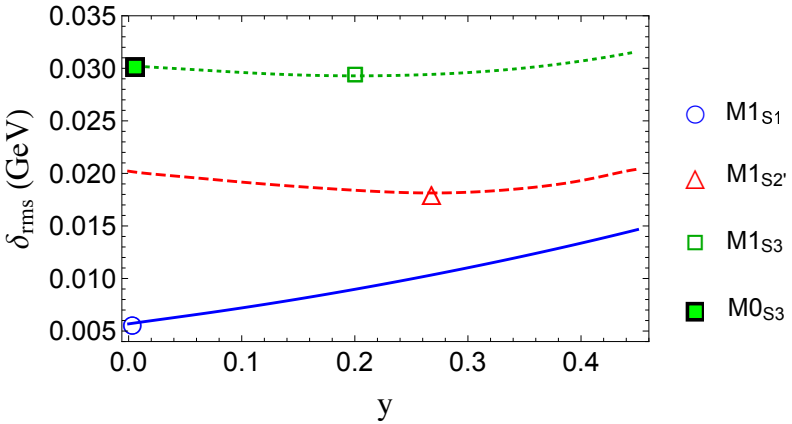

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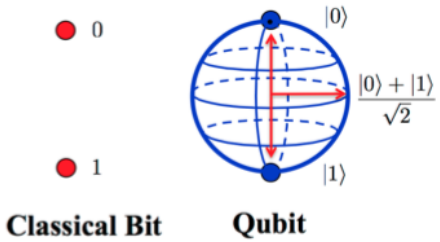
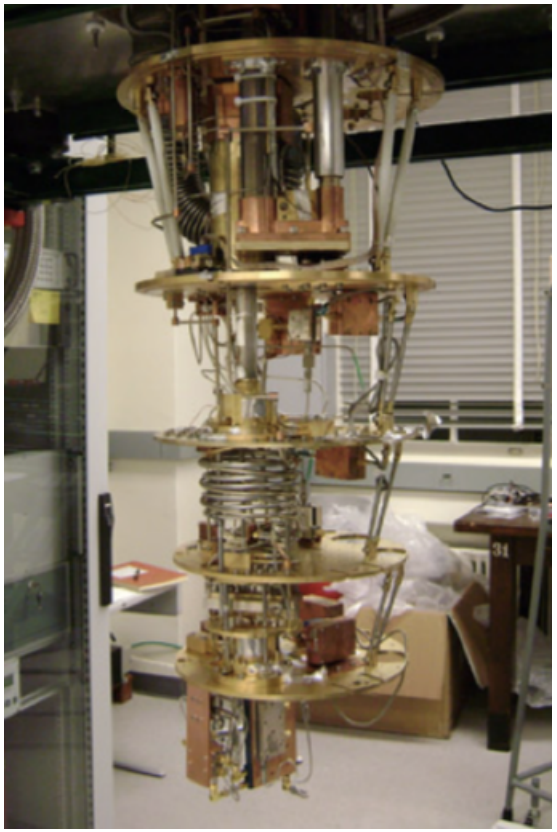
- To investigate wether or not other physical observables (e.g. decay constants) are more stringent with respect to y and the masses.

New beginnings...

Recent developments in Quantum Computing

- A quantum computer (QC) is a device that processes information exploiting QM properties $\rightsquigarrow$ superposition, entanglement, ...





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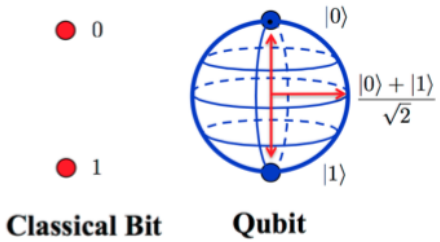
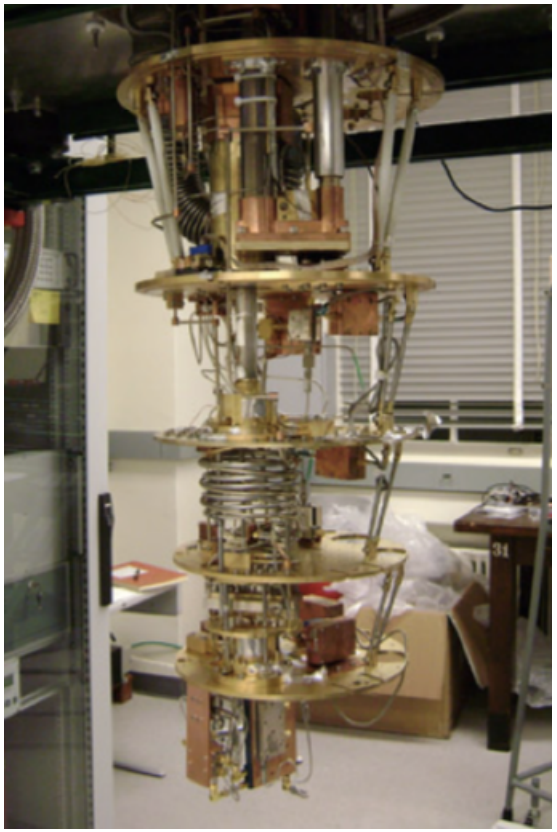


- Technical hurdles to create a QC:
  – *qubits* were difficult to create,
  – superconducting quantum processors needed to be cooled,
  – significant shielding required.
  $\hookrightarrow$ Currently, 72 qubits (Google) $\rightsquigarrow$ go to thousands and beyond.
  – significant error correction.
  – create a truly fault-tolerant quantum computer.



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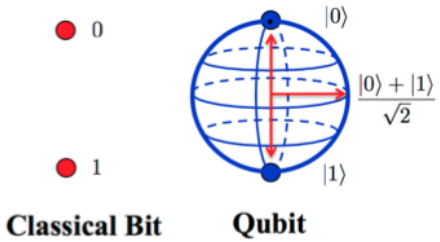

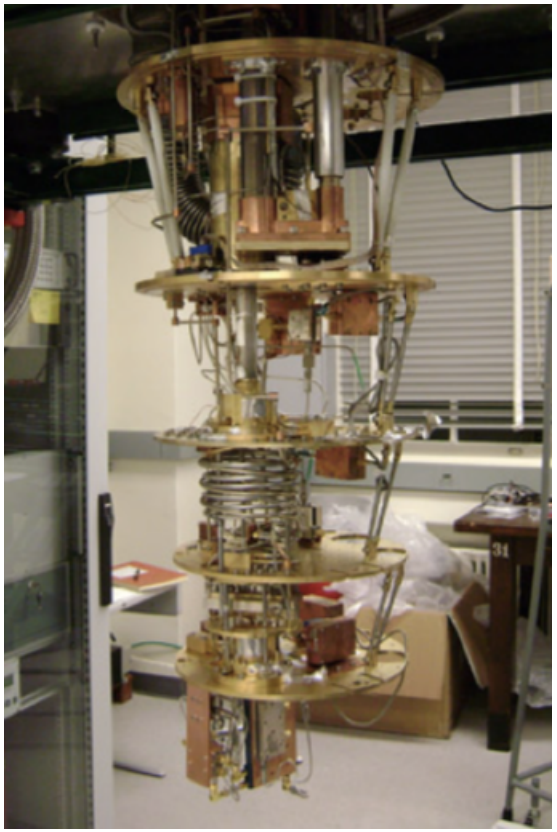

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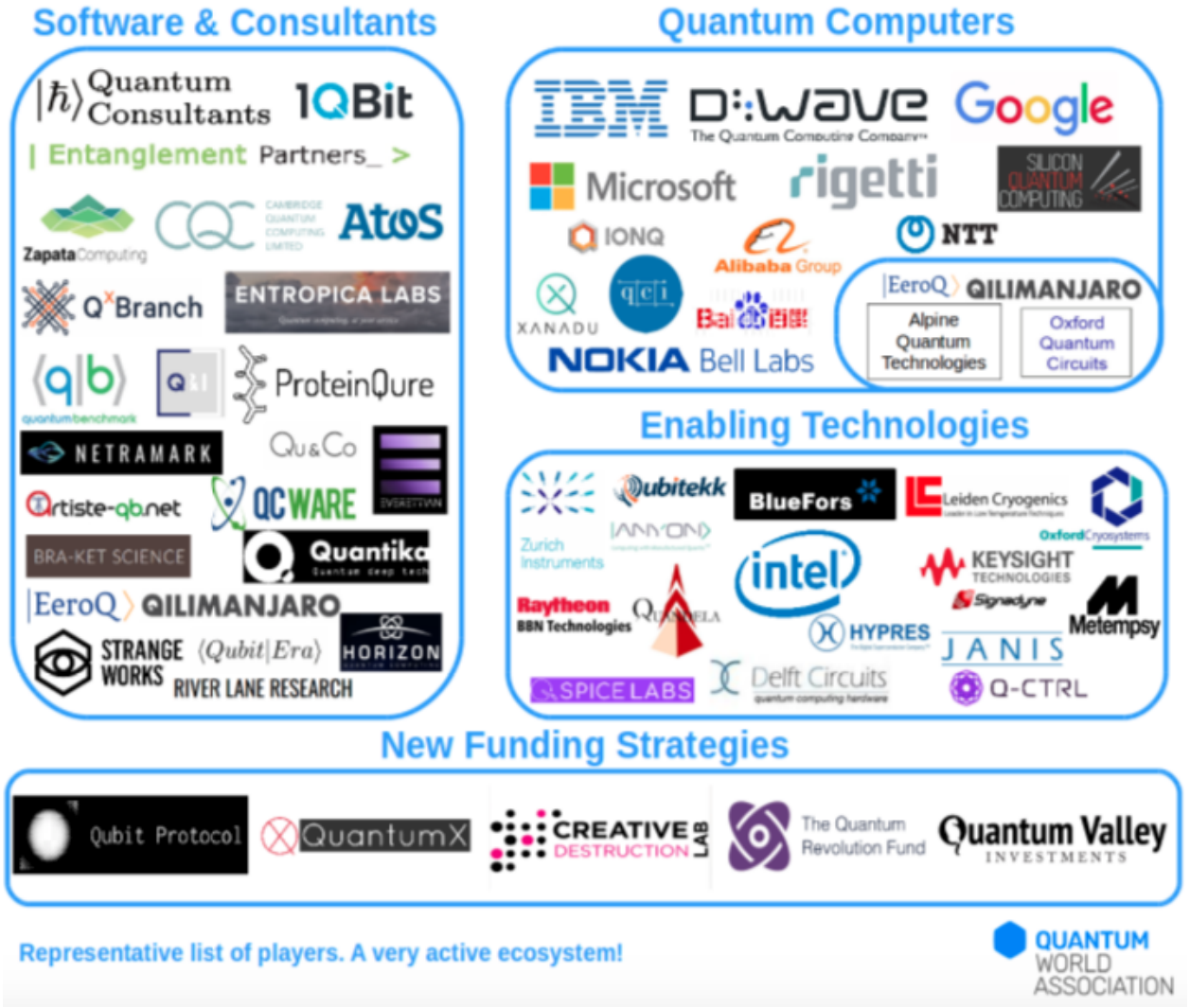
- Recent key developments
  - new hardware and online resources.
  - increasing business interest in future commercial application.
  - significant discussion of "quantum supremacy".

Recent developments in Quantum Computing



- Quantum Flagship $\rightsquigarrow$ a large-scale European research program for quantum technologies (>1 billion €).

What is a QC good for?

- Factoring large numbers
  $15 = 5 \times 3$, $21 = 3 \times 7$, $8193 = 3 \times 2731$ $\rightsquigarrow$ Schor's Algorithm

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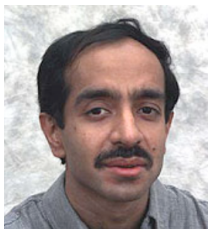

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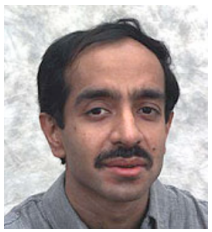
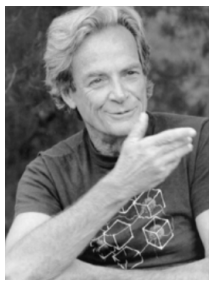


- Simulate quantum systems $\rightsquigarrow$ original Feynman's proposal



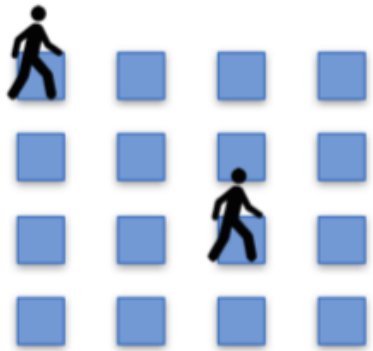
"... because nature isn't classical, dammit,
and if you want to make a simulation of nature,
you'd better make it quantum mechanical."

Quantum simulation

- *Why?*

Quantum simulation

- *Why?*
- Imagine a simple scenario...



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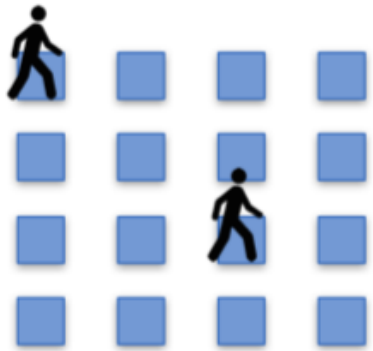

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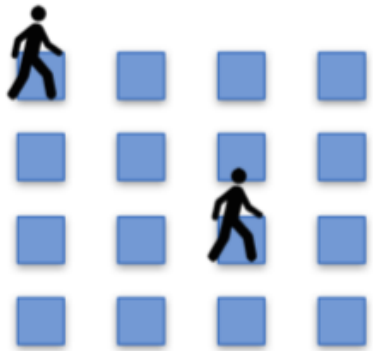

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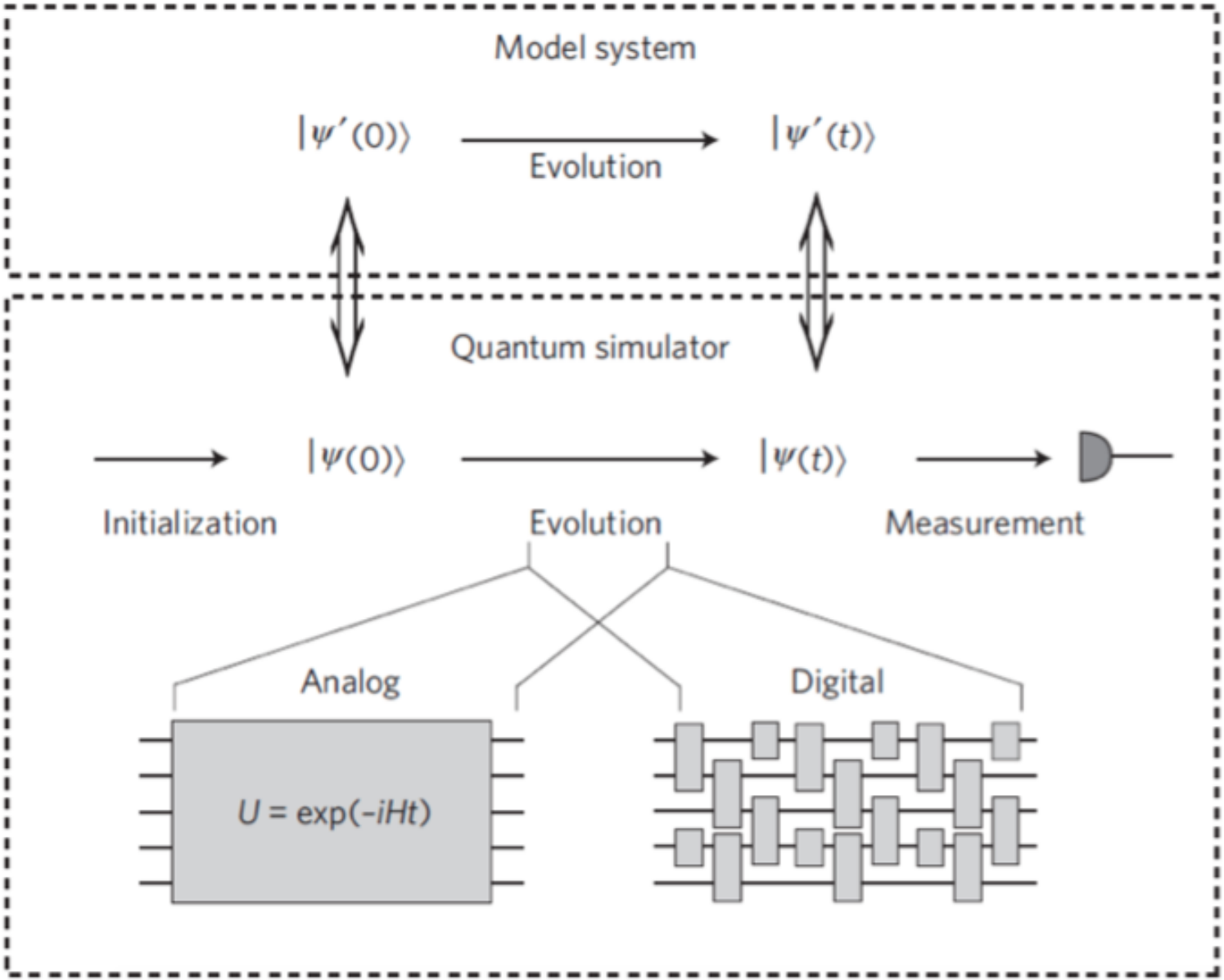
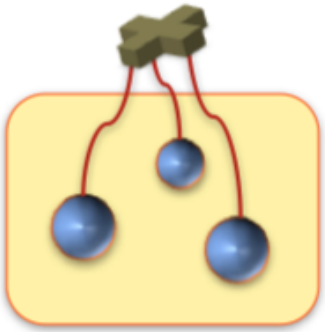
- For a complex system, *"highly entangled"*, a classical probabilistic computing machine simply **cannot reproduce** the required quantum probability distributions!
- In fact, it is *precisely* the chance of preparing and manipulating **entangled states**, together with the **superposition principle**, that allows for the *computational quantum advantage*.

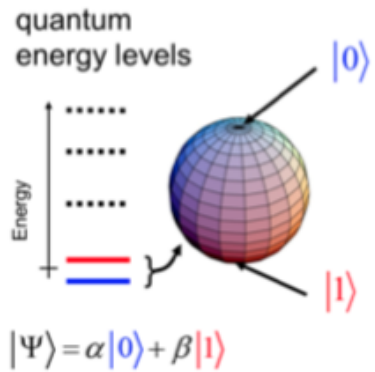
Quantum simulation - time evolution of a system



Richard Feynman - *Simulating Physics with computers*

- *"If you had discrete quantum systems, what other discrete quantum systems are exact imitators of it, and is there a class against which everything can be matched?"*





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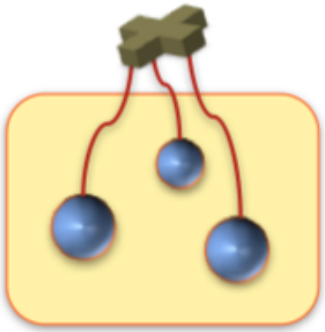
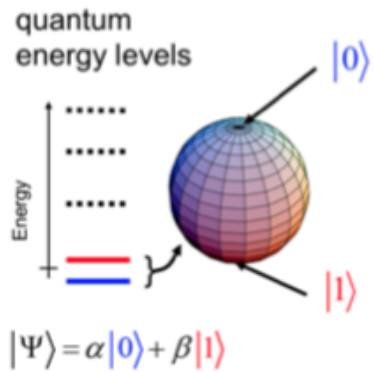




- .... *Yes!* $\rightsquigarrow$ *Digital quantum computing*

  Seth Loyd 1998: efficient technique for the quantum simulation of time-evolving physical systems

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle, \qquad \hat{U}(t) = e^{-i\hat{H}t/h},$$

  using Lie-Trotter expansions $\hat{U}(t) = \left[\hat{U}(t/n)\right]^n$

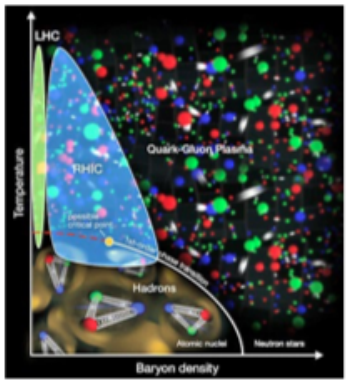
$$\hat{U}(t/n) = e^{-i\hat{H}t/nh} \approx e^{-i\hat{H}_1 t/nh} e^{-i\hat{H}_2 t/nh} \ldots,.$$

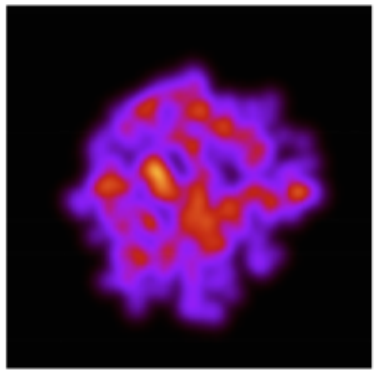
  with $\hat{H} = \hat{H}_1 + \hat{H}_2 + \ldots$ $\rightsquigarrow$ *quantum gates, quantum circuits*

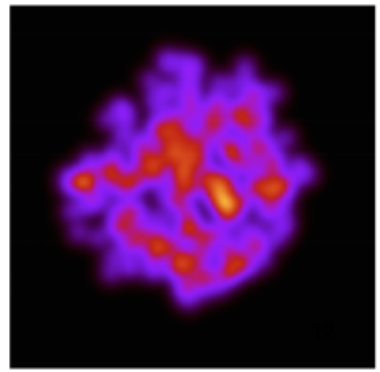
Motivation from QCD

Even with some *remarkable* improvements over the last years, Lattice QCD faces some challenges:

- the well-known sign problem.
  $\hookrightarrow$ If we are interested in the time evolution of systems with baryon number, isospin, electric charge, strangeness, etc. *...or* currents, viscosity, non-equilibrium dynamics $\rightsquigarrow$ real-time evolution.







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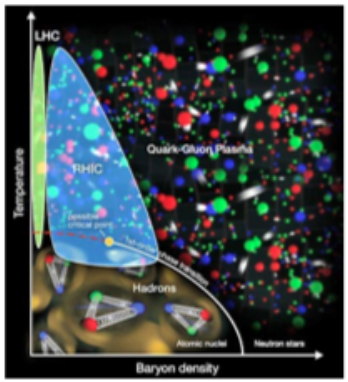

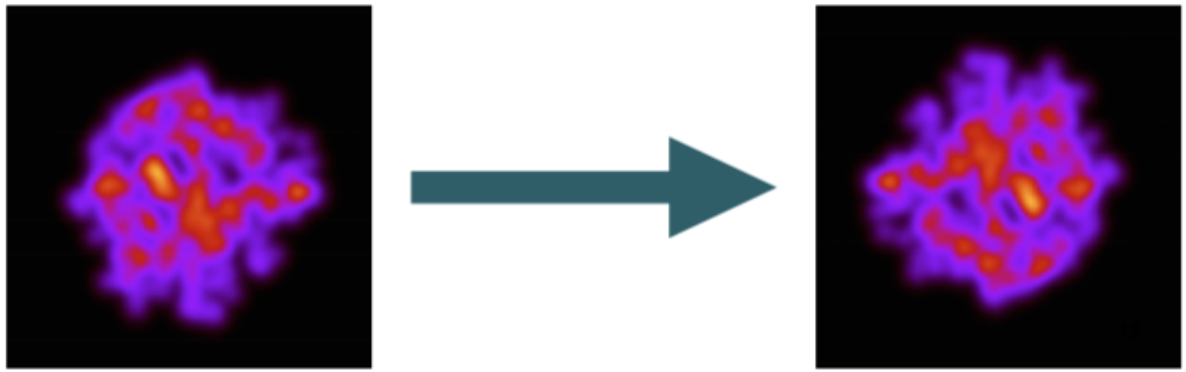

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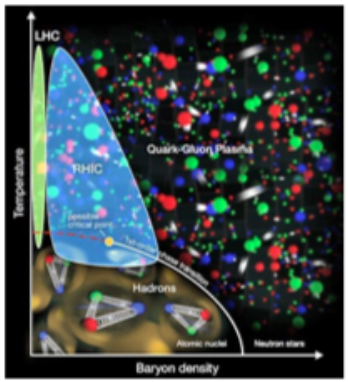
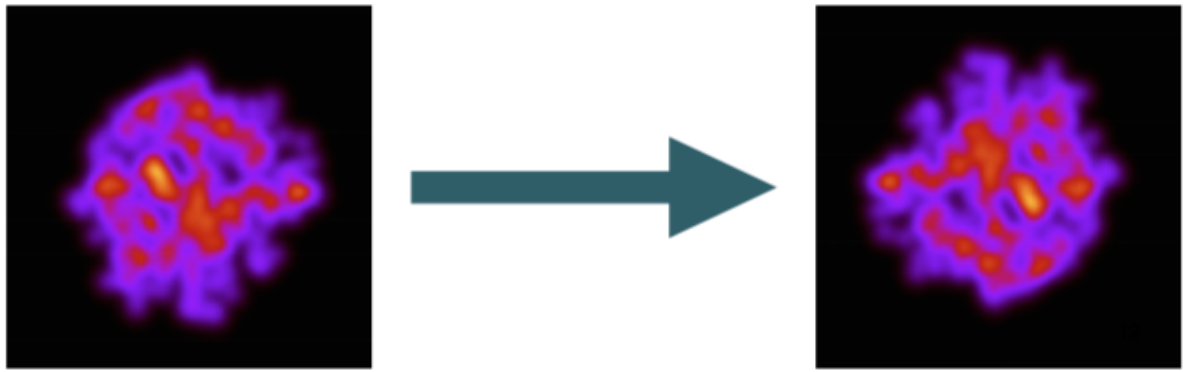


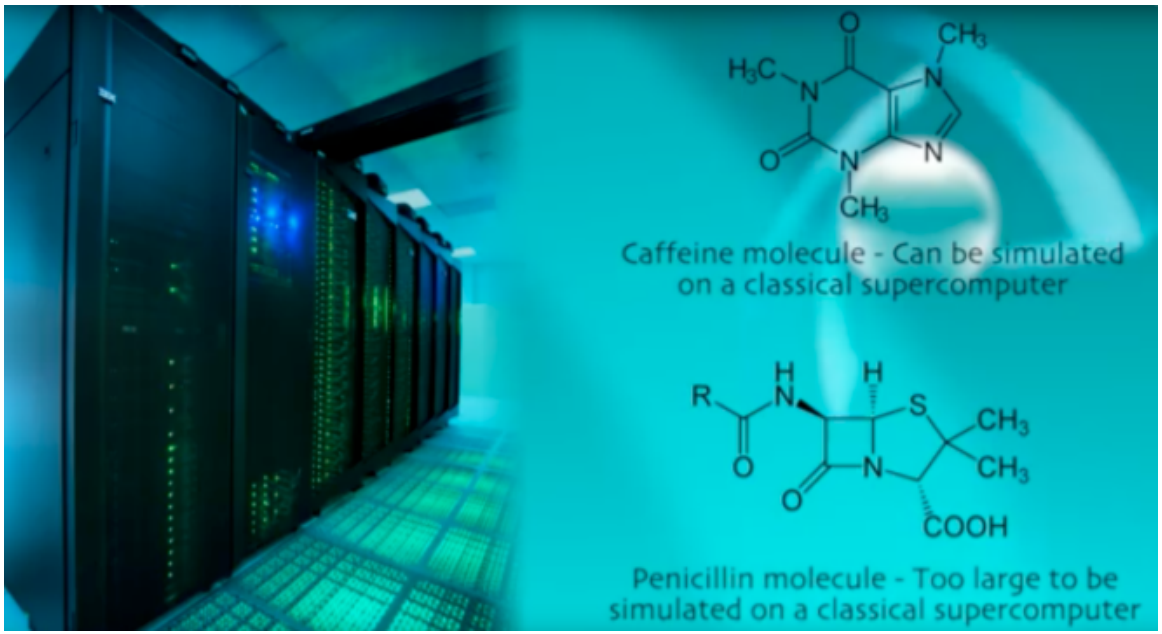


- Required computational power can be excessive, even for the current most powerful superconductors
  $\hookrightarrow$ *Can we make use of quantum supremacy in the future?*
- What about bound-states in equilibrium?
  $H_{eff.}|\Psi\rangle = E|\Psi\rangle \rightarrow$ for instance, finding lowest **E**?
  $\hookrightarrow$ *Can we simulate hadrons on a quantum computer?*

Ideal systems for quantum simulation - Molecules

Why ideal?... $H|\Psi\rangle = E|\Psi\rangle$

- *"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."* - P.Dirac



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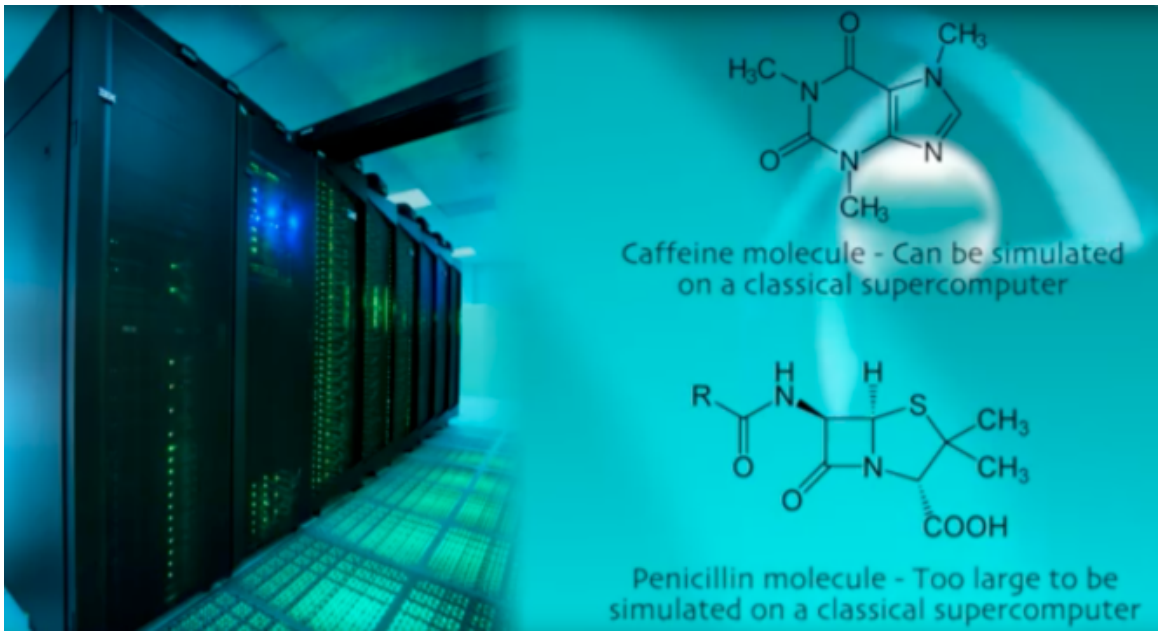
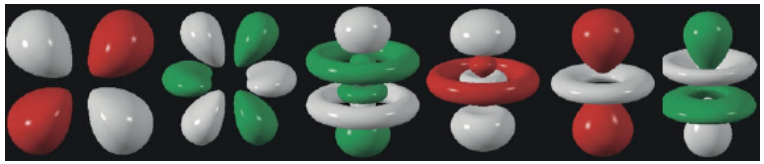


- Molecular electronic Hamiltonian (in Born Oppenheimer approx.):

$$H = \sum_{i=1}^{n_e} \left(-\frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_A^{n_N} \frac{Z_A}{4\pi\epsilon_0|\vec{r}_i - \vec{R}_A|} \right) + \sum_{i<j}^{n_e} \frac{e^2}{4\pi\epsilon_0|\vec{r}_i - \vec{r}_j|}$$

Ideal systems for quantum simulation - Molecules

- To represent as a N-qubit problem we must discretize $\rightsquigarrow$ basis of Molecular orbitals



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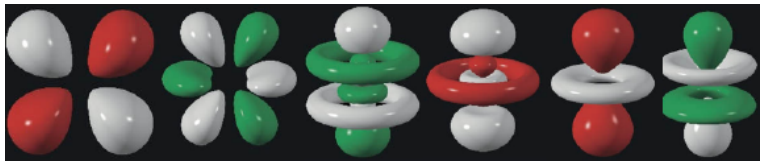

- For each orbital define $\hat{a}_k$ and $\hat{a}_k^\dagger$ satisfying:

$$\{\hat{a}_j, \hat{a}_k\} = \{\hat{a}_j^\dagger, \hat{a}_k^\dagger\} = 0, \quad \{\hat{a}_j, \hat{a}_k^\dagger\} = \delta_{jk}\mathbb{I}$$

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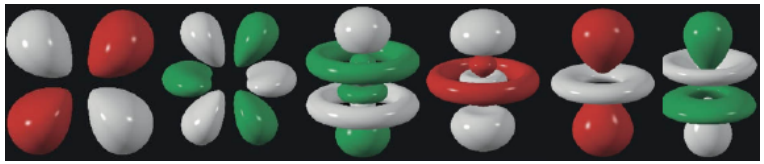

- For each orbital define $\hat{a}_k$ and $\hat{a}_k^\dagger$ satisfying:

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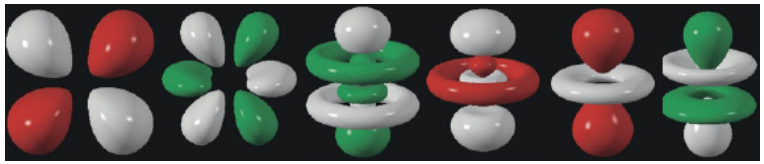

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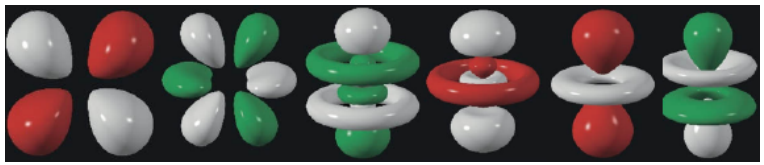

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- Obtain an Hamiltonian expressed in the basis of Pauli operators $\{\mathbb{I}^i, \sigma_\alpha^i\}$, for each nuclear configuration R. Example for $N = 2$:

$$\hat{H}(R) = \sum_{ij}^{\alpha\beta} g_{ij}(R)\hat{\sigma}_\alpha^i \hat{\sigma}_\beta^j.$$

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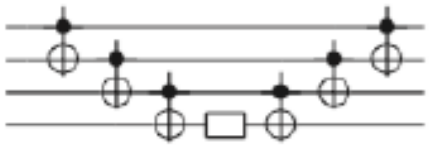
- Construct the associated quantum circuit.



Variational Quantum Eigensolver (VQE)

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     ✓ **Easy task for a QC...** *ex: Measurements of* $< \sigma_i^z >, < \sigma_1^z \sigma_2^z ... \sigma_n^z >, ...$
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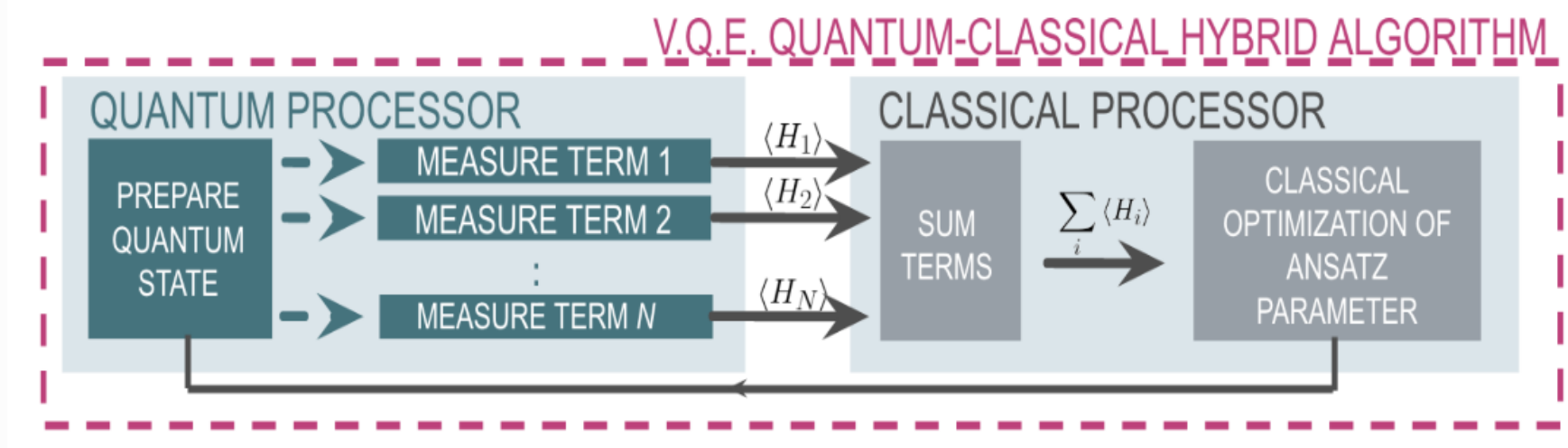
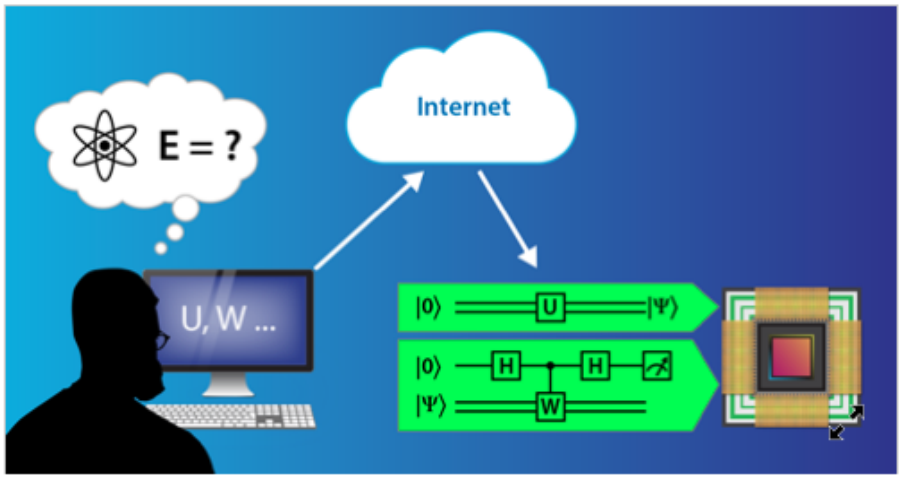
- We get an expectation value dependent on $\vec{\theta}$ parameters. This value can be minimized with a gradient-free optimization method such as Nelder-Mead method on the classical computer.

VQE Quantum-classical hybrid algorithm

- In summary...

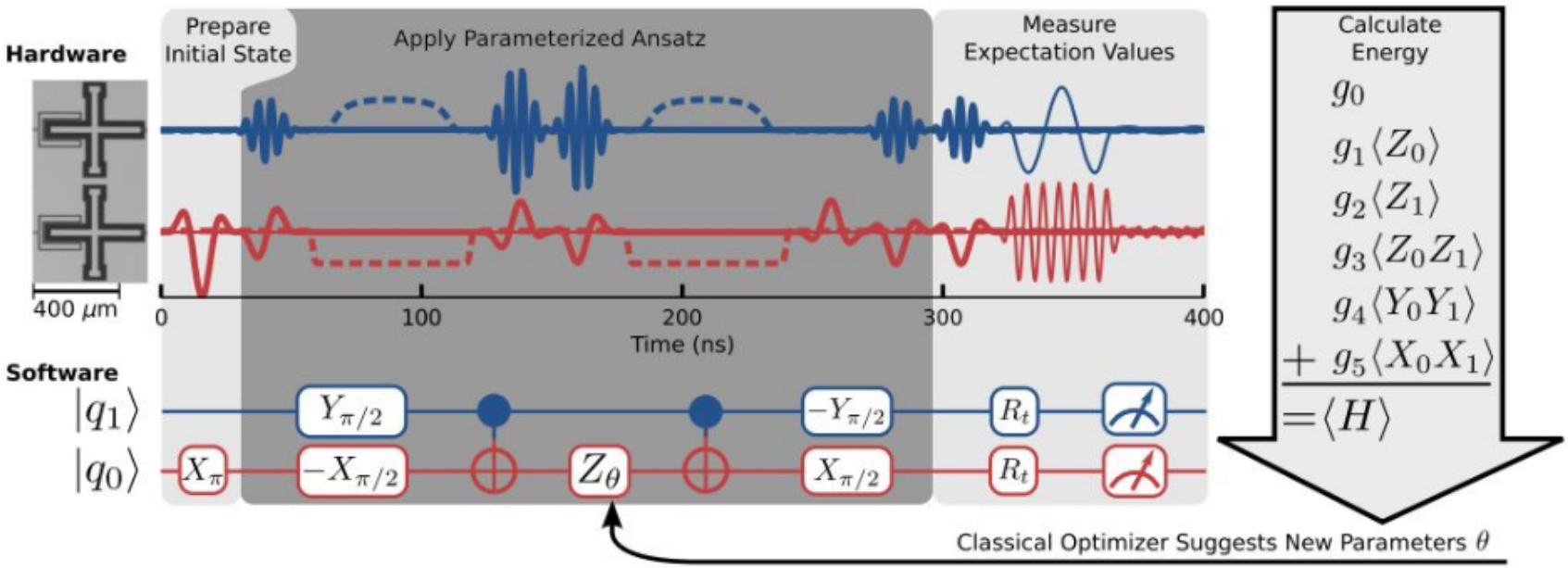


- It is *now a reality*, to use a cloud-based quantum computing (Google, D-Wave, Rigetti, IBM, ...)

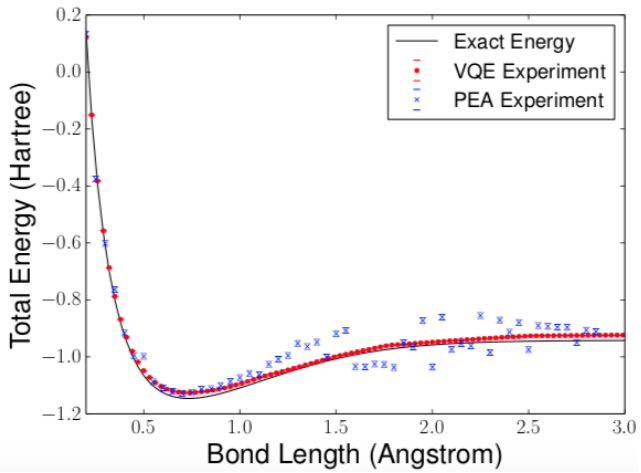


Results using VQE

- H2 molecule using Google's quantum computer (only 2 qubits)

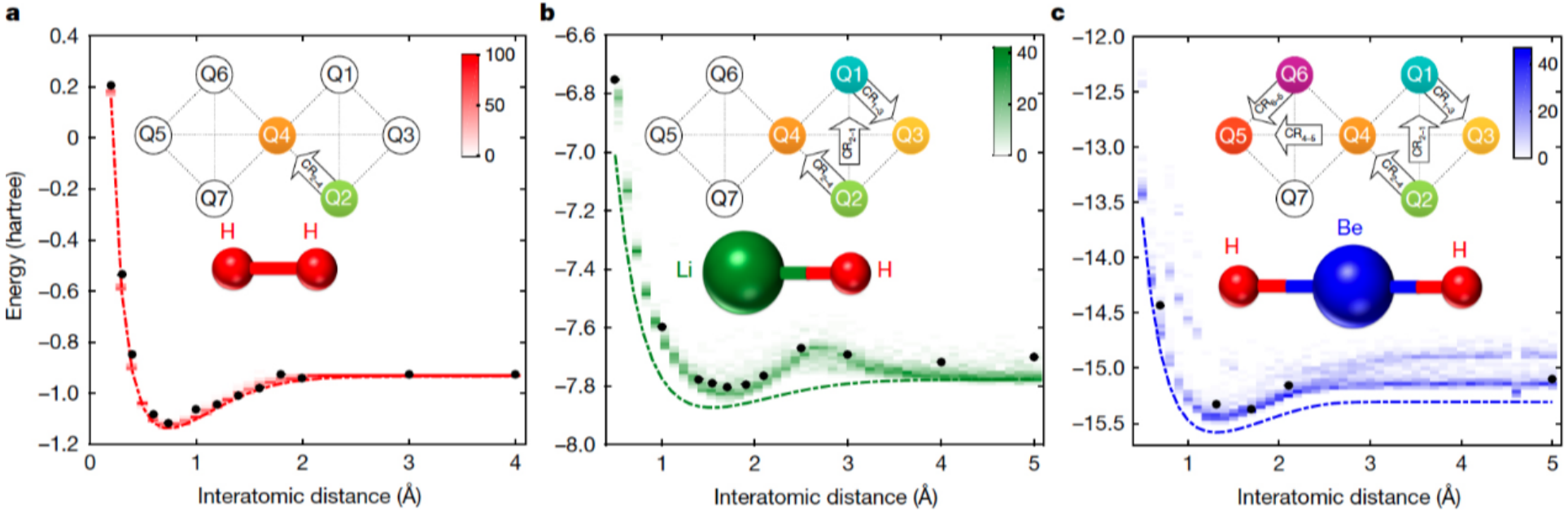


P.J.J. O'Malley et al. *Scalable Simulation of Molecular Energies* Physical Review X (2016). DOI: 10.1103/PhysRevX.6.031007



Results using VQE

- Results using the IBM quantum computer (up to 6 qubits)



Abhinav Kandala et al. *Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets*, Nature (2017). DOI: 10.1038/nature23879

Quantum simulation of the deuteron

PHYSICAL REVIEW LETTERS **120,** 210501 (2018)

Editors' Suggestion | Featured in Physics

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,†]

[1]*Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
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[3]*Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[4]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
[5]*National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

(Received 12 January 2018; published 23 May 2018)

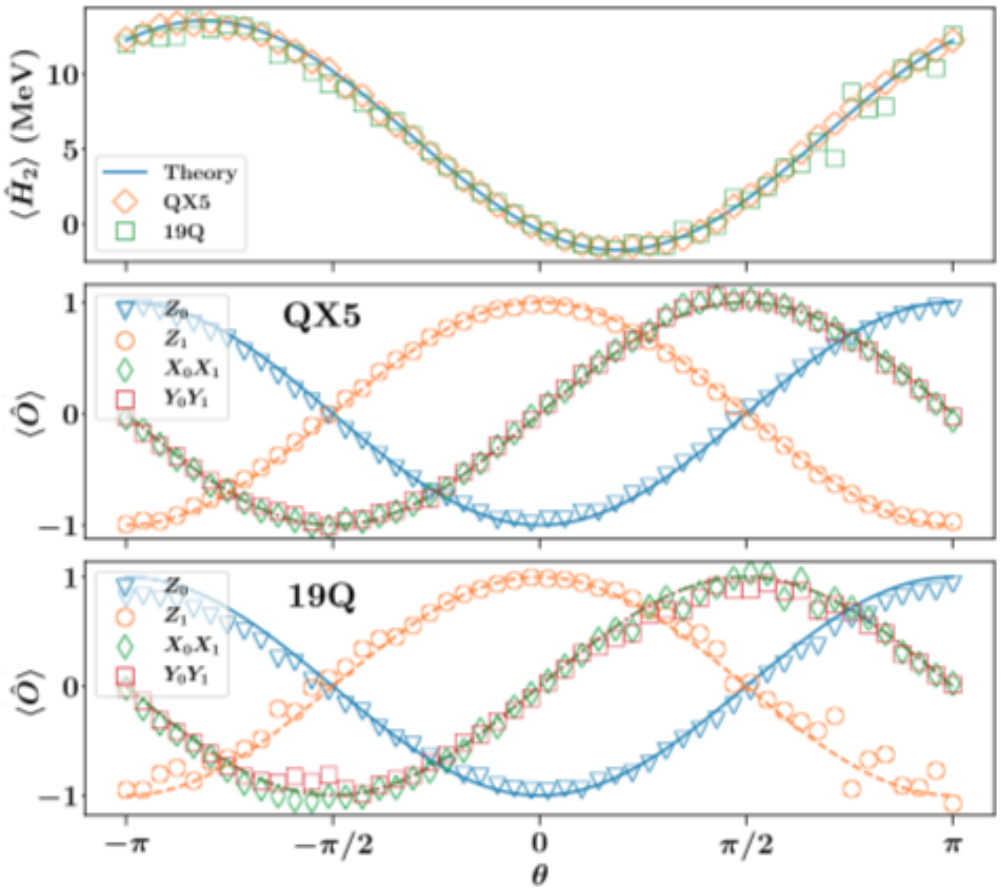
We report a quantum simulation of the deuteron binding energy on quantum processors accessed via cloud servers. We use a Hamiltonian from pionless effective field theory at leading order. We design a low-depth version of the unitary coupled-cluster ansatz, use the variational quantum eigensolver algorithm, and compute the binding energy to within a few percent. Our work is the first step towards scalable nuclear structure computations on a quantum processor via the cloud, and it sheds light on how to map scientific computing applications onto nascent quantum devices.

DOI: 10.1103/PhysRevLett.120.210501

- Results using IBM QX5 and Rigetti 19Q quantum chips, using 2 and 3 qubits.

Quantum simulation of the deuteron

- The deuteron ground-state energy is -2.22 MeV $\rightsquigarrow$ extrapolation to infinite space is within 3% of the exact result.



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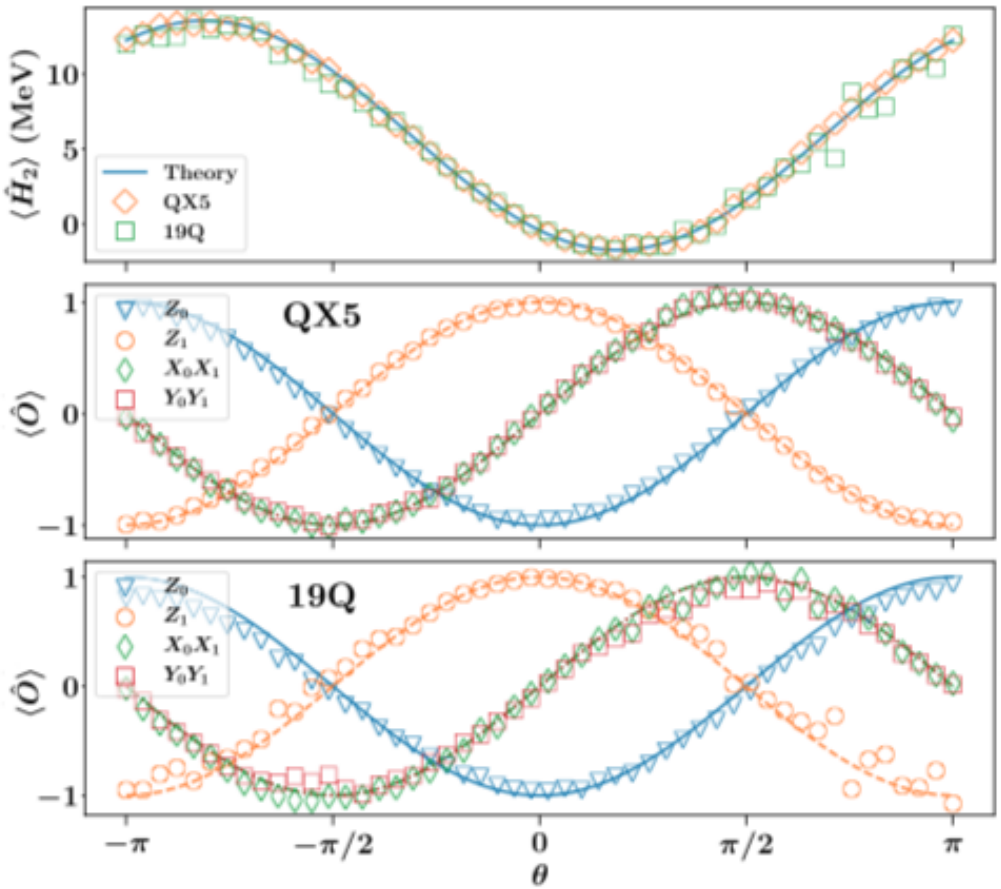

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- *Can we compute binding energies of hadrons on a quantum computer?... Yes!*

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- The future is both challenging and promising!

Acknowledgements

Thank you for your attention!

We gratefully acknowledge the support from:

John Templeton Foundation

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FCT Fundação para a Ciência e a Tecnologia
MINISTÉRIO DA EDUCAÇÃO E CIÊNCIA

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IST, 26 September 2018

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