Quantum algorithms for Nuclear Physics II

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FRIB
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LEADERSHIP COMPUTING FACILITY

Outline

Scale invariance

Quantum scale anomalies

Realization with trapped ions

Discrete scale invariance for two bosons

Time fractals

Variational quantum eigensolver

Cloud quantum computing of the deuteron

Scale invariance

Start with a one-dimensional classical Hamiltonian $H(p, r)$ with momentum p and position r. Suppose that the Hamiltonian can be written in the form

$$H(p, r) = p^{\gamma} h(pr)$$

We can show that this classical system is scale invariant. Consider any simultaneous rescaling of p and r where

$$r \rightarrow r' = \lambda r, \; p \rightarrow p' = \lambda^{-1} p$$

The Hamiltonian transforms as

$$H(p, r) \rightarrow H(p', r') = \lambda^{-\gamma} H(p, r)$$

D.L., Watkins, Frame, Given, He, Li, Lu, Sarkar, PRA 100, 011403(R) (2019)

Let us also rescale time t as

$$t \to t' = \lambda^{\gamma} t$$

The equations of motion are

$$\frac{dp}{dt} = -\frac{\partial H(p,r)}{\partial r}, \quad \frac{dr}{dt} = \frac{\partial H(p,r)}{\partial p}$$

Exactly the same equations of motion hold for the rescaled variables with the same functional form for the Hamiltonian H,

$$\frac{dp'}{dt'} = -\frac{\partial H(p',r')}{\partial r'}, \quad \frac{dr'}{dt'} = \frac{\partial H(p',r')}{\partial p'}$$

We conclude that the system is scale invariant.

Quantum scale anomalies

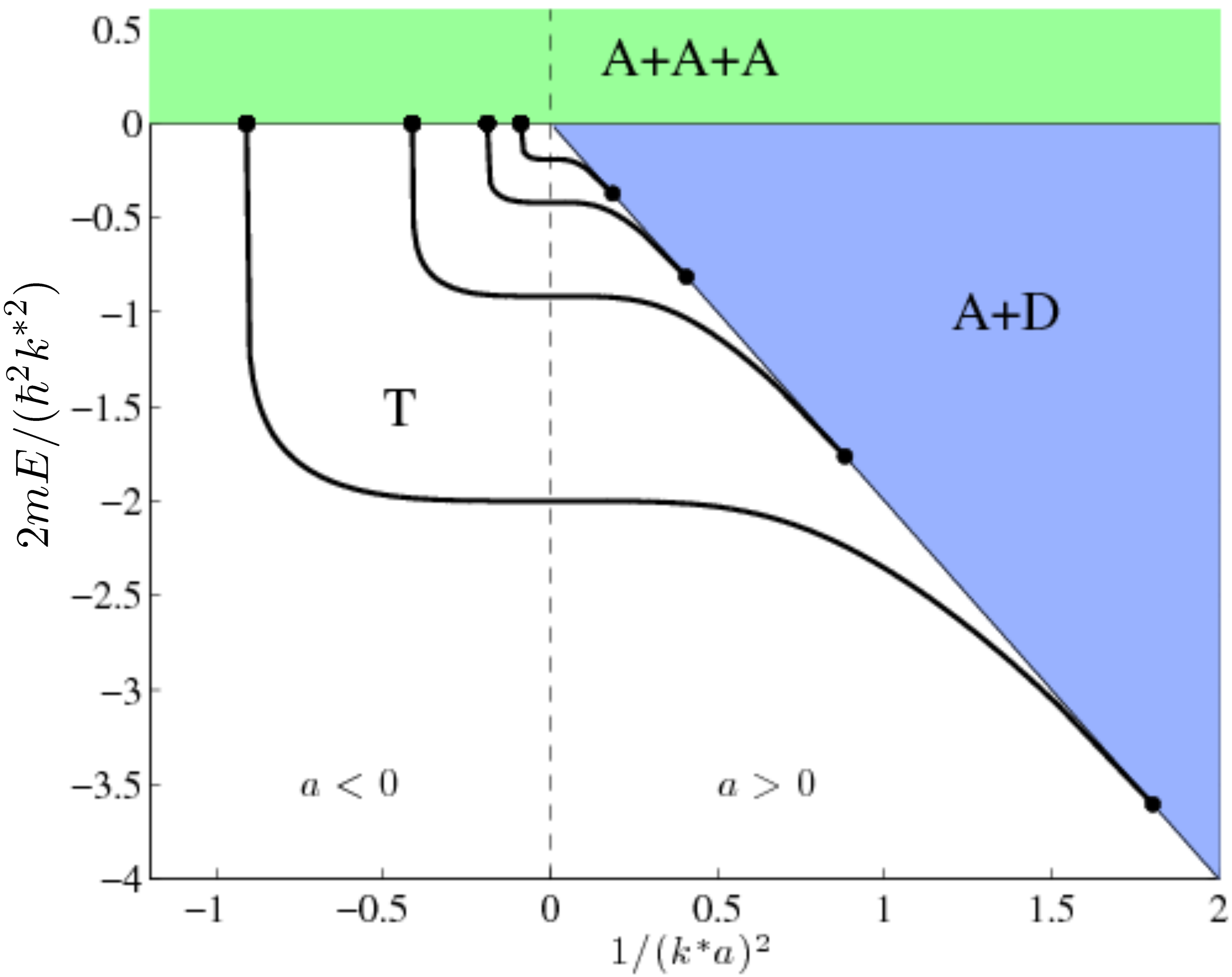
In quantum mechanics and quantum field theory, scale invariance can be spoiled by quantum scale anomalies. This happens when there are bound states, which necessarily correspond to discrete energy levels.

Nevertheless it may happen that a discrete subgroup of the scale symmetry is preserved for the dynamics of certain sectors of the Hilbert space.

This phenomenon was first noted by Efimov for bound states of three bosons when the two-body interactions are pointlike and the interaction strength is tuned to produce a zero-energy two-body resonance.

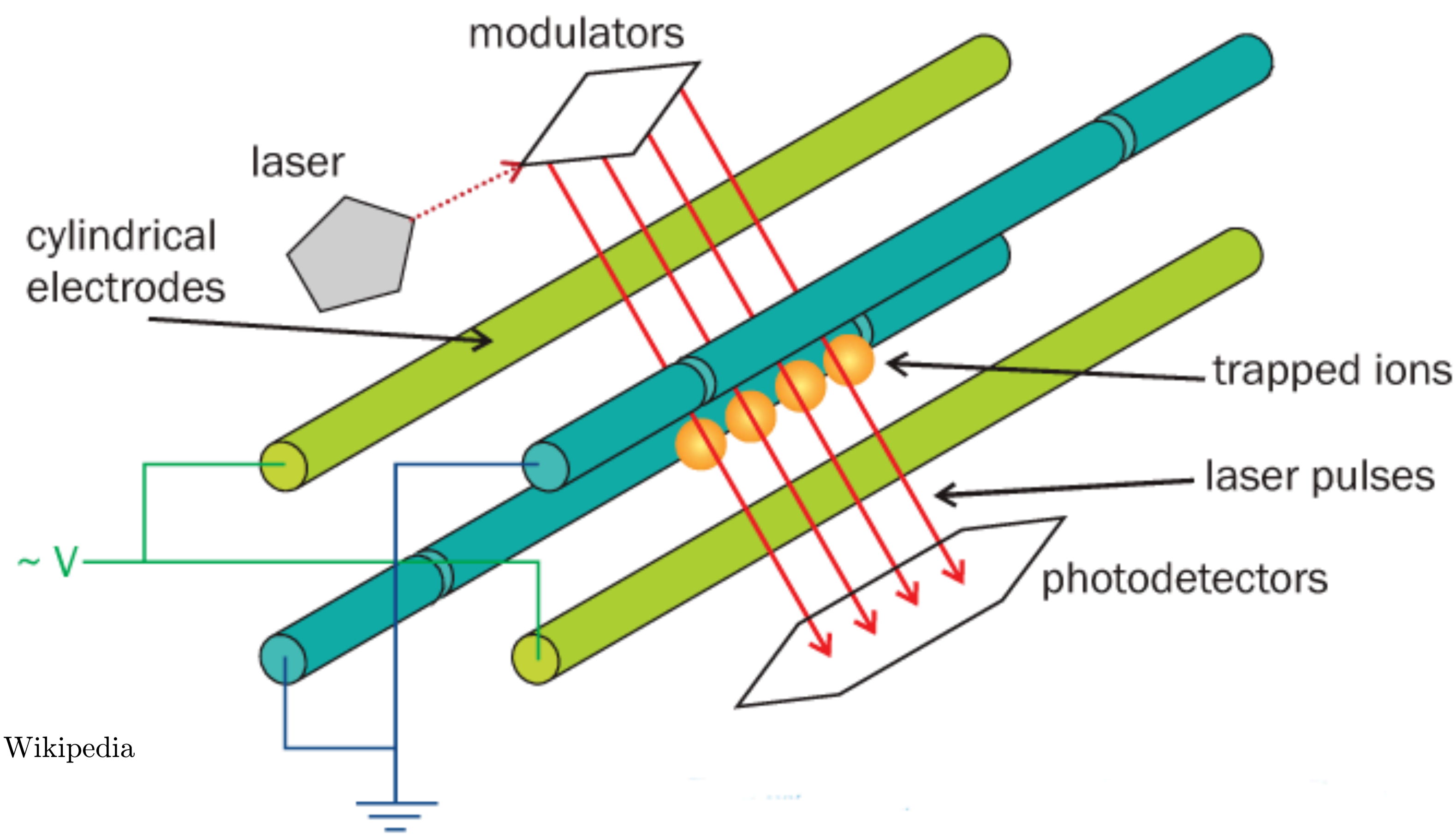
Efimov, Sov. J. Nucl. Phys. 12, 589 (1971); Efimov, Phys. Rev. C47 1876 (1993)
Bedaque, Hammer, van Kolck, Phys. Rev. Lett. 82 463 (1999)

Efimov trimers

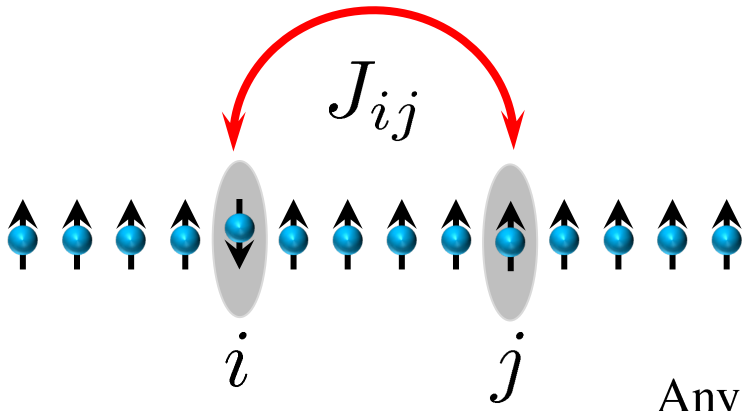


Zinner *et al.*, J. Phys. G40 053101 (2013)

Realization with trapped ions

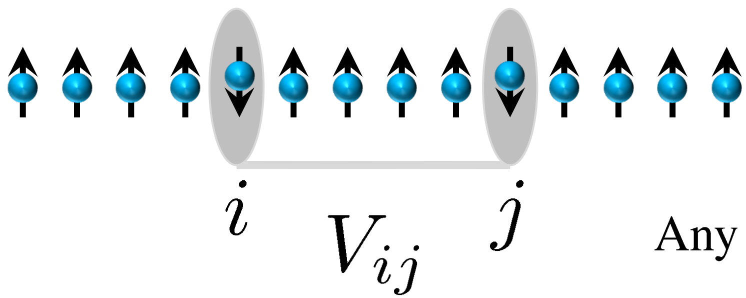


Wikipedia



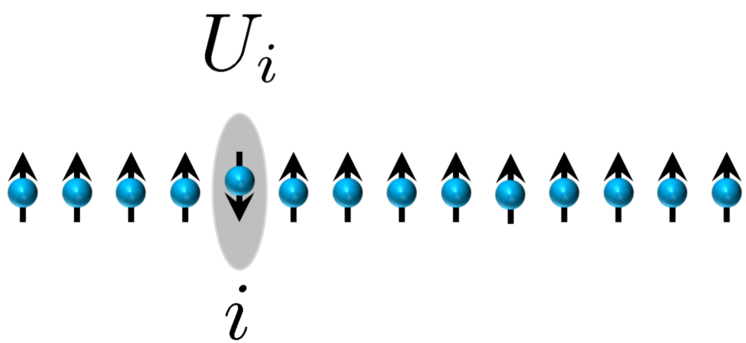
$$J_{ij} = \frac{J_0}{|r_i - r_j|^\alpha}$$

Any $0 < \alpha < 3$, but $0.5 < \alpha < 1.8$ favored.



$$V_{ij} = \frac{V_0}{|r_i - r_j|^\beta}$$

Any $0 < \beta < 3$, but $0.5 < \beta < 1.8$ favored.



Zhang *et al.*, Nature 543, 217 (2017), Zhang *et al.*, Nature 551, 601 (2017)

Our trapped ion Hamiltonian has the form

$$H = T + V_2 + U + C$$

where

$$T = \frac{1}{4} \sum_i \sum_{j \neq i} J_{ij} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y)$$

$$V_2 = \frac{1}{8} \sum_i \sum_{j \neq i} V_{ij} (1 - \sigma_i^z)(1 - \sigma_j^z)$$

$$U = \frac{1}{2} \sum_i U_i (1 - \sigma_i^z)$$

and C is a constant.

We can rewrite the Ising-like terms in the Hamiltonian as

$$V_2 + U = \frac{1}{8}\sum_i \sum_{j\neq i} V_{ij}\sigma_i^z \sigma_j^z - \frac{1}{2}\sum_i U_i' \sigma_i^z + C'$$

where

$$U_i' = U_i + \frac{1}{2}\sum_{i\neq j} V_{ij}$$

$$C' = \frac{1}{8}\sum_i \sum_{j\neq i} V_{ij} + \frac{1}{2}\sum_i U_i$$

We will regard the state with all spins pointing in the positive z direction as the vacuum state. Then any spin in the negative z direction can be regarded as a hardcore boson. It is not possible to have more than one hardcore boson on the same site.

In terms of the hardcore boson annihilation and creation operators, our Hamiltonian is now

$$H = \frac{1}{2}\sum_i \sum_{j\neq i} J_{ij}[b_i^\dagger b_j + b_j^\dagger b_i] + \frac{1}{2}\sum_i \sum_{j\neq i} V_{ij} b_i^\dagger b_i b_j^\dagger b_j + \sum_i U_i b_i^\dagger b_i + C$$

Let us now take

$$U_i = -\sum_{j\neq i} J_{ij} = -\sum_{j\neq i} \frac{J_0}{|r_i - r_j|^\alpha}$$

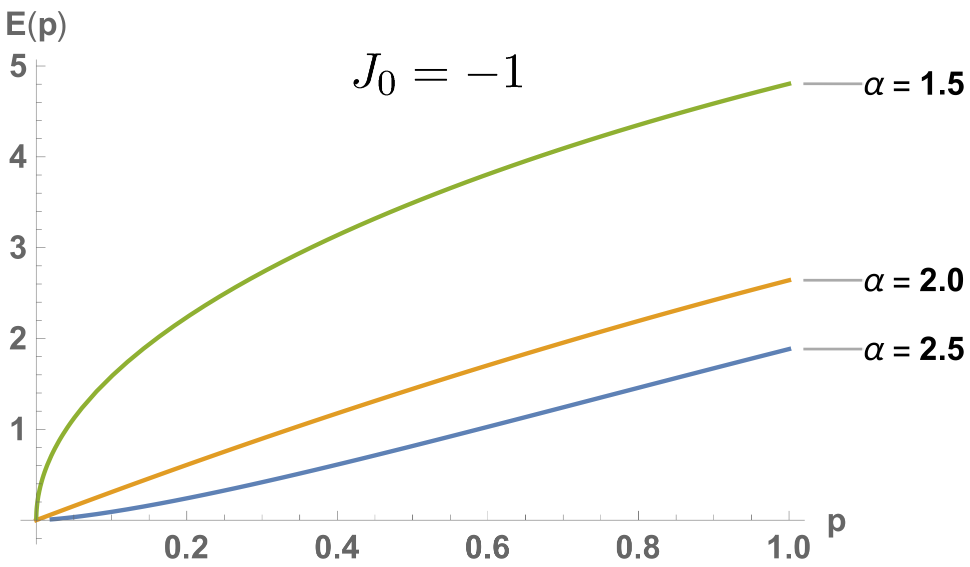
This choice ensures that a zero-momentum boson has zero energy. We now consider the dispersion relation for one boson.

For a boson with momentum p, the energy is

$$E(p) = 2J_0 \sum_{n>0} \frac{\cos(pn) - 1}{n^\alpha} = J_0 \left[\mathrm{Li}_\alpha(e^{ip}) + \mathrm{Li}_\alpha(e^{-ip}) - 2\mathrm{Li}_\alpha(1)\right]$$

At low momenta, this can be simplified as

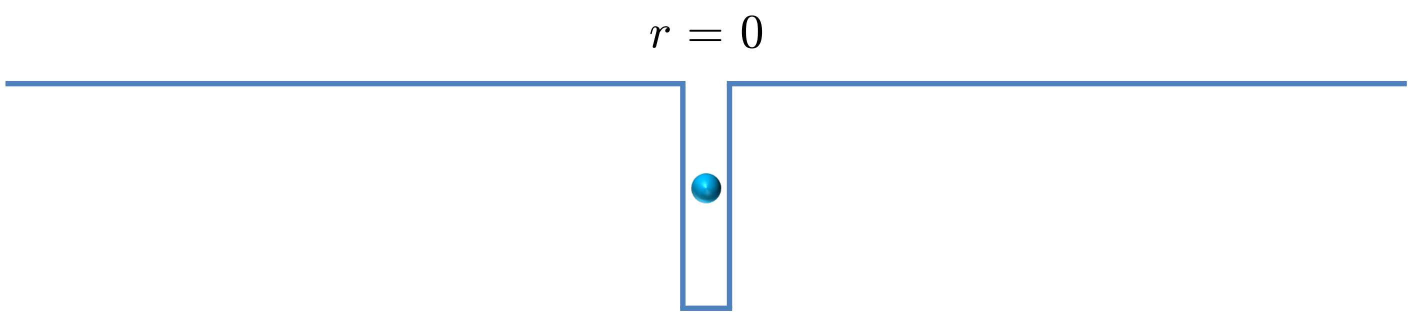
$$E(p) = 2J_0 \sin(\alpha\pi/2)\Gamma(1-\alpha)|p|^{\alpha-1} + J_0\zeta(\alpha-2)p^2 + O(p^4) \;\text{ for } \alpha < 3$$



We now introduce a single-site deep trapping potential that traps one boson at some site i_0

$$U_i = -\sum_{j\neq i} \frac{J_0}{|r_i - r_j|^\alpha} - u\delta_{i,i_0} \qquad \text{for } u \gg 1$$

We choose the position of site i_0 to be $r = 0$. We subtract a constant from the Hamiltonian so that the energy of this state is exactly zero.



For future reference, we call this state $|o\rangle$.

Discrete scale invariance for two bosons

We now add one more boson to the system. We regard the immobile boson at $r = 0$ as a static source.

The low-energy effective Hamiltonian for the mobile boson is

$$H(p, r) = 2J_0 \sin(\alpha\pi/2)\Gamma(1-\alpha)|p|^{\alpha-1} + \frac{V_0}{|r|^{\beta}}$$

where we have dropped terms of $O(p^2)$. We will consider the case where both J_0 and V_0 are negative. In order that the Hamiltonian have classical scale invariance, we take $\beta = \alpha - 1$.

Therefore

$$H(p, r) = 2J_0 \sin(\alpha\pi/2)\Gamma(1-\alpha)|p|^{\alpha-1} + \frac{V_0}{|r|^{\alpha-1}}$$

In the limit of zero energy, the bound-state wave functions have the following forms for even and odd parity

$$\psi_+(r) = \frac{1}{2}\left(|r|^{i\delta_+} + |r|^{-i\bar{\delta}_+}\right)$$
$$\psi_-(r) = \frac{1}{2}\,\mathrm{sgn}(r)\left(|r|^{i\delta_-} + |r|^{-i\bar{\delta}_-}\right)$$

where

$$2J_0\delta_+\Gamma(1-\alpha)\sin(\alpha\pi/2)\Gamma(i\delta_+)\sinh(\delta_+\pi/2) = V_0\Gamma(2-\alpha+i\delta_+)\cos((\alpha-i\delta_+)\pi/2)$$

$$2J_0\delta_-\Gamma(1-\alpha)\sin(\alpha\pi/2)\Gamma(i\delta_-)\cosh(\delta_-\pi/2) = iV_0\Gamma(2-\alpha+i\delta_-)\sin((\alpha-i\delta_-)\pi/2)$$

The case $\alpha = 2$ corresponds to a Hamiltonian of the form

$$H(p,r) = -\pi J_0|p| + \frac{V_0}{|r|}$$

For the case $\alpha = 2$,

$$\delta_+ = \frac{V_0}{J_0 \pi} \coth(\delta_+ \pi/2), \quad \delta_- = \frac{V_0}{J_0 \pi} \tanh(\delta_- \pi/2)$$

We can rewrite the zero-energy bound-state solutions as

$$\psi_+(r) = \cos[\delta_+ \ln(|r|)], \quad \psi_-(r) = \mathrm{sgn}(r) \cos[\delta_- \ln(|r|)]$$

Under the scale transformations $r \to \lambda_\pm r$,

$$\psi_+(r) \to \cos[\delta_+ \ln(|r|) + \delta_+ \ln(\lambda_+)]$$

$$\psi_-(r) \to \mathrm{sgn}(r) \cos[\delta_- \ln(|r|) + \delta_- \ln(\lambda_-)]$$

The wave functions exhibit discrete scale invariance when the scale factors are

$$\lambda_+ = \exp(\pi/\delta_+), \quad \lambda_- = \exp(\pi/\delta_-)$$

The bound state energies form a geometric progression

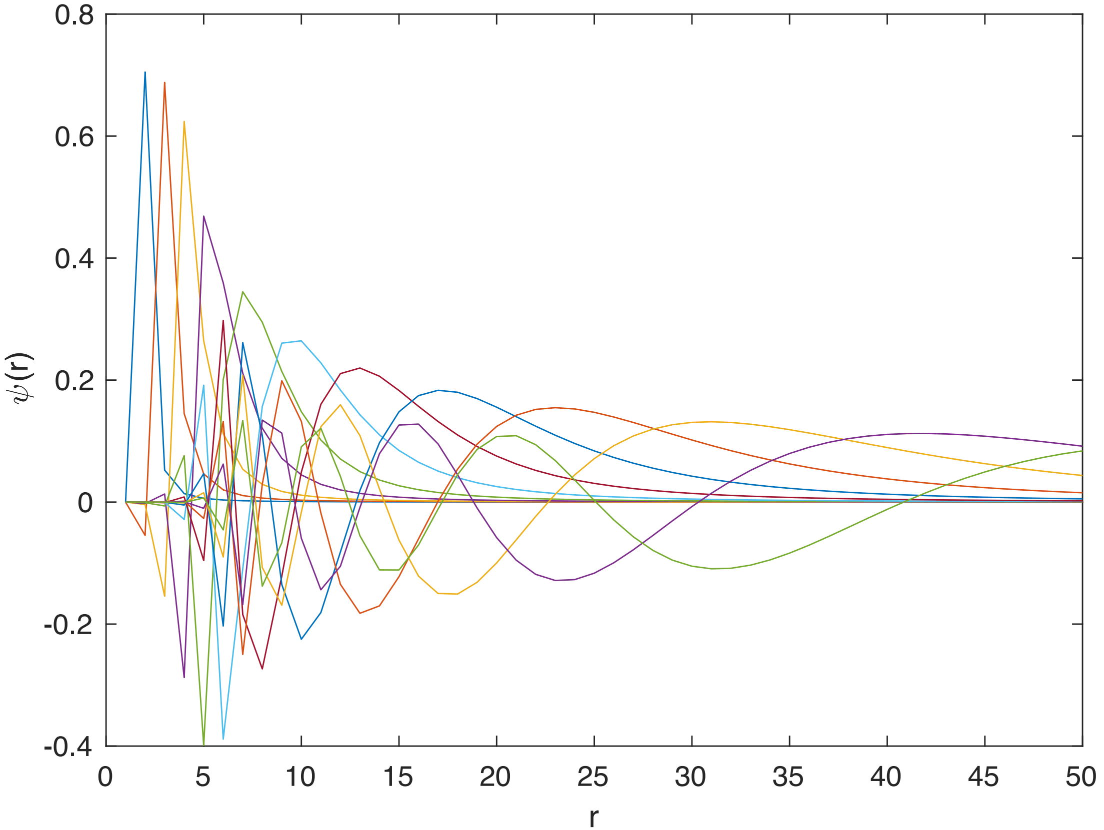
$$E_+^{(n)} = \epsilon_+ \lambda_+^{-n}, \quad E_-^{(n)} = \epsilon_- \lambda_-^{-n}$$

The general formulae are

$$\lambda_+ = \exp(\pi/\mathrm{Re}\,\delta_+), \quad \lambda_- = \exp(\pi/\mathrm{Re}\,\delta_-)$$

$$E_+^{(n)} = \epsilon_+ \lambda_+^{-(\alpha-1)n}, \quad E_-^{(n)} = \epsilon_- \lambda_-^{-(\alpha-1)n}$$

The first twelve even-parity bound-state wave functions:



$\alpha = 2$, $\beta = 1$, $J_0 = -1$, and $V_0 = -30$

n	$E_+^{(n)}$	$E_+^{(n-1)}/E_+^{(n)}$	$E_-^{(n)}$	$E_-^{(n-1)}/E_+^{(n)}$
0	-27.05304149	–	-26.5188669	–
1	-11.93067205	2.267520336	-11.79861873	2.247624701
2	-6.977774689	1.709810446	-6.919891389	1.705029468
3	-4.553270276	1.5324754	-4.521425357	1.530466798
4	-3.139972298	1.450098869	-3.120231851	1.449067112
5	-2.233327278	1.405961557	-2.220194049	1.405386998
6	-1.617052389	1.381110033	-1.607920414	1.380786033
7	-1.182654461	1.367307563	-1.176124883	1.367134084
8	-0.869406941	1.360300229	-0.864656962	1.360221377
9	-0.640405903	1.357587332	-0.636916042	1.357568195
10	-0.471738446	1.357544438	-0.469161911	1.357561276
11	-0.347112043	1.359037968	-0.345207121	1.359073675
12	-0.254996818	1.361240684	-0.253589633	1.361282464
13	-0.187011843	1.363532996	-0.18597462	1.363571189
theory	–	$\lambda_+ = 1.3895595319$	–	$\lambda_- = 1.3895595319$

Time fractals

We use a phase convention where all of the bound-state wave functions are real valued. Let us construct a coherent superposition of the first N even-parity bound states, where N is large.

$$|S\rangle = \sum_{n=0}^{N-1} |\psi_{+}^{(n)}\rangle$$

We could have just as easily chosen odd-parity bound states. We now consider the amplitude

$$A(t) = \mathrm{Re}[Z(t)], \quad Z(t) = \langle S| \exp(-iHt)|S\rangle$$

Aside from corrections of relative size $1/N$ from endpoint terms at $n = 0$ and $n = N - 1$, the amplitude is invariant under the discrete rescaling of time.

$$t \to \lambda_+^{\alpha-1} t$$

$$A(t) \to A(\lambda_+^{\alpha-1} t) = A(t) \cdot [1 + O(1/N)]$$

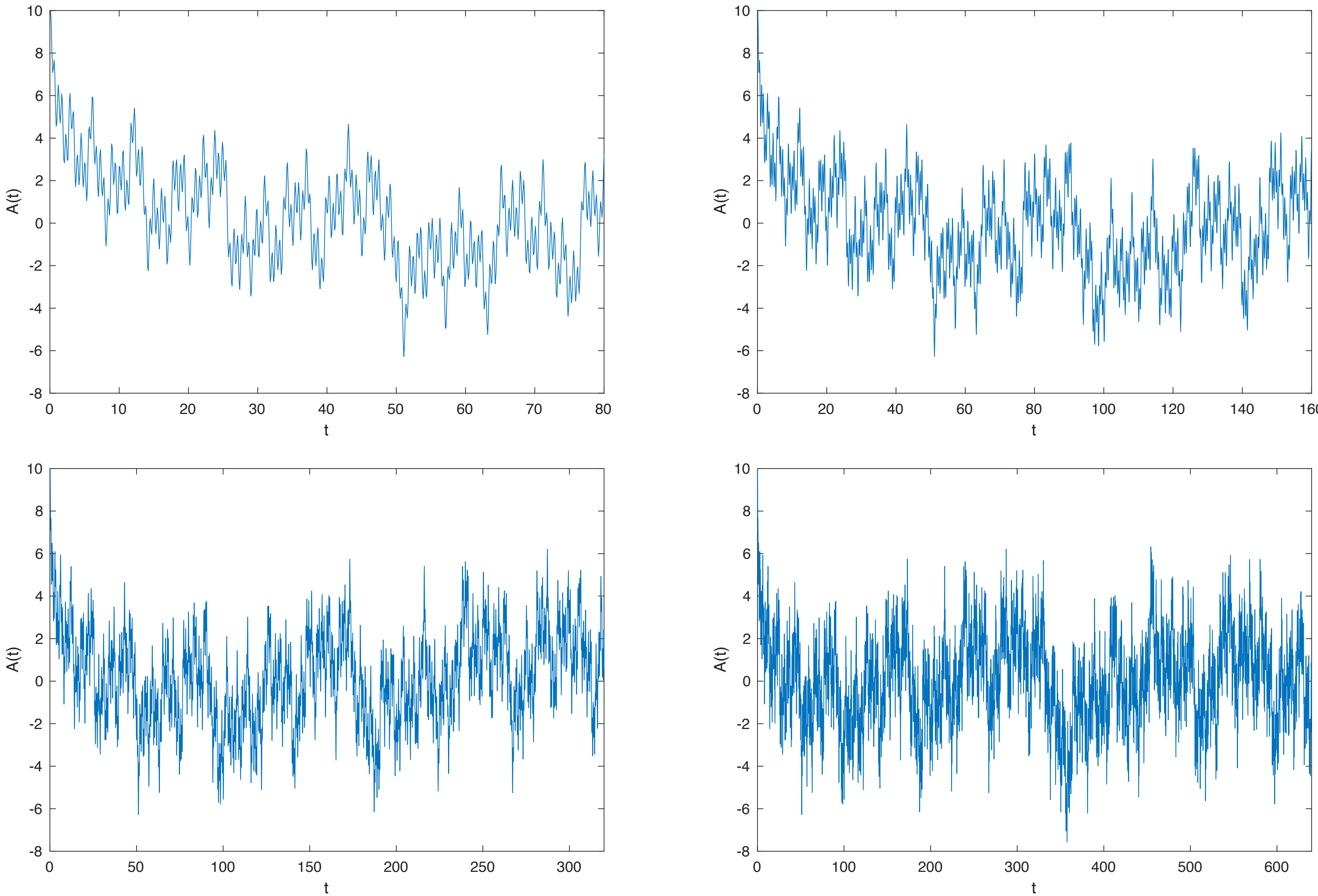
Given the self-replicating behavior of the amplitude under time rescaling, we call it a time fractal.

We choose an integer time scaling factor

$$\lambda_+^{\alpha-1} = 2$$

by taking the parameters

$$\alpha = 2, \quad J_0 = -1, \quad V_0 = -14.2388293$$



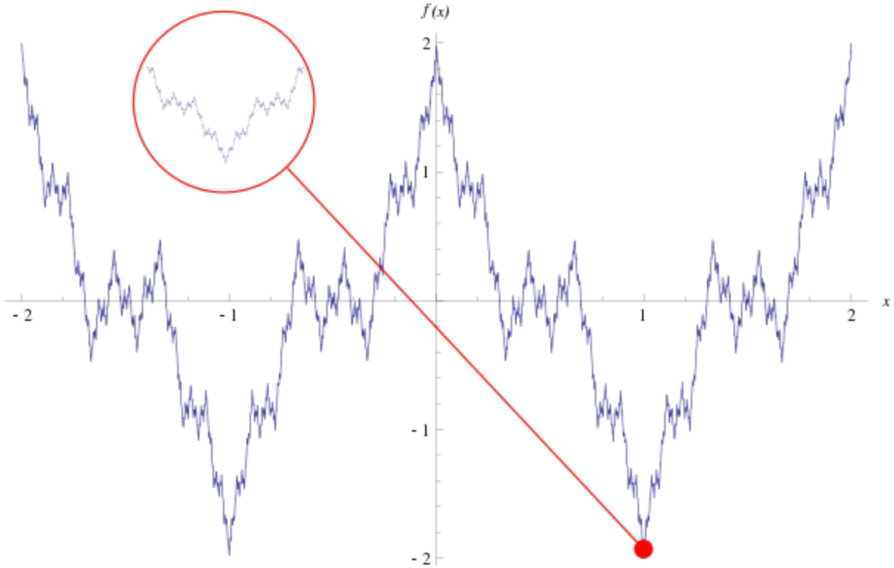
D.L., Watkins, Frame, Given, He, Li, Lu, Sarkar, PRA 100, 011403(R) (2019)

This is a particular case of the Weierstrass function,

$$w(t) = \sum_{k=0}^{\infty} a^k \cos(2\pi b^k t) \qquad 0 < a < 1 < b \text{ with } ab \geq 1$$

In our case we take $a \to 1$, $b = 2$ and truncate after a finite number of terms. The next slide shows a picture of the Weierstrass function for $a = 0.5$, $b = 3$.

$$a = 0.5, \quad b = 3$$



The Weierstrass function has fractal dimension

$$D = 2 + \frac{\log a}{\log b}$$

Hardy, Trans. Amer. Math. Soc. 17, 301 (1916)
Hunt, Proc. Amer. Math. Soc. 126, 791 (1998)

We now show how to produce time fractals directly with the trapped ion quantum simulator. We start with the function $S(r)$ defined as

$$|S\rangle = \sum_{r\neq 0} S(r)|r\rangle$$

Using this function, we define the following product of single-qubit rotations

$$U(\epsilon) = \prod_{r\neq 0} \exp[-i\epsilon\sigma_r^y S(r)]$$

When acting on the state with one boson immobilized at $r = 0$, we get

$$U(\epsilon)|o\rangle = \left[1 - \frac{\epsilon^2}{2}\langle S|S\rangle + O(\epsilon^3)\right]|o\rangle + \epsilon|S\rangle + O(\epsilon^2)|X\rangle$$

Recall that we added a constant to the Hamiltonian so that

$$\langle o|\exp[-iHt]|o\rangle = \langle o|o\rangle = 1$$

We can now use the quantum simulator to determine

$$B(\epsilon,t) = |\langle o|U^\dagger(\epsilon)\exp[-iHt]U(\epsilon)|o\rangle|^2$$

This corresponds to measuring the projection operator $|o\rangle\langle o|$ on the state

$$U^\dagger(\epsilon)\exp[-iHt]U(\epsilon)|o\rangle$$

If we expand in ϵ we get

$$B(\epsilon,t) = \left|1 - \epsilon^2\langle S|S\rangle + \epsilon^2 Z(t) + O(\epsilon^3)\right|^2$$

This can be rewritten as

$$\begin{aligned} B(\epsilon, t) &= 1 - 2\epsilon^2 \langle S|S \rangle + \epsilon^2 [Z(t) + Z^*(t)] + O(\epsilon^3) \\ &= 1 - 2\epsilon^2 \langle S|S \rangle + 2\epsilon^2 A(t) + O(\epsilon^3), \end{aligned}$$

We can therefore extract the time fractal amplitude $A(t)$.

Variational quantum eigensolver

A variational quantum eigensolver is a variational method where unitary transformations with several free parameters are used to construct an approximate ground state wave function. The expectation value of each of the terms in the Hamiltonian are computed on a quantum computer for various values of free parameters. The parameters are chosen to minimize the expectation value of the Hamiltonian.

T. Papenbrock

Game plan ("simplest deuteron")

1. Hamiltonian from pionless EFT at leading order; fit to deuteron binding energy; constructed in harmonic-oscillator basis of $^3S_1$ partial wave [à la Binder et al. (2016); **Aaina Bansal et al. (2017)**]; cutoff at about 150 MeV.

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^\dagger a_n$$

$$\langle n'|V|n\rangle = V_0 \delta_n^0 \delta_n^{n'}$$

$$V_0 = -5.68658111 \text{ MeV}$$

2. Map single-particle states |n⟩ onto qubits using |0⟩ = |↑⟩ and |1⟩ = |↓⟩. This is an analog of the Jordan-Wigner transform.

$$a_p^\dagger \leftrightarrow \sigma_-^{(p)} \equiv \frac{1}{2}(X_p - iY_p) \qquad a_p \leftrightarrow \sigma_+^{(p)} \equiv \frac{1}{2}(X_p + iY_p)$$

3. Solve H_1, H_2 (and H_3) and extrapolate to infinite space using harmonic oscillator variant of Lüscher's formula [More, Furnstahl, TP (2013)]

$$E_N = -\frac{\hbar^2 k^2}{2m}\left(1 - 2\frac{\gamma^2}{k}e^{-2kL} - 4\frac{\gamma^4 L}{k}e^{-4kL}\right) + \frac{\hbar^2 k \gamma^2}{m}\left(1 - \frac{\gamma^2}{k} - \frac{\gamma^4}{4k^2} + 2w_2 k \gamma^4\right)e^{-4kL}$$

Dumitrescu et al., Phys. Rev. Lett. 120, 210501 (2018)

Variational wave function

Wave functions on two qubits

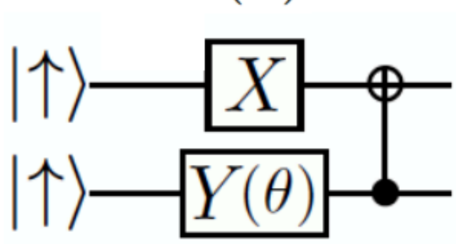
$U(\theta)|\downarrow\uparrow\rangle$ $$U(\theta) \equiv e^{\theta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)} = e^{i\frac{\theta}{2}(X_0 Y_1 - X_1 Y_0)}$$

Wave functions on three qubits

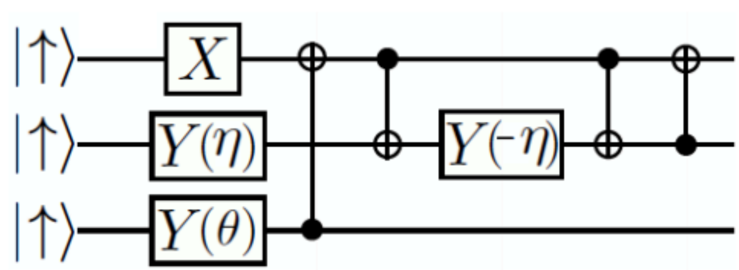
$U(\eta,\theta)|\downarrow\uparrow\uparrow\rangle$ $$U(\eta,\theta) \equiv e^{\eta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right) + \theta\left(a_0^\dagger a_2 - a_2^\dagger a_0\right)}$$

Minimize number of two-qubit CNOT operations to mitigate low two-qubit fidelities (construct a "low-depth circuit")

$U(\theta)$

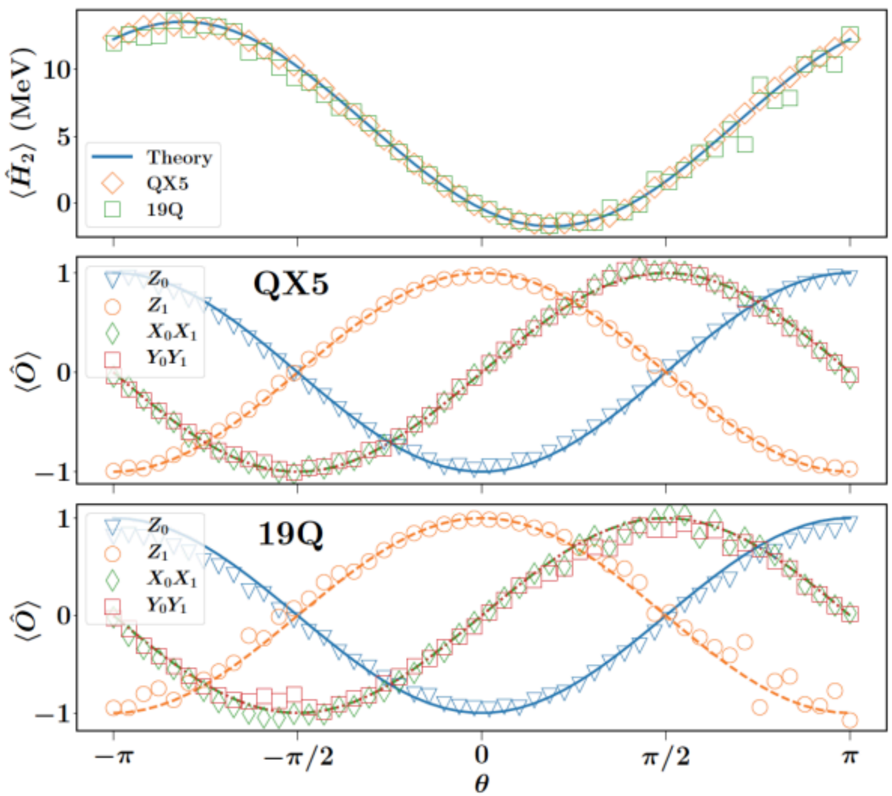


$U(\eta,\theta)$



Hamiltonian expectation value on two qubits

$$H_2 = 5.906709 I + 0.218291 Z_0 - 6.125 Z_1 - 2.143304\,(X_0 X_1 + Y_0 Y_1)$$

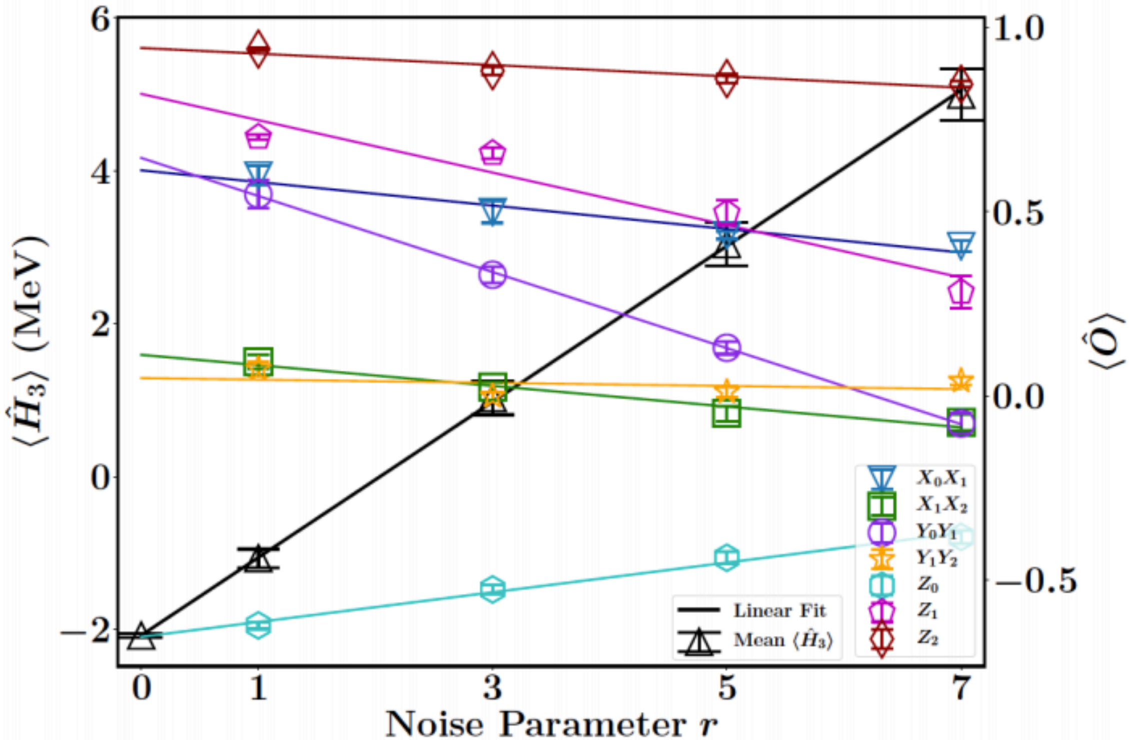


Quantum-classical hybrid algorithm VQE [Peruzzo et al. 2014; McClean et al 2016]:

Expectation values on QPU.
Minimization on CPU.

Three qubits

$$H_3 = H_2 + 9.625(I - Z_2) - 3.913119\,(X_1X_2 + Y_1Y_2)$$



Three qubits have more noise. Insert *r* pairs of CNOT (unity operators) to extrapolate to *r*=0. [See, e.g., Ying Li & S. C. Benjamin 2017]

Final results

Deuteron ground-state energies from a quantum computer compared to the exact result, E_∞=-2.22 MeV.

E from exact diagonalization				
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	-1.749	-2.39	-2.19	
3	-2.046	-2.33	-2.20	-2.21
E from quantum computing				
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	$-1.74(3)$	$-2.38(4)$	$-2.18(3)$	
3	$-2.08(3)$	$-2.35(2)$	$-2.21(3)$	$-2.28(3)$

$$E_N = -\frac{\hbar^2 k^2}{2m}\left(1 - 2\frac{\gamma^2}{k}e^{-2kL} - 4\frac{\gamma^4 L}{k}e^{-4kL}\right) + \frac{\hbar^2 k \gamma^2}{m}\left(1 - \frac{\gamma^2}{k} - \frac{\gamma^4}{4k^2} + 2w_2 k \gamma^4\right)e^{-4kL}$$

Dumitrescu et al., Phys. Rev. Lett. 120, 210501 (2018)

Recap of lecture

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