Inelastic Reactions on a Quantum Computer

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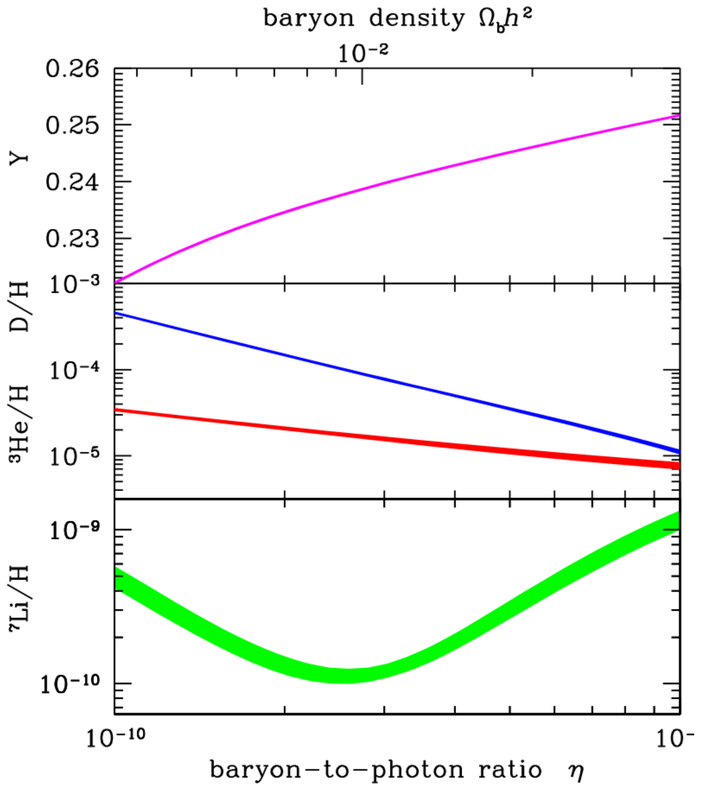
Outline

- Motivation
- Nuclear interactions and (some) approach to reaction calculations
- Reactions on quantum computers
- Conclusions

Motivation

Nuclear reactions at BBN and stellar conditions are input for Astrophysical models. Theory uncertainty quantification is crucial.

BBN reaction involves lighter nuclei at sub MeV energies.

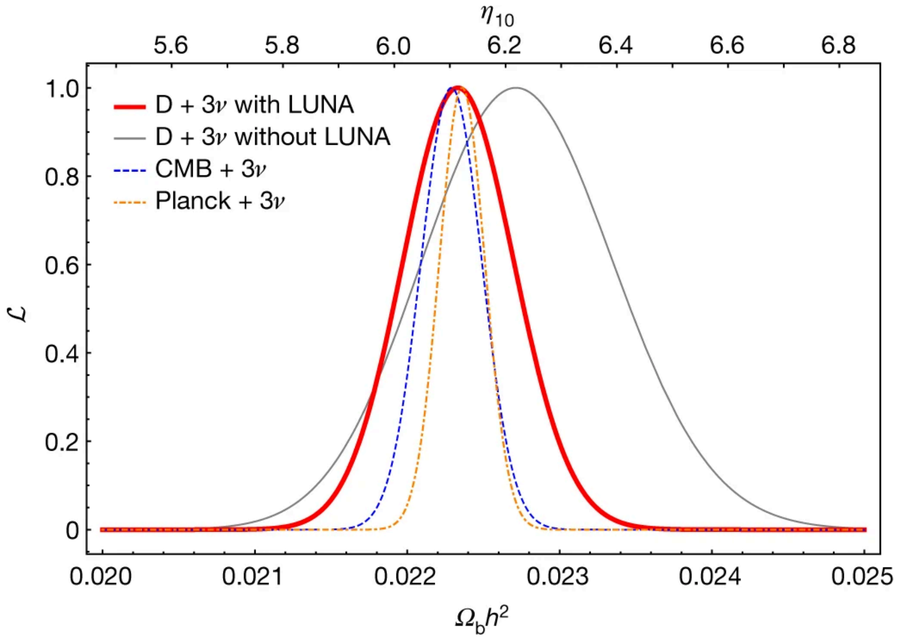


Cyburt, Fields, Olive, Yeh,
RMP 88, 015004 (2016)

TABLE I. For each reaction and nuclide, the energies (in keV, center-of-mass) at which the sensitivity functions for D and ^{7}Li attain half their maximum value; these intervals indicate the energies relevant for BBN ($\Omega_B h^2 = 0.019$).

Reaction	D	^{7}Li
p(n,γ)d	25–200	17–153
d(p,γ)^{3}He	53–252	65–270
d(d,p)^{3}H	55–242	134–348
d(d,n)^{3}He	62–258	79–282
^{3}He(α,γ)^{3}Be	no effect	157–376
^{3}He(d,p)^{4}He	187–325	107–283
^{3}He(n,p)^{3}H	52–228	24–188
^{7}Li(p,α)^{4}He	no effect	57–208
^{7}Li(p,n)^{7}Be	no effect	1649–1690
^{3}H(α,γ)^{7}Li	no effect	62–162
^{3}H(d,n)^{4}He	176–338	167–285

Burles, Nollett, Truran, Turner,
PRL 82, 4176 (1999)

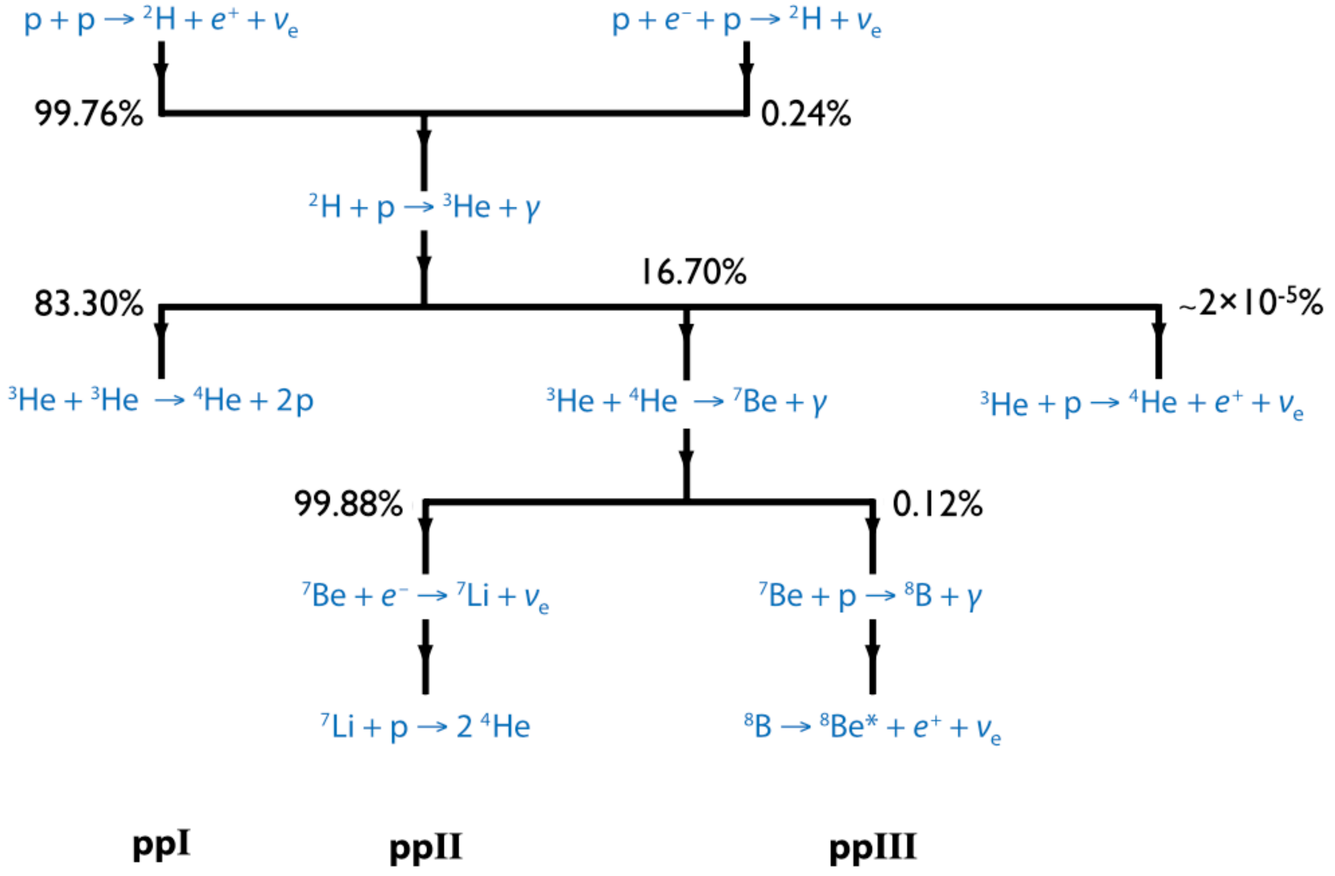


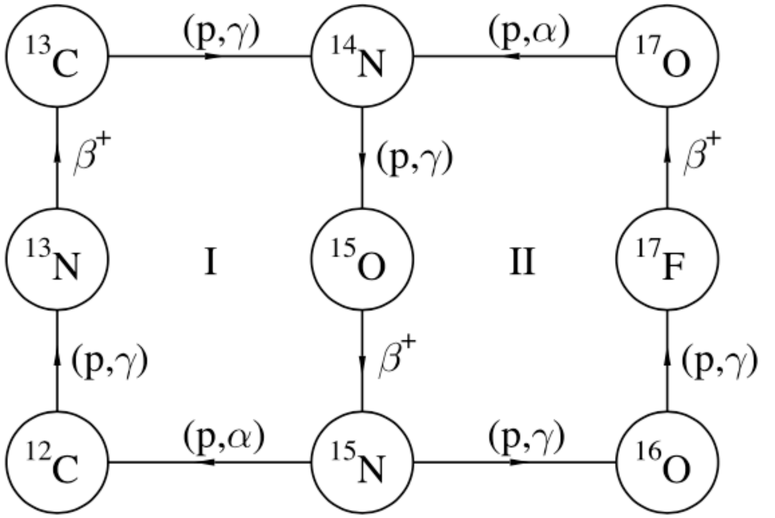
Mossa et al. Nature 587, 210 (2020)

Pionless EFT with short range interactions should be sufficient.

Radiative capture and charge exchange reactions

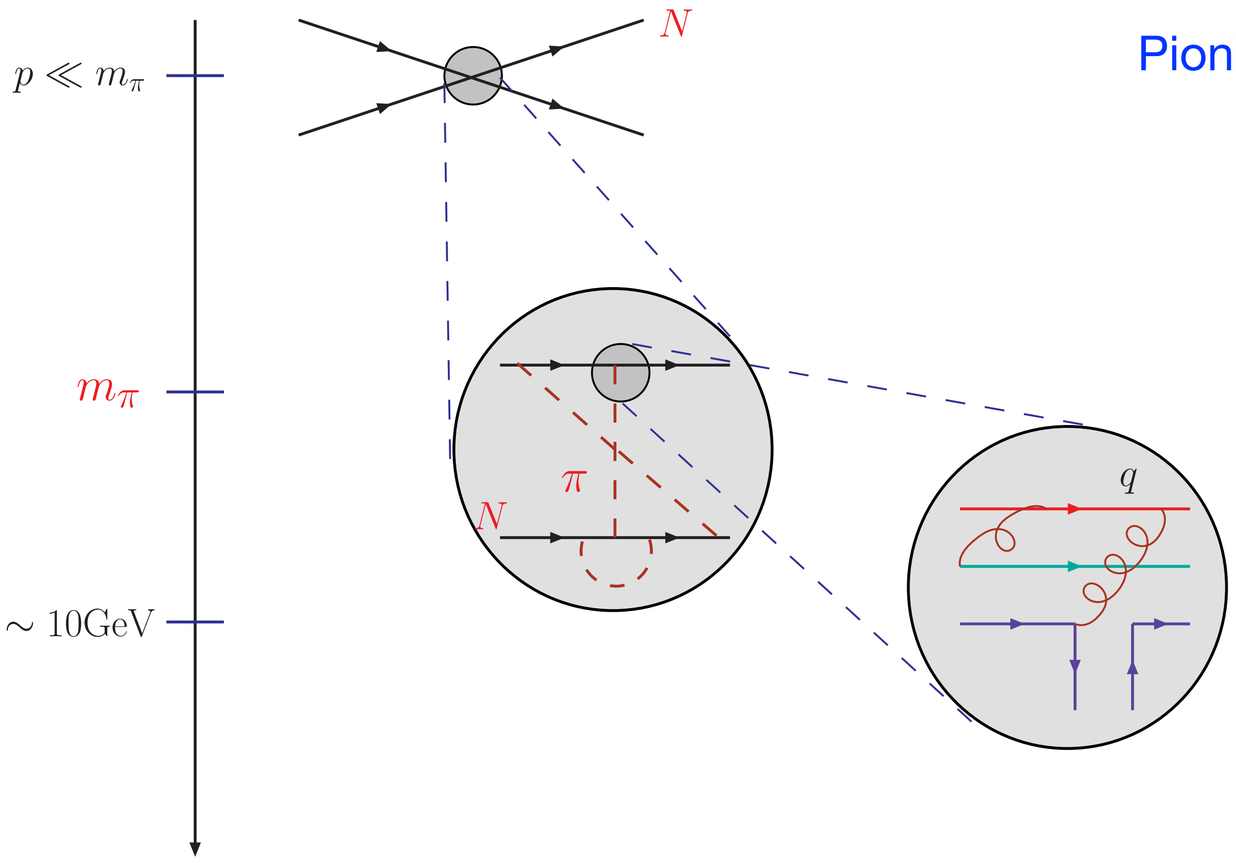
Stellar evolution involves a host of reactions including heavier nuclei depending on stellar mass.





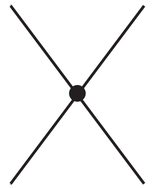
Adelberber et al., Solar Fusion II, RMP 83, 195 (2011)

Nuclear Forces



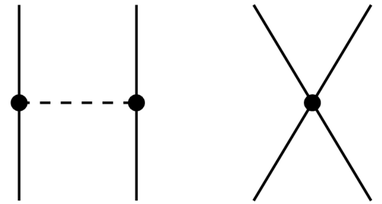
$m_\pi \sim 140$ MeV $\ll m_N \sim 1000$ MeV, *etc.*

Pionless/Halo/Cluster EFT

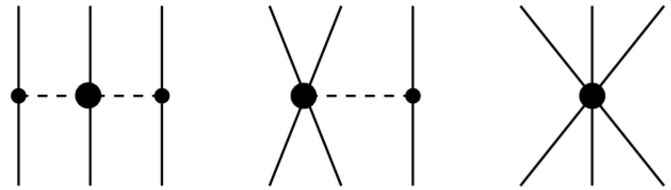


Chiral EFT

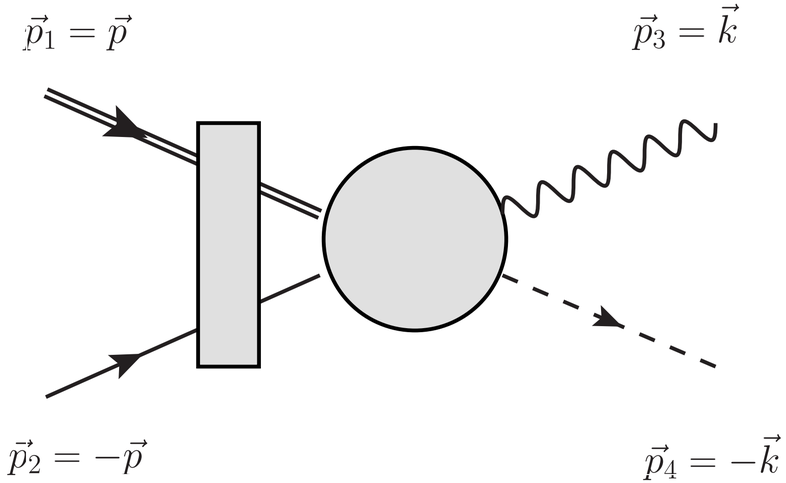
LO $\sim \left(\frac{Q}{M_{\rm hi}}\right)^0$:



NNLO $\sim \left(\frac{Q}{M_{\rm hi}}\right)^3$:



Anatomy of a Capture Reaction



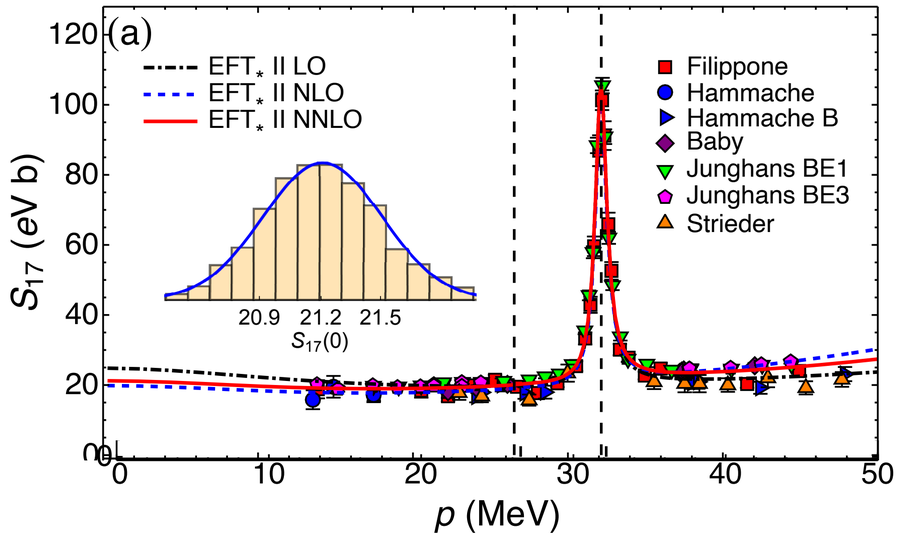
$$\langle \psi_B | \, \mathrm{O}_{\mathrm{EM}} \, | \psi_i \rangle$$

Initial state: Phase shifts provide a model-independent description

Final state: Again phase shifts (affects overall normalization)

EM currents: Usually one-body (Siegert/Ward-Takahashi theorem)

$^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$ in halo EFT



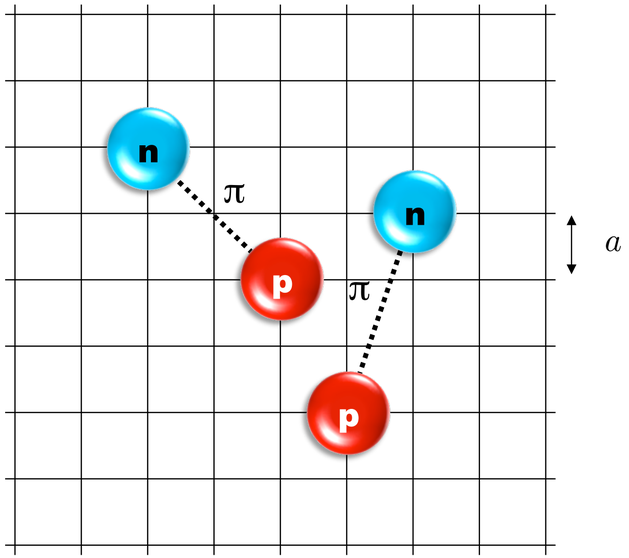
Solar II [3] is $S_{17}(0) = 20.8(16)\,\mathrm{eV\,b}$

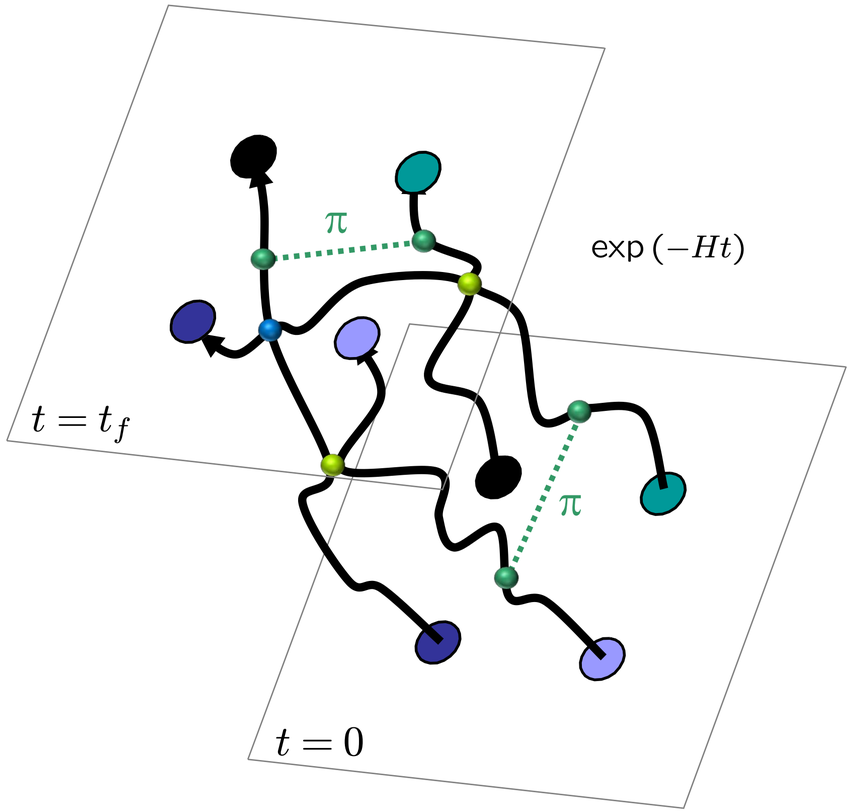
Adelberber et al., Solar Fusion II, RMP 83, 195 (2011)

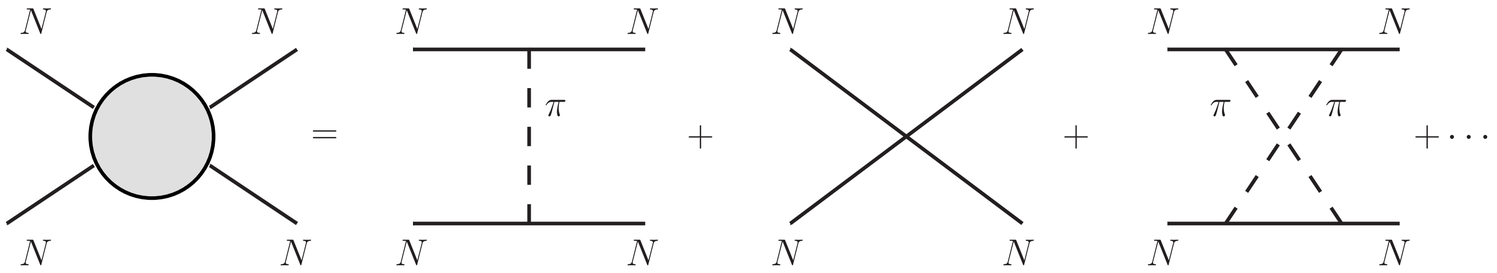
Reduced theory error by factor of 2 $S_{17}(0) = 21.0(7)\,\mathrm{eV\ b}$

Higa, Premarathna, Rupak (2022)

Lattice EFT



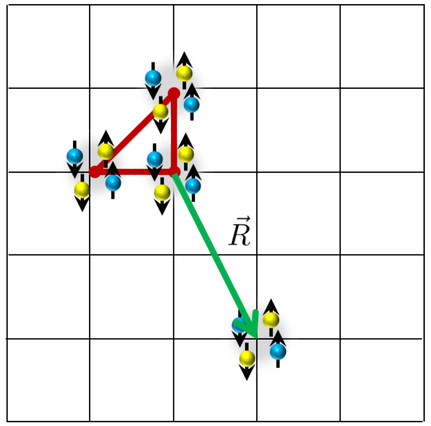




Static properties are easiest to calculate. However, ...

Reaction in Lattice EFT

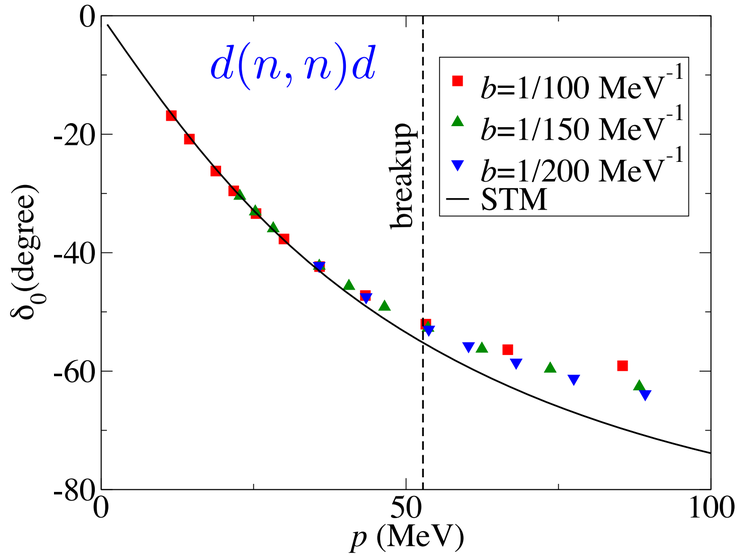
- Consider reactions: $a(b,\gamma)c$; $a(b,c)d$
- Derive a "cluster" Hamiltonian—acts in cluster coordinates, spins, etc.
- Use cluster Hamiltonian with other continuum methods

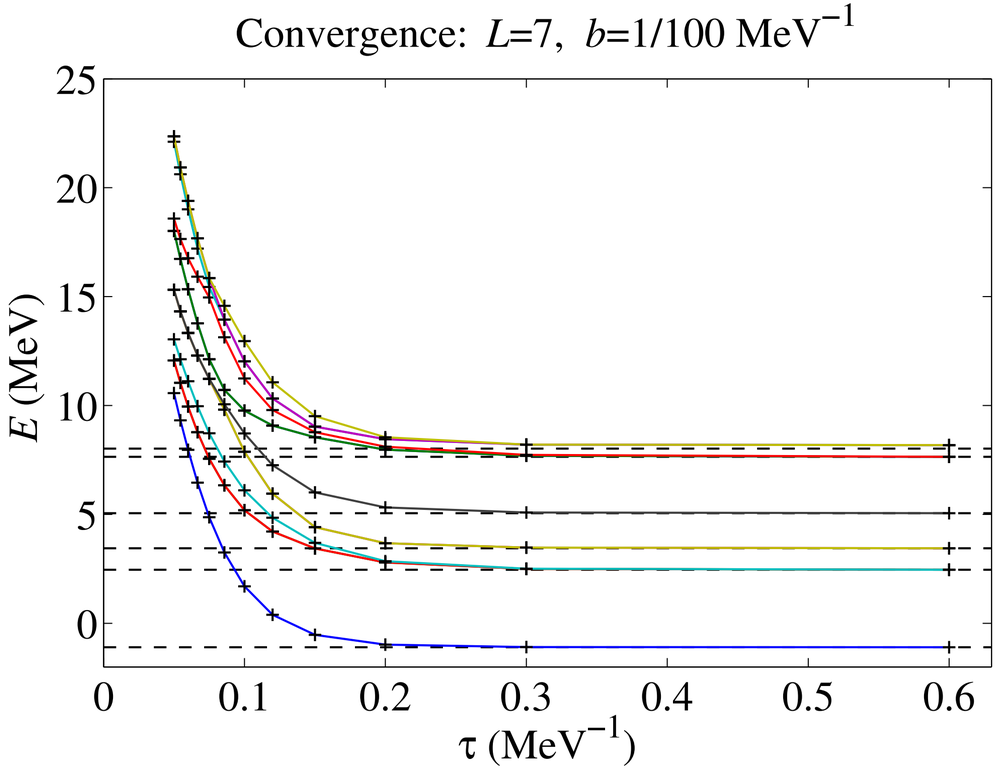


Initial state $|\vec{R}\rangle$

Evolved state $|\vec{R}\rangle_\tau = e^{-\tau H}|\vec{R}\rangle$

Cluster hamiltonian $_\tau\langle\vec{R}'|H|\vec{R}\rangle_\tau$

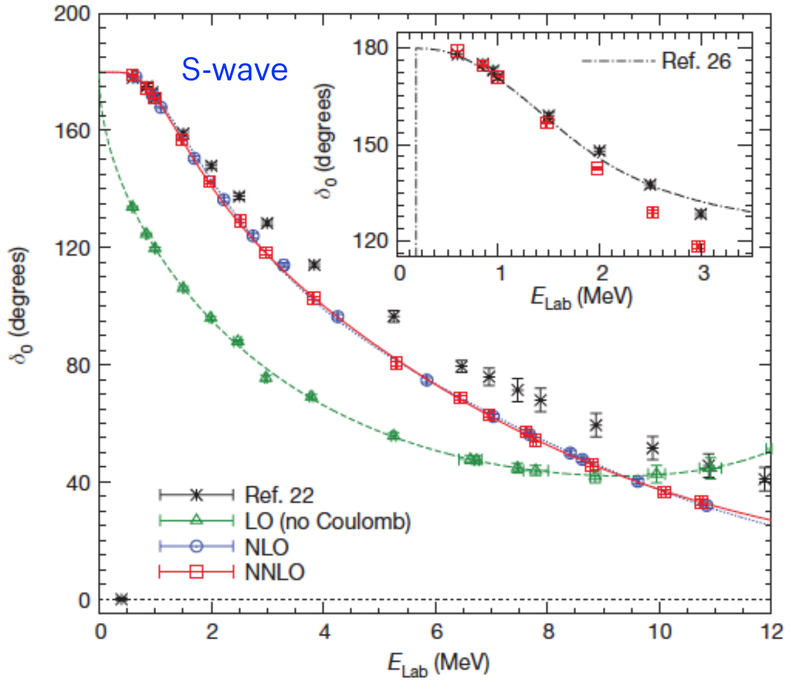


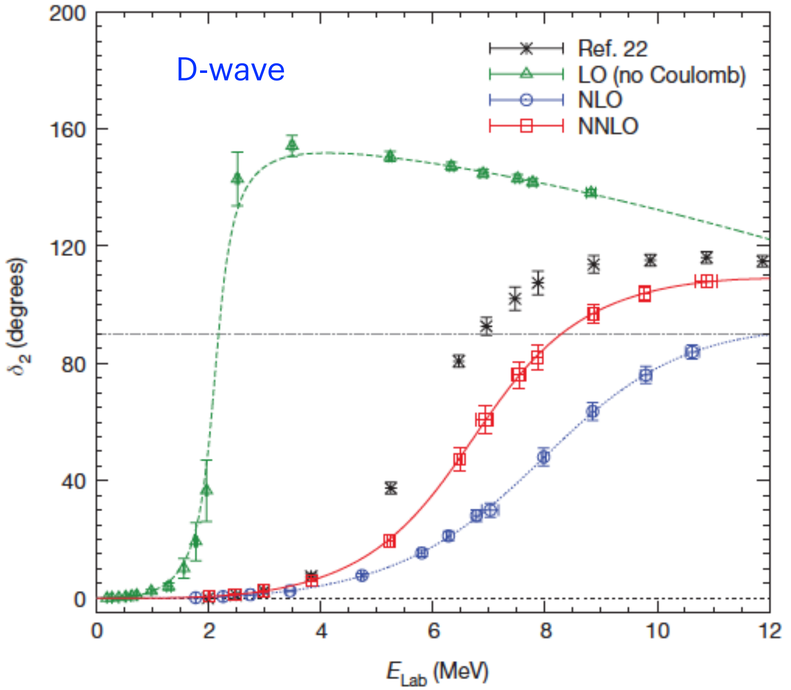


Proof of principle calculation in pionless EFT

Rupak, Lee (2013)
Pine, Rupak, Lee (2013)

^{4}He-^{4}He Scattering



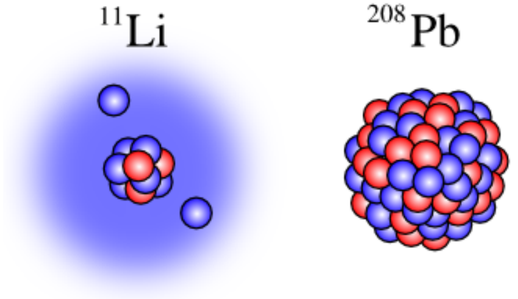


Calculation in chiral EFT

Ref. 22: Afzal et al. (1969)
Ref. 26: Higa et. al. (2008)

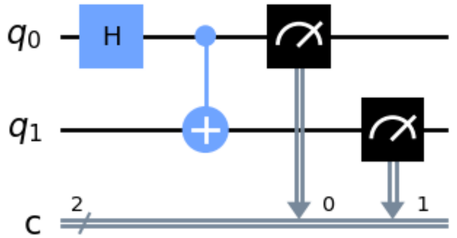
Elhatisari, Lee, Rupak, Epelbaum, Kerbs, Läde, Luu, Meißner, Nature 528, 111 (2015)
Lattice EFT Collaboration

Maybe connect back to halo/cluster EFT



Need for Quantum Computation

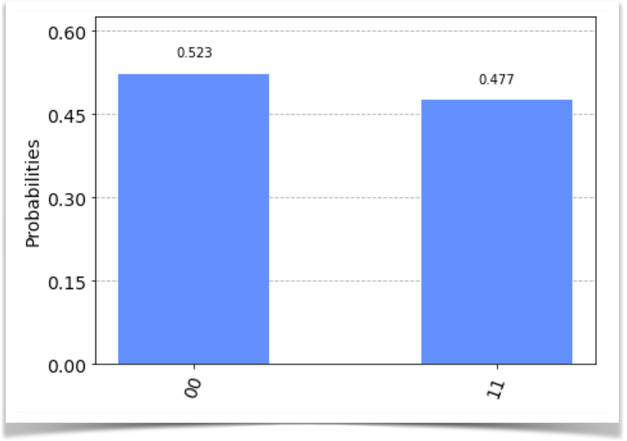
Realistic many-nucleon computation rely on stochastic methods. These methods use the imaginary time formulation.



$$\beta_{00} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

1. Scattering is a real-time phenomena

2. Sign problem becomes severe as the system size increases



Benioff (1980) suggested Quantum Mechanics as a model for computation.
Feynman (1980) showed quantum phenomena such as entanglement cannot be efficiently simulated classically.

Physics problem: How to calculate inelastic processes such as $a(b,\gamma)c$ or $a(b,c)d$?

How to calculate transition matrix elements $\langle E_f|O_T|E_i\rangle$?

Nuclear Theory

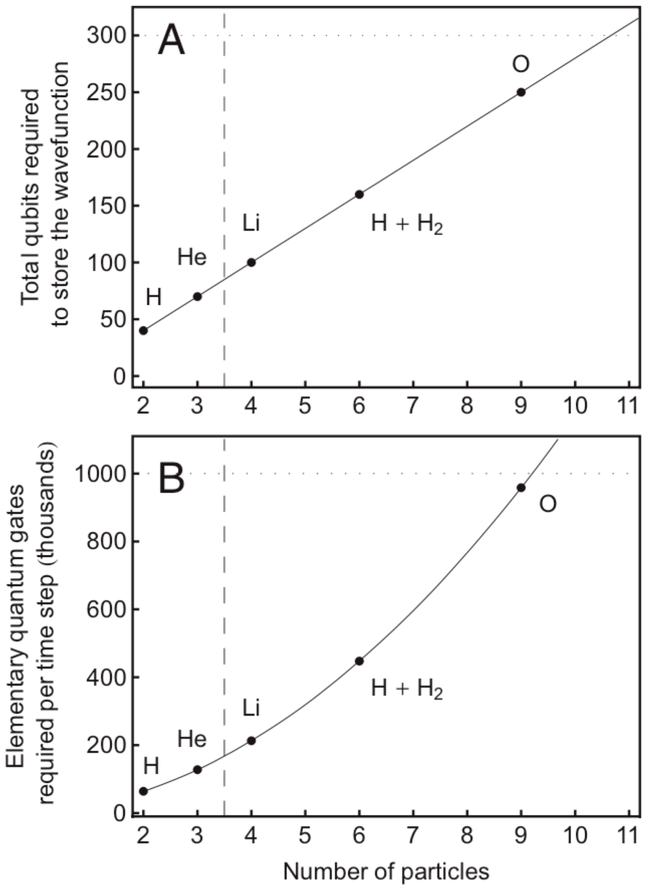
- Where do we start? Pionless EFT seems like a good place since we only have short range interaction. Theory well studied. RG understood.

- First or second quantization? We would like to know how resource need scales with system size.

First quantization computationally faster in quantum chemistry beyond few particles
Cody Jones et al. (2012)

Make this for Nuclear Physics

Kassal et al. (2008), for Quantum Chemistry



Mapping fermions to qubits (Jordan-Wigner, Bravyi-Kitaev, Verstraete-Cirac), initial state preparation (adiabatic theorem?) are issues that also needs attention.

Entanglement with the Environment

In nature, entanglement is a friend and $a(b,\gamma)c \leftrightarrow c(\gamma,b)a$ *is negligible.*

Moreover, the photon is a boson with many allowed modes (qubits?)

Rabi oscillations is something we have to live with in unitary evolution. Use this to measure matrix elements.

Algorithm for Inelastic Reactions

The algorithm we propose is as follows:

1: Encode the system and add an extra "photon" qubit.

2: Prepare the initial state as $|1\rangle \otimes |E_i\rangle$.

3: Evolve initial state with $e^{-iH_T t}$.

4: Measure the photon qubit.

Counting register

$$H_T = \mathbb{1} \otimes H + \frac{\omega}{2}(\mathbb{1} - Z) \otimes \mathbb{1} + c_0 \left(\phi^\dagger + \phi\right) \otimes O_T$$

"Photon" energy

"Photon" creation and annihilation, an X gate

Bedaque, Khadka, Rupak, Yusf (2022)

MRI Scan of Transition Matrix Elements

The algorithm works like a Nuclear Magnetic Resonance. We drive the system to resonance with photon energy $\omega \approx E_f - E_i$. Near the resonance

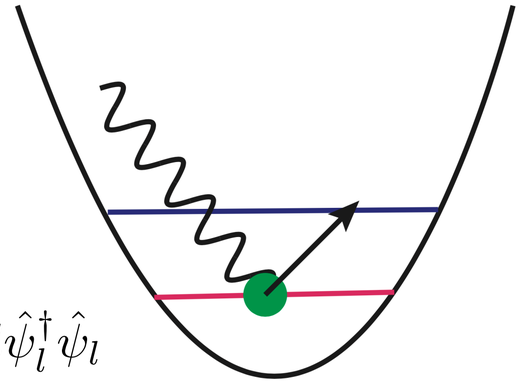
$$H_T^{\text{eff}} = \begin{pmatrix} E_f & \omega_1/2 \\ \omega_1/2 & E_i + \omega \end{pmatrix}, \qquad \text{with} \qquad \omega_1 = 2c_0 \langle E_f | O_T | E_i \rangle$$

Transition probability: $$P(t) = \frac{\omega_1^2}{(E_f - E_i - \omega)^2 + \omega_1^2} \sin^2 \frac{\sqrt{(E_f - E_i - \omega)^2 + \omega_1^2}\, t}{2}$$

Why does it work? Tuning ω near the resonance, the H_T^{eff} eigenstates $|0\rangle_x$, $|1\rangle_x$ (physics $|\pm\rangle_x$) are orthogonal to the initial state $|1\rangle$ (physics $|-\rangle$). Time evolution then efficiently mixes $|0\rangle = \frac{|0\rangle_x + |1\rangle_x}{2}$ and $|1\rangle = \frac{|0\rangle_x - |1\rangle_x}{2}$

First Calculation: 1-particle E1 Transition in SHO

Single particle in a 1-dimensional SHO, inside a box of size aL, lattice size a



$$\hat{H} = -\frac{1}{2\hat{m}} \sum_l [\hat{\psi}_l^\dagger \hat{\psi}_{l+1} + \hat{\psi}_{l+1}^\dagger \hat{\psi}_l - 2\hat{\psi}_l^\dagger \hat{\psi}_l] + \sum_l \hat{V}_l \hat{\psi}_l^\dagger \hat{\psi}_l + \frac{\omega}{2}(\mathbb{1} - Z) + qe\sigma^2 X \sum_l l \hat{\psi}_l^\dagger \hat{\psi}_l$$

Kinetic energy, Jordan-Wigner transformation

SHO potential

"Photon" energy

E1 dipole transition

Transition operator motivated by minimal coupling:

$$\boldsymbol{P} \to \boldsymbol{P} + qe\boldsymbol{A} \to \frac{qe}{m}\boldsymbol{A}(\boldsymbol{r}) \cdot \boldsymbol{P}$$

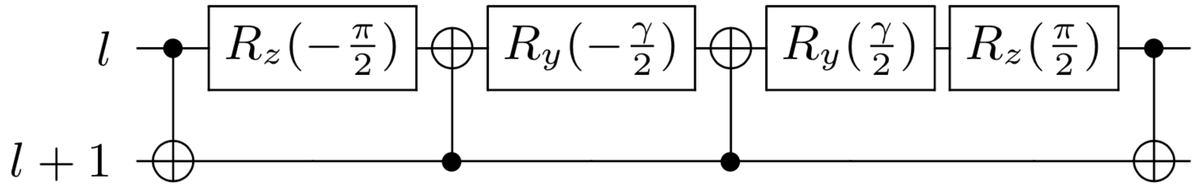
$$\frac{i}{m}\boldsymbol{P} = [\boldsymbol{R}, H] \to (E_f - E_i)\boldsymbol{A}(\boldsymbol{r}) \cdot \boldsymbol{R}$$

Coordinate Space Quantum Circuit

For the simulation we take $V_l = \frac{1}{2}\omega_0^2 l^2$ for $l = -\frac{L-1}{2}, \ldots, \frac{L-1}{2}$ for odd L

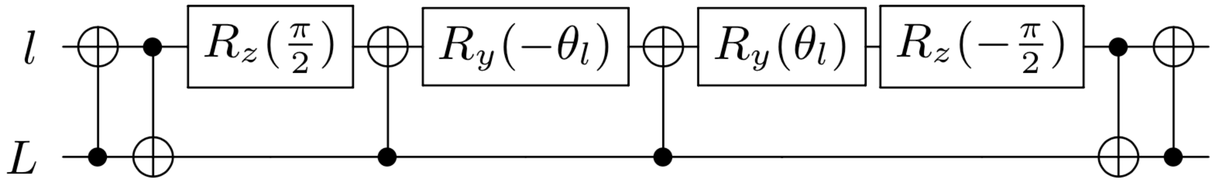
$L+1$ qubits with the "photon" in the highest qubit.

Kinetic energy circuit



Hopping parameter $\gamma = -\frac{\Delta t}{m}$

E1 dipole transition circuit



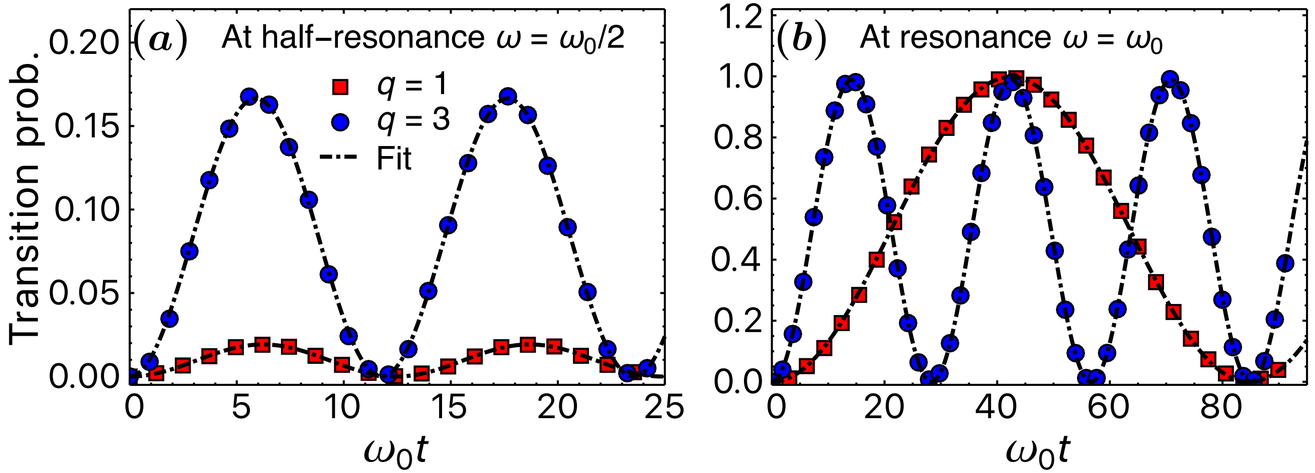
$\theta_l = qe\hat{\sigma}^2 l \Delta\hat{t}$

E1 Transition Rates from Qulacs Simulations

Nuclear physics motivated number:

$$m = 940\,\mathrm{MeV}\,,$$
$$\omega_0 = 8\,\mathrm{MeV}\,,$$
$$\sigma = 11\,\mathrm{MeV}\,,$$
$$L = 21\,, a = 0.6\,\mathrm{fm}\,.$$

5000 shots



Charge/coupling q we can choose conveniently

Fit Rabi oscillation transition amplitude parameter $\Delta E = E_f - E_i$ and ω_1

$$P(t) = \frac{\omega_1^2}{(E_f - E_i - \omega)^2 + \omega_1^2} \sin^2 \frac{\sqrt{(E_f - E_i - \omega)^2 + \omega_1^2}\, t}{2}$$

Continuum, infinite volume limit:

$$\frac{1}{2}\omega_1^{(\mathrm{th})} \equiv qe\sigma^2 \int_{-\infty}^{\infty} dx\, x\phi_1^*(x)\phi_0(x) = \frac{qe\sigma^2}{\sqrt{2m\omega_0}}$$

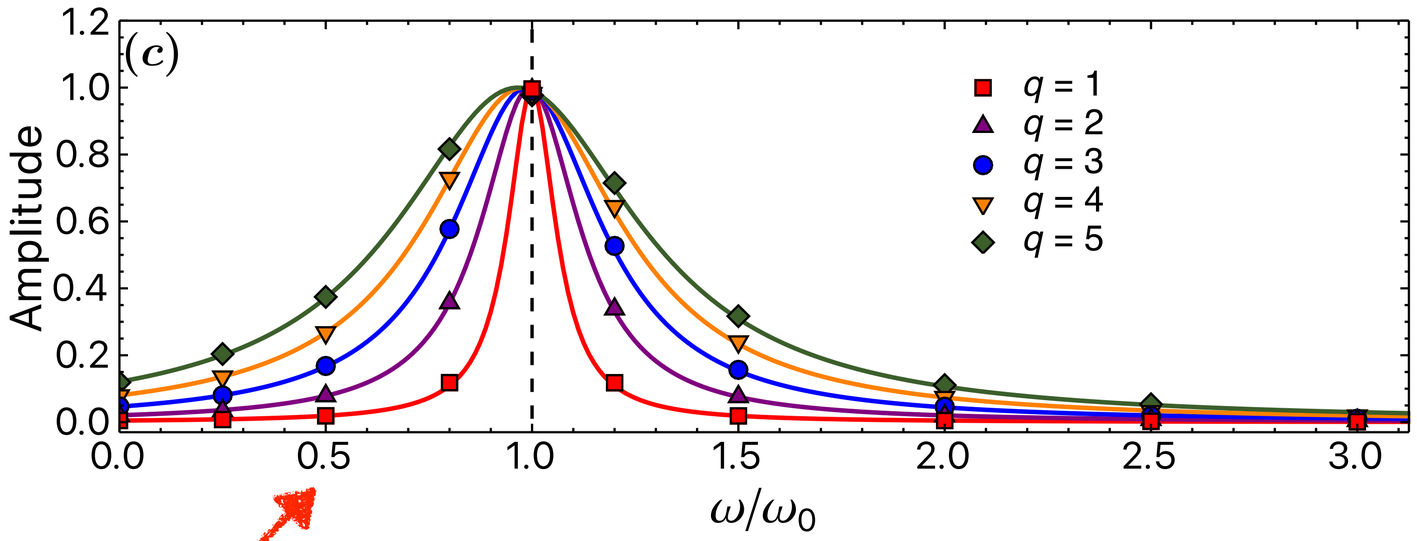
Qulacs simulator: Suzuki et al. Quantum 5, 559 (2021)

TABLE I. Fit parameter $\Delta\bar{E}$ and $\bar{\omega}_1$ for SHO normalized to expected oscillator frequency $\omega_0 = 8\,\mathrm{MeV}$ and $\omega_1^{(\mathrm{th})}$, respectively. The first set of $(\Delta\bar{E}, \bar{\omega}_1)$ is from fits at $\omega = \omega_0/2$ and the second set with the superscript R is at resonance $\omega = \omega_0$.

q	$\Delta\bar{E}$	$\bar{\omega}_1$	$\Delta\bar{E}^{(R)}$	$\bar{\omega}_1^{(R)}$
1	1.000(6)	0.936(2)	0.996(8)	0.9911(6)
2	0.994(5)	0.967(4)	0.988(11)	0.9866(10)
3	0.987(3)	0.972(3)	0.976(8)	0.9834(9)
4	0.977(2)	0.966(2)	0.961(10)	0.9793(13)
5	0.965(2)	0.958(2)	0.940(10)	0.9735(16)

Lorentzian Amplitude

Rabi oscillation formula $A(\omega) = \dfrac{\omega_1^2}{(E_f - E_i - \omega)^2 + \omega_1^2}$



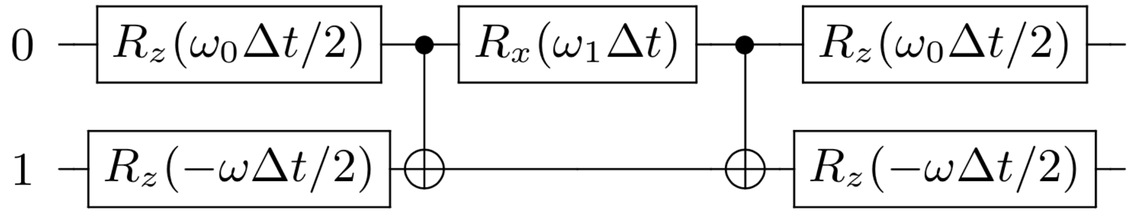
Fit at $\omega = \dfrac{1}{2}\omega_0$ predicts simulation data at other frequencies.

Reaction Calculation on IBMQ

Two-level system/charge exchange/SHO in abstract linear vector space

$$H_T = \frac{\omega_0}{2}\mathbb{1}\otimes Z + \frac{\omega}{2}(\mathbb{1}-Z)\otimes\mathbb{1} + c_0\, X\otimes X$$

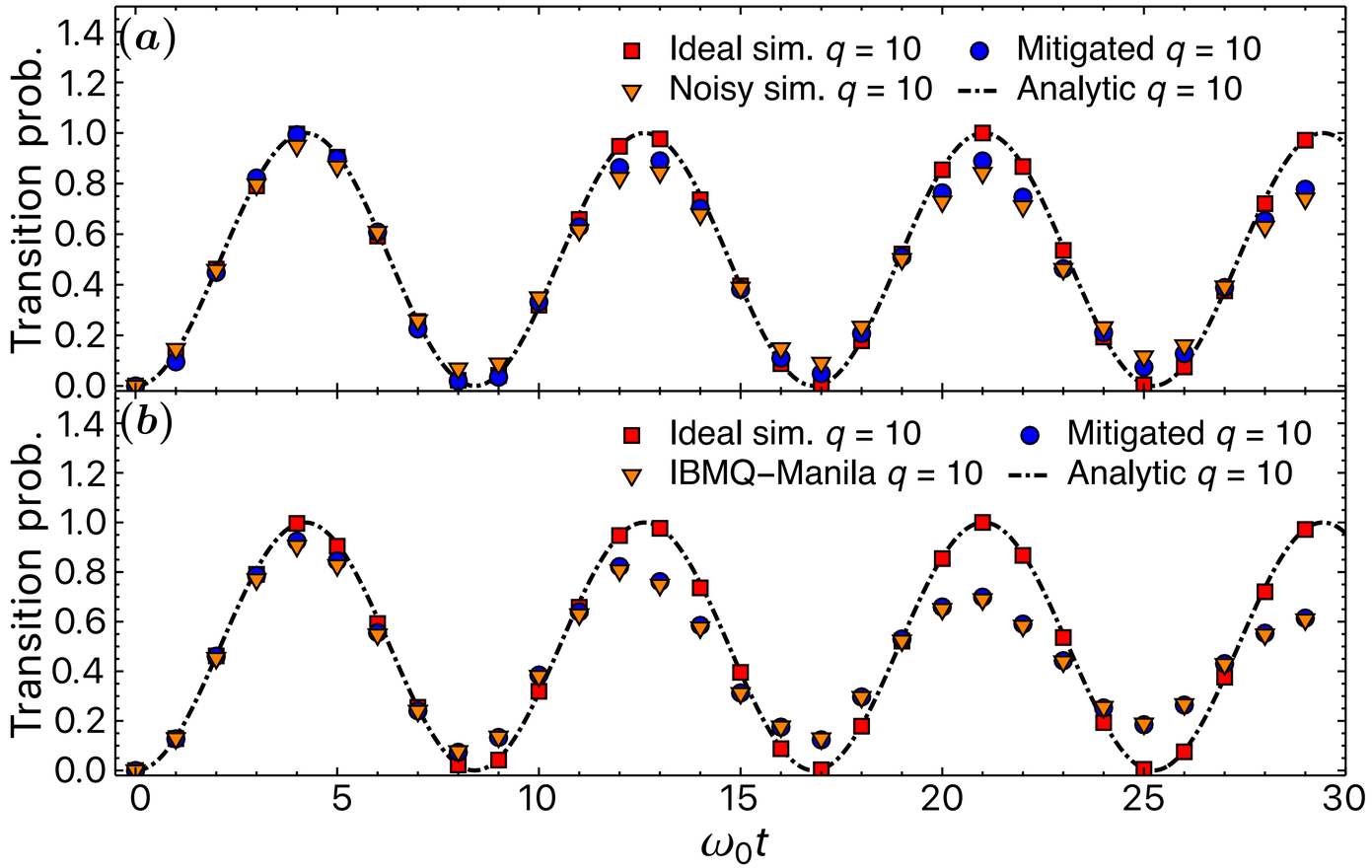
$$c_0 = \frac{qe\sigma^2}{\sqrt{2m\omega_0}} \equiv \frac{1}{2}\omega_1$$



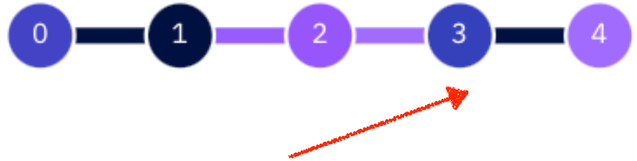
The two-level Hamiltonian can be any transition operator. Coupling to a photon is not necessary. The "photon" in this algorithm is motivated by E1 transition but it is just a counting register for transition.

This circuit has similarity to Roggero, Carlson (2018) except the crucial "photon" qubit energy term that drives the system to resonance and gives 100% transition probability.

IBMQ Results



Two-level results from IBMQ-Manila



Qubits 3 and 4 were used for 1024 measurements

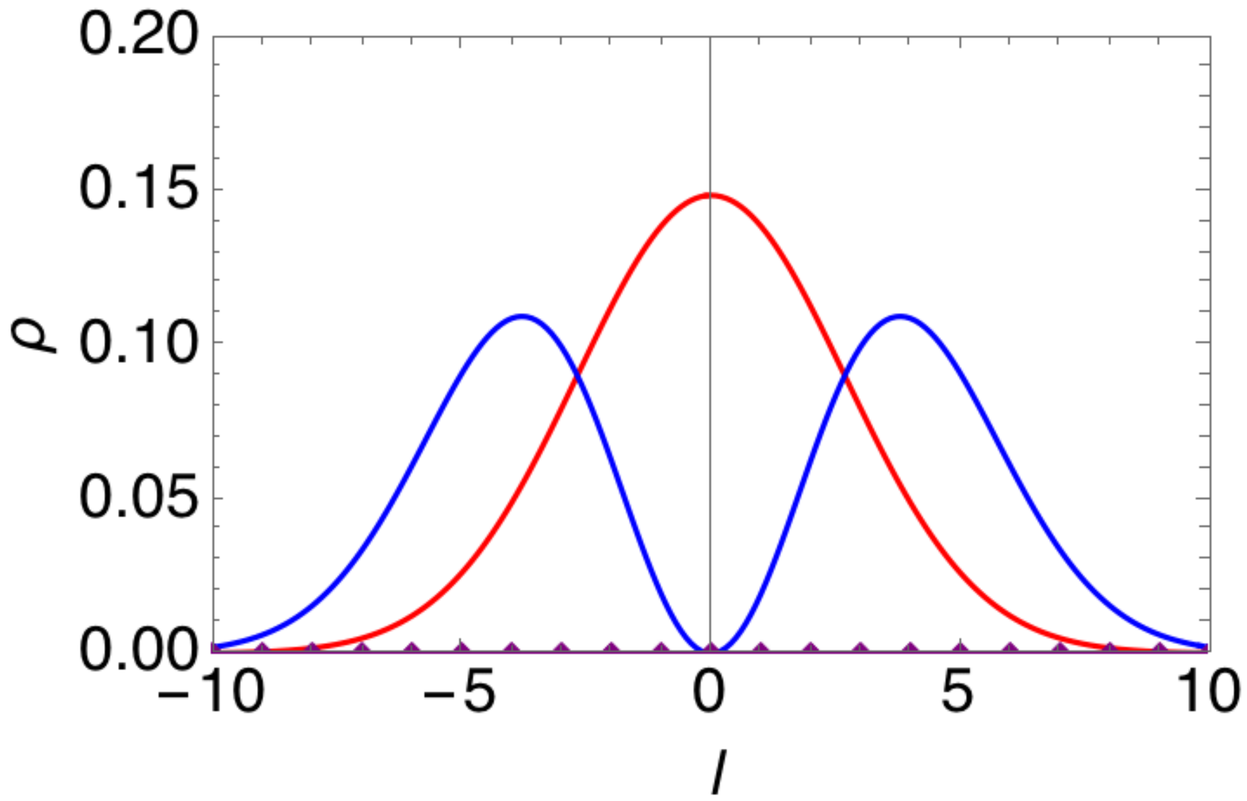
Algorithm is robust: Only require the locations of maxima $(2n+1)\pi/t_{\max}$ or minima $2(n+1)\pi/t_{\min}$ for matrix element measurement.

We get $\omega_1^{(\text{meas.})} = 1.03(3)\,\omega_1^{(\text{th})}$

Excited State Preparation

Note that the algorithm can also generate excited state with high probability by tuning near the resonance.

Initial state preparation is still expensive through adiabatic evolution.



$$l = -\frac{L-1}{2}, \cdots, \frac{L-1}{2}, L = 21$$

Conclusions

1. Quantum computing might provide an advantage in real-time calculation of electro-weak processes.
   Efforts in this direction is important.

2. A generic algorithm for inelastic processes, final/excited state preparation was presented.

3. Work is in progress to calculate $p(n,\gamma)d$, building from lower to higher dimensions.

4. Green's function approach to calculate binding energies.

5. Initial state preparation, higher dimension.