# AI/Deep Learning for extrapolations and prospects for applications with quantum computers

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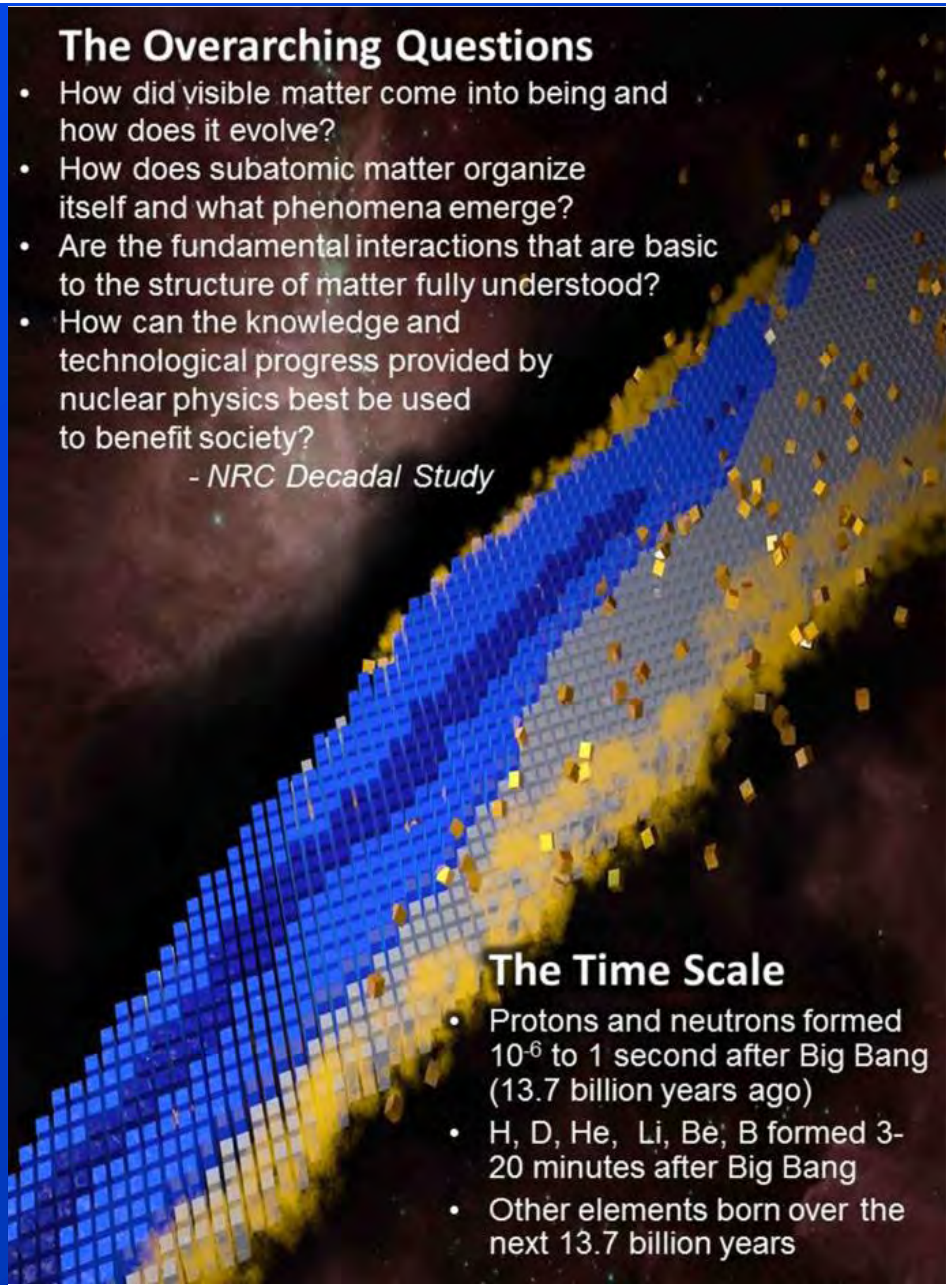
**LENPIC**
**Annual Meeting Workshop**
**Bochum, Germany**

Aug. 24 - 26, 2022

1. NCSM/NCCI with Daejeon16
2. ANN Topology and strategy
3. Spectroscopy, radii, quadrupole moments, . . .
4. Issues and Challenges
5. Quantum Computing in NP
6. Issues and Challenges



## Machine Learning to predict ab initio No-Core Shell Model (NCSM) results

"Feed-forward ANNs can be viewed as universal non-linear function approximators [Hornik 1989 & 1991]. Moreover, ANNs can find solution when algorithmic methods are computationally intensive or do not exist. For this reason, ANNs are considered a more powerful modeling method for mapping complex nonlinear input-output problems."

"Training/testing data" supplied by ab initio NCSM results obtained on Leadership-Class supercomputers

↓

ANN

↓

Predictions of exact NCSM results in the continuum limit

G.A. Negoita, G.R. Luecke, J.P. Vary, P. Maris, A.M. Shirokov, I.J. Shin, Y. Kim, E.G. Ng and C. Yang, in Proceedings of the Ninth International Conference on Computational Logics, Algebras, Programming, Tools, and Benchmarking COMPUTATION TOOLS 2018; arXiv: 1803.03215

G.A. Negoita, J.P. Vary, G.R. Luecke, P. Maris, A.M. Shirokov, I.J. Shin, Y. Kim, E.G. Ng, C. Yang, M. Lockner and G.M. Prabhu, Phys. Rev. C 99, 054308 (2019); arXiv: 1810.04009

# No Core Shell Model
# A large sparse matrix eigenvalue problem

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet\bullet\bullet$$

$$H|\Psi_i\rangle = E_i|\Psi_i\rangle$$

$$|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle$$

$$\text{Diagonalize } \{\langle\Phi_m|H|\Phi_n\rangle\}$$

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral EFT interactions and Daejeon16
- Adopt the 3-D Harmonic Oscillator (HO) for the single-nucleon basis states, α, β,…
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (manages the bookkeepping of anti-symmetrization)
- Diagonalize this sparse many-body H in its "m-scheme" basis where [$\alpha = (n,l,j,m_j,\tau_z)$]

$$|\Phi_n\rangle = [a_\alpha^+ \bullet\bullet\bullet a_\varsigma^+]_n|0\rangle$$

$$n = 1,2,\ldots,10^{10} \text{ or more!}$$

- HO basis defined by $(N_{\max}, \hbar\Omega)$ where $\sum(2n_\alpha + l_\alpha)_{\text{occ}} \le N_0 + N_{\max}$
- Evaluate observables and compare with experiment

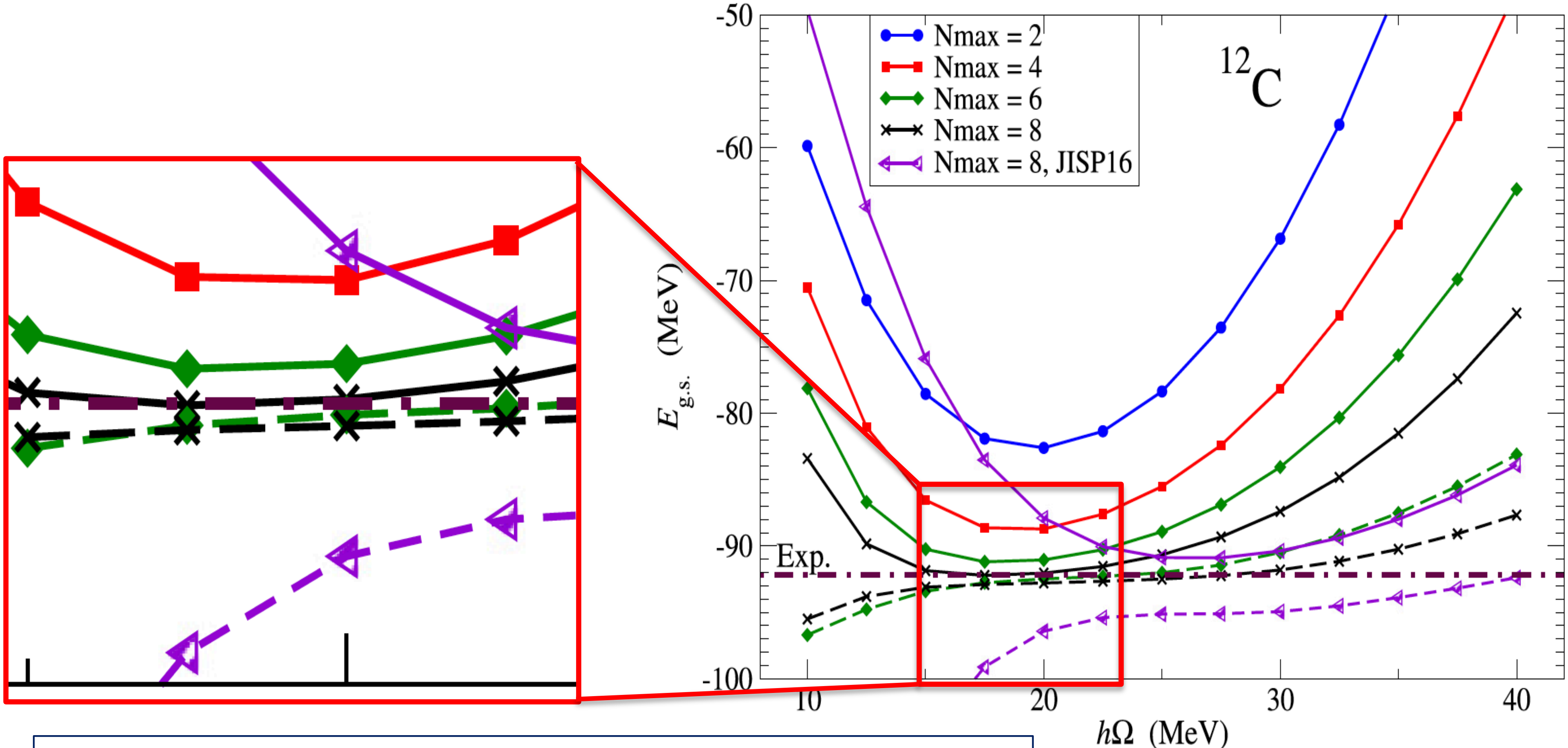
## Comments

- Straightforward but computationally demanding => new algorithms/computers
- Requires convergence assessments and extrapolation tools
- Achievable for nuclei up to A=16 (40) today with largest computers available

# Daejeon16 NN interaction

Based on SRG evolution of Entem-Machleidt “500” chiral N3LO to $\lambda = 1.5\ \text{fm}^{-1}$ followed by Phase-Equivalent Transformations (PETs) to fit selected properties of light nuclei.

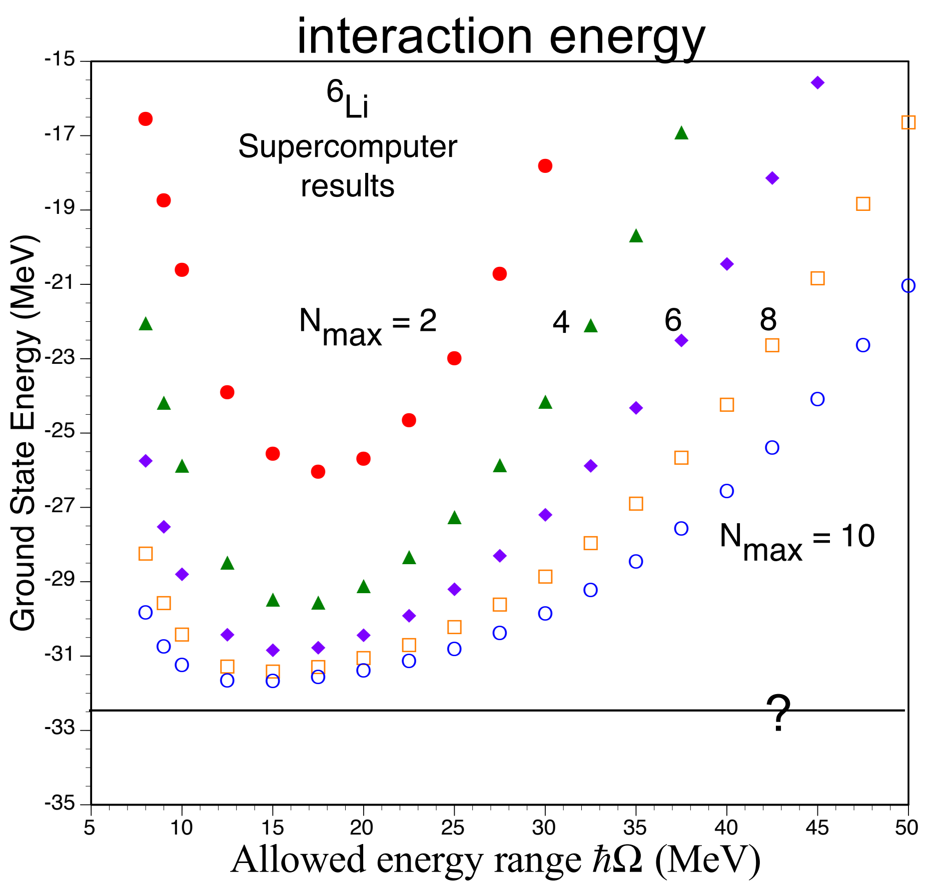
A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris and J.P. Vary, “N3LO NN interaction adjusted to light nuclei in ab exitu approach,” Phys. Letts. B 761, 87 (2016); arXiv: 1605.00413

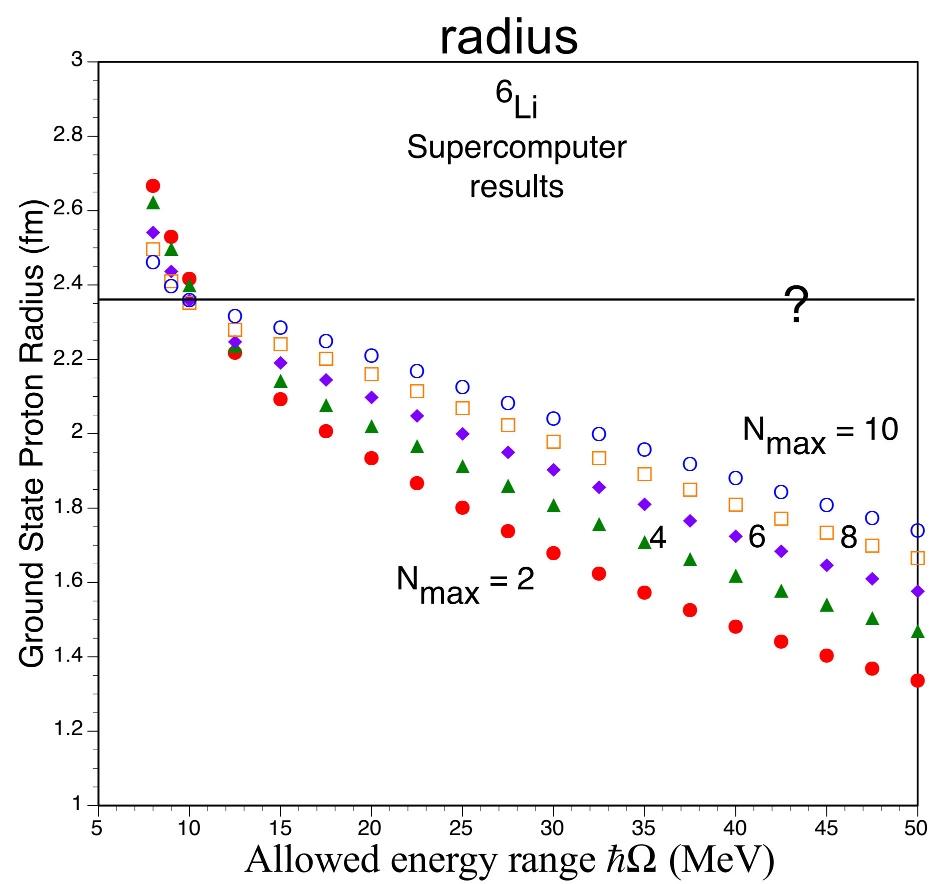



GS radius also agrees with experiment to within 1%

Consider the goal of solving for the interaction energy and the radius of $^6$Li. These are important test cases since available supercomputer calculations can be used to train and test the validity of an ANN for predicting the first principles results.

Results of supercomputer calculations up to $N_{max}$ = 10 used for training/testing

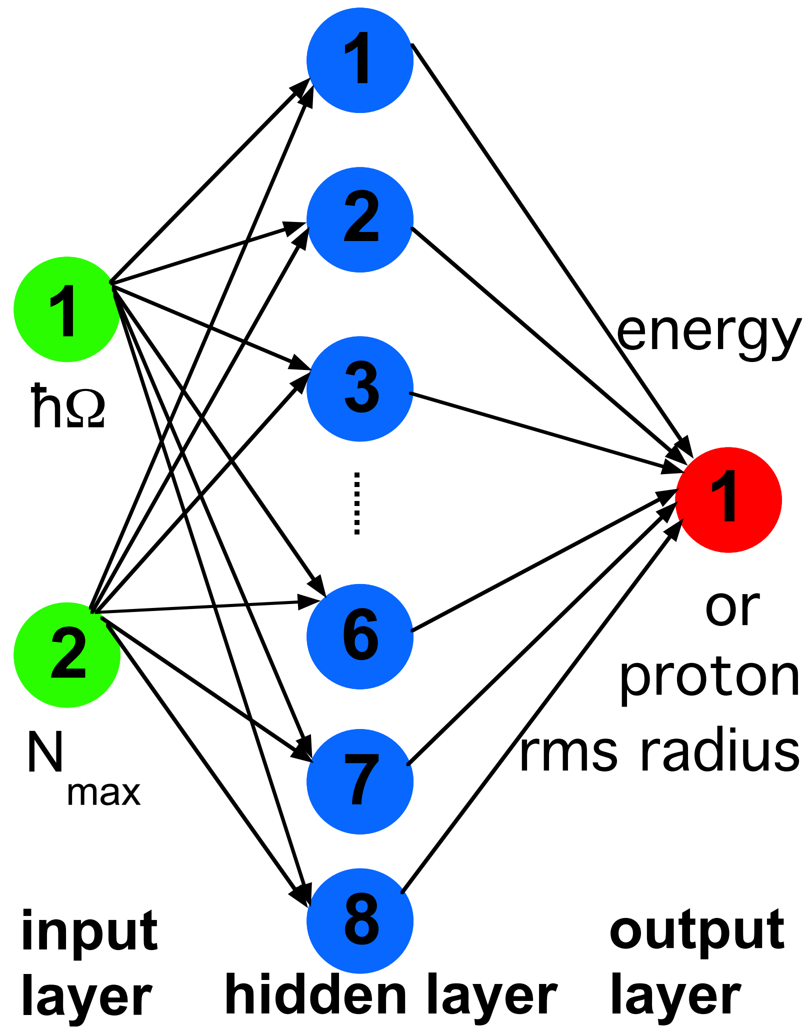


# ANN Design

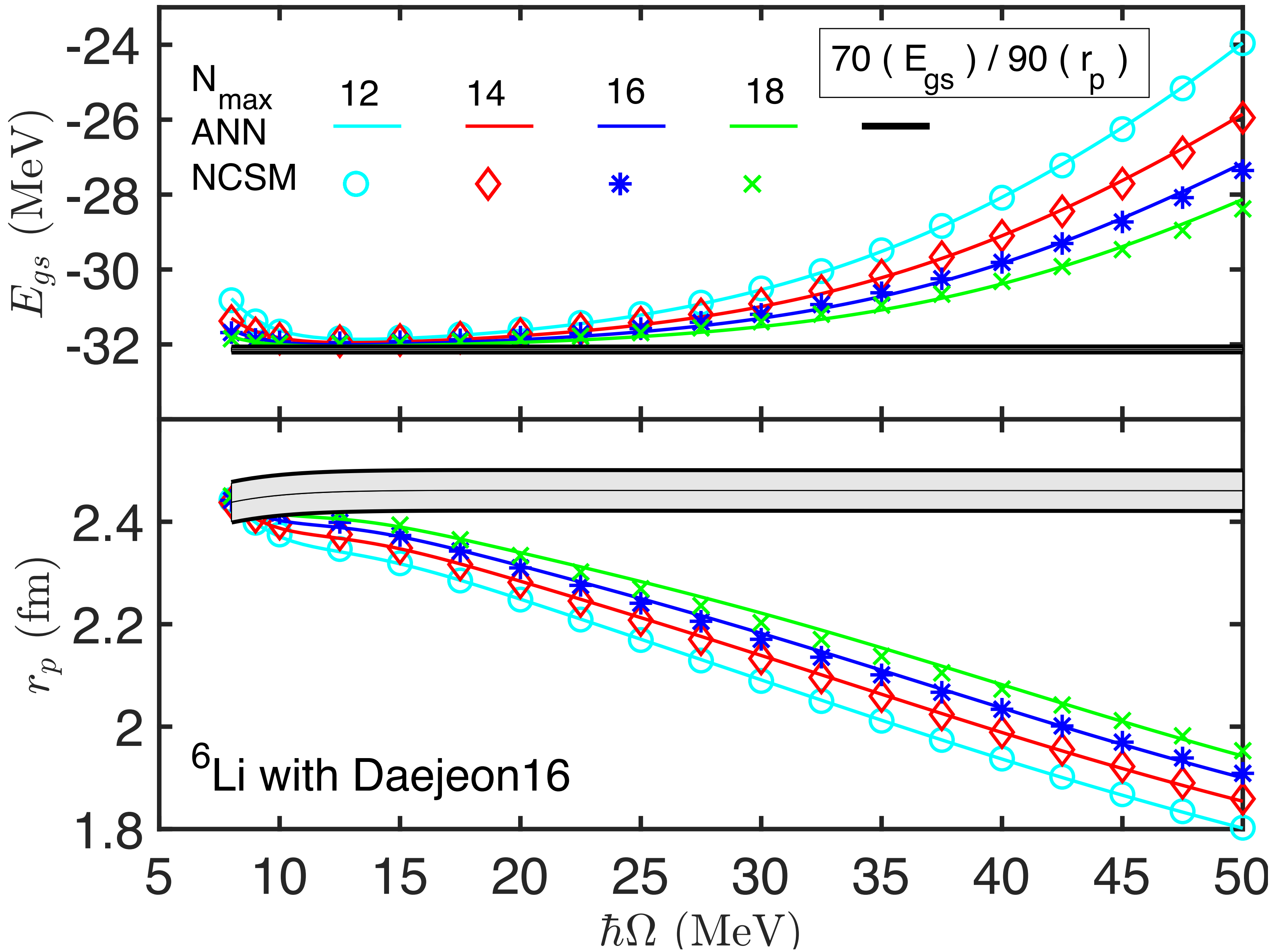
- Topology:
  - hidden layer: *hyperbolic tangent sigmoid* activation function
  - output layer: linear activation function
- The original dataset:
  - NCSM calculation results with MFDn code using Daejeon16 at 19 selected values of $\hbar\Omega = 8 - 50$ *MeV* for all $N_{\max} \leq$ threshold
  - test set $(3/19 \approx 16\%)$
    - 3 random points for each $N_{\max}$
  - design set $(16/19 \approx 84\%)$
    - 90% training
    - 10% testing
- Performance function: MSE

*Feed-forward* three-layer ANN:



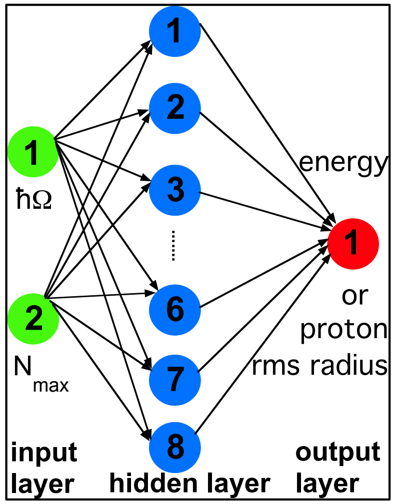

Gianina Alina Negoita, James P. Vary, Glenn R. Luecke, Pieter Maris, Andrey M. Shirokov, Ik Jae Shin, Youngman Kim, Esmond G. Ng, Chao Yang, Matthew Lockner and Gurpur M. Prabhu, "Deep Learning: Extrapolation Tool for Computational Nuclear Physics," PRC 99, 054308 (2019); arXiv: 1810.04009

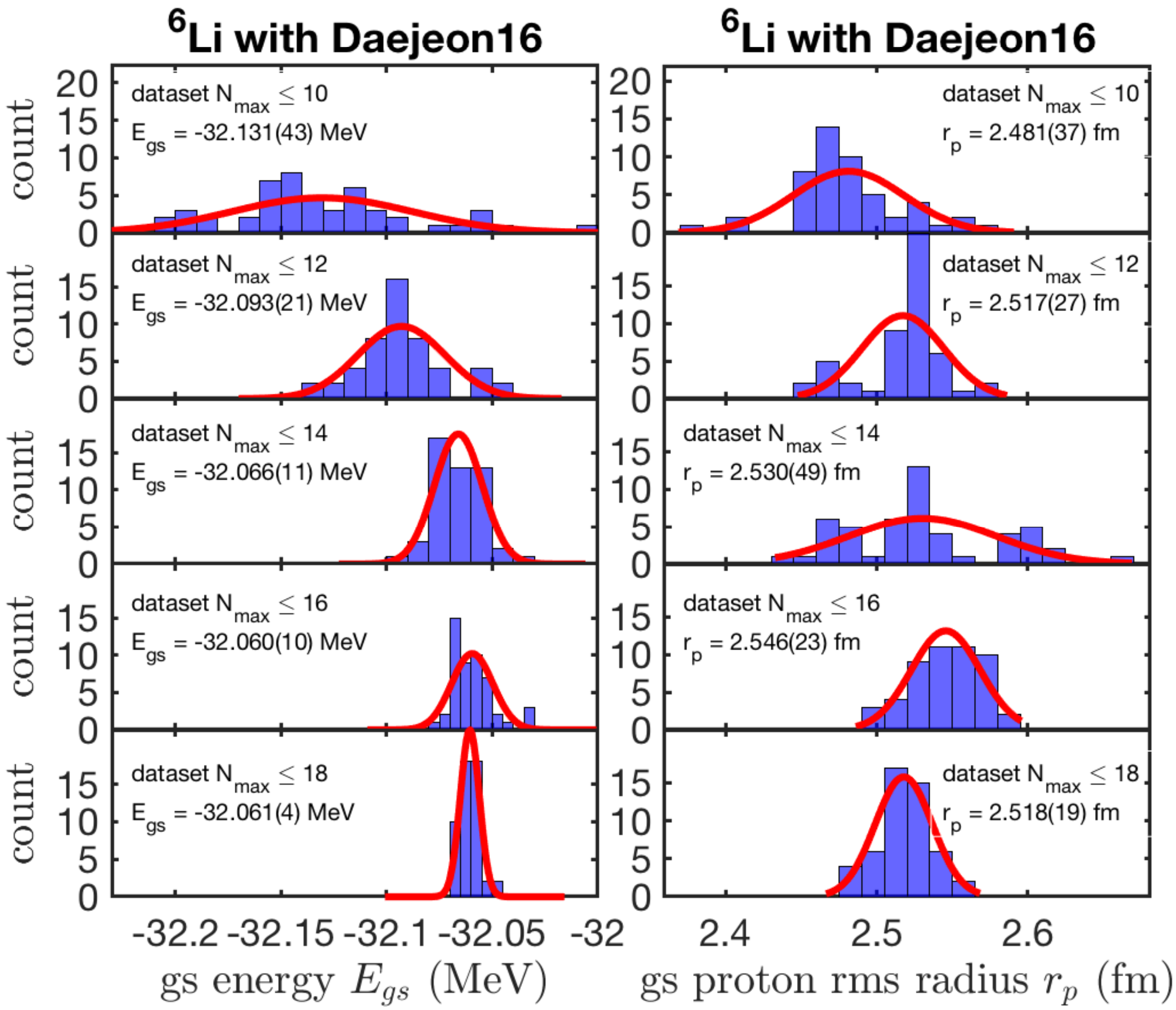
## ANN results when training & testing data limited to Nmax ≤ 10

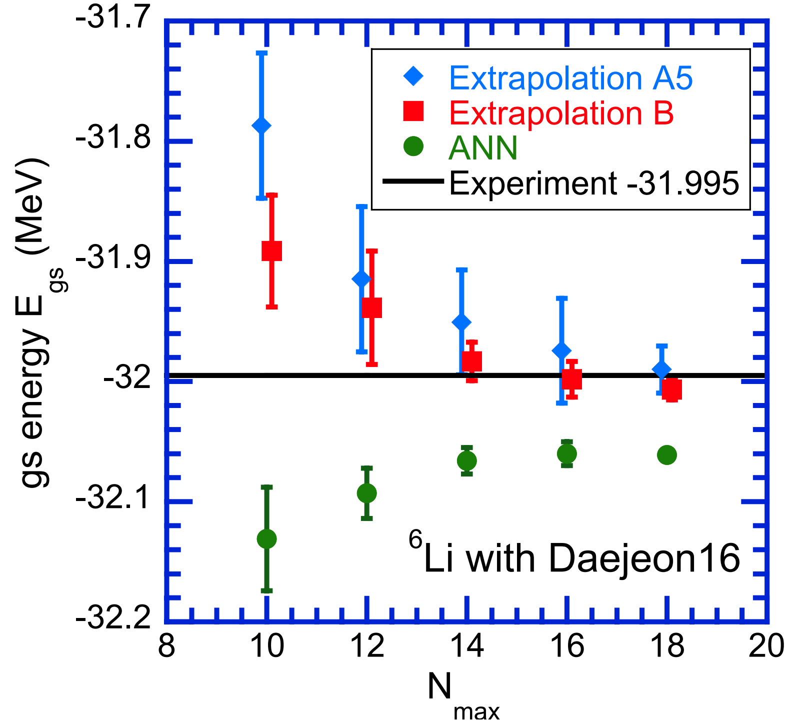


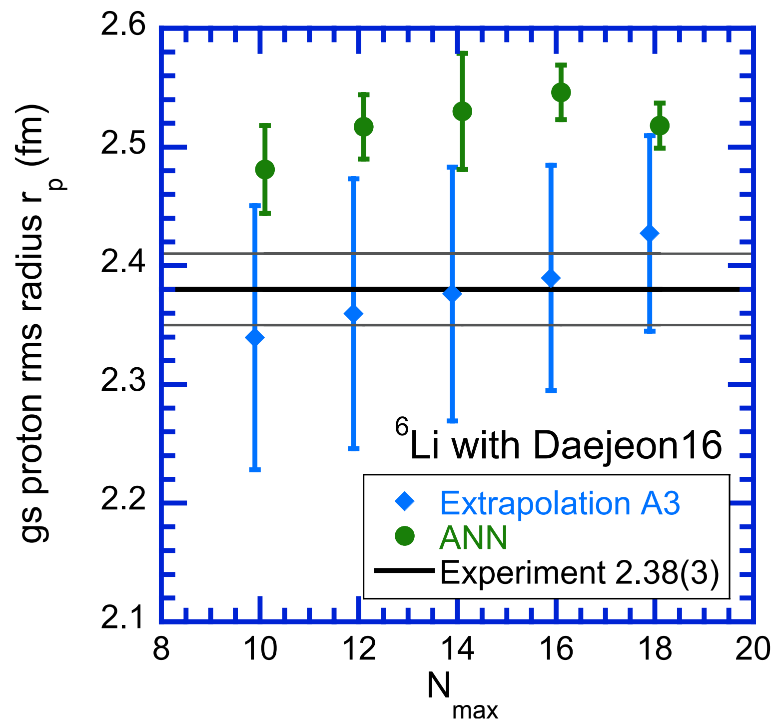

G.A. Negoita, et al., "Deep Learning: Extrapolation Tool for Computational Nuclear Physics," PRC 99, 054308 (2019); arXiv: 1810.04009

"Deep Learning: Extrapolation Tool for Ab Initio Nuclear Theory," G.A. Negoita, et al., PRC 99, 054308 (2019); arXiv:1810.04009

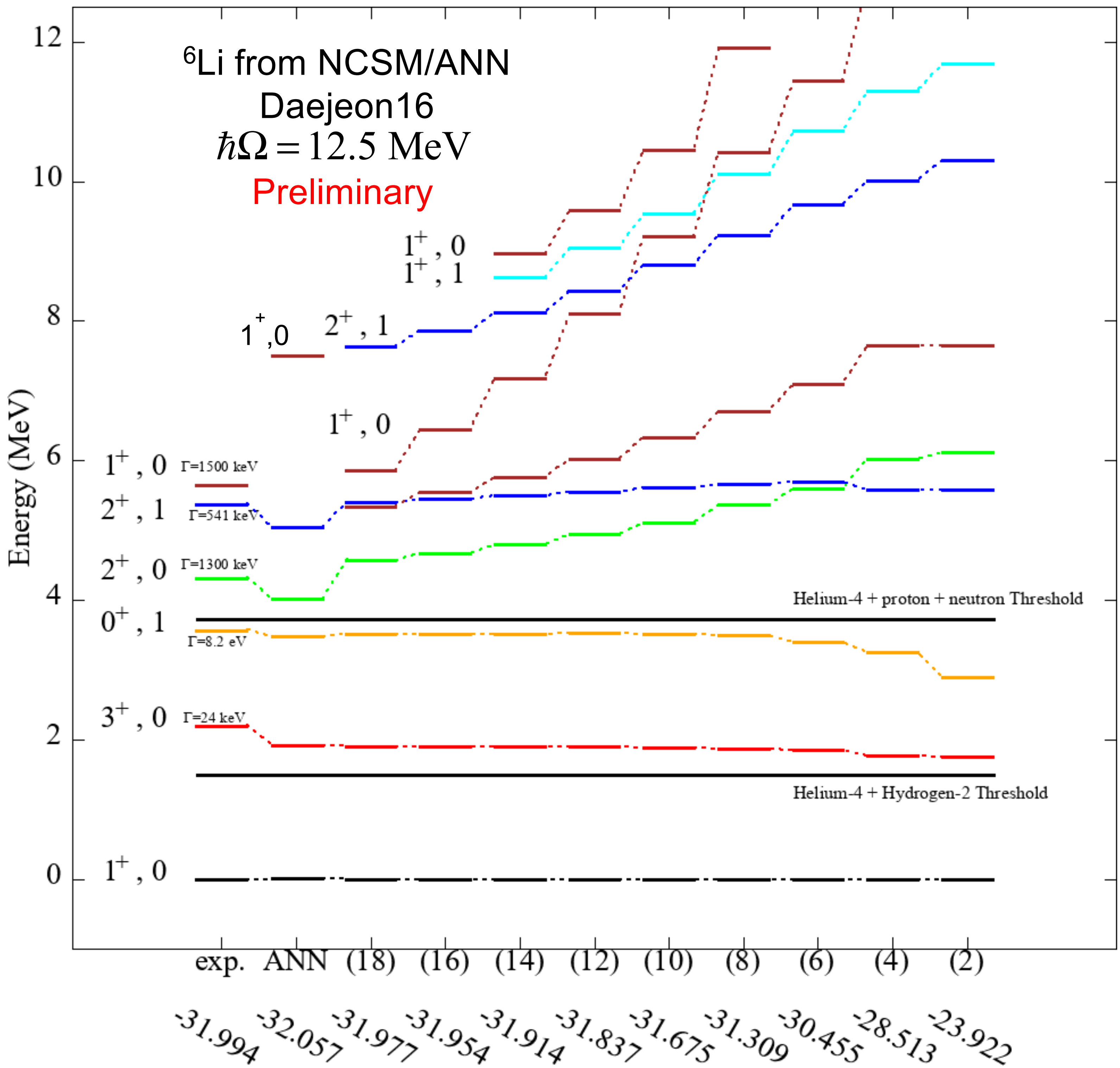


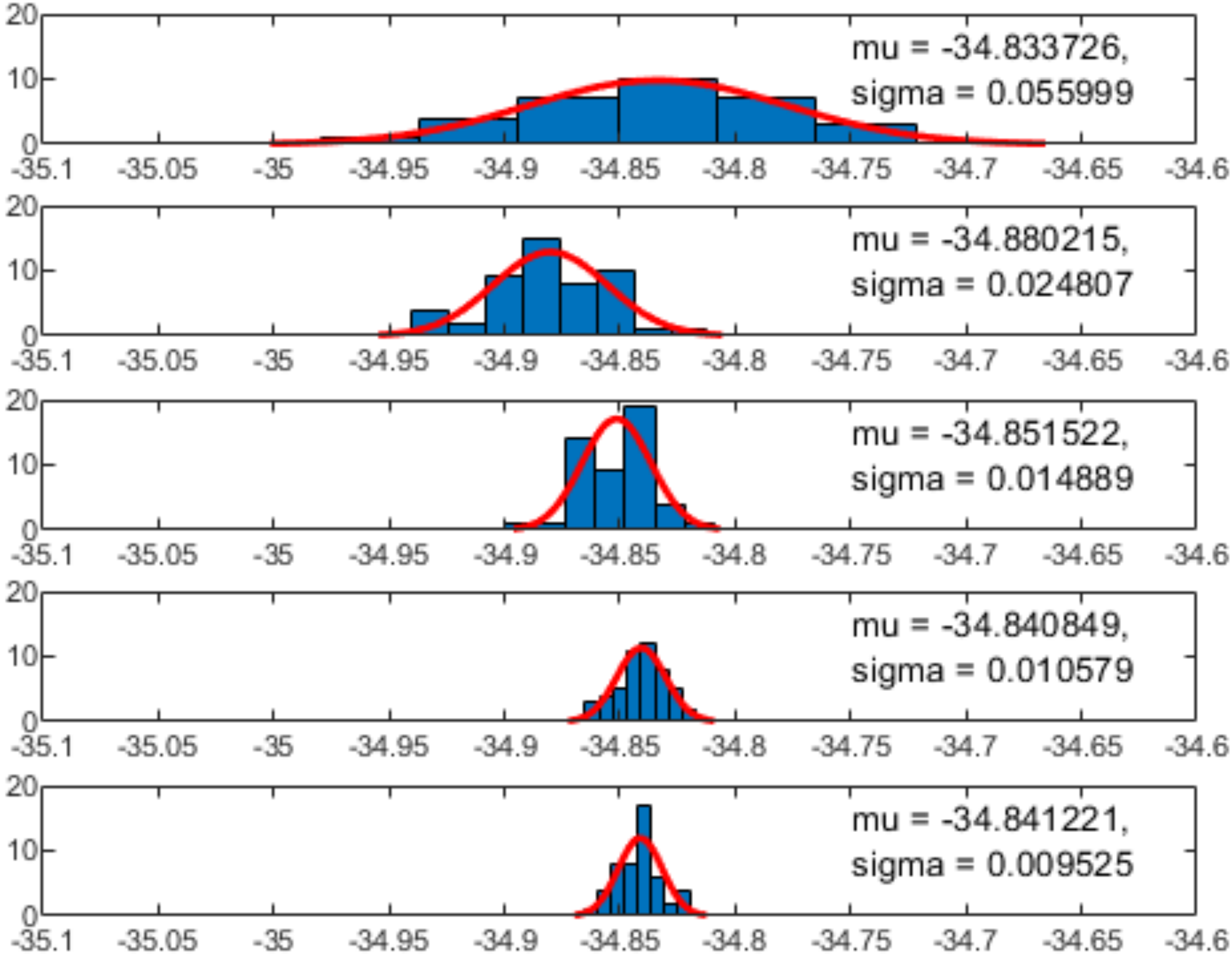



New application: excited states incl. resonances R. McCarty, et al., in preparation

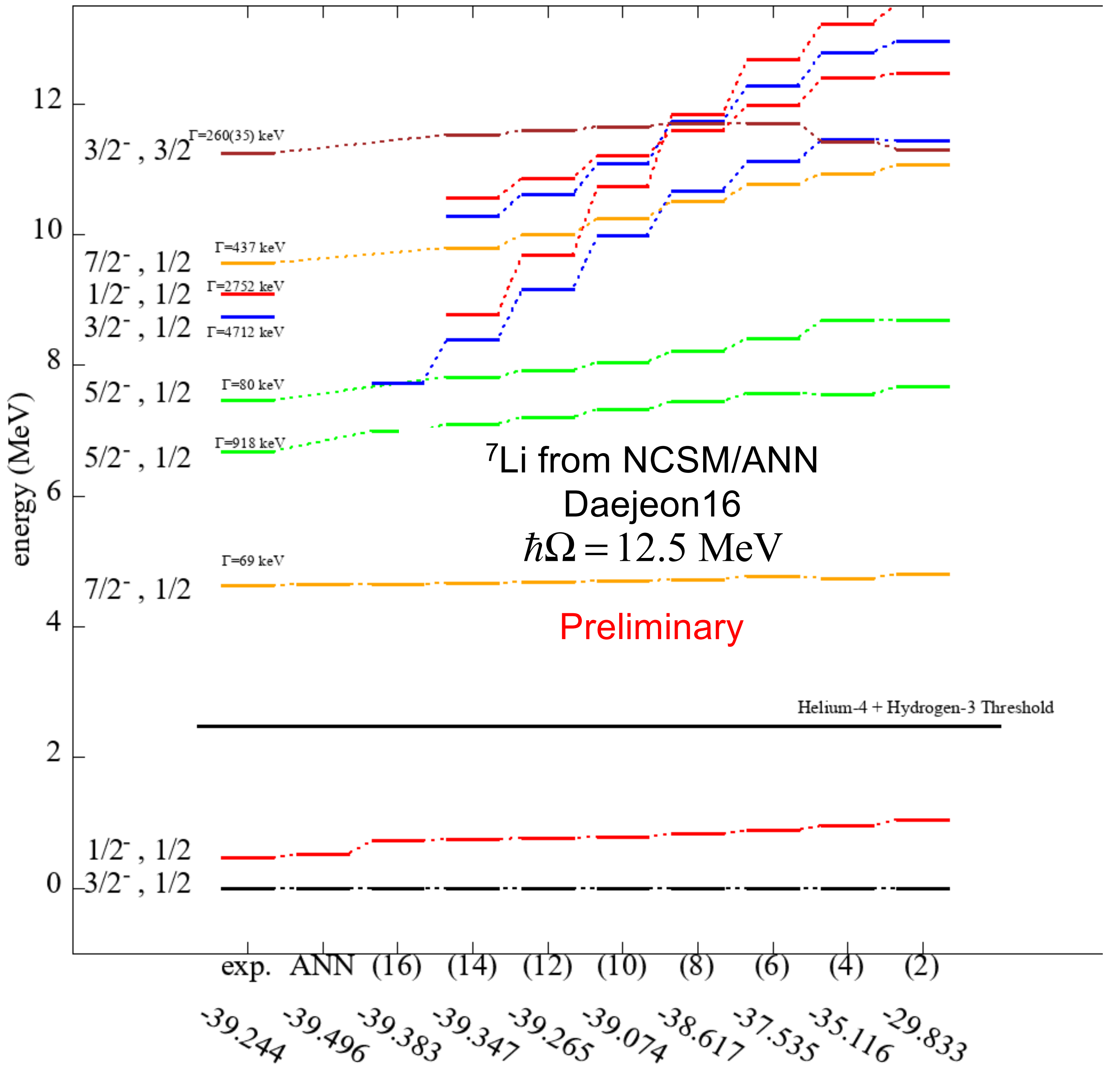


$^7$Li from NCSM/ANN second excited state (7/2$^-$)
Daejeon16, $\hbar\Omega = 12.5$ MeV
Preliminary

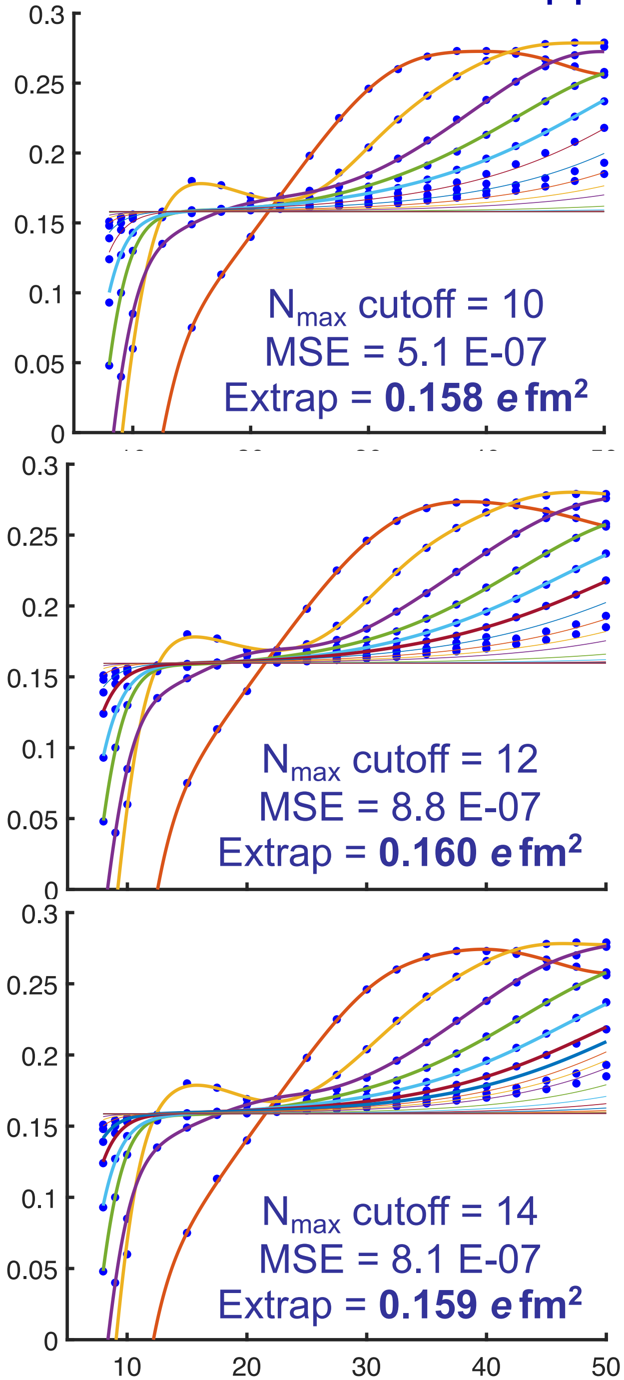


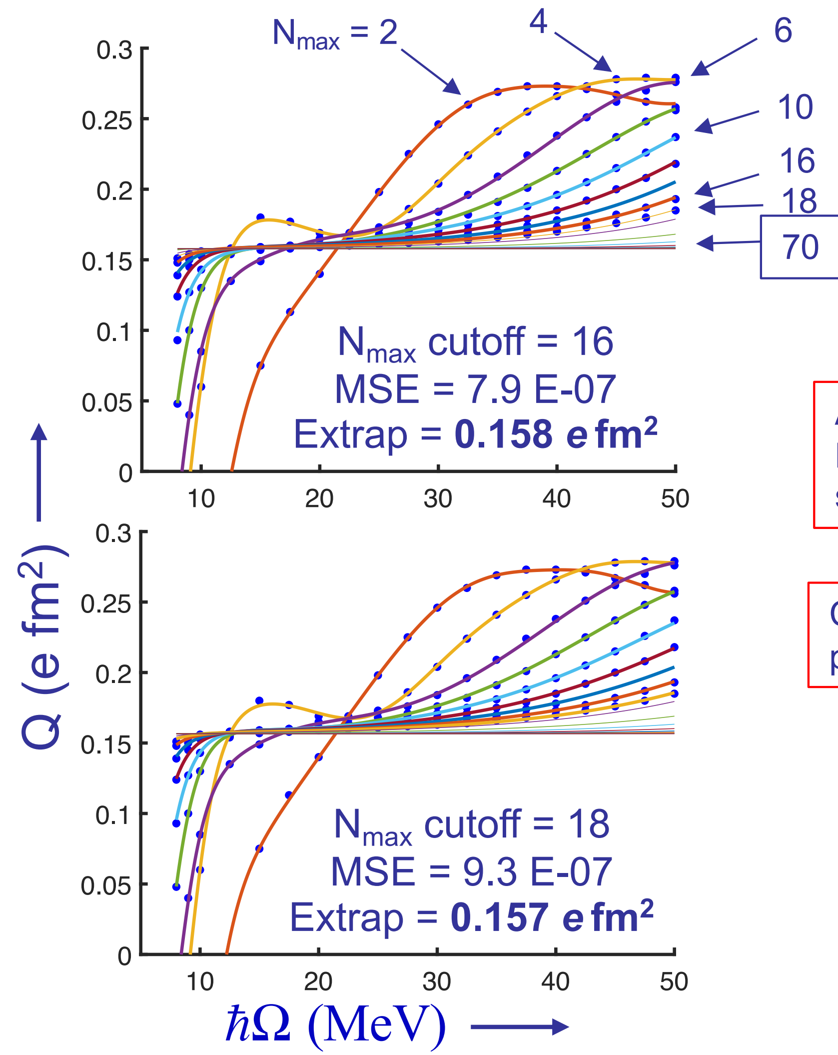

M. Lockner, et al., in preparation

Excited states
incl. resonances
R. McCarty, et al.,
in preparation



# Initial application to the $^6$Li ground state quadrupole moment
## "Best in Class"



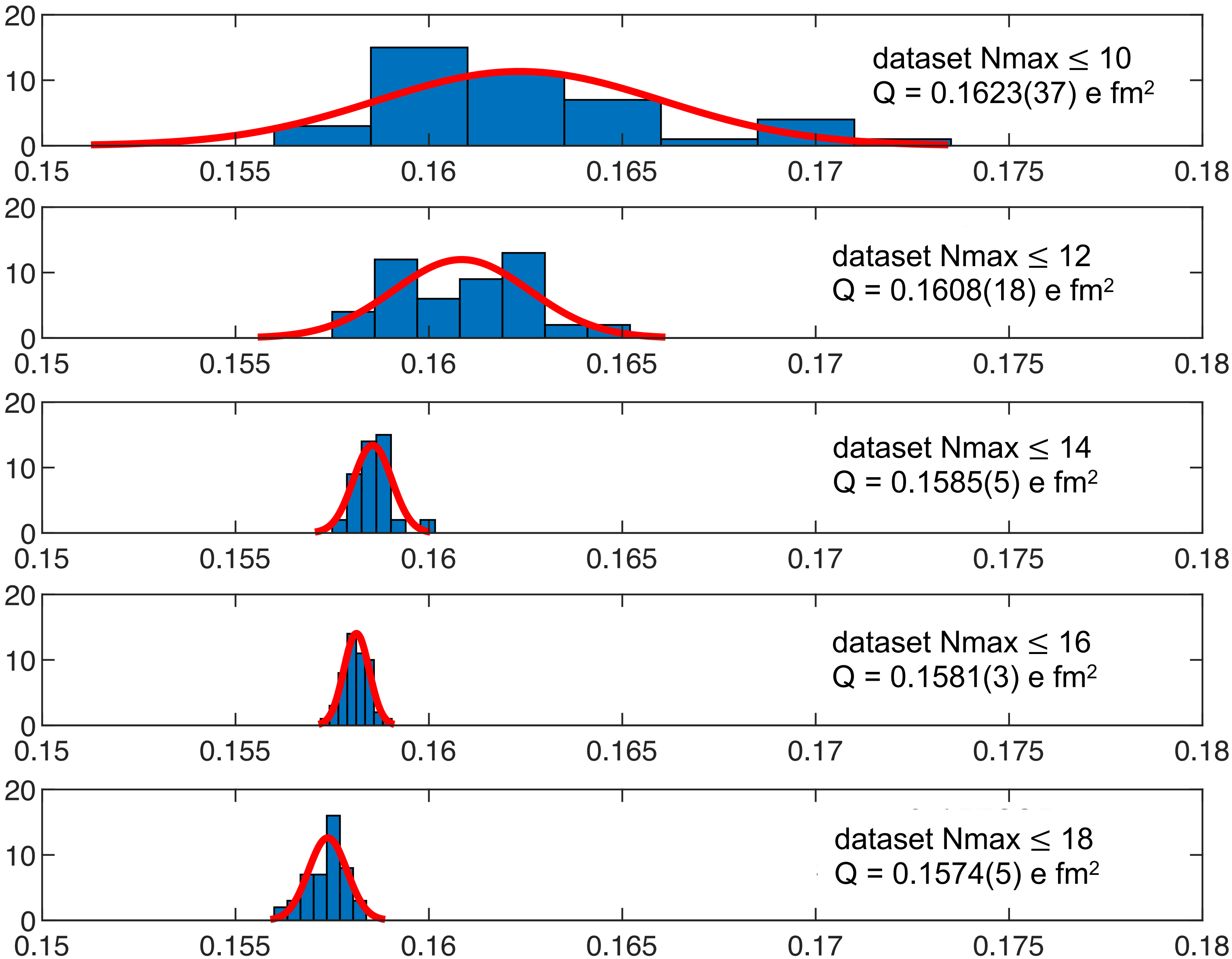




ANN predictions for $N_{max}$ = 20, 25, . . . 65, 70 shown in all graphs

Converged sequence of ANN predictions: Q = 0.157(2) *e* fm$^2$

M. Lockner, et al., in preparation

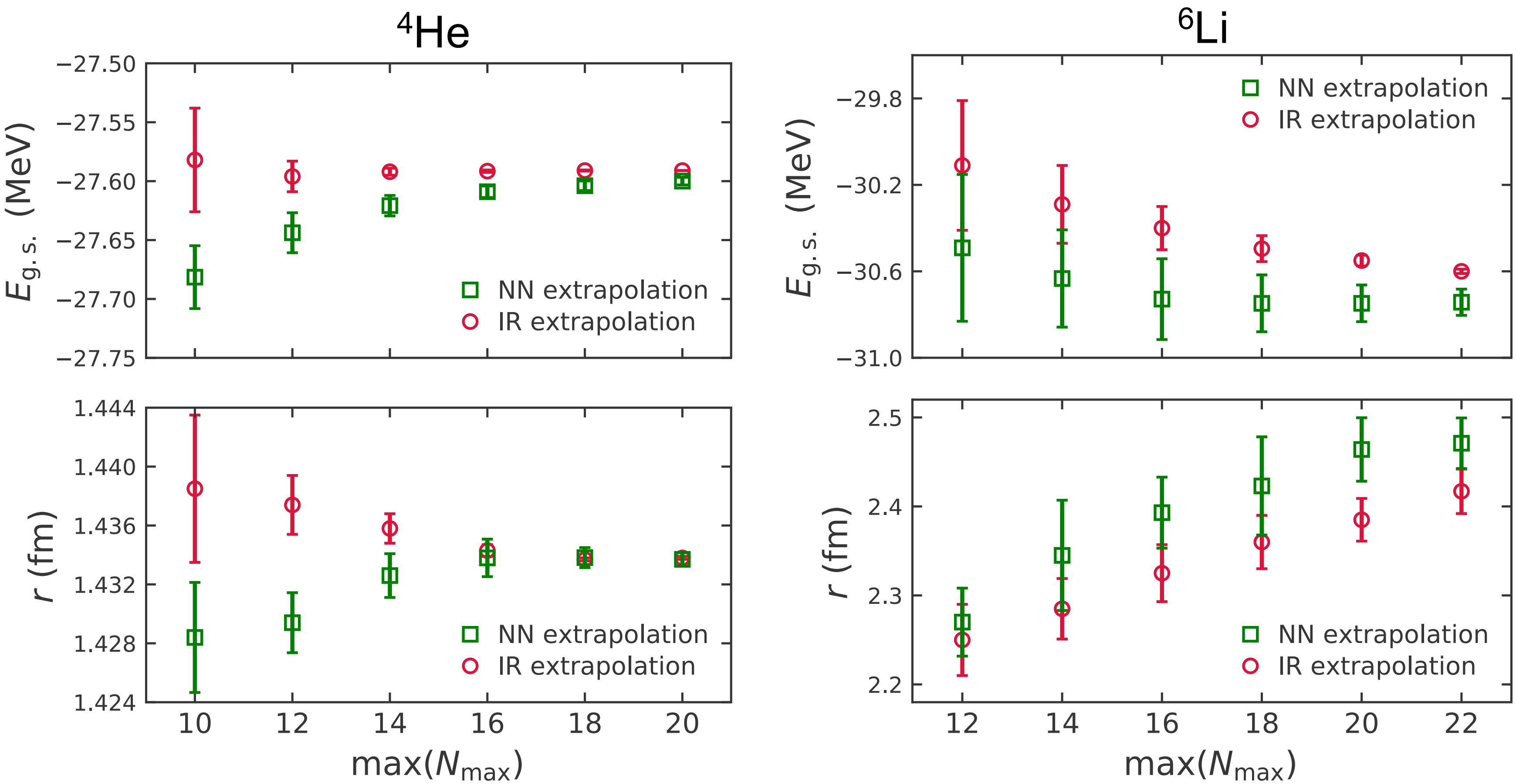
# $^6$Li with Daejeon16
# Ground state quadrupole moment
# Ensembles of ANN results




M. Lockner, et al., in preparation

# Artificial Neural Networks applied to both No-Core Shell Model and Coupled Cluster results

- $NNLO_{opt}$ used for nucleon-nucleon interaction
- Adopts a sigmoid activation function $(1 + e^{-x})^{-1}$
- Uses interpolation to augment the training data set
- Uses a Gaussian to downweight training data in the UV and IR regions
  ~ employing a prior in Bayesian statistics



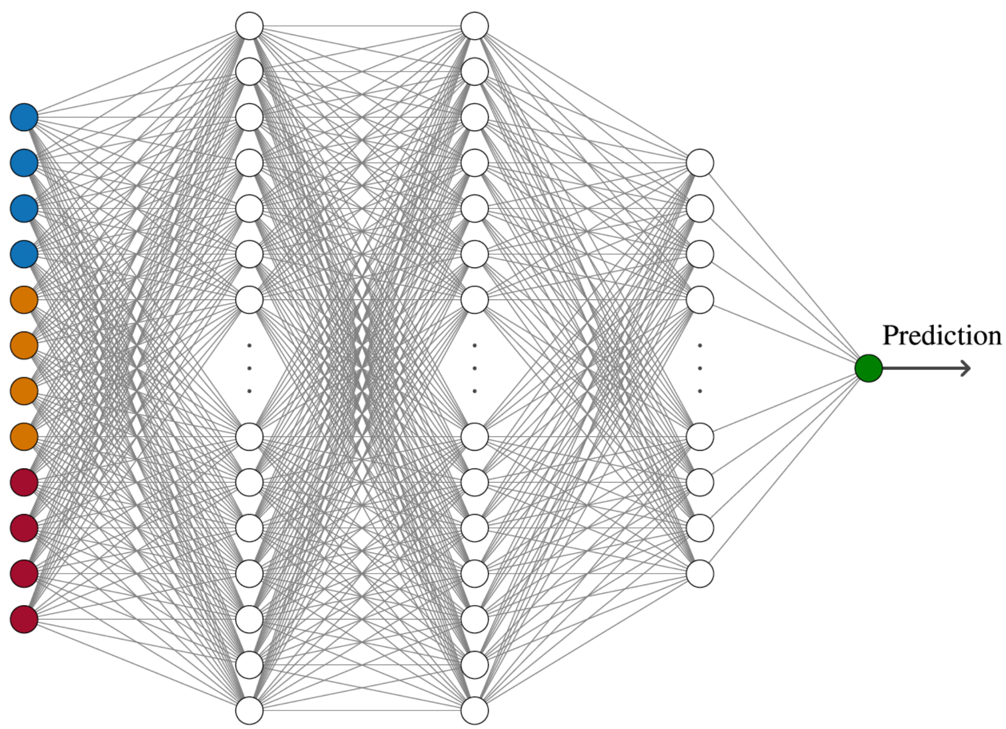

W.G. Jiang, G. Hagen and T. Papenbrock, Phys. Rev. C 100, 5 (2019)

# Machine Learning for the Prediction of Converged Energies from Ab Initio Nuclear Structure Calculations

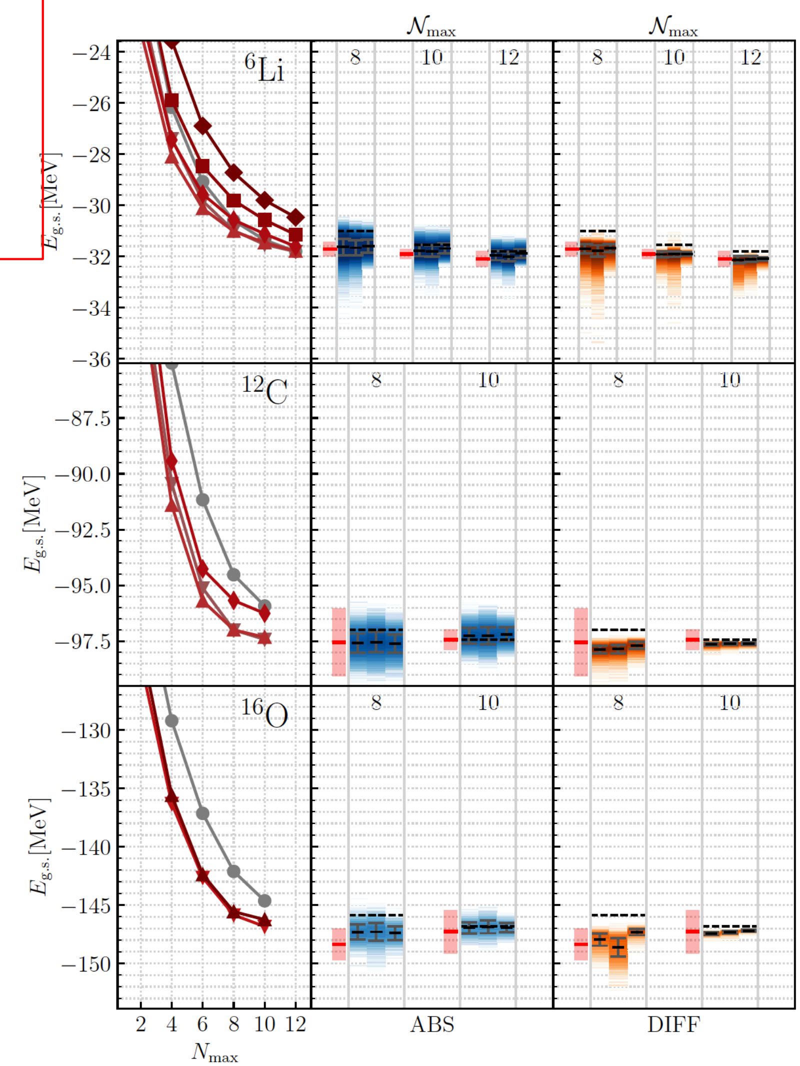
arXiv: 2207.03828

Marco Knöll[a], Tobias Wolfgruber[a], Marc L. Agel[a], Cedric Wenz[a], Robert Roth[a,b]

Use NCSM g.s. energy results for multiple interactions and A = 2, 3 and 4 for training/testing -> predict g.s. energies of heavier nuclei with $N_{max} \leq 12$ NCSM results as input




Topology




Conclusion: Use energy differences for training/testing

Predictions

# Machine Learning – Issues & Challenges

- **Discovering the best ML approach: a research project in its own right**
- **Opening the black box: from application success to physics insights**
- **Gaining trust in ML results: uncertainty quantification, benchmarking**
- **Quantifying network bias: model studies, multiple approaches - GP vs NN**
- **Sharing “expensive” simulated data sets: a community resource**
- **Limited computational resources: ML-friendly architectures**
- **Trained workforce considerations: career path, sustainability**
- **Sharing experiences: improving exchanges with private sector**


## Funding Sources

DOE NP Division

DOE NP/ASCR Divisions (SciDAC/UNEDF SciDAC/NUCLEI)

DOE ASCR Division INCITE Awards on Leadership Class Supercomputers

DOE ASCR Division NERSC Annual Awards

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

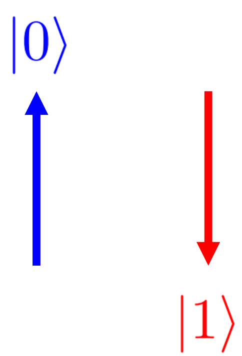
[Int. J. Theor. Phys. Vol. 21, pp. 467-488, (1982)]

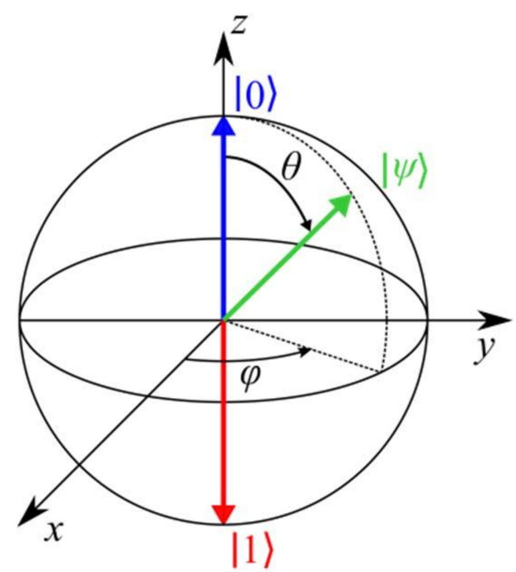
"I'm not happy with all the analyses that go with the classical theory, because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy." --- R. P. Feynman's vision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

# From classical to quantum mechanical

| Classical bit | Quantum bit (qubit) |
| --- | --- |
| $\lvert 0\rangle$ or $\lvert 1\rangle$ | $\lvert\psi\rangle = a\lvert 0\rangle + b\lvert 1\rangle$ |
| **2 states** | **infinite number of states** |

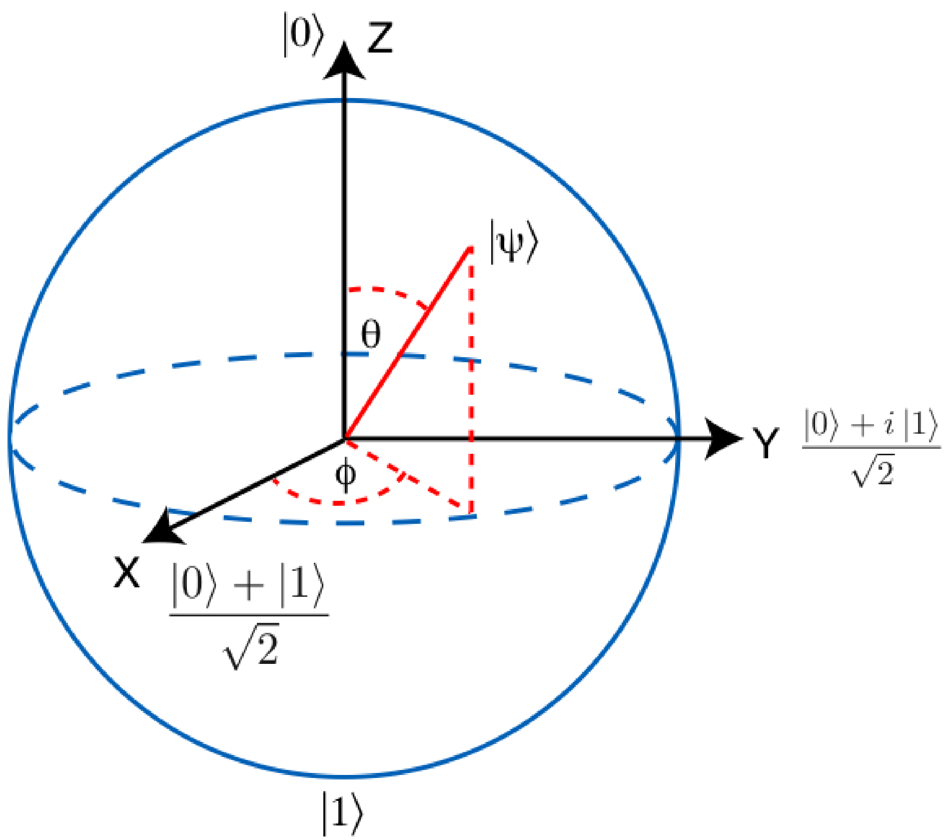
**transistor ON or OFF**




Adapted from Weijie Du, QCGSS Seminar 2020

# Qubit on the Bloch Sphere




- Some use the notation $|\pm\rangle = \frac{|0\rangle \pm |1\rangle}{\sqrt{2}}$ and $|\circlearrowright / \circlearrowleft\rangle = \frac{|0\rangle \pm i|1\rangle}{\sqrt{2}}$

Adapted from Bo Basili, ISU Seminar 2020

# Quantum Mechanics 101: Entanglement

Quantum single-particle states as a column vector: $|\psi_1\rangle = a|0\rangle + b|1\rangle \rightarrow \begin{bmatrix} a|0\rangle \\ b|1\rangle \end{bmatrix}$,

used to define quantum two-particle states as a "tensor product":

$$|\psi\rangle = |\psi_1\rangle|\psi_2\rangle = \begin{bmatrix} a|0\rangle \\ b|1\rangle \end{bmatrix} \otimes \begin{bmatrix} c|0\rangle \\ d|1\rangle \end{bmatrix} \rightarrow \begin{bmatrix} \alpha|00\rangle \\ \beta|01\rangle \\ \gamma|10\rangle \\ \delta|11\rangle \end{bmatrix} \ni |\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1$$

Qubit #1 Qubit #2

Entangled Qubits #1 and #2

Entanglement:

- Multiple Particles can be in "entangled" states that cannot be described independently.
  - Example: $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$
- Entanglement may be thought of as the extension of superposition to many-particle states.

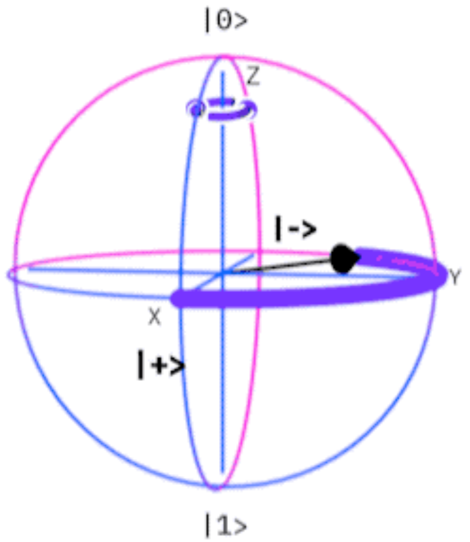
When we measure the state of two qubits, we find one of these four possible states

Adapted from Bo Basili, ISU Seminar 2020

# 1-qubit logic gate examples

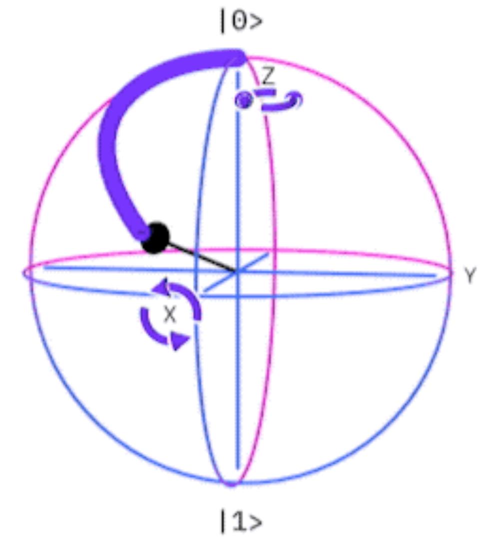
$$Z|+\rangle = |-\rangle \quad \text{or} \quad \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}}|0\rangle \\ \frac{1}{\sqrt{2}}|1\rangle \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}}|0\rangle \\ -\frac{1}{\sqrt{2}}|1\rangle \end{bmatrix}$$

**Z:**




|+⟩ → |-⟩

**H:**

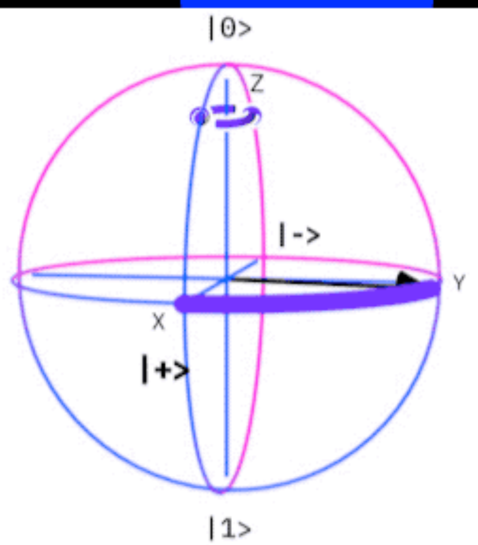



|0⟩ → |+⟩

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

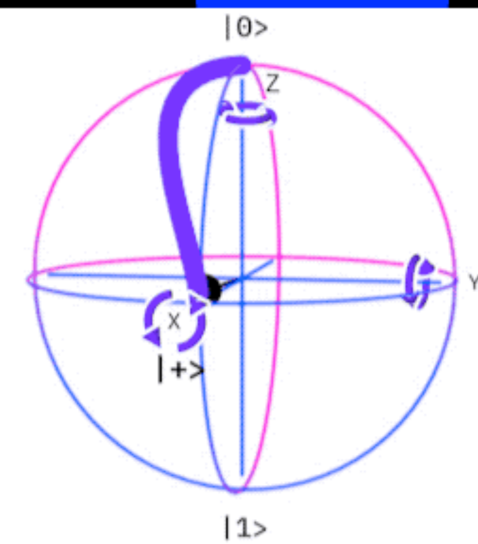
$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

**Rz:**




|+⟩ Rz(π/2) → (|0⟩+i|1⟩)/√2

**U3:**




|0⟩ U3(π/2,π/2,π/2) → |+⟩

$$R_z(\phi) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}$$

$$U_3(\theta, \phi, \lambda) = \begin{bmatrix} \cos\theta/2 & -e^{i\lambda}\sin\theta/2 \\ e^{i\phi}\sin\theta/2 & e^{i\lambda+i\phi}\sin\theta/2 \end{bmatrix}$$

IBM Quantum Experience

Adapted from Bo Basili, ISU Seminar 2020

# Quantum Logic Gates

- Quantum logic gates must correspond to **Unitary** operators.
- Infinite number of logic gates exist, but only a finite number are required to form a "universal gate set".
- Some standard 1-qubit gates:
  - $I|\psi\rangle = |\psi\rangle$ (identity)
  - $X|0/1\rangle = |1/0\rangle$ (flip)
  - $Y|\circlearrowleft / \circlearrowright\rangle = |\circlearrowright / \circlearrowleft\rangle$
  - $Z|\pm\rangle = |\mp\rangle$
  - $H|0/1\rangle = |\pm\rangle$
- These may be defined using the "number" and "complement" operators $n|q\rangle = q|q\rangle$ and $\tilde{n} = I - n$:
  - $Z = n - \tilde{n}$
  - $Y = iXZ$
  - $H = \frac{1}{\sqrt{2}}(X + Z)$
- Note $X$, $Y$, and $Z$ are equivalent to the Pauli matrices.
- The Hadamard gate, $H$, functions as a fourier transform.

Adapted from Bo Basili, ISU Seminar 2020

# Encoding Many-Body basis states on qubits

**Direct encoding** = one qubit for each single-particle state

Advantages:
Simplicity
Minimizes the circuit depth

Disadvantage:
While good for FCI applications (esp. Quantum Chemistry and valence-space Shell Model applications) it is not particularly useful for $N_{max}$ truncations of the NCSM

**Compact encoding** = qubits assigned as digital counter of many-body states so that, with $N_q$ qubits, one encodes $2^{N_q}$ many-body states

Advantages:
Works well for non-FCI truncation schemes such as the NCSM with $N_{max}$ truncation
Suitable for non-Slater determinant basis such as employed in tBFq and tBLFQq

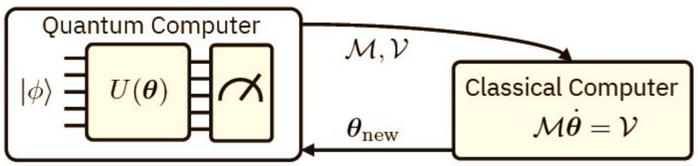
Disadvantage:
Greater circuit depth than direct encoding

# Applications in HEP/NP

Two main directions:

- **Variational Approaches**: Variational Quantum Eigensolver (VQE), hybrid optimization algorithm, many variants, widely-used in quantum chemistry, lead to Q machine learning

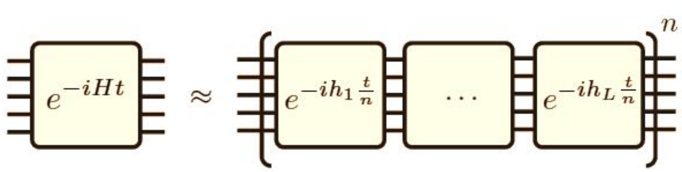
Peruzzo et al., 1304.3061 (2013)
Bharti et al., 2101.08448 (2021)



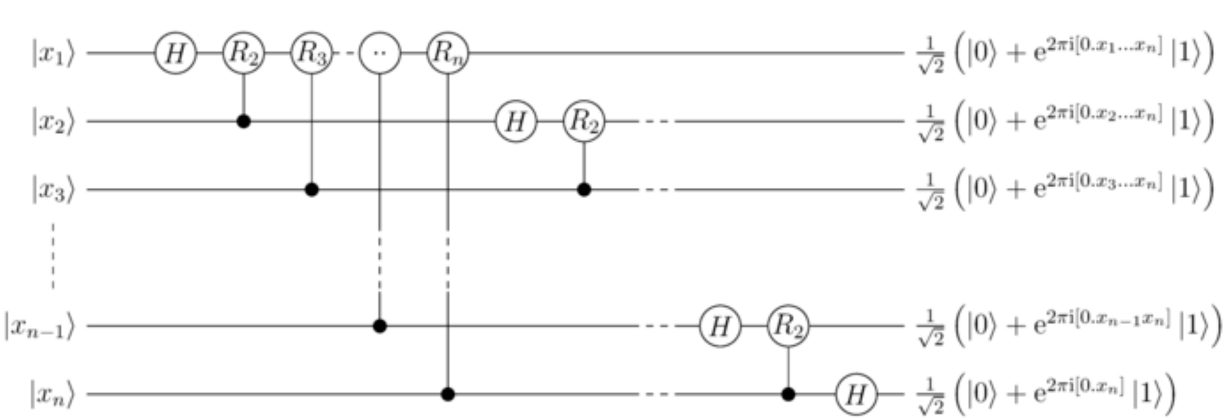

- **Decomposition Approaches**: Quantum Simulation Algorithms, prepare, evolve, fourier transform, measure to find quantum state of the system

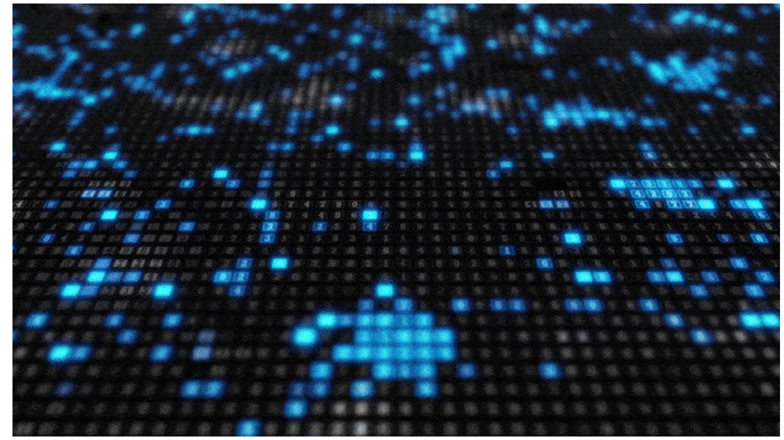
Wiesner, 9603028 (1996); Zalka, 9603026 (1996)

Image from Miessen's talk at QGSS 2022



# Algorithm development

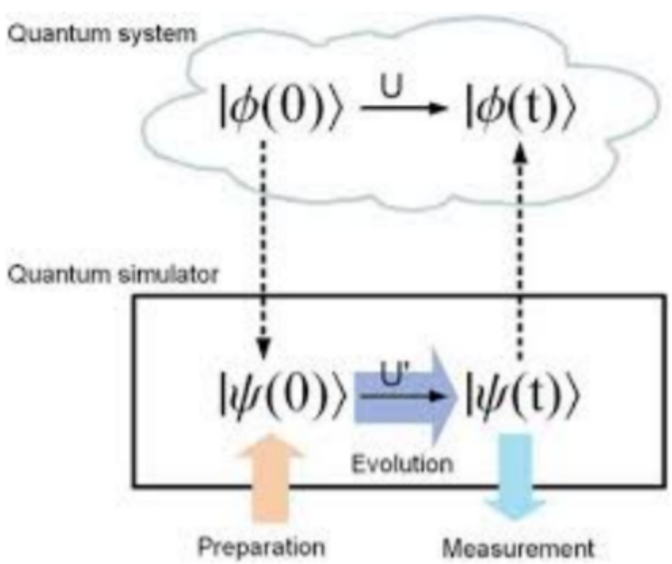


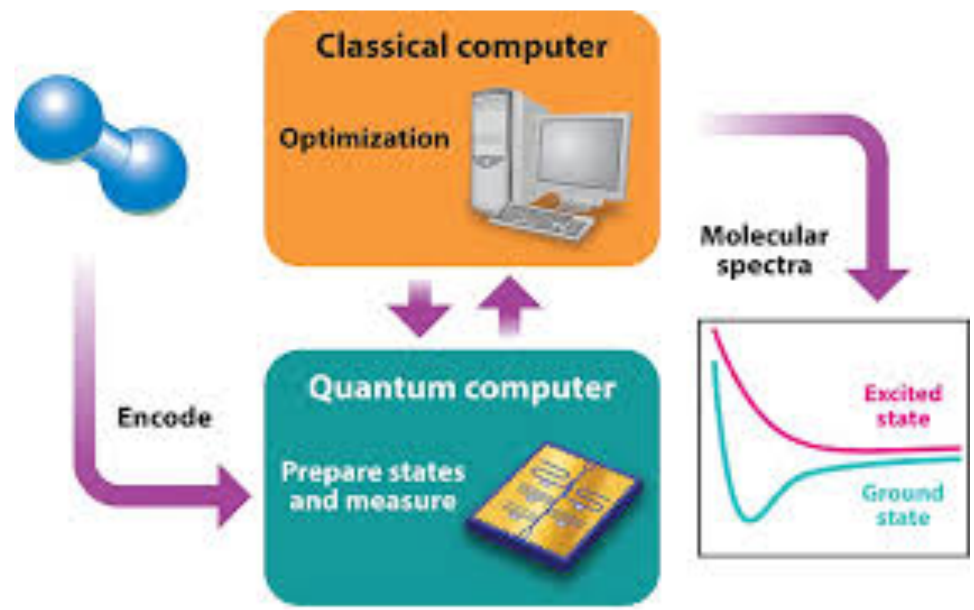
https://quantumalgorithmzoo.org/

Andrew Childs et al., Rev. Mod. Phys. **82**, 1

**some algorithms of interest to nuclear physics**




- **Hamiltonian simulation** (for dynamics, real-time evolution)




- **Eigensolver** (for structure calculations)

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

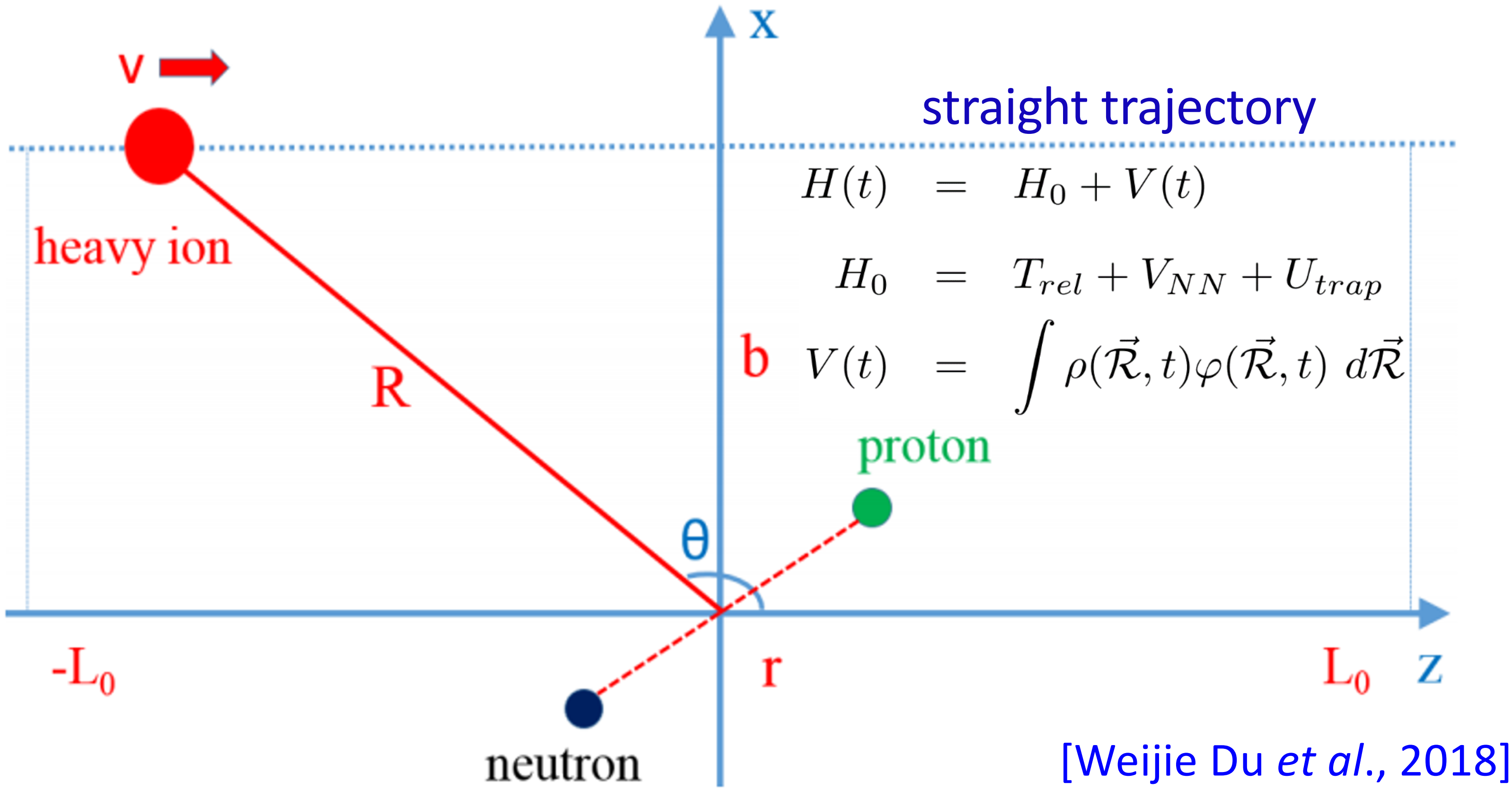
- Unified structure and reaction theory
- Based on successful *Ab initio* nuclear structure theory
- Non-perturbative scattering method
- Retaining full quantal coherence & entanglement
- Circumventing the exponential cost in computation resource in simulating real-time many-body dynamics

*Theoretical scattering method (tBF) introduced and solved on classical computers:*
W. Du, P. Yin, Y. Li, G. Chen, W. Zuo, X. Zhao and J.P. Vary, "Coulomb Excitation of Deuteron In Peripheral Collisions with a Heavy Ion," Phys. Rev. C 97, 064620 (2018); arXiv: 1804.01156

*tBF solved for deuteron inelastic scattering by simulation of a quantum computer:*
W. Du, J.P. Vary, X. Zhao and W. Zuo, "Quantum Simulation of Nuclear Inelastic Scattering," Phys. Rev. A 104, 012611 (2021); arXiv: 2006.01369

*tBF provides a parameter-free deuteron elastic scattering cross sections on classical computers:*
P. Yin, W. Du, W. Zuo, X. Zhao and J.P. Vary, "Sub-Coulomb barrier d+208Pb scattering in a Time-dependent basis function approach," J. Phys. G. 2022 (in press); arXiv: 1910.10586

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




- $H_0$: 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

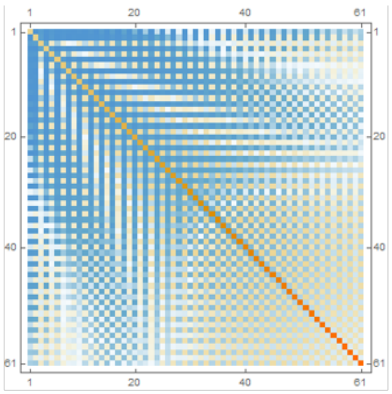
## Construct the basis representation from *ab initio* nuclear structure calculation

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

$$H_0 = T_{rel} + V_{NN} + U_{trap}$$

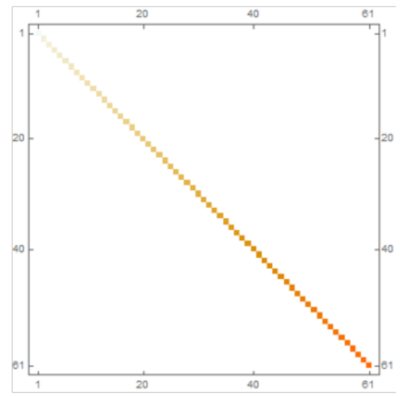
**Basis representation**

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



**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

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

## 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

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

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

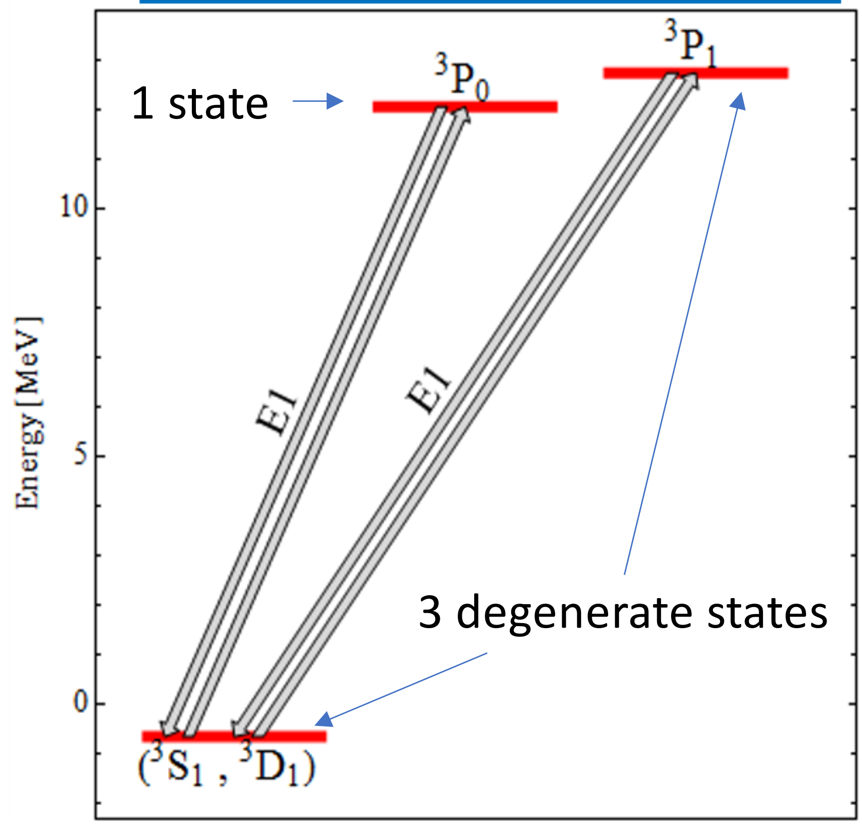
$\langle \beta_j | U_I(t;t_0) | \beta_i \rangle$ ➡ **Quantum circuit**

# 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**

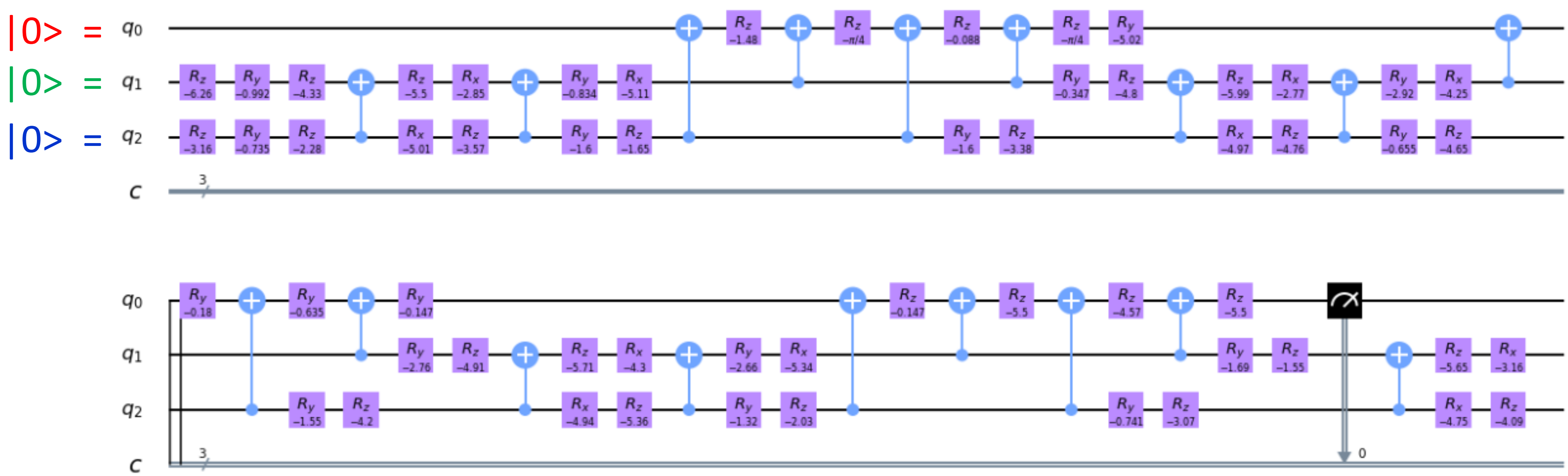


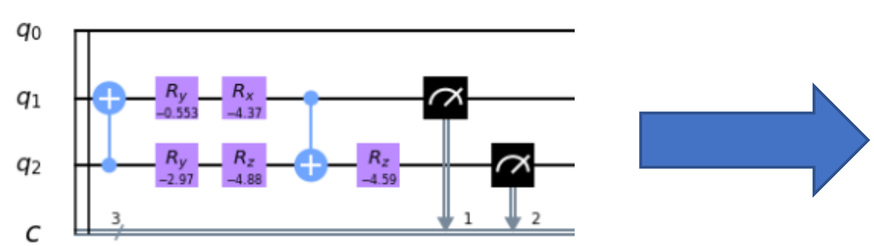

1. 7 basis states of the target solved via *ab initio* structure calculation
2. Initial state set to be antiparallel to z-axis
3. E1 radiative transitions retained in dynamics (time-evolution operator)
4. Trotterization; 7 basis states ***mapped*** to 3 qubits

[Weijie Du et al., 2017]

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

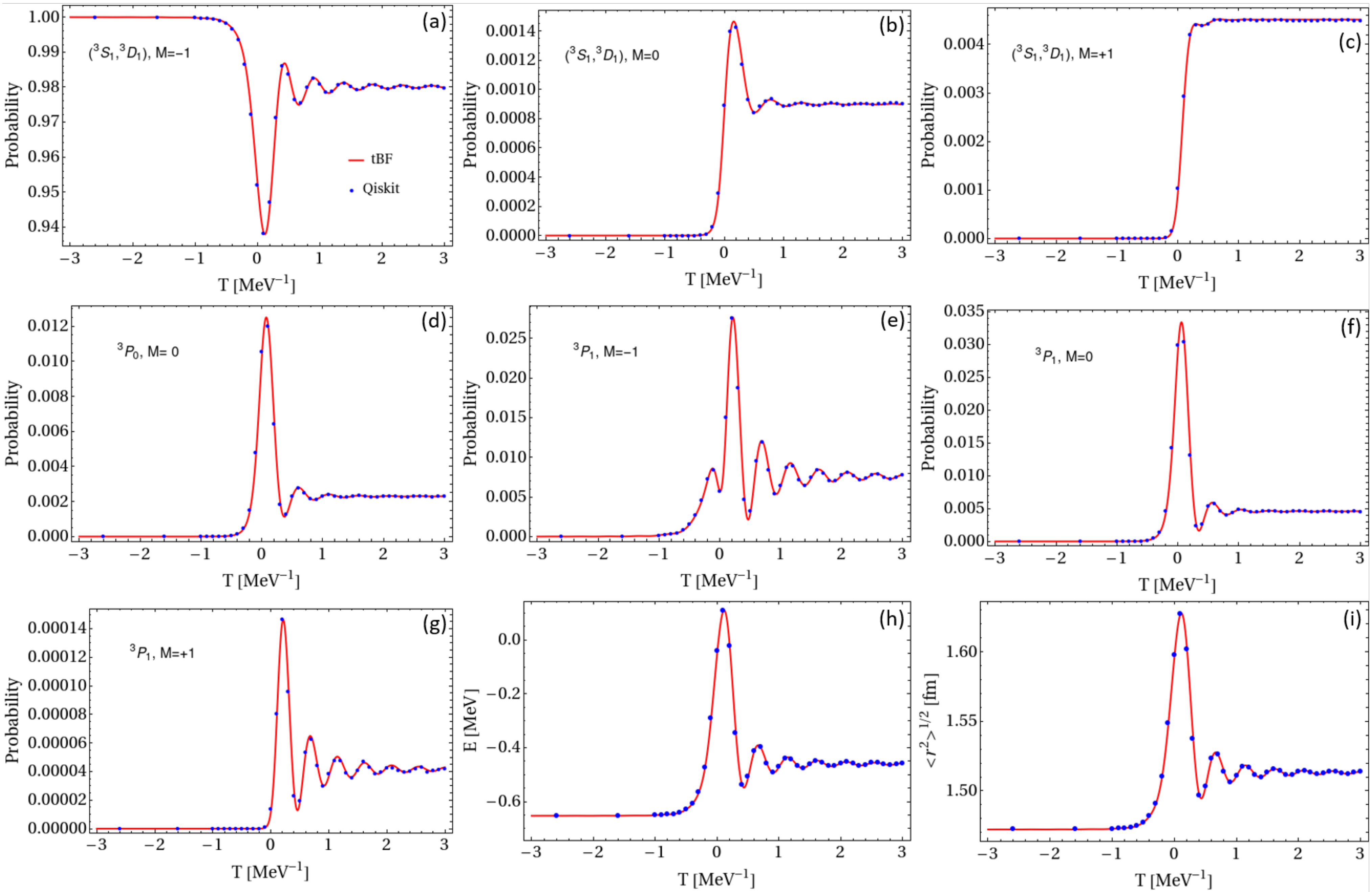
- The initial state in the qubit representation is |000>
- The quantum circuit is constructed by Quantum Shannon Decomposition




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

# Transition probabilities and observables on a simulated QC (dots)




Weijie Du et al., Phys. Rev. A 104, 012611 (2021); arXiv:2006.01369

# Dynamics of many-nucleon system on quantum computer

**Problem:** **exponential scaling** in computing resources of quantum many-body problems
**Goal:** quantum algorithm for the structure and dynamics of the many-nucleon systems

**Focus:** to develop **input model** for the second-quantized many-nucleon Hamiltonian

**Hamiltonian:** $$H = \sum_{p<q,r<s} \langle pq|H|rs\rangle a_p^\dagger a_q^\dagger a_s a_r \qquad H_{pqrs} = T_{pqrs}^{\text{rel}} + V_{pqrs}^{\text{NN}} + H_{pqrs}^{\text{CM}}$$

**Direct encoding scheme:** one-on-one mapping between single-nucleon bases and qubits

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| neutron state | **qubit index** | **0** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** | **11** |
| | occupancy | **1** | 0 | 0 | 0 | **1** | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| proton state | **qubit index** | **12** | **13** | **14** | **15** | **16** | **17** | **18** | **19** | **20** | **21** | **22** | **23** |
| | occupancy | 0 | **1** | 0 | 0 | 0 | 0 | **1** | 0 | 0 | 0 | 0 | 0 |

Fock state **encoded as** binary string
$|0,4,13,18\rangle$
$\rightarrow$ 100010000000 010000100000

**Hamiltonian input model:** to construct the isometry $\mathcal{T}$ via oracle queries

$$\mathcal{T}|\mathcal{F}\rangle|b\rangle = |\mathcal{F}\rangle|b\rangle|\phi_{\mathcal{F},b}\rangle$$
$$\mathcal{T}^\dagger S \mathcal{T}|\lambda_j\rangle|0\rangle = \left[\frac{\epsilon}{||H||_1} H \otimes |0\rangle\langle 0| + |0\rangle\langle 0| \otimes |1\rangle\langle 1|\right]|\lambda_j\rangle|0\rangle = \widetilde{\lambda}_j|\lambda_j\rangle|0\rangle$$

[Berry and Childs, Quantum Inf. Comput. 12, 29 (2012)]

# High precision eigenvalues and phase shift via Rodeo algorithm

$H_0 = T + V_{NN}$

Discretization by an external harmonic oscillator potential

$H(\omega) = H_0 + \frac{1}{2}\mu\omega^2 r^2$

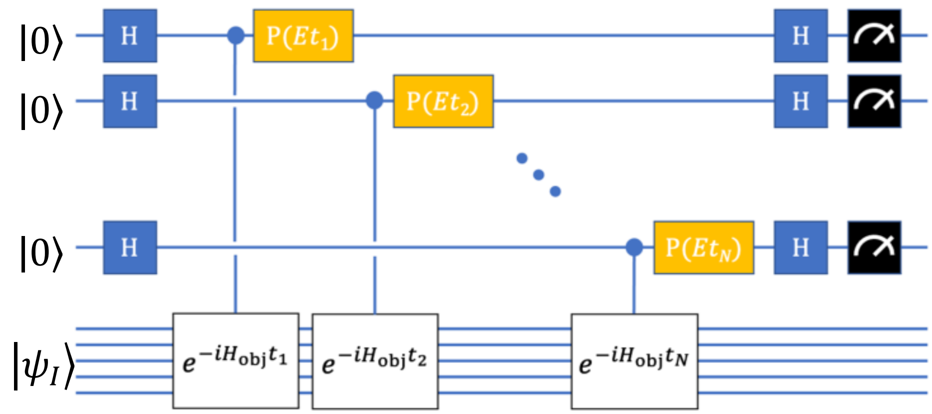
Rodeo algorithm for e-values

$E_n = E_n(\omega)$

Zero-range relation[1], fitting

$\delta = \delta(\omega)|_{\omega\to 0}$

Scattering phase shift of free scattering system of $H_0$




The probability of the measurement 0 for m-th state:

$$P\left(|0\rangle, |\phi_m\rangle\right) = \frac{1}{4}|c_m|^2 \left|1 + e^{i(E-E_m)t_1}\right|^2 = |c_m|^2 \left|\cos\left(\frac{E-E_m}{2}t_1\right)\right|^2$$

$$p^{2l+1}cot\delta_l(p) = (-1)^{l+1}\,(2\mu\omega)^{l+\frac{1}{2}}\,\frac{\Gamma(\frac{2l+3}{4} - \frac{\varepsilon}{2})}{\Gamma(\frac{1-2l}{4} - \frac{\varepsilon}{2})}, \varepsilon = \frac{E}{\omega}, p = \sqrt{\mu E}$$

W. Du, et al., in preparation


[T. Busch et al., Found. Phys. 28, 549 (1998)]
[K. Choi, D. Lee et al., PRL 127, 040505 (2021)]
[Z. Qian et al., PRL, arXiv:2110.07747 (2021)]

# *NN* scattering phase shift via quantum computing

## Demonstration problem:

1. $V_{NN}$ as spherical well potential:

$$V_{NN} = \begin{cases} -V_0, & x \leq R_0 \\ 0 \;\;\;, & x > R_0 \end{cases}$$

$$V_0 = 48.0002 \text{ MeV}, R_0 = 1.70134 \text{ fm}.$$

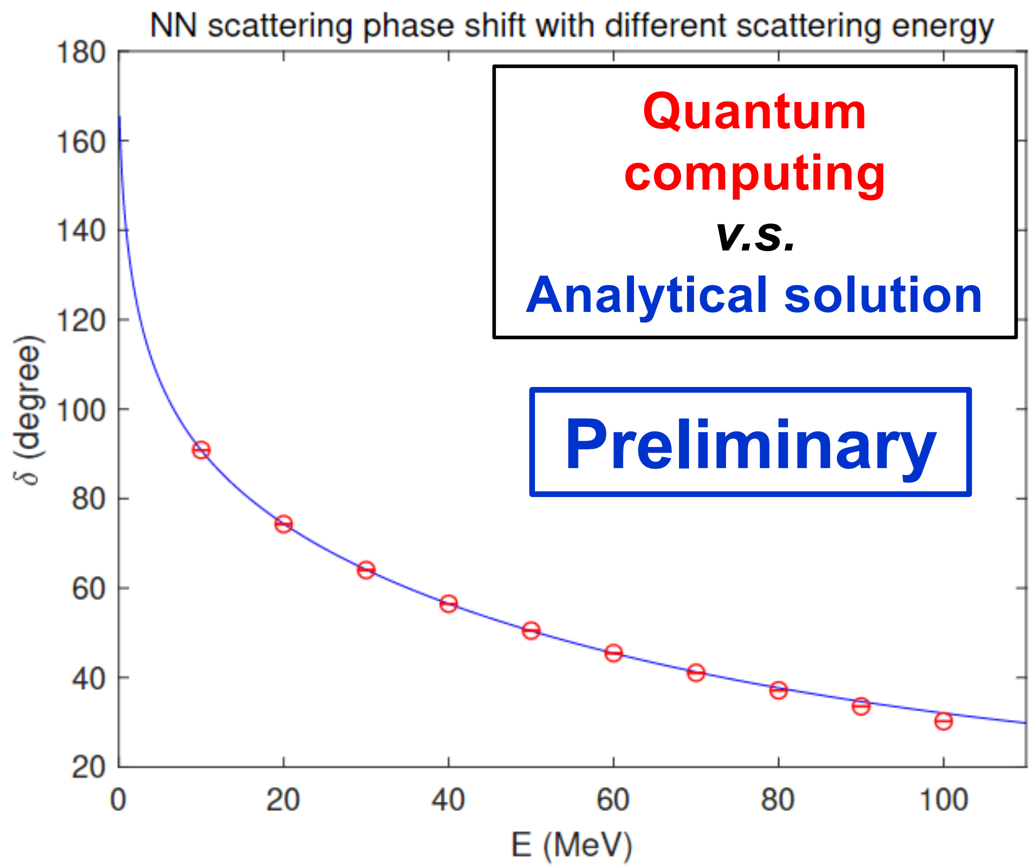
2. 3DHO basis:

$$\omega = 60 \text{ MeV}, N_{max} = 600.$$

3. Analytical solution:

$$\delta = \arctan\left[\frac{k}{p}\tan(pR_0)\right] - kR_0 + n\pi$$

$$k = \sqrt{2\mu E}, p = \sqrt{2\mu(E + V_0)}.$$




[Peiyan Wang, Weijie Du et al., in preparation]

# SSVQE Application to BLFQ

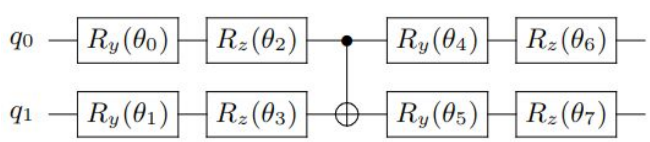
J.P. Vary et.al., 0905.1411 (2009)
W. Qian, S. Jia, Y. Li, J.P. Vary, 2005.13806 (2020)

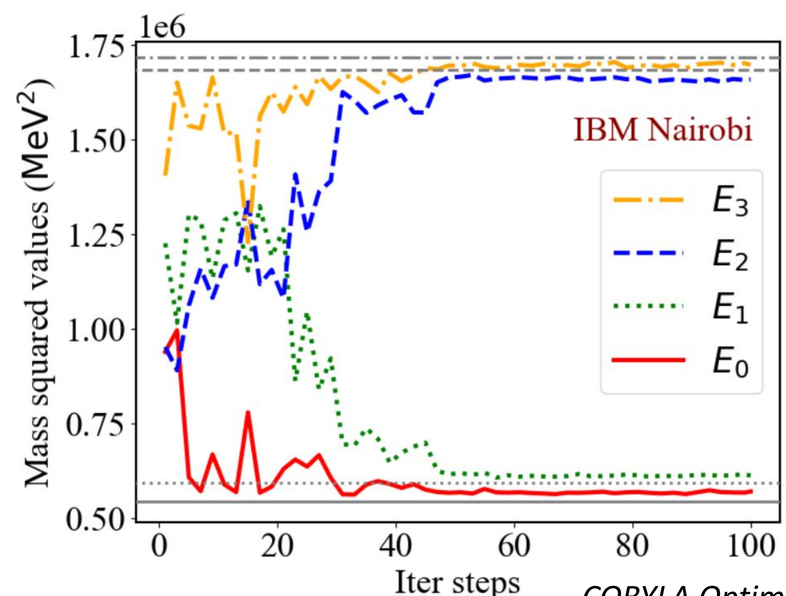
The SSVQE approach can be naturally applied to BLFQ hadron structure calculations, where we look at problem Hamiltonian of reduced basis representation. For example, the smallest non-trivial Hamiltonian of BLFQ light meson system:

$$
\begin{aligned}
H^{(1,1)}_{\text{direct}} &= 2269462\,\text{IIII} - 284243\,(\text{ZIII} + \text{IIZI}) \\
&- 850488\,(\text{IZII} + \text{IIIZ}) \\
&+ 12714\,(\text{XZXI} + \text{YZYI}) \\
&- 7883\,(\text{IXZX} + \text{IYZY}),
\end{aligned}
$$

$$
\begin{aligned}
H^{(1,1)}_{\text{compact}} &= 1134731\,\text{II} - 566245\,\text{IZ} \\
&+ 4831\,\text{XI} + 20598\,\text{XZ},
\end{aligned}
$$

In particular, we use compact encoding, orthogonal basis formed by Pauli strings under trace, and hardware-efficient heuristic ansatz, to represent the Hamiltonian economically on quantum circuit.



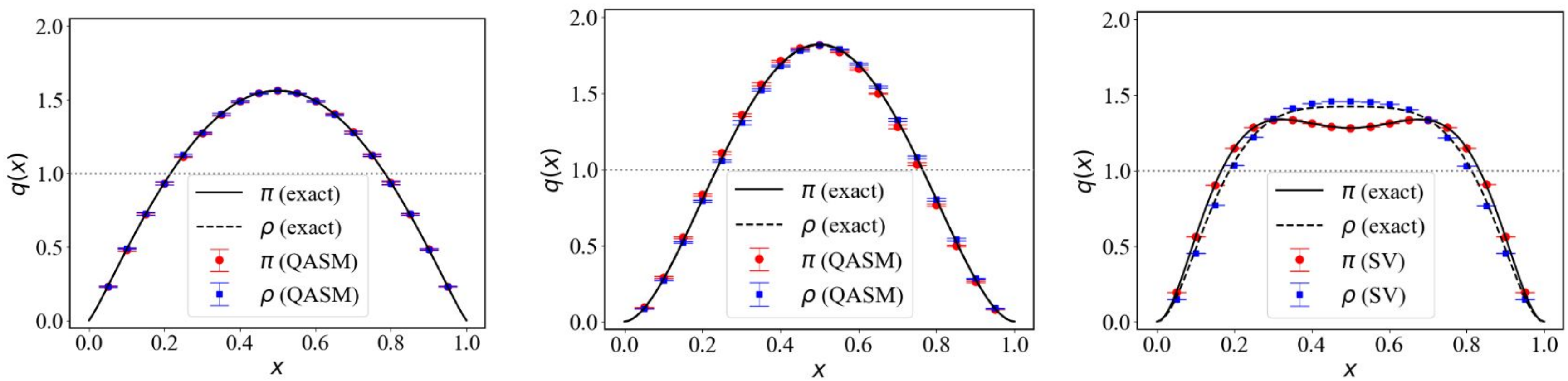

*COBYLA Optimizer*

W. Qian, R. Basili, S. Pal, G. Luecke, J. P. Vary, 2112.01927 (2021)

# Additional hadron properties

W. Qian, R. Basili, S. Pal, G. Luecke, J. P. Vary, 2112.01927 (2021)

With obtained quantum states for hadron states, we can directly evaluate observables by mapping BLFQ operator to quantum operator on the circuit, such as decay constants, parton distribution functions (PDF), and more




$N_{\max} = 1, L_{\max} = 1$ $N_{\max} = 4, L_{\max} = 1$ $N_{\max} = 4, L_{\max} = 3$

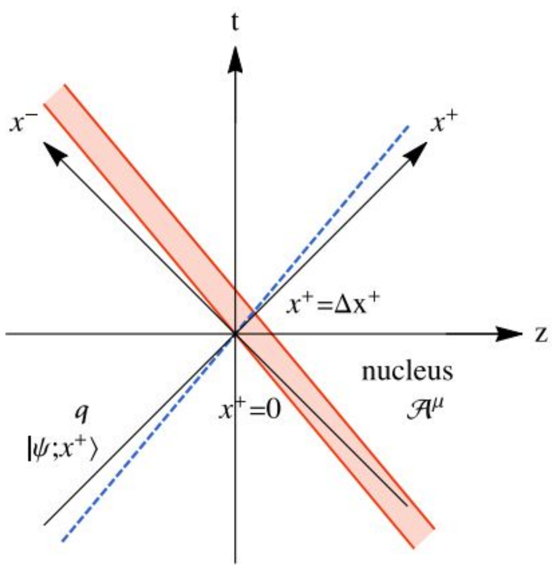
IBM QASM and statevector (SV) simulators results for PDF: longitudinal excitations emerging from increasing basis cutoffs

Transition amplitudes, such as radiative transitions, can also be computed in SSVQE

# Medium induced jet broadening in a quantum computer

Barata, Salgado, 2104.04661 (2021)
Barata, Du, Li, Salgado, Qian (2022, TBA)

High-energy quark moving close to the light cone scattering on a dense nucleus medium

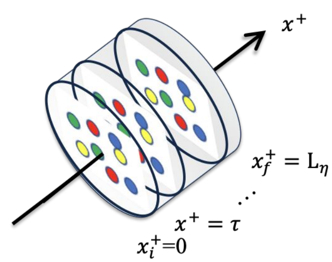



M. Li, Zhao, Maris, Chen, Y. Li, Tuchin, Vary, 2002.09757 (2020)

The light-front Hamiltonian consists of kinetic and potential term:

$$P^-(x^+) = P^-_{\rm KE} + V_{\rm A}(x^+) = \frac{p_\perp^2}{p^+} + gA(x^+)\cdot T$$

The stochastic background field uses the McLerran-Venugopalan (MV) model




$$(m_g^2 - \nabla_\perp^2)A_a^-(x^+, \boldsymbol{x}) = \rho_a(x^+, \boldsymbol{x})$$

$$\langle\langle \rho_a(x^+, \boldsymbol{x})\rho_b(y^+, \boldsymbol{y})\rangle\rangle$$
$$= g^2\mu^2(\boldsymbol{x})\delta_{ab}\delta^2(\boldsymbol{x}-\boldsymbol{y})\delta(x^+-y^+)$$

Time evolution of the probe:

$$|\psi_{L_\eta}\rangle = U(L_\eta; 0)\,|\psi_0\rangle$$
$$\equiv \mathcal{T}_+ e^{-i\int_0^{L_\eta} {\rm d}x^+\, P^-(x^+)}\,|\psi_0\rangle$$

$$U(L_\eta;0) = \prod_{k=1}^{N_t} U(x_k^+; x_{k-1}^+)$$



W. Qian, M. Li, et al, in preparation

# Quark scattered in a colored background field by quantum simulation

**Problem:** a quark scattered by the colored background field generated by a heavy nucleus.

**Method:** time-dependent basis light-front quantization (tBLFQ) on quantum computer.

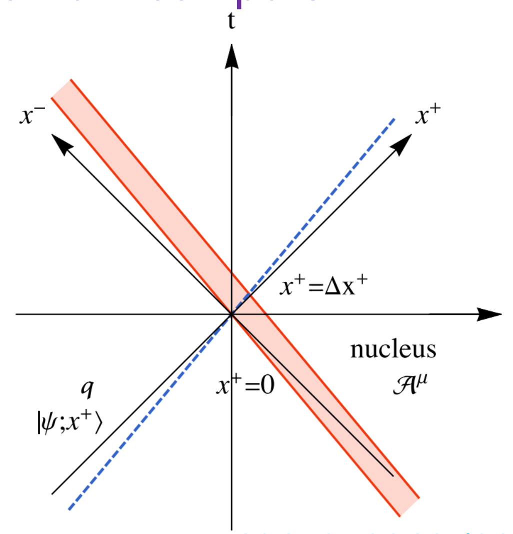
Fock sector truncation: $|q\rangle = a|\tilde{q}\rangle + \sout{b|\tilde{q}g\rangle + \cdots}$

EOM on the light front: $$i\frac{\partial}{\partial x^+}\left|\psi; x^+\right\rangle = \frac{1}{2}\boldsymbol{P}^-\left|\psi; x^+\right\rangle,$$

Time evolution unitary: $$\boldsymbol{U} = \mathcal{T}\exp\left\{-\frac{i}{2}\int_0^{x^+}\boldsymbol{P}^-(s)\,ds\right\}$$

Light-front Hamiltonian:

$$\boldsymbol{P}^- = \int dx^- d^2x_\perp \left\{\frac{1}{2}\overline{\Psi}\gamma^+\frac{m^2-\nabla_\perp^2}{i\partial^+}\Psi + g\overline{\Psi}\gamma^\mu T^a\Psi\mathcal{A}_\mu^a\right\}$$
$$= \boldsymbol{P}_{\mathrm{QCD}}^-\left(\boldsymbol{k}^\perp\right) + \boldsymbol{V}\left(x^+, \boldsymbol{x}^\perp, c\right).$$




[Meijian Li, et al., PRD 101, 076016 (2020)]
[McLerran, et al., PRD 50, 2225 (1994)]

Background field via the McLerran-Venugopalan model

**momentum *eigen* basis rep.**

$$\boldsymbol{P}^- = \boldsymbol{P}_{\mathrm{QCD}}^-\left(\boldsymbol{k}^\perp\right) + \mathcal{F}^\dagger\boldsymbol{V}\left(x^+, \boldsymbol{k}^\perp, c\right)\mathcal{F}$$

Quantum simulation

1. **Encoding**
2. **State preparation**
3. **Time evolution**
4. **Measurement**

Sihao Wu, Weijie Du et al., in preparation

## Quantum algorithm: Truncated Taylor series (TTS)

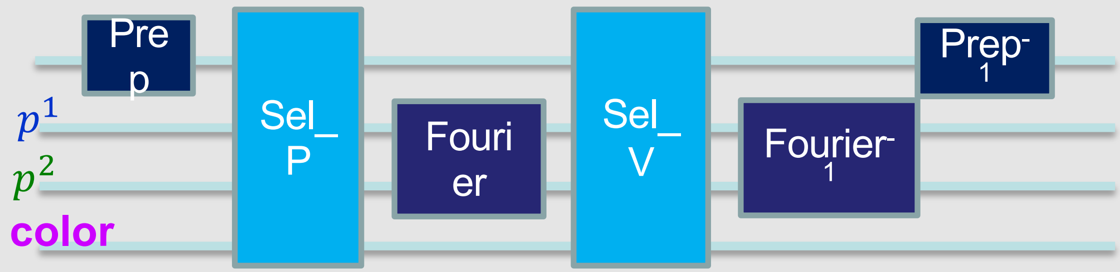
[Berry, et al., PRL 114, 090502 (2015)]

$$P^- = P^-_{\mathrm{QCD}} + \mathcal{F}^\dagger \widetilde{V} \mathcal{F} = \sum_{l=1}^{L} \alpha_l H_l$$

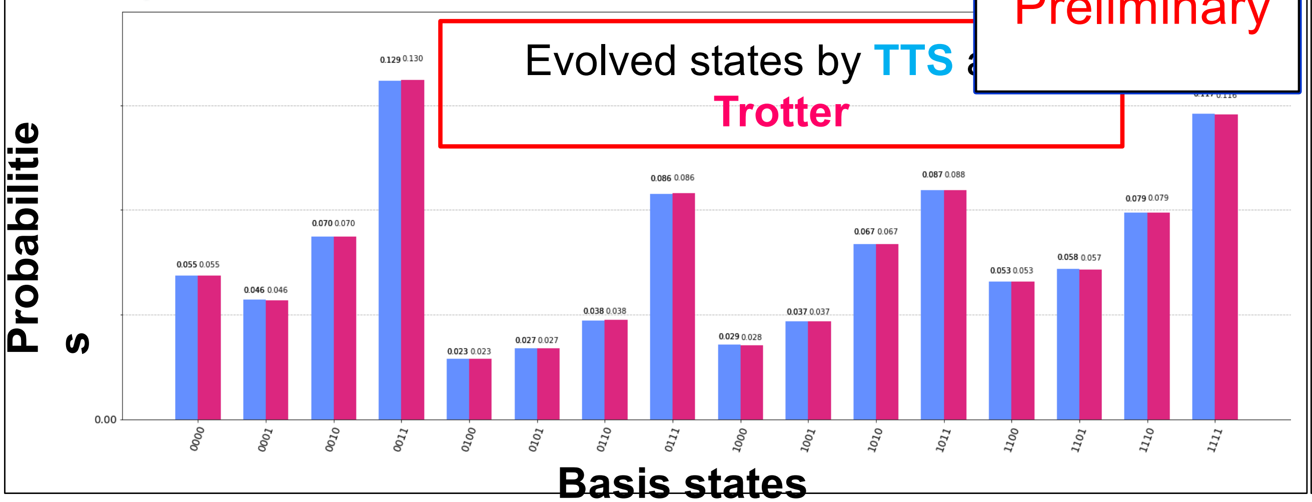
**Time evolution Op.**

$$U_r \approx \sum_{k=0}^{K} \sum_{\ell_1,\dots,\ell_k=1}^{L} \frac{(-it/r)^k}{k!} \alpha_{\ell_1} \cdots \alpha_{\ell_k} H_{\ell_1} \cdots H_{\ell_k}$$

## Circuit structure:




## Sample simulation result:




## Complexity analysis:

**TTS** better than **Trotter**

**Trotter:** $t_{\mathrm{run}} \sim \frac{LT^2}{\epsilon}$

**TTS:** $t_{\mathrm{run}} \sim T \frac{\log(T/\epsilon)}{\log\log(T/\epsilon)}$

$$T := ||P^-||t$$

[Sihao Wu, Weijie Du et al., in preparation]

## Some key QC papers by our group - some in collaboration with other groups

Michael Kreshchuk, Shaoyang Jia, William M. Kirby, Gary Goldstein, James P. Vary and Peter J. Love,
"Simulating Hadronic Physics on NISQ devices using Basis Light-Front Quantization,"
Phys. Rev. A 103, 062601 (2021); arXiv: 2011.13443

Michael Kreshchuk, Shaoyang Jia, William M. Kirby, Gary Goldstein, James P. Vary and Peter J. Love,
"Light-Front Field Theory on Current Quantum Computers,"
Entropy 23, 597 (2021); Special Issue NISQ Technologies; arXiv: 2009.07885

Weijie Du, James P. Vary, Xingbo Zhao and Wei Zuo,
"Quantum Simulation of Nuclear Inelastic Scattering",
Phys. Rev. A 104, 012611 (2021); arXiv: 2006.01369

Robert A.M. Basili, Wenyang Qian, Shuo Tang, Austin Castellino, Mary Eshaghian-Wilner, Ashfaq Khokhar,
Glenn Luecke and James P. Vary,
"Performance Evaluations of Noisy Approximate Quantum Fourier Arithmetic," arXiv: 2112.09349

Wenyang Qian, Robert Basili, Soham Pal, Glenn Luecke and James P. Vary,
"Quantum Computing for Hadron Structures," arXiv: 2112.01927

Weijie Du, James P. Vary, Xingbo Zhao and Wei Zuo,
"Ab initio nuclear structure via quantum adiabatic algorithm," arXiv: 2105.08910

# Quantum Computing – Issues & Challenges

- **Discovering the best QC algorithm: a research project in its own right**
- **New/improved QC algorithms emerging for Nuclear Structure, Reactions & Dynamics**
- **Need improved noise mitigating strategies for NISQ era and beyond**
- **Anticipating industry developments - # qubits, gate suites, topologies (“volume”)**
- **Trained workforce considerations: career path, sustainability**
- **Sharing experiences: improving exchanges with private sector**


## Funding Sources

DOE NP Division

DOE NP/ASCR Divisions (SciDAC/UNEDF SciDAC/NUCLEI)

DOE ASCR Division INCITE Awards on Leadership Class Supercomputers

DOE ASCR Division NERSC Annual Awards