Toward quantum simulation of nuclear reactions: from state preparation to cross-section extraction

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Outline

- nuclear dynamics for quantum computing
    - the case for quantum computation
- novel algorithm based on wave-packets for nuclear reactions
    - physical and qubit representation, other supporting algorithms
- summary and outlook

Quantum advantage: nuclear structure vs. dynamics

Nuclear structure / statics

- Targets ground and low-lying excited states
- Often confined to a low-energy subspace
- Benefits from truncations, symmetries, and variational methods
- Imaginary-time projection can isolate relevant states
- Bound-state methods are often sufficient
- Correlations often remain organized around a reference state

Nuclear dynamics / reactions

- Requires real-time many-body evolution
- Can explore a much larger fraction of Hilbert space
- Low-energy truncations can become dangerous
- Phases and coherence must be preserved
- Continuum, breakup, transfer, and open channels are essential
- Entanglement and configuration mixing can grow rapidly

Quantum advantage may emerge sooner in nuclear reactions, where coherent real-time evolution explores a rapidly growing many-body space beyond the reach of many low-energy approximations.

Quantum computing implementations for nuclear dynamics

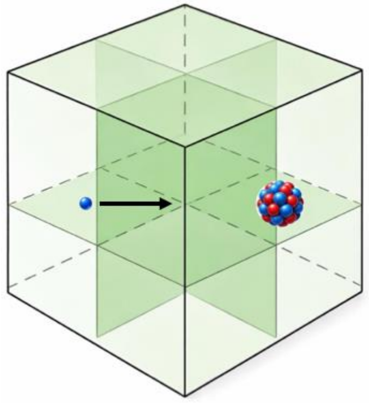
	Nuclear problem	Quantum approach	Status / scale
Roggero et al. (2020)	Neutrino-nucleus response	Ground-state preparation plus real-time evolution for response functions	Triton-scale demonstration; early hardware/resource study
Du et al. (2021)	Coulomb excitation of deuteron	Time-dependent basis-function approach	Qiskit demonstration; externally driven inelastic scattering
Baroni et al. (2022)	Electron/neutrino nuclear response	Real-time two-point correlation functions	Three distinguishable nucleons on four lattice sites; quantum hardware plus error mitigation
Turro et al. (2023)	Two-neutron scattering	Hybrid classical-coordinate / quantum-spin real-time propagation	Hardware demonstration at LBNL Advanced Quantum Testbed
Turro et al. (2024)	Elastic scattering phase shifts	Direct real-time evolution with variational improvement	Tested on IBM quantum processors
Wang et al. (2024)	Elastic scattering of two nuclei	Trap the continuum, calculate discrete energies, and extrapolate the phase shift	Rodeo algorithm on Qiskit simulator; hybrid quantum/classical
Sharma et al. (2024)	Two-nucleon scattering, deuteron $^3S_1$ channel	VQE + quantum subspace expansion; finite-volume spectrum converted to scattering phase shifts using a Lüscher-type relation	Quantum simulator and superconducting hardware; up to ~5 qubits gave acceptable results

Quantum computing implementations for nuclear dynamics

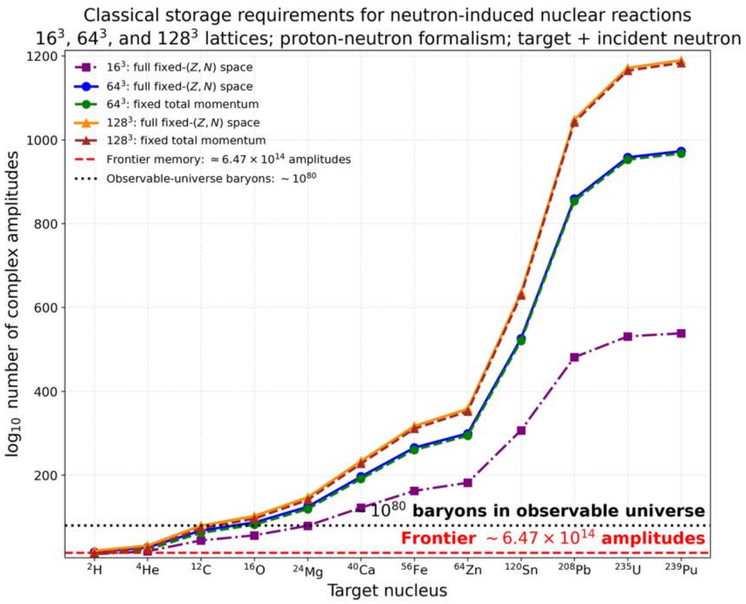
	Nuclear problem	Quantum approach	Status / scale
Yusf et al. (2025)	Two-particle elastic scattering	Harmonic trap plus ground-state energy / VQE	Schmidt decomposition reduces the example to two-qubit circuits
Spagnoli et al (2025)	Real-time low-energy nuclear dynamics / scattering with LO pionless EFT	**First-quantized** Hamiltonian simulation using product formulas and quantum signal processing	Fault-tolerant resource analysis; polynomial in particle number, logarithmic in basis size; few hundred logical qubits and ~10^7 T gates for representative scattering problems
Weiss et al. (2025)	Nuclear reaction response functions	First-quantized lattice; Trotter evolution plus QPE	Two-body electron-scattering example with detailed depth/noise estimates
Rule & Stetcu (2026 preprint)	Elastic and inelastic two-cluster reactions	Real-time wave packets on a finite Cartesian lattice; extract the S matrix from time-dependent overlaps	Classical numerical demonstrations of a proposed first-quantized quantum algorithm
Guo et al. (2026)	Elastic phase shifts	Integrated real-time correlation functions in a finite/trapped system	IBM hardware: good two-qubit result; three-qubit calculation limited by hardware errors
Watson et al. (2023/26 preprint)	Nuclear dynamics with pionless, static-pion, and dynamical-pion EFTs	Second-quantized lattice EFT; product-formula time evolution and QPE; detailed Trotter/resource analysis	Resource study; pionless cheapest, OPE intermediate, dynamical pions most costly; exploits locality and parallelization
Platter et al. (2026 preprint)	Two-body s- and p-wave scattering	Finite-volume **real-time wave-packet evolution**; detector observables combined with ML to infer infinite-volume scattering	2D lattice model, algorithmic/numerical study

Lattice representation for nuclear dynamics simulations

- **Natural for real-space dynamics**: collisions, transfer, breakup, and fragment separation are represented directly in coordinate space.
- **Local nuclear interactions are simple to apply on the lattice**, especially short-range and local chiral interactions.
- **Continuum channels arise naturally** without preselecting a reaction or fragmentation basis.
- **No need to assume a specific cluster structure**: the same representation can describe entrance, compound, and exit configurations.
- **Momentum-space** operations remain **efficient through quantum Fourier transforms**, allowing accurate treatment of kinetic energy.
- **Scales systematically**: spatial resolution and box size can be improved by refining the lattice.
- **Well-matched to first quantization**: each nucleon is represented by compact position and spin registers, with qubit cost growing only as $A(\log_2(V) + 1)$.
- **Complements finite-volume approaches:** unlike Lüscher-type methods, which infer scattering information from discrete finite-volume spectra and are best suited to relatively simple few-channel situations, real-time lattice dynamics can access strongly inelastic, multichannel reactions directly.



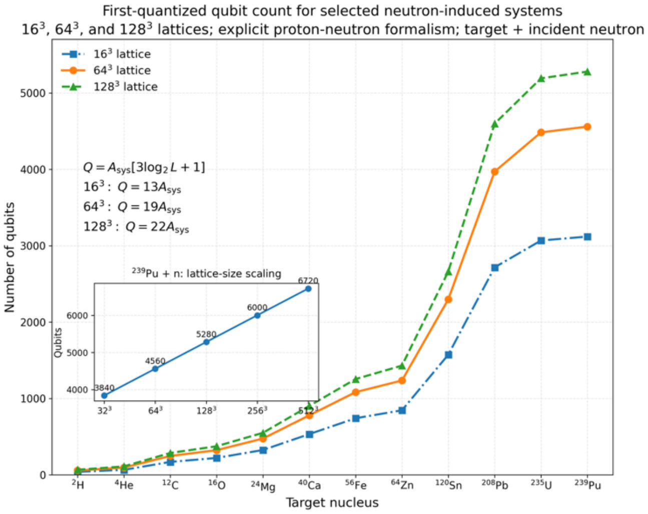
Many-body scaling using classical computing



- Classical storage grows combinatorially with nucleon number.
- Larger lattices rapidly increase the many-body space.
- Fixing total momentum helps but does not remove the exponential growth.
- Frontier’s memory is exceeded for very light nuclei.
- Around C–O, amplitudes already exceed $\sim 10^{80}$, the number of baryons in the observable universe.

Many-body simulations scaling in quantum computing

- **First quantization scales linearly with nucleon number**: Q∝A, rather than with the exponentially large Hilbert-space dimension.
- **Spatial resolution enters only logarithmically**: $Q = A_{sys}(3\log_2 L + 1)$.
  - Increasing the lattice from 16^3 to 128^3 produces only a modest increase in qubit count.
- Even heavy systems such as ^{239}Pu+n require only a few thousand physical-state qubits.
- The contrast with classical amplitude storage is dramatic: **exponential classical memory growth versus polynomial quantum storage.**
- Compared with **second quantization**, where **the qubit count scales with the volume**, **first quantization scales with the number of particles times the logarithm of the lattice size**, making it potentially much more compact for large real-space lattices.



NB: physical register only

Challenges

- **Hardware gap**: no existing quantum computer is close to the qubit count, fidelity, connectivity, and circuit depth needed for realistic nuclear reactions.
- **Fault-tolerant requirements**: useful calculations will require error-corrected logical qubits, far beyond today's NISQ devices.
- **Long coherent evolution**: reaction times translate into deep circuits, amplifying both hardware noise and algorithmic errors.
- **Realistic interactions**: tensor, spin-orbit, Coulomb, and three-body terms **substantially increase circuit complexity**.
- **State preparation and readout**: preparing antisymmetric nuclear states and extracting S-matrix observables are nontrivial.
- **Large spatial volumes**: reactions require enough lattice volume for incoming and outgoing fragments, increasing resource demands.

The algorithms are becoming credible, but the required hardware is still far beyond current quantum computers. There could also be unforeseen challenges.

Wish list for a nuclear reaction algorithm

- Scalability to many-particle systems, without constructing an exponentially large channel basis.
- Simple real-time propagation, with kinetic and potential evolution that map naturally onto quantum circuits.
- Direct access to scattering observables, rather than only finite-volume energy levels.
- Elastic and inelastic reactions within the same framework, without fundamentally changing the algorithm.
- Minimal dependence on enumerating final states, especially as the number of open channels grows.
- Efficient access to inclusive observables: ideally, the total cross section should not require calculating every individual exit channel.
- A formulation compatible with large spatial volumes, since incoming and outgoing fragments must be well separated.
- A path toward realistic many-body interactions and composite projectile/target states.

Inspiration

RESEARCH ARTICLE | MARCH 01 1993

Wave packet correlation function formulation of scattering theory: The quantum analog of classical *S*-matrix theory

David J. Tannor; David E. Weeks

Check for updates

J. Chem. Phys. 98, 3884–3893 (1993)
https://doi.org/10.1063/1.464016

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Classical

$$\langle \phi_\beta^- | \phi_\alpha^+ \rangle \xrightarrow{FT} \langle \psi^-_{\beta,E'} | \psi^+_{\alpha,E} \rangle = S_{\beta\alpha}(E)\,\delta(E-E')$$

Quantum estimate using a wave packet formulation

Wave-packet implementation

Rule and Stetcu, arXiv:2603.26881 (2026)

- Prepare states for projectile and target wave packets in their desired internal states on separate target and projectile registers
  - Antisymmetrization inside target (and projectile) Rule et at, Quantum **10**, 2056 (2026)
  - Target and projectile on top of each other Tanner and Weeks, J. Chem. Phys **98**, 3894 (1993)
  - State preparation (ground/excited state) Stetcu et al, Phys. Rev. C **108**, L031306 (2023)
  - Controlled on ancilla, prepare incoming and outgoing states
- Evolve the incoming/outgoing states controlled on ancilla $\exp(\pm iH_0T_0)$ until well separated
- Perform antisymmetrization between target and projectile Stetcu, arXiv:2512.16138 (2025)

- Evolve incoming/outgoing states with the full Hamiltonian $\exp(\mp iHT_0)$ to produce scattering states $|\phi^{\pm}\rangle$
- Project $|\phi^{-}\rangle$ on fixed CM momentum
- Evolve $|\phi^{+}\rangle$ and take the overlap with projected $|\phi^{-}\rangle$ state: $\langle\phi^{-}|P\exp(-iHt)|\phi^{+}\rangle$
- Repeat above to sample different times and then perform the Fourier transform to extract the full S matrix

Localization and *S*-matrix extraction

- Initial state: wave packet in the CM of all particles, average momentum zero:

$$|\phi_{k_0,\alpha}\rangle \propto |\psi_{\alpha_1}^{target}\rangle|\psi_{\alpha_2}^{proj}\rangle \exp(-ik_{target}Z_{CM}^{target})\exp\left(-\frac{Z_{CM}^{target\,2}}{2\sigma_{target}^2}\right) \exp(-ik_{proj}Z_{CM}^{proj})\exp\left(-\frac{Z_{CM}^{proj\,2}}{2\sigma_{proj}^2}\right)$$

  - Integral over impact parameters automatically performed
  - Scattering angles are selected through the momentum of the outgoing wave packets: adding transverse fixed CM momentum rotates the outgoing relative momentum away from the incident direction

- Moller operators construct scattering states with incoming and outgoing boundary conditions

$$\Omega_\pm = \lim_{t\to\mp\infty} e^{iHt}e^{-iH_0t}$$

- Application: time evolution with free and full Hamiltonians produce wave packet scattering states
- The plane-wave Moller-evolved states are given by

$$|\psi_{k,\alpha}^{\pm}\rangle = \frac{k_z}{2\pi\mu\eta(k_z)}\sqrt{\frac{\mu}{k}}\int_{-\infty}^{\infty} e^{-iHt}|\phi_{k_0,\alpha}^{\pm}\rangle e^{iEt}\,dt$$

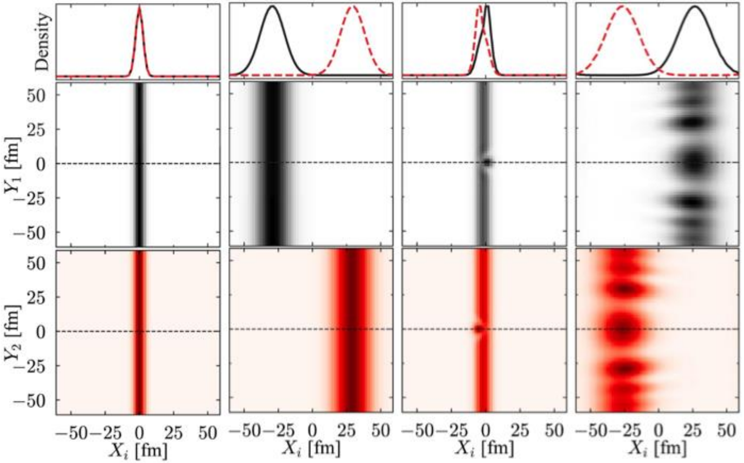
- Hence, the full S matrix writes is proportional with the Fourier transform of the time-dependent correlation function

$$C_{\beta\alpha}(k_0,k_0';t) \equiv \langle\phi_{k_0',\beta}^{-}|e^{-iHt}|\phi_{k_0,\alpha}^{+}\rangle$$

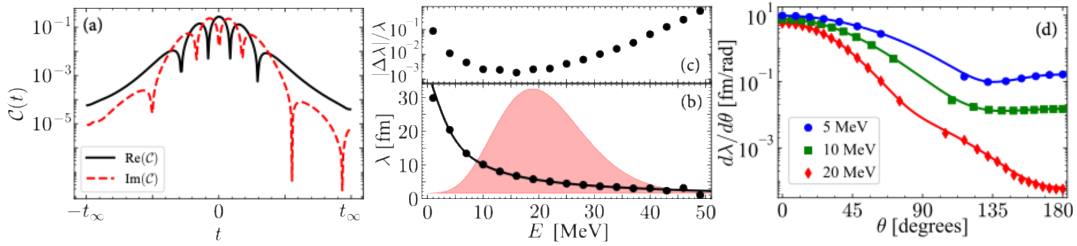
- *S* matrix provides the differential cross section; optical theorem: total cross section from the forward amplitude

Rule and Stetcu, arXiv:2603.26881 (2026)

Classical numerical simulations for short-range interactions



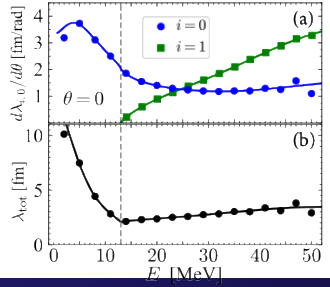
Elastic differential scattering/total cross section



$$V(|\vec{r}_1 - \vec{r}_2|) = V_0 U(r) = V_0 \exp\left(-\frac{r^2}{2R_0^2}\right)$$

Inelastic scattering/total cross section

$$H = \begin{pmatrix} T + V_0 U(r) & \bar{V}_0 U(r) \\ \bar{V}_0 U(r) & T + \Delta + V_0 U(r) \end{pmatrix}$$



Rule and Stetcu, arXiv:2603.26881 (2026)

Challenges

- **Realistic nuclear interactions**: tensor, spin-orbit, Coulomb, and three-body terms can substantially increase circuit complexity.
- **Long evolution times**: low-energy reactions, compound-nucleus formation, or well-separated outgoing fragments may require very deep time evolution.
- **Large spatial volumes**: incoming and outgoing wave packets must remain well separated from boundaries and periodic images.
- **State preparation**: realistic antisymmetric projectile and target states may be costly to prepare.
- **Observable extraction**: accurate S-matrix elements require precise real and imaginary overlap measurements over many times.
- **Many exit channels**: inelastic, transfer, and breakup reactions may require multiple outgoing-state preparations and measurements.
- **Error accumulation**: Trotterization and hardware errors must remain controlled throughout long coherent evolutions.
- **Hardware requirements**: realistic applications are well **beyond current noisy quantum devices** and will likely require fault-tolerant hardware.

Continued algorithmic advances may overcome many of the current bottlenecks and bring realistic nuclear-reaction simulations within reach

A first-quantization survival guide

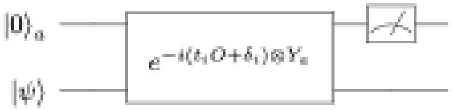
- ✓ Work directly with particle registers for position, spin, and species.
- ✓ Resist the temptation to expand the full interaction into Pauli strings — this can destroy the locality and simplicity of the physics. Use Pauli decompositions selectively, not as the default implementation strategy.
- ✓ Apply local interactions directly in coordinate space using particle separations.
- ✓ Apply kinetic energy efficiently in momentum space using quantum Fourier transforms.
- ✓ Use reversible arithmetic and phase operations rather than enumerating large operator expansions.
- ✓ Keep spin and isospin operations local to the small internal-state registers.
- ✓ Preserve physical locality whenever possible for contact and finite-range interactions.

First quantization is most powerful when the algorithm acts on particle coordinates directly, rather than translating everything into Pauli strings

Summary

- **Nuclear dynamics offers a compelling opportunity for quantum advantage**, where classical calculations rapidly become intractable.
- For many-body reactions, avoiding severe truncations may ultimately require quantum simulation to retain the **full coherent dynamics without uncontrolled approximations**.
- **Real-space lattice representations are a natural framework for reactions**, and may also benefit nuclear structure near the **driplines**, where coupling to the continuum is essential.
- **First quantization provides a compact and physically transparent encoding** for many-body dynamics, particularly when the number of particles is modest compared with the size of the spatial basis.
- **Substantial algorithmic development is still needed**, especially for reactions beyond “simple” 2→2 processes, including breakup, transfer, and many-channel dynamics. We have ideas, we welcome ideas, **we look for talent**
- **Our LANL group is actively advancing this program**, improving existing algorithms and developing new approaches toward realistic quantum simulations of nuclear reactions.

Selected references from our group



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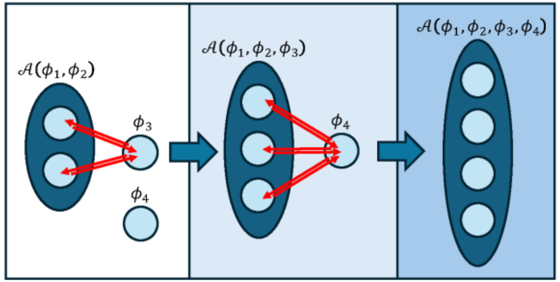

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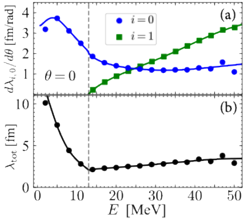

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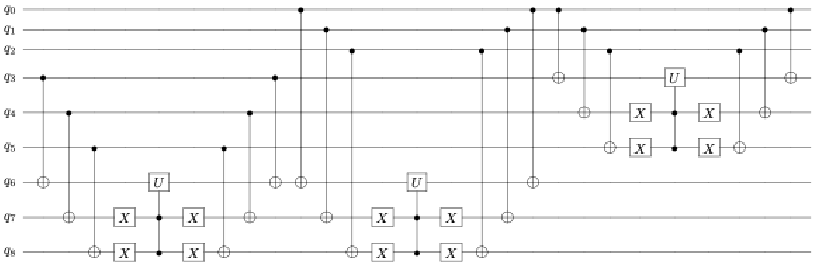

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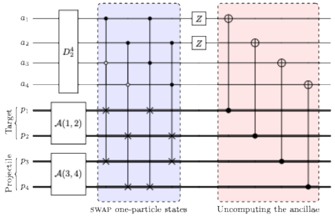
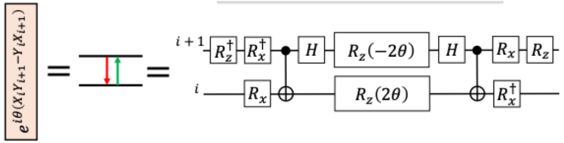


Stetcu, arXiv:2512.16138 (2025)



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Collaborators

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Nuclear Theory Postdoctoral Researcher in Quantum Computing

APPLY

What You Will Do

The T-2 group (Nuclear and Particle Physics, Astrophysics and Cosmology) in the Theoretical Division at Los Alamos National Laboratory invites applications for two postdoctoral positions in theoretical modeling of nuclear dynamics using quantum computing. Candidates are expected to have obtained a PhD in Physics or closely related field by the beginning of the postdoctoral appointment (within five years of receiving their PhD). This appointment is for two years. Extension for a third year may be considered, contingent on performance and funding.

Interested applicants should submit their application (CV, research statement) and arrange for three letters of recommendation to be sent by email (t2-pdsearch-q@lanl.gov). Applications will be reviewed on a rolling basis, and evaluation will begin immediately upon receipt. The advertisement will remain open until October 16, 2026, but one or both positions could be filled before this deadline.

The successful candidate will:

- Design algorithms specific for implementing quantum nuclear dynamics on quantum hardware
- Publish research in leading scientific journals
- Develop strong programming skills
- Work both independently and in a team environment to solve problems in support of Laboratory missions

https://lanl.jobs/search/jobdetails/nuclear-theory-postdoctoral-researcher-in-quantum-computing/a3968411-2f6d-47e2-ab75-376551ae098c