New method for determining few-body resonance poles in finite volume

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In Collaboration with:

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Frontiers in NLEFT, Beijing, 01/03/2025

Outline

- Background
  - Resonance in finite volume
- Method and examples
  - The method
  - Example 1: two particles
  - Example 2: three particles
- Discussion
  - Wave packet propagation velocity
  - Twisted boundary conditions
  - In a large volume
  - Spectral functions
- Summary and outlook

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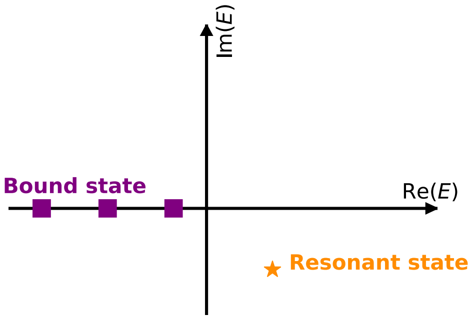
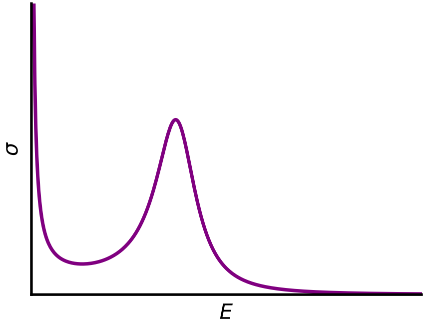
(Quantum)resonance

- Quasi-bound; Finite lifetime; Barrier tunneling
- Theoretically, a non-physical S-matrix pole in the complex energy plane $(E_0 - i\,\Gamma/2)$
- Experimentally, a peak in the cross section

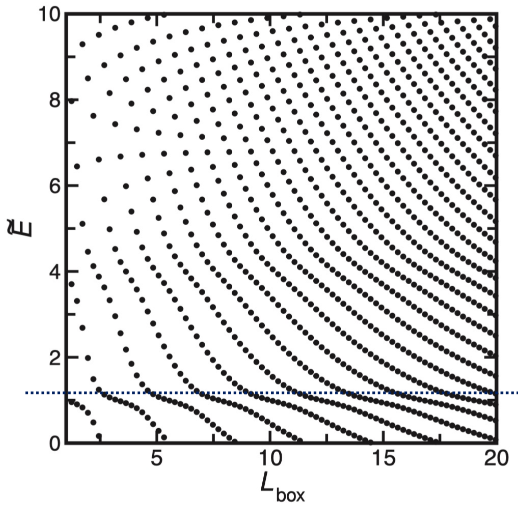




Hermitien Hamiltonian in Finite Volume (FV)

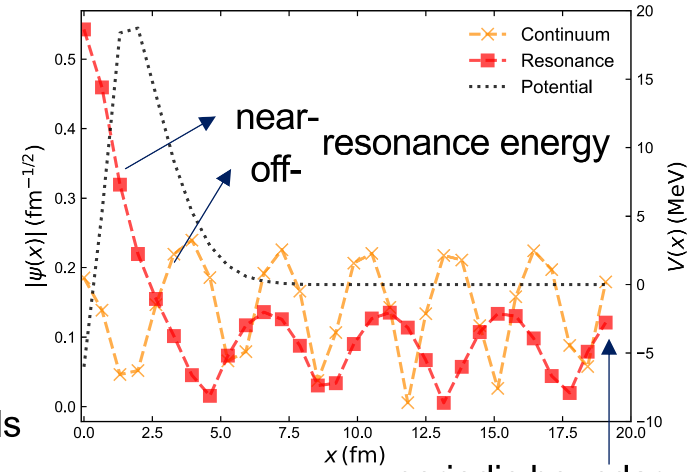
- Stabilization method

eigenvalues:



E_0: flat and avoid crossing energy levels

eigenfunctions:



periodic boundary condition

from: N. Moiseyev, Non-Hermitian Quantum Mechanics (Cambridge University Press, 2011)

- Few-body cases in periodic cubic box are similar:

P. Klos, S. König, H.-W. Hammer, J.E. Lynn, A. Schwenk, PRC 98, 034004 (2018)

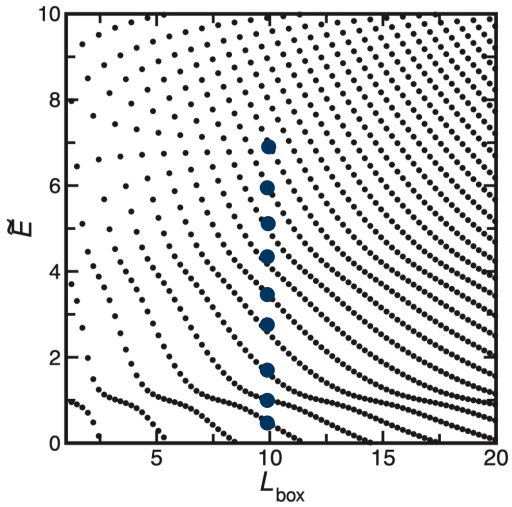
"Resonance" embedded in discretized continuum states:

- No exponential divergence (unlike the Gamow/Siegert resonant state)
- More localized spatially than the "continuum"

Hermitien Hamiltonian in Finite Volume (FV)

- Lüscher method

eigenvalues:



from: N. Moiseyev, Non-Hermitian Quantum Mechanics (Cambridge University Press, 2011)

Finite volume

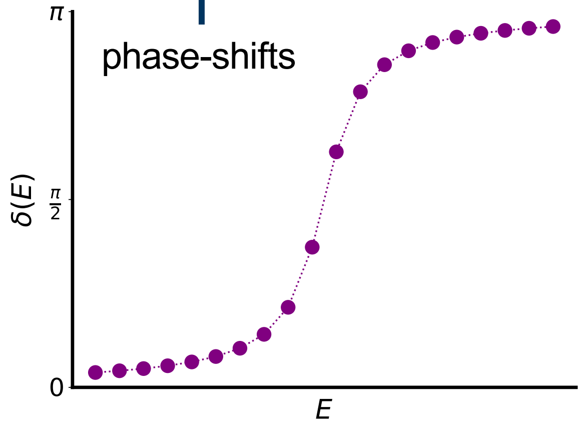
Quantization Condition

M. Lüscher, NPB 354, 531 (1991)
M. Lüscher, Comms. Math. Phys. 105, 153 (1986)
…

resonance poles

analytical continuation

phase-shifts



Infinite volume

- Requires precise energy levels B.-N. Lu, T. Lähde, D. Lee, U.-G. Meißner , PLB 760, 309-313 (2016)
  → hard to implement successfully in NLEFT
- Difficult when beyond more than two-body resonances

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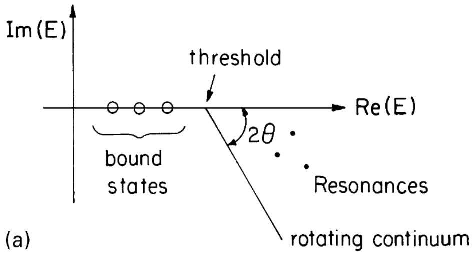
Non-Hermitien Hamiltonian in FV

- Complex scaling method:

complexed Hamiltonian

$$H^\theta = H(r \to re^{i\theta})$$

$$H^\theta \Psi^\theta = E^\theta \Psi^\theta$$



from: N. Moiseyev, Phys. Rept. 302, 212293 (1998)

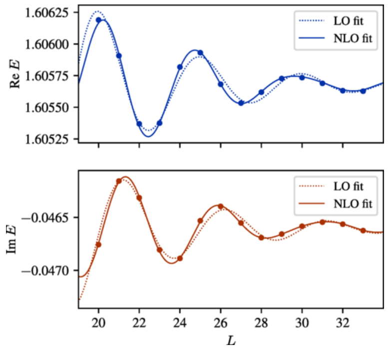
- Implemented in nuclear models:
  - Cluster model
  - No-core shell model

  ...

A.T.. Kruppa, N. Michel, X.-L. Shang, W. Zuo, arXiv:2501.11294
H.-T. Zhang, B. Dong, Z. Wang, Z.-Z. Ren, PRC 105, 054317 (2022)
T. Myo, Y. Kikuchi, H. Masui, K. Kato, PTEP 2020, 12A101 (2014)
...

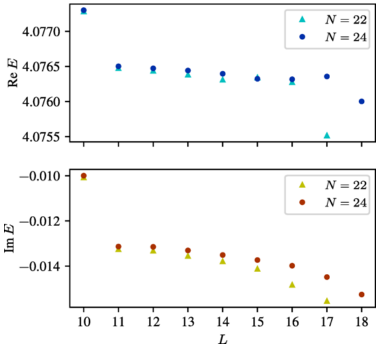
- Implemented in finite volume (continuum):

Two-body:



H. Yu, N. Yapa, S. König, PRC 109, 014316 (2024)

Three-body:



"Since the volume dependence of this state is unknown, this figure does not include any fitted curves"

Challenges:
- Numerical potential (chiral EFT nuclear potential)
- On lattice
- Three-body resonances

...

A new method is needed

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Persistent state method for determining resonance poles in finite-volume

Hermitian quantum mechanics from time-dependent perspective

- Survival amplitude for a resonant state:

decomposed as scattering states: N. S Krylov, V. A. Fock, JETP 17, 93 (1947)

$$|\psi_{\text{res.}}\rangle = \int dE\, a(E)|E\rangle$$

for usual Breit-Wigner:

$$a(E) \propto \frac{1}{E - E_0 + i\ \Gamma/2}$$

$$f(t) = \langle\psi_{\text{res.}}|e^{-iHt}|\psi_{\text{res.}}\rangle \longrightarrow f(t) = \int dE\, |a(E)|^2 e^{-iEt} \propto e^{-iE_0 t - \Gamma t/2}$$

- Ansatz: simple persistent state approximating the resonant state
  - Persistent state: compact spatially (e.g., Gaussian) and decaying slowly

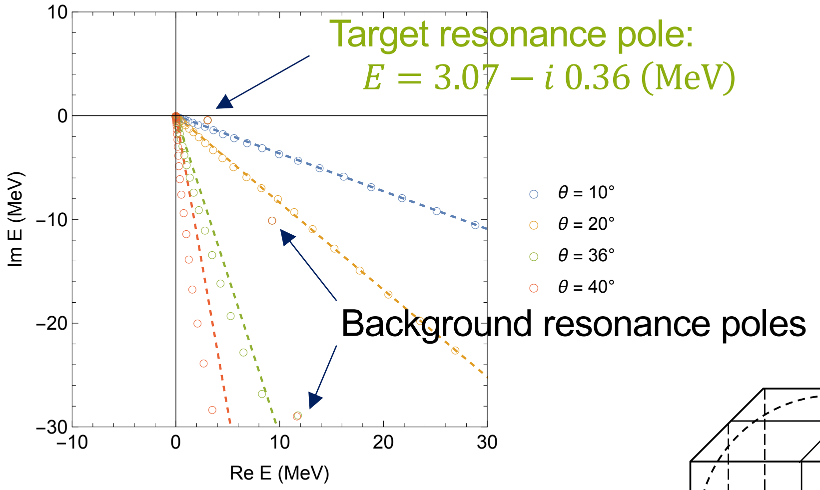
input: $\langle\psi_{\text{persis.}}|e^{-iHt}|\psi_{\text{persis.}}\rangle$ (Finite volume) → fit function: $f(t)$ (Infinite volume) → output: E_0 Γ (Infinite volume)

Extract resonance poles without any eigenvalues or eigenstates

Euclidean time evolution is in progress (by Avik Sarkar et al.)

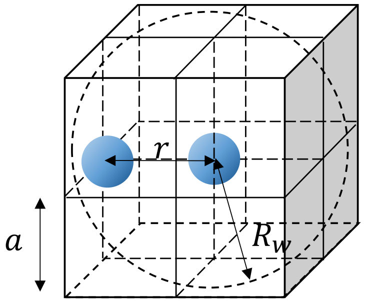
Benchmark 1: two particles in 3D

- Toy model: Two spinless particles in s-wave
  - Potential: $V(r) = 30\, e^{-\left(\frac{r}{2\text{ fm}}\right)^2} - 40\, e^{-\left(\frac{r}{1.5\text{ fm}}\right)^2}$ (MeV), $\mu = 6 * 938.92$ (MeV)



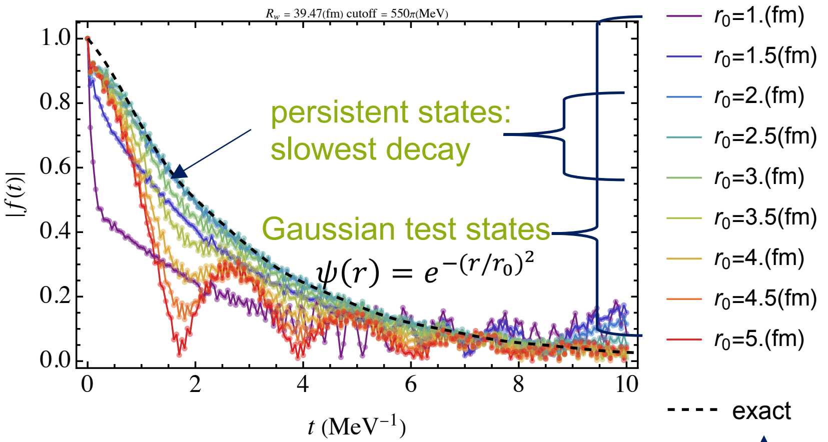
- Finite volume setup: lattice with a spherical wall
  - Spherical wall for restoring rotational symmetry

B. Borasoy, et al., EPJA 34, 185-196 (2007) $V \to V + \Lambda\,\theta(r - R_w), \quad \Lambda \to \infty$



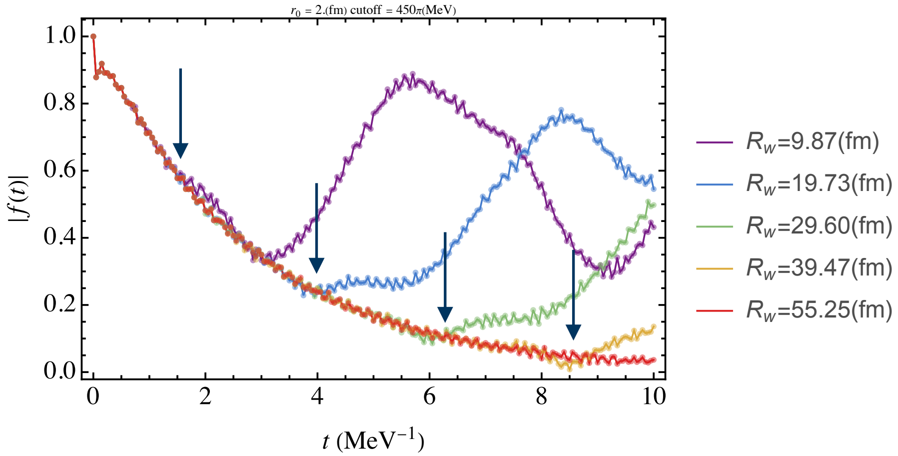
Survival amplitudes in FV

- Selection of persistent states



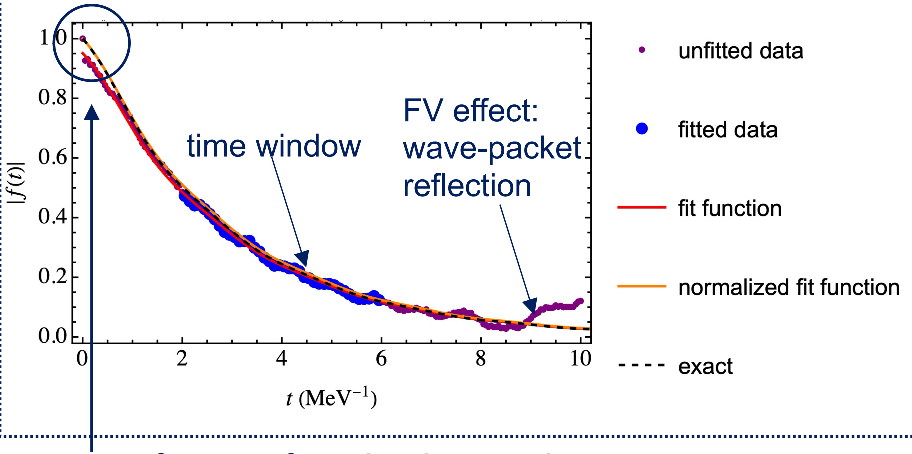
theoretical f(t) of the exact pole in infinite volume

- Volume “independence”

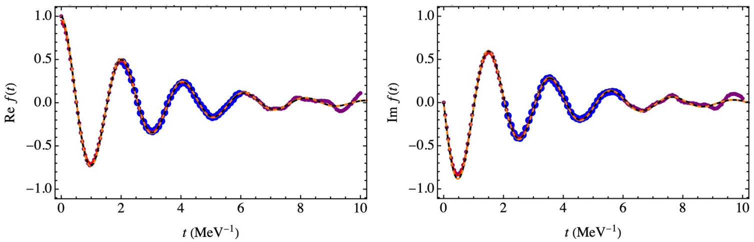


Extraction on the resonance pole

- Abs.



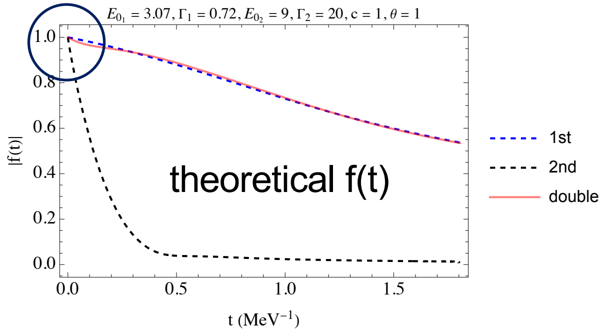
- Re.
- Im.

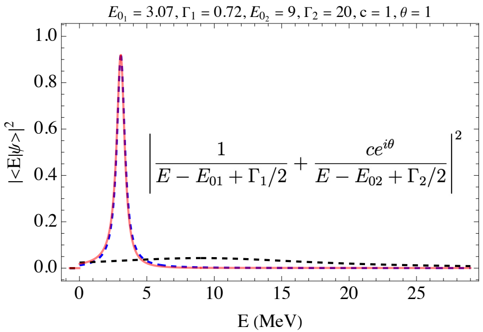


- Jacknnife fit result:

$$E_0 = 3.073 \pm 0.001(\mathrm{MeV})$$
$$\Gamma = 0.707 \pm 0.001(\mathrm{MeV})$$

- Interference from background resonance poles





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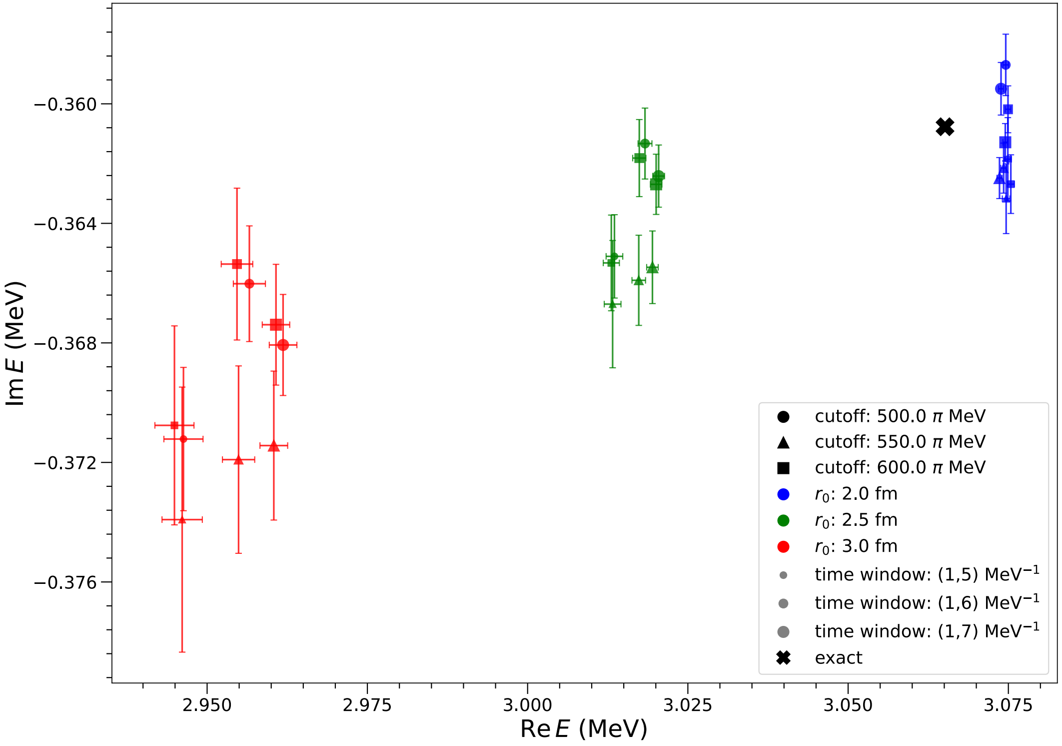
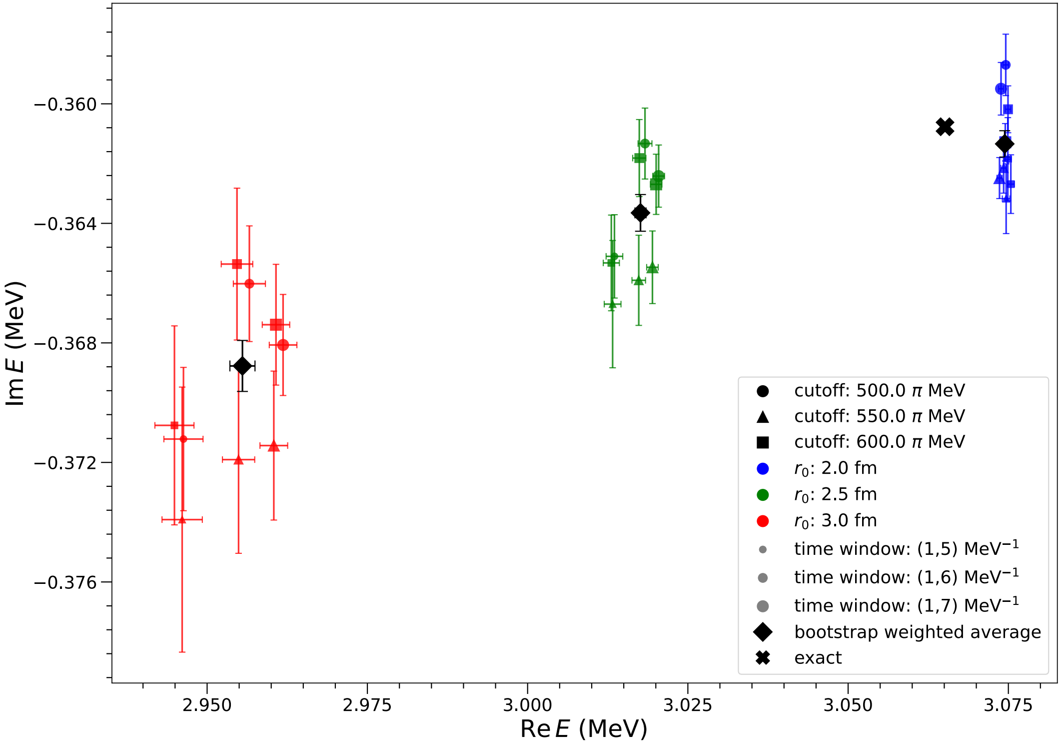
Extraction on the resonance pole

Dependences:
- persistent states
- fitting time window
- cutoff (lattice spacing) (fixed in NLEFT calculations)



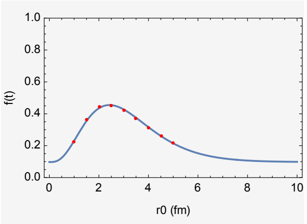
Extraction on the resonance pole

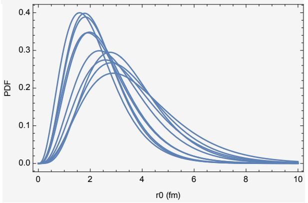
Bootstrap weighted average on vary cutoffs and fitting time windows



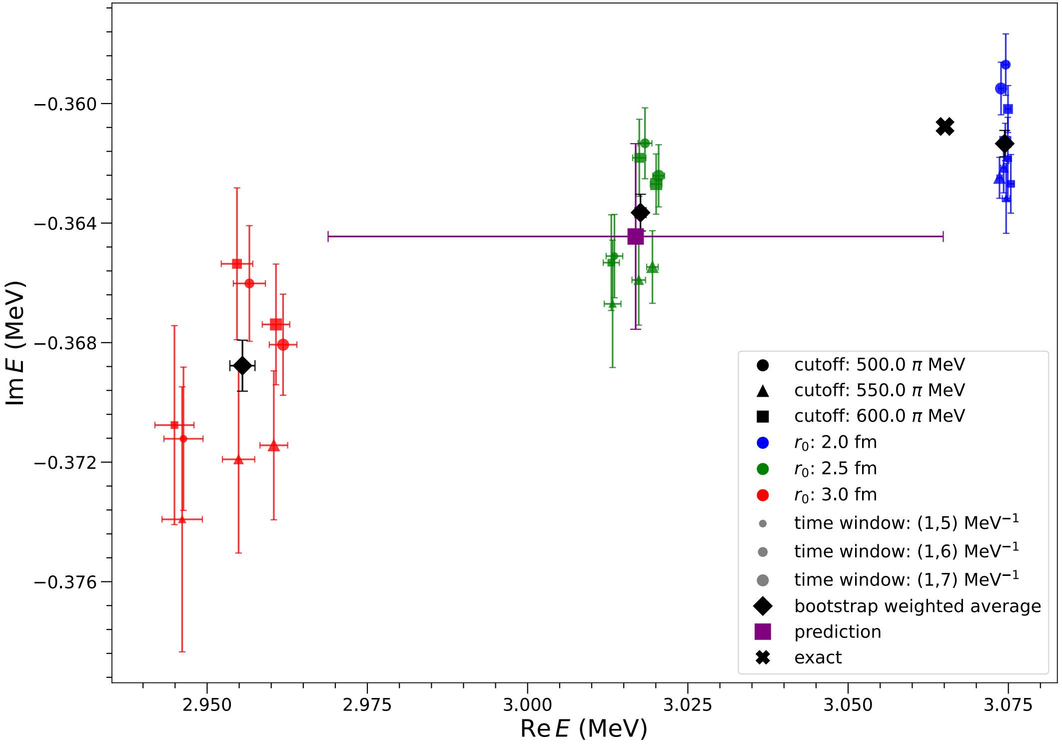
Extraction on the resonance pole

Bayesian analysis
on persistent states





Gamma distribution ansatz
for the prior probability



final result:

$$E_0 = 3.02 \pm 0.05 \text{ (MeV)}$$
$$\Gamma = 0.73 \pm 0.01 \text{(MeV)}$$

exact value:

$$E_0 = 3.07 \text{ (MeV)}$$
$$\Gamma = 0.72 \text{ (MeV)}$$

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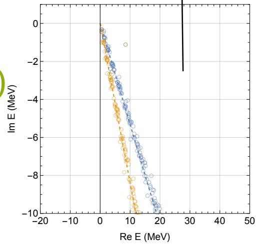
Benchmark 2: three particles in 1D FV continuum

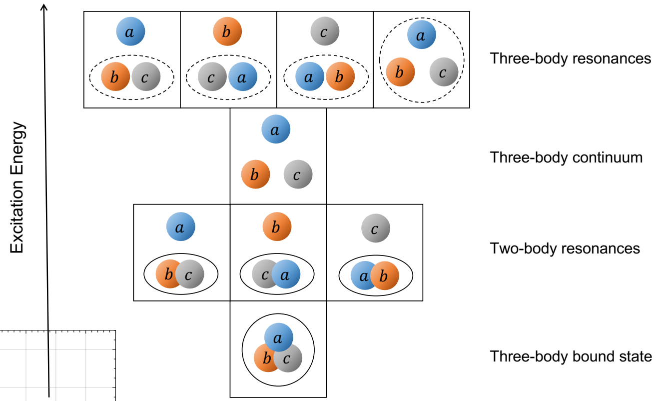
- Toy model: three-body resonance

  - $\text{mass} = 938.92\ (\text{MeV})\,,\ V_{2\text{B}}(x) = 30\ e^{-\left(\frac{x}{1\ \text{fm}}\right)^2}\ (\text{MeV}),$
    $V_{3\text{B}}(x_1, x_2, x_3) = -100\ e^{-((x_1-x_2)^2+(x_2-x_3)^2+(x_3-x_1)^2)/(2\ \text{fm})^2}\ (\text{MeV})$

  - The exact pole value solved by the Gaussian expansion method + complex scaling method
    E. Hiyama, Y. Kino, M. Kamimura, PPNP 55(1), 223-307 (2003)
    N. Moiseyev, Phys. Rept. 302, 212293 (1998)

  - Single three-body resonance pole: $E = 8.51 - i\ 1.09\ (\text{MeV})$

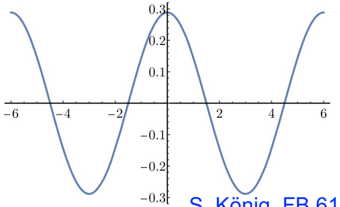




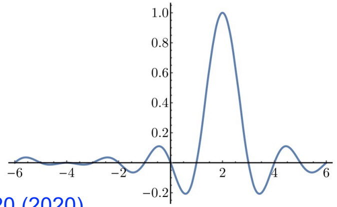
- FV setup: continuum with periodic boundary condition

  - Solving the eigenvalue problem by the plane-wave based discrete variable representation (DVR)

plane wave basis



DVR basis

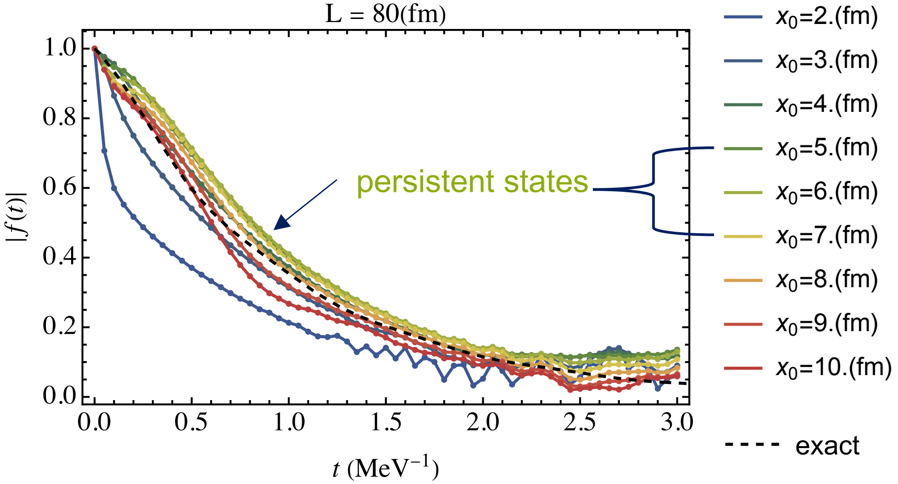


S. König, FB 61, 20 (2020)

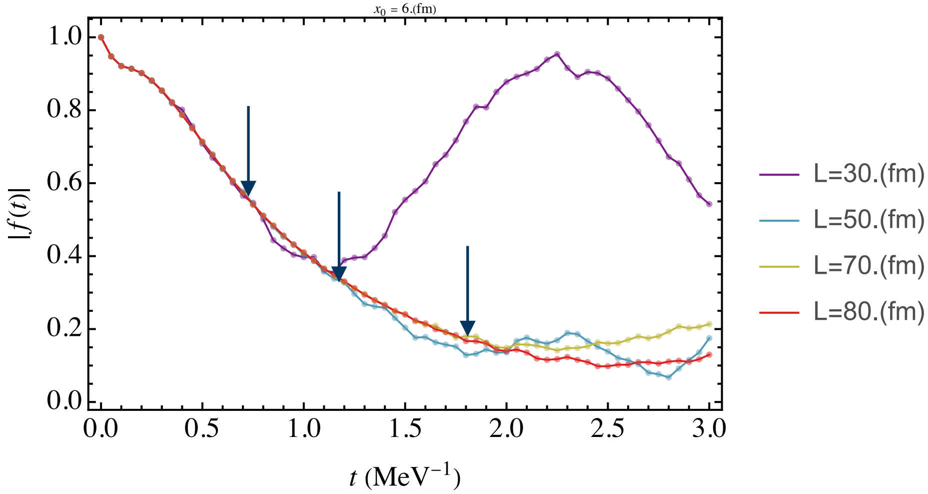
Survival amplitudes in FV (3 body)

Similar to the two-body case

- Selection of persistent states



- Volume “independence”



- Natural generalization of test states to the three-body case:

$$\psi(x_{12}, x_{13}) = e^{-(x_{12}^2+x_{23}^2)/x_0^2}$$

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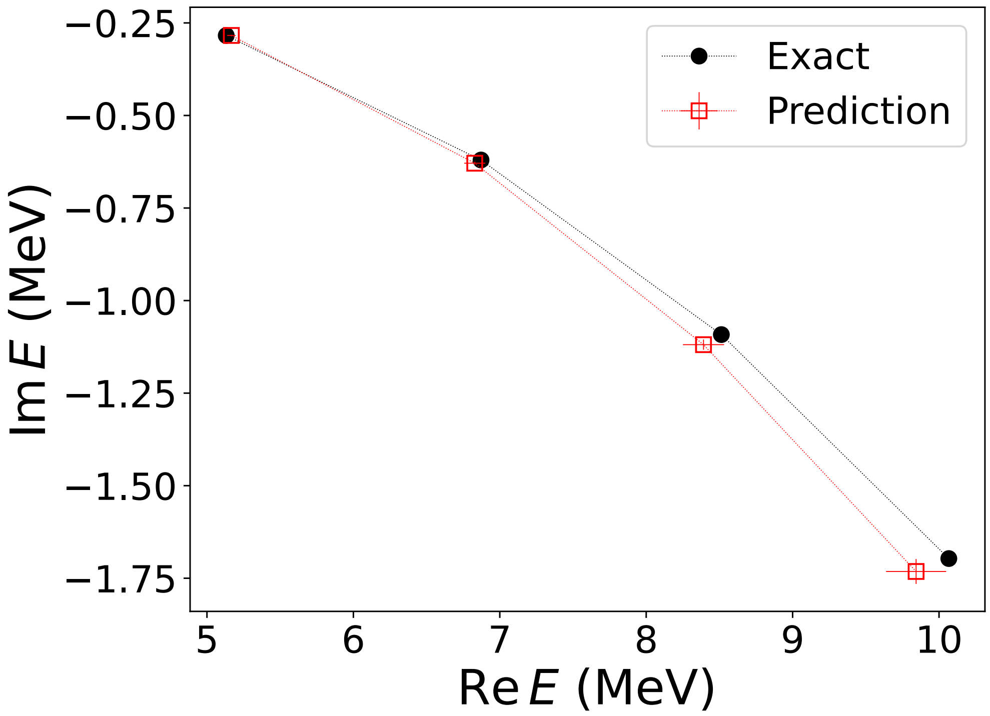
Extracting resonance poles from time evolution



Pole trajectory for varying three-body potential strength

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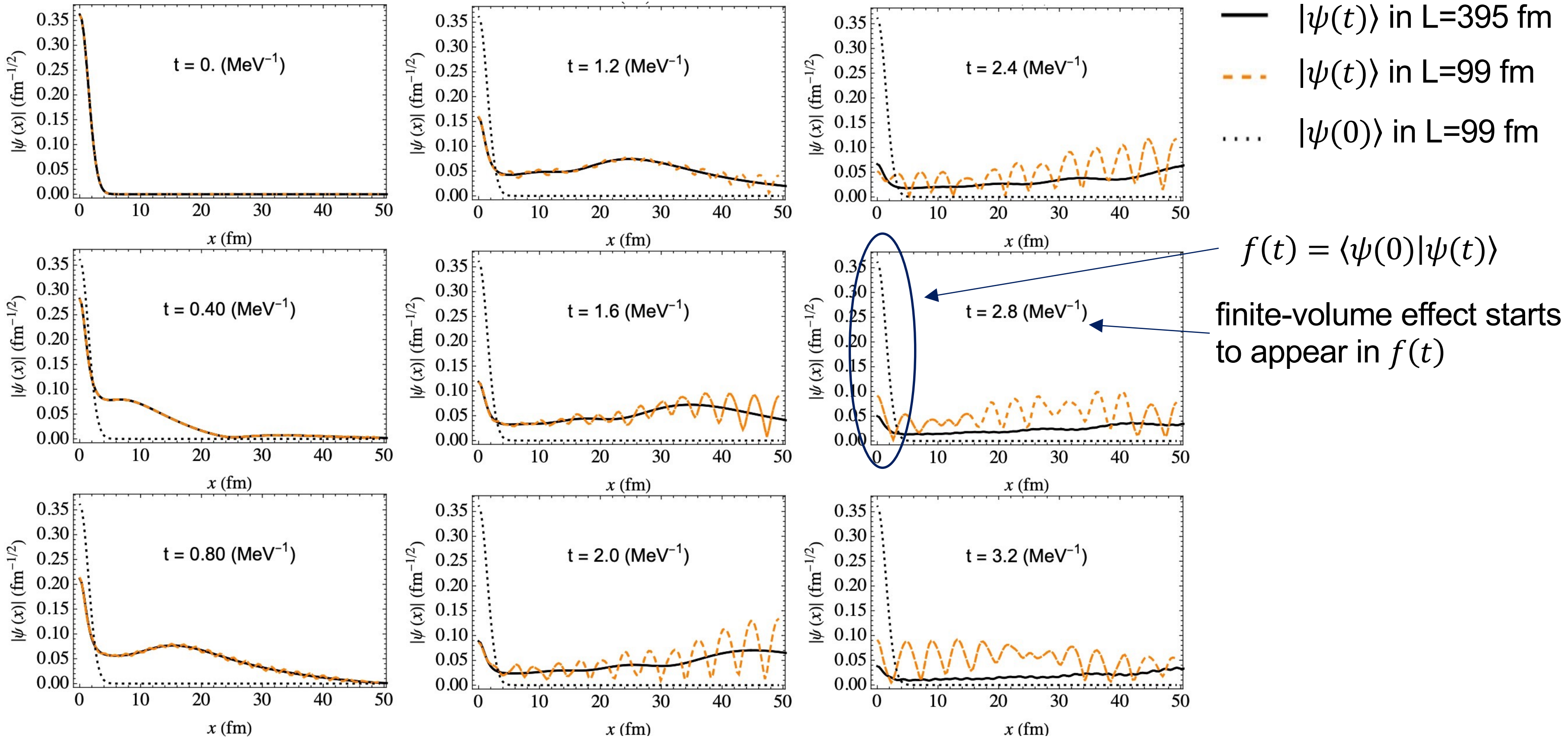
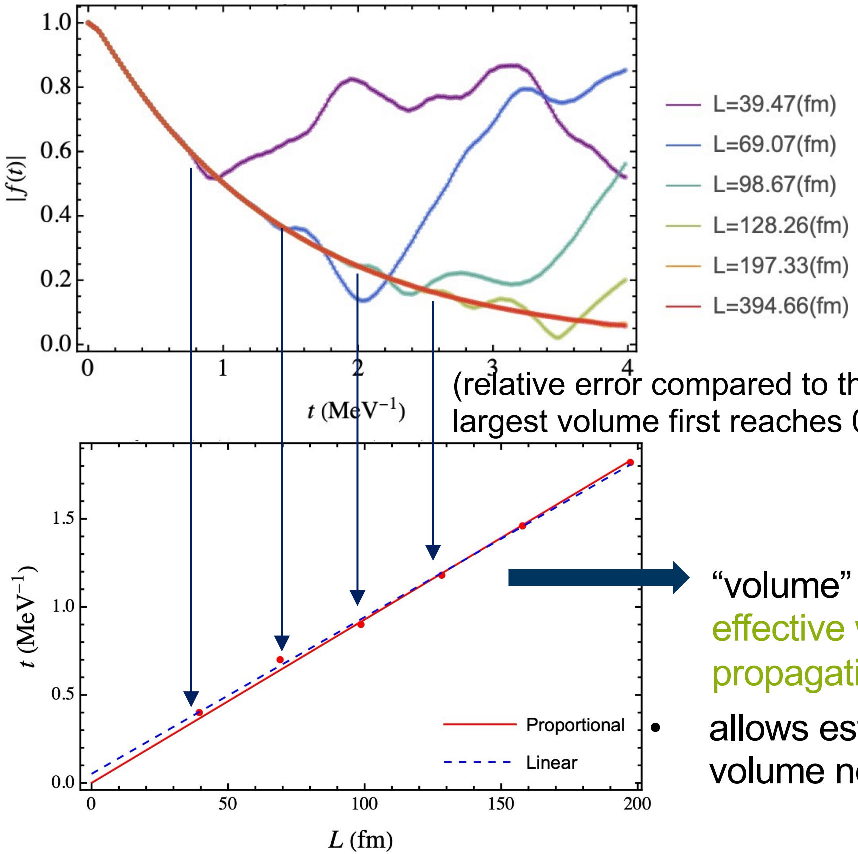
- In example of two particles in 1D

Wave-packet propagation in FV



Wave-packet propagation in FV



(relative error compared to the largest volume first reaches 0.001)

x_0 (fm)	v	v_{err}	G.O.F.
0.5	1.37	$1.08 \cdot 10^{-2}$	0.996
1	0.71	$2.15 \cdot 10^{-3}$	0.999
2	0.56	$5.05 \cdot 10^{-3}$	0.996
4	0.52	$4.64 \cdot 10^{-3}$	0.996
6	0.51	$1.42 \cdot 10^{-3}$	0.999

$$\psi(x) = e^{-(x/x_0)^2} \leftrightarrow \tilde{\psi}(k) = e^{-(kx_0/2)^2}$$

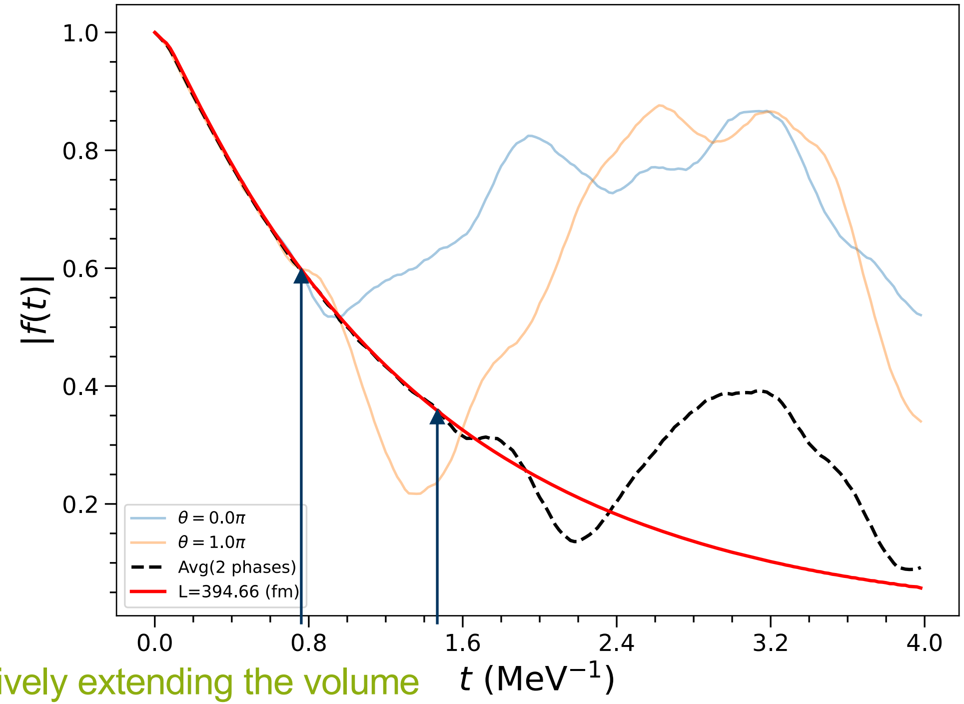
- broader test state causes lower required volume, while may contain more continuum components.

“volume” in proportional to “time”: effective wave-packet propagation velocity

- allows estimation of the volume needed for the f(t)-fit

Survival amplitudes with twisted boundary conditions

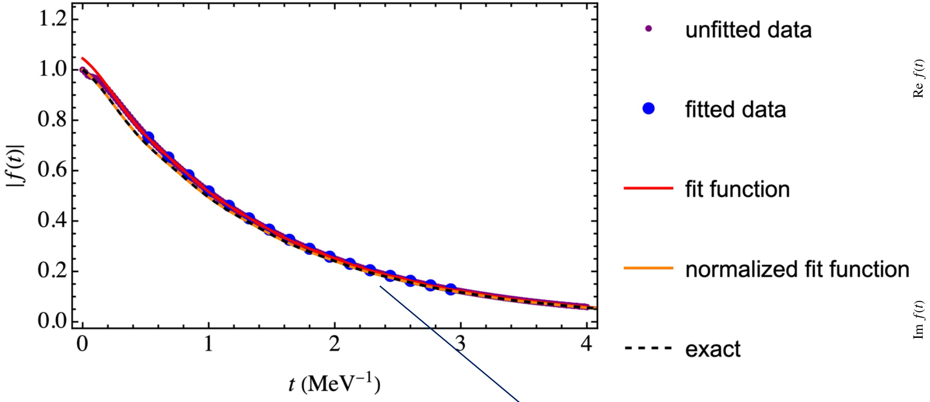
$$\psi(x+L) = e^{i\theta}\psi(x)$$

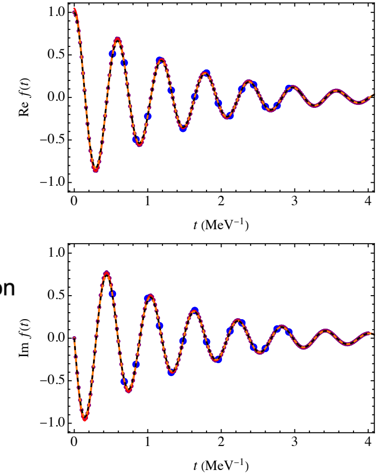


effectively extending the volume

courtesy of Avik Sarkar

Persistent state method in a large volume





L = 395 fm;
FV continuum;
$V(x) = 30\, e^{-\left(\frac{x}{3\text{ fm}}\right)^2} - 36\, e^{-\left(\frac{x}{1\text{ fm}}\right)^2}$ (MeV),
$\mu = 938.92$ (MeV);

persistent state:

x_0 (fm)	time window (MeV^{-1})	E_0 (MeV)	Γ (MeV)
2.0	0.5 – 2.0	10.605 ± 0.002	1.452 ± 0.003
	0.5 – 3.0	10.596 ± 0.001	1.450 ± 0.001
	0.5 – 4.0	10.593 ± 0.001	1.450 ± 0.001
2.5	0.5 – 2.0	10.554 ± 0.001	1.451 ± 0.003
	0.5 – 3.0	10.553 ± 0.001	1.449 ± 0.001
	0.5 – 4.0	10.553 ± 0.001	1.449 ± 0.001
3.0	0.5 – 2.0	10.492 ± 0.003	1.448 ± 0.002
	0.5 – 3.0	10.502 ± 0.002	1.448 ± 0.001
	0.5 – 4.0	10.506 ± 0.001	1.449 ± 0.001

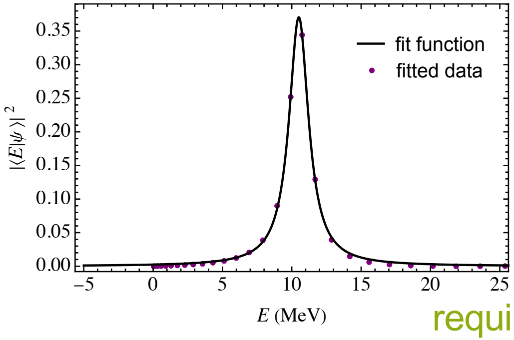
exact sol.:
$E_0 = 10.550$ (MeV)
$\Gamma = 1.449$ (MeV)

Resonance pole from spectral (overlap) function

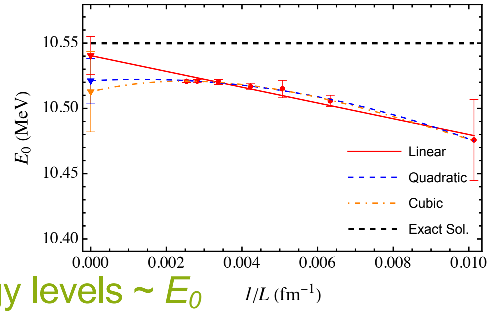
$$|\psi_{\text{res.}}\rangle = \int dE\, a(E)|E\rangle$$

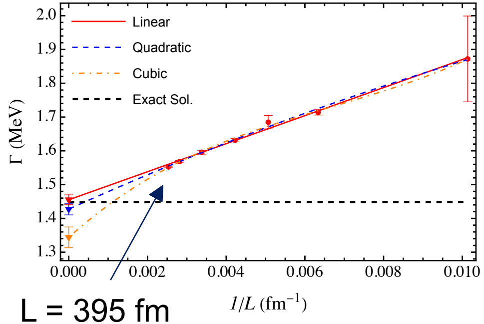
input: overlap $\langle\psi_{\text{persis.}}|E\rangle$ → fit function: spectral function $a(E)$ → output: E_0 Γ

- Persistent state



- Volume dependence (different from survival amplitudes):





require dense energy levels ~ E_0
→large volume

- Extracted resonance poles:

x_0 (fm)	E_0 (MeV)	extrapolation	Γ (MeV)	extrapolation
2.5	10.586 ± 0.020	quad.(vol.)	1.397 ± 0.020	quad.(vol.)
3.0	10.521 ± 0.017	quad.(vol.)	1.428 ± 0.017	quad.(vol.)
3.5	10.443 ± 0.037	quad.(vol.)	1.484 ± 0.012	lin.(vol.)

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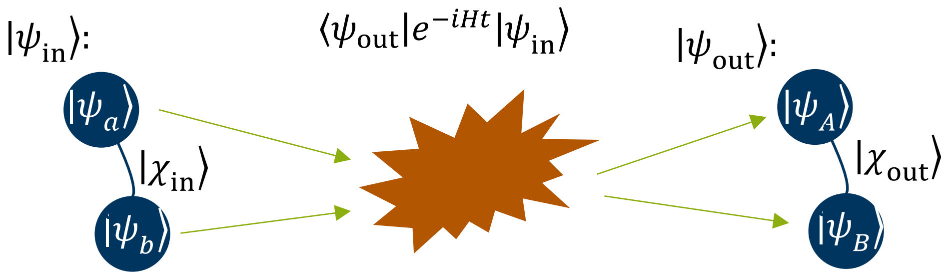
Outlook

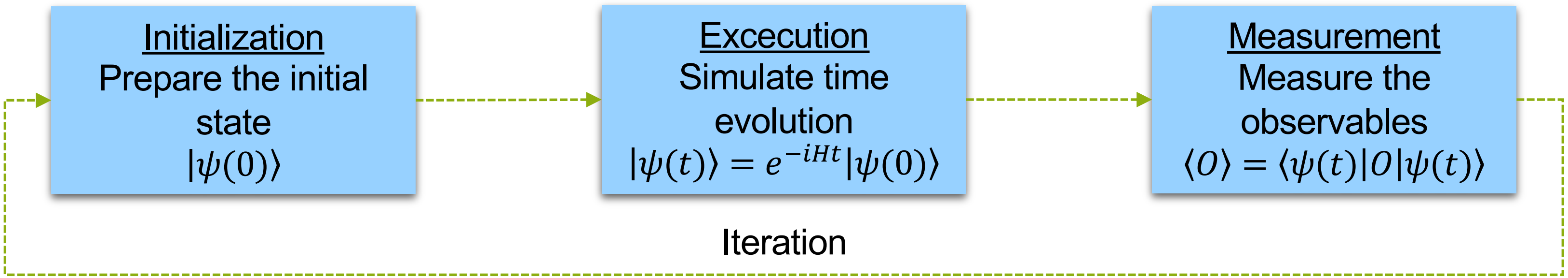
- (In)elastic scattering simulation
  - Resonance poles encoded in: $\langle\psi|e^{-iHt}|\psi\rangle$
  - Scattering process simulation by time evolution:



- Realistic nuclear resonances
  - Resonance poles from: $\langle\psi|e^{-Ht}|\psi\rangle$

- Resonance (and scattering) via quantum computing

typical quantum simulation process:



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Summary

- Persistent-state method is proposed and benchmarked in few-body models

- Advantages:
  - straightforward generalization to few-body resonances
  - extendable to scattering processes

- Challenges:
  - reducing finite-volume effect
  - handling multiple narrow resonances

Thank you!