Nuclear few- and many-body systems in a discrete variable representation basis

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***with**

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INT program: Universality in few-body systems, 03/31/2014

Outline

Motivation:

Consistent nuclear structure calculations at N^3LO in chiral EFT

Dialogue with lattice QCD

Lattice methods for nuclear few- and many-body systems

Discrete variable representation (DVR) basis

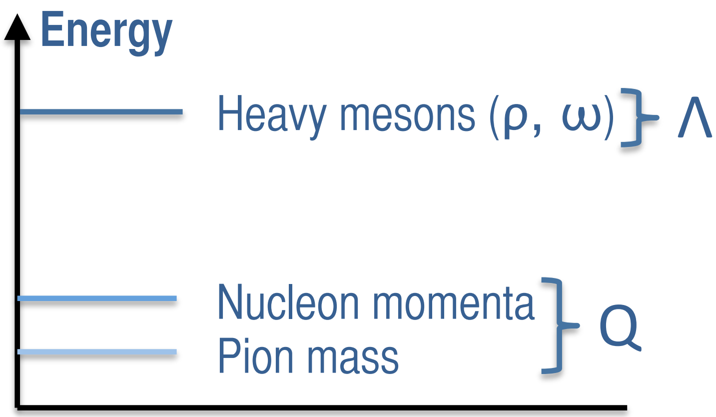
Construction of consistent chiral nuclear potentials

Applications to light nuclei

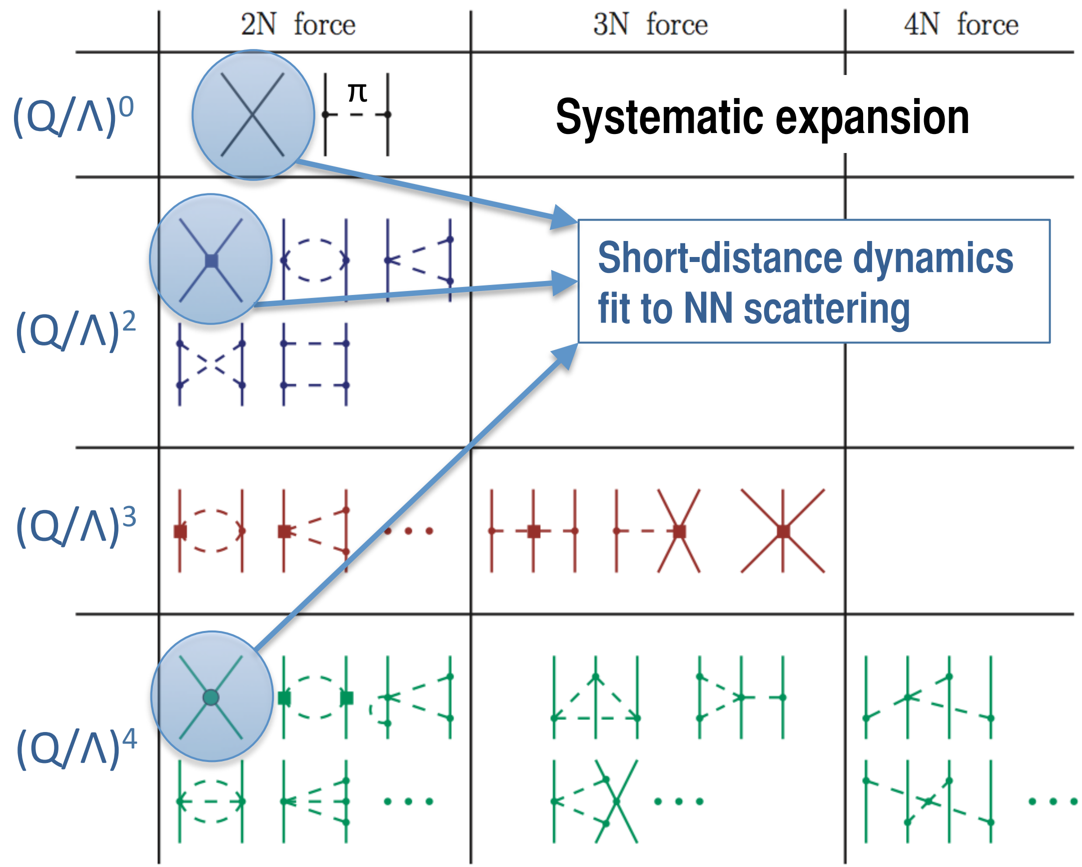
Applications to infinite neutron matter

Chiral effective field theory and nuclear forces

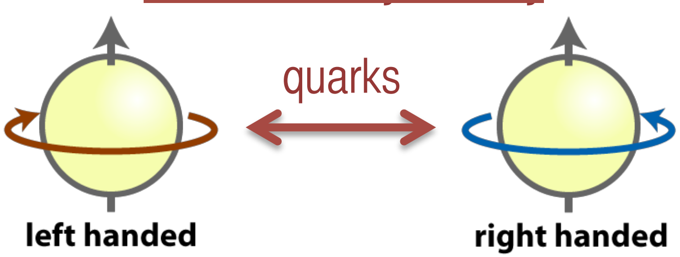
SEPARATION OF SCALES + SYMMETRIES



Low-energy theory of nucleons and pions



QCD chiral symmetry



Constrains pion dynamics

Chiral effective field theory and nuclear forces

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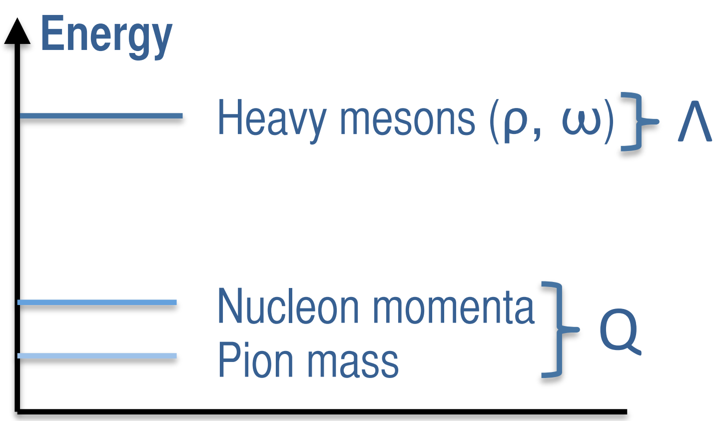

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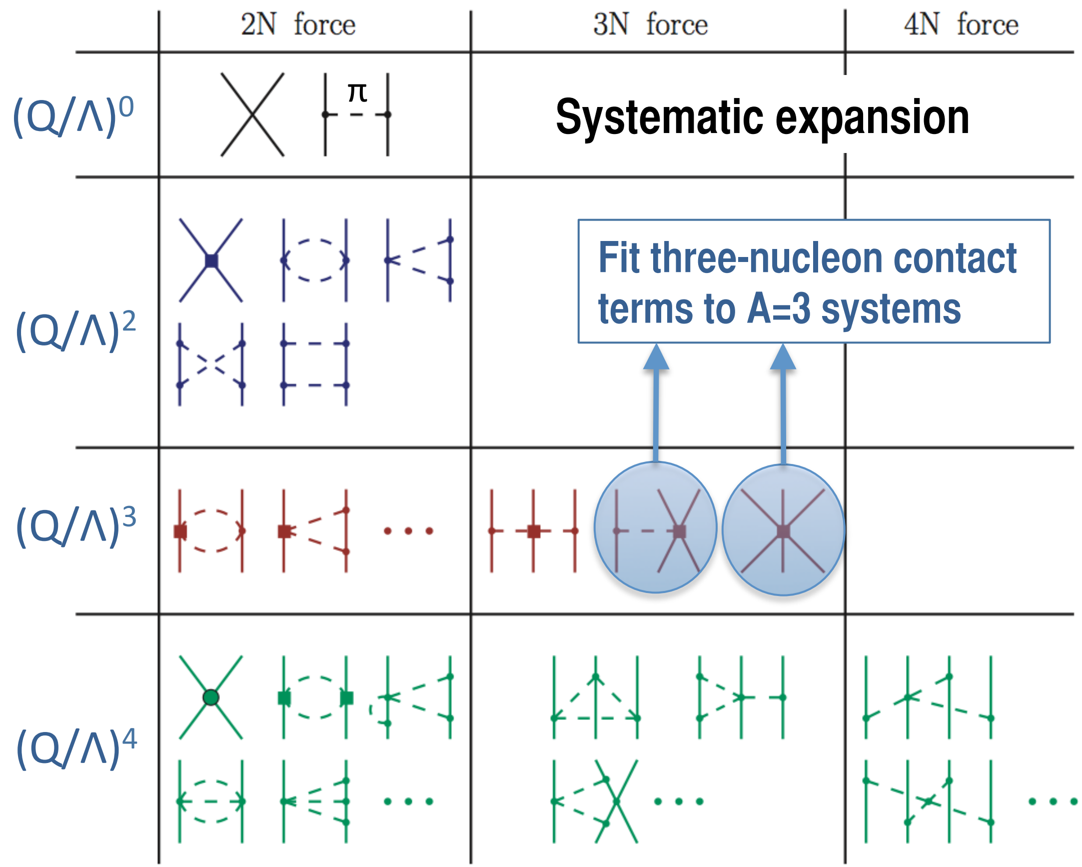

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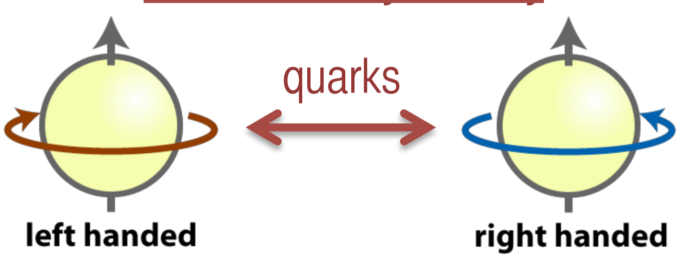

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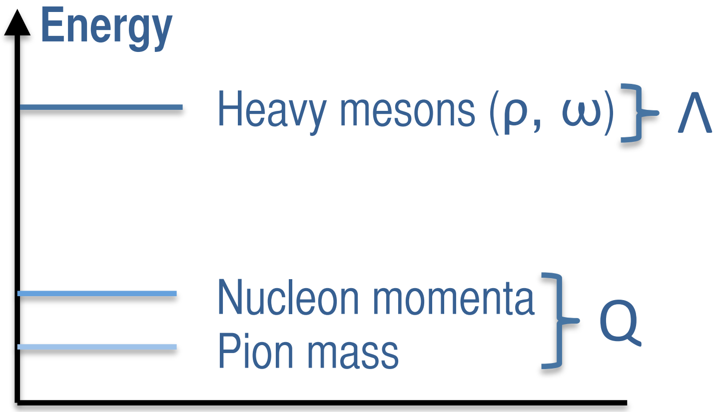

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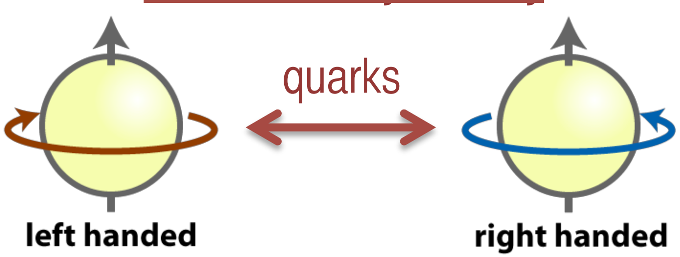

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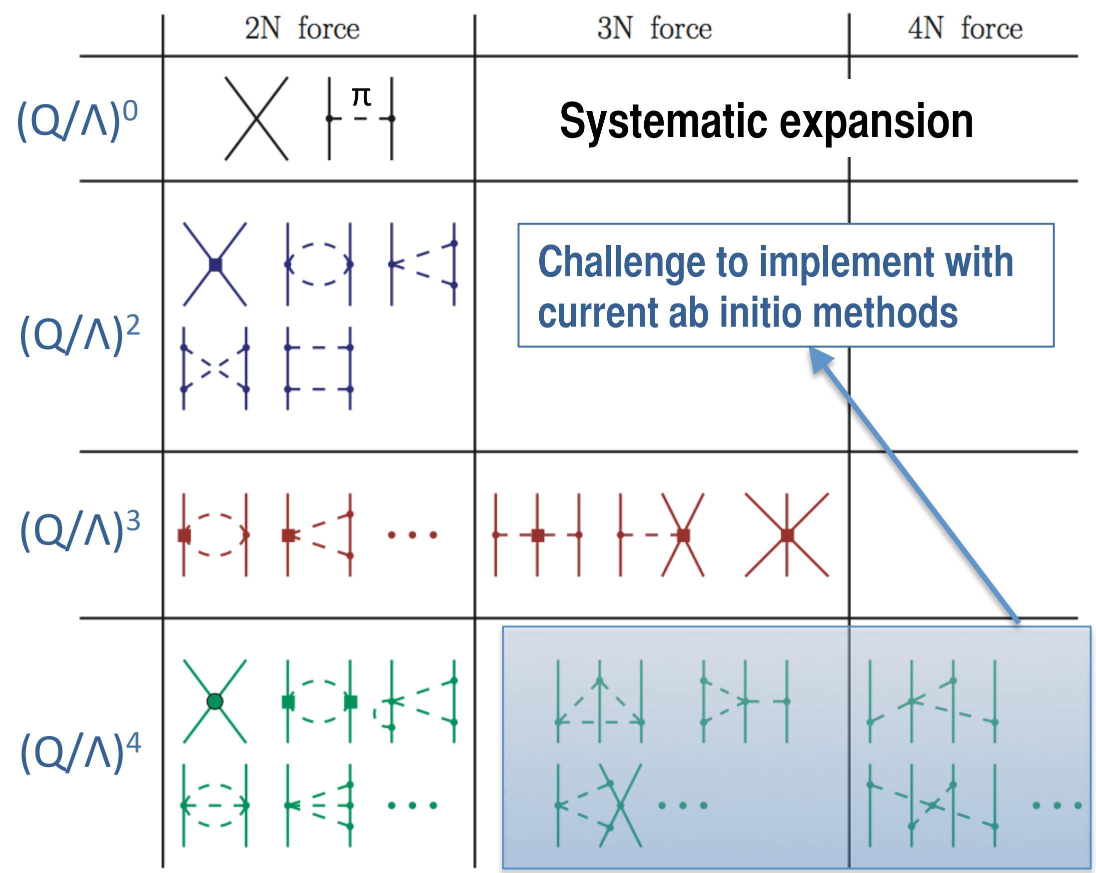
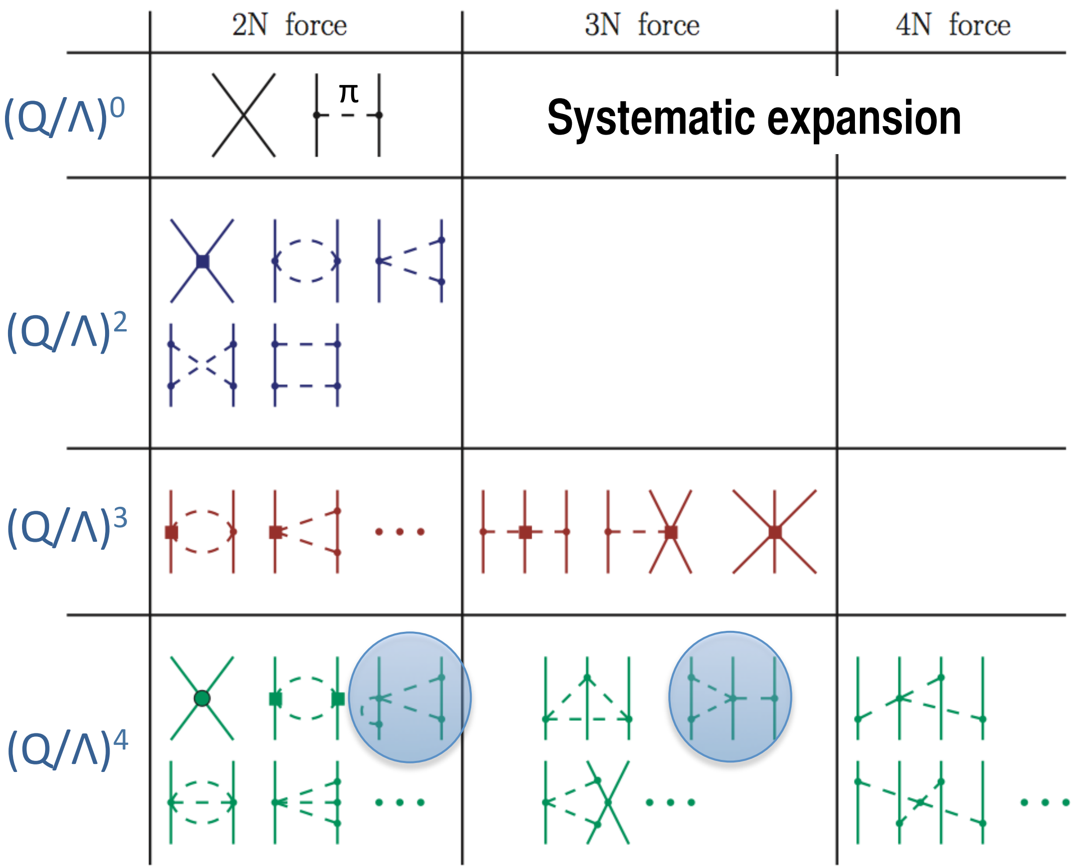
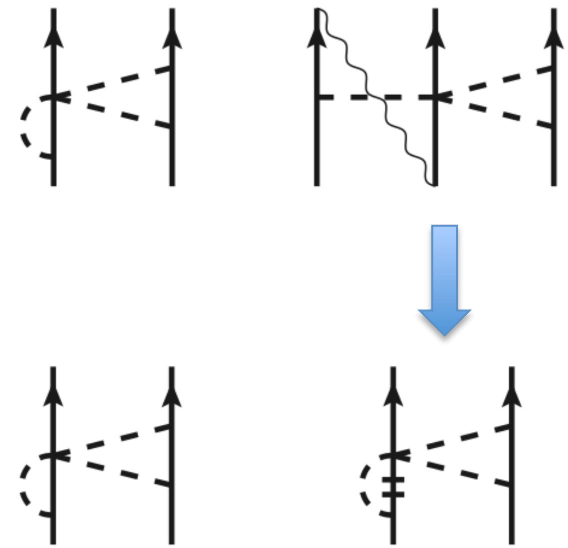


Pauli principle consistency

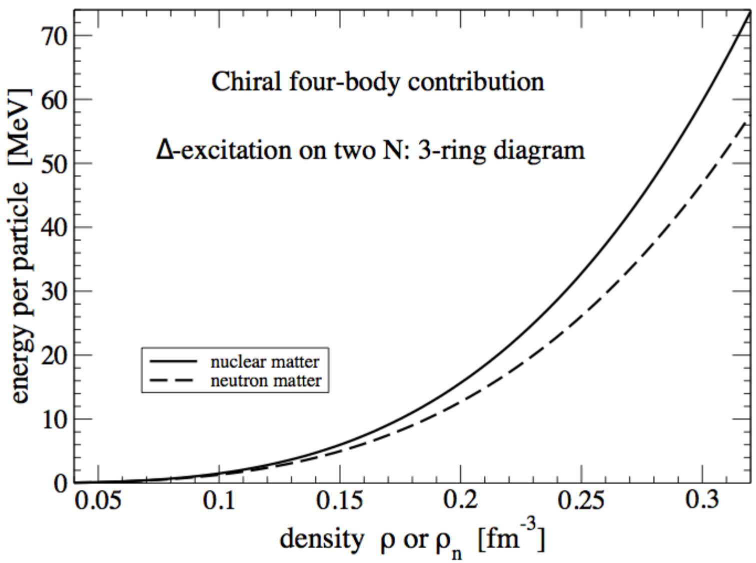


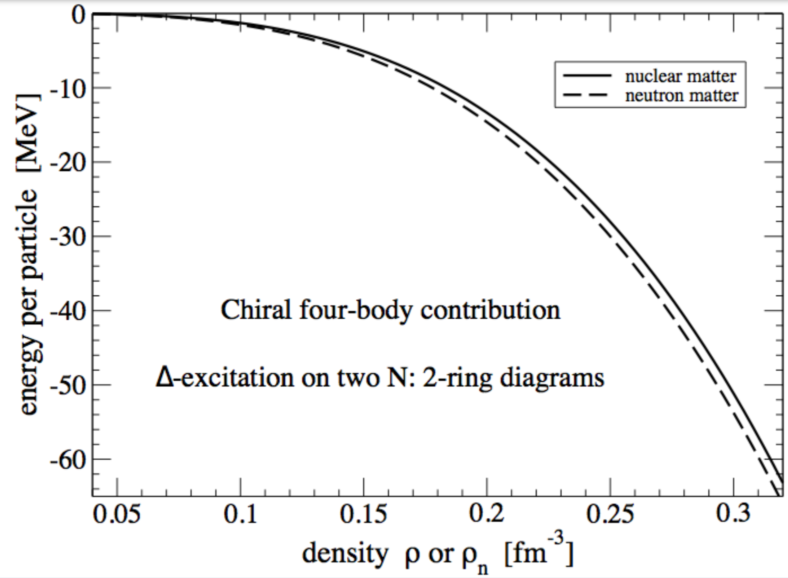


$$G(p_0,\vec{p}) = \frac{i}{p_0 - \vec{p}^{\,2}/2M + i\epsilon}$$

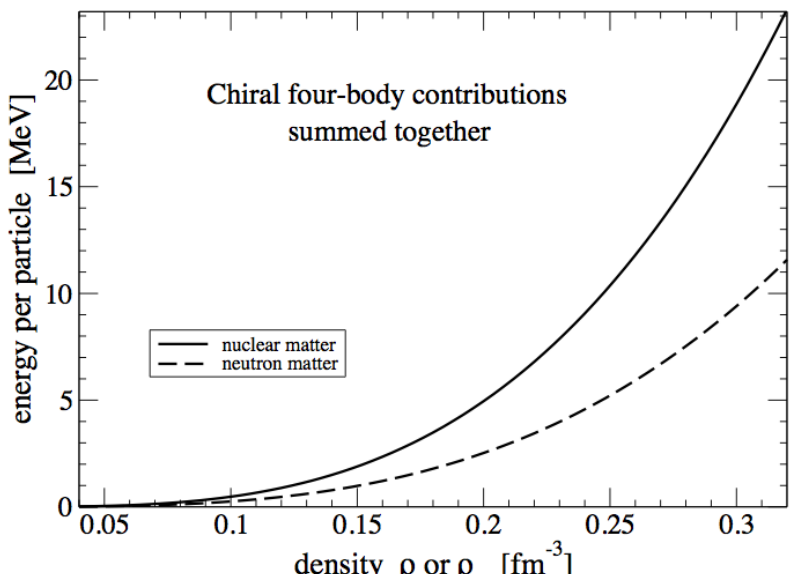
$$-2\pi\delta(p_0 - \vec{p}^{\,2}/2M)\theta(k_f - |\vec{p}|)$$

Strength of nuclear four-body forces





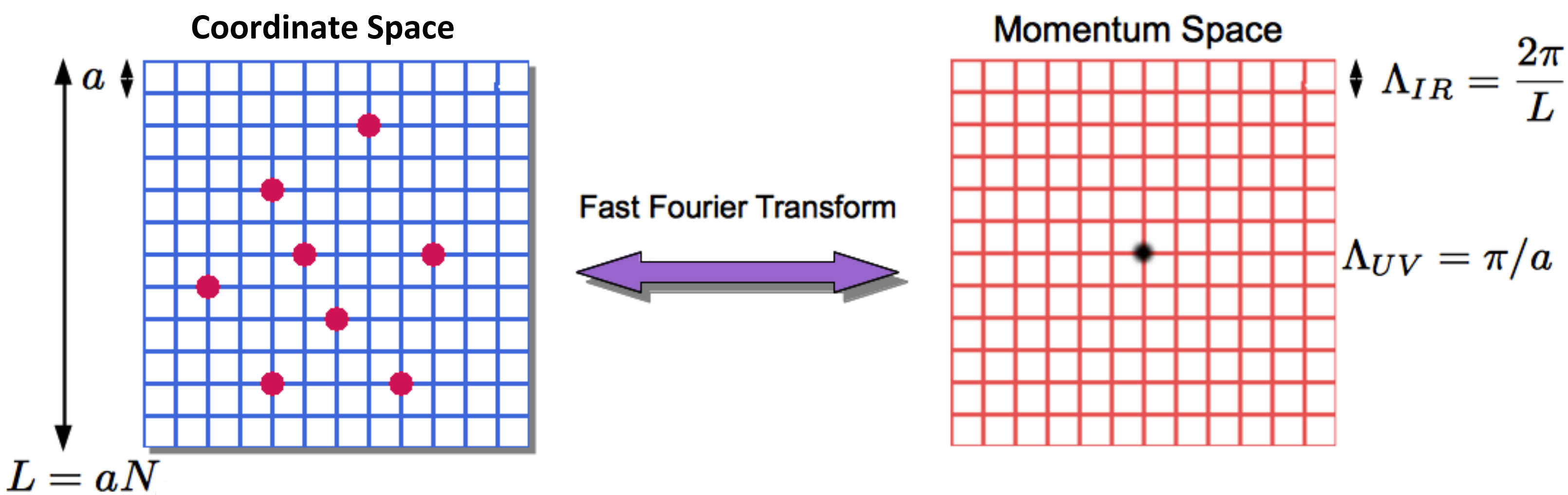
4NF with explicit Δ



N. Kaiser, EPJA (2013)

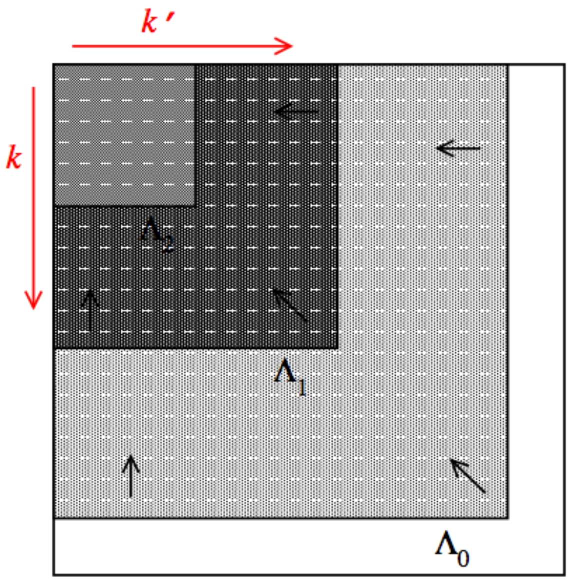
Nucleons on a lattice

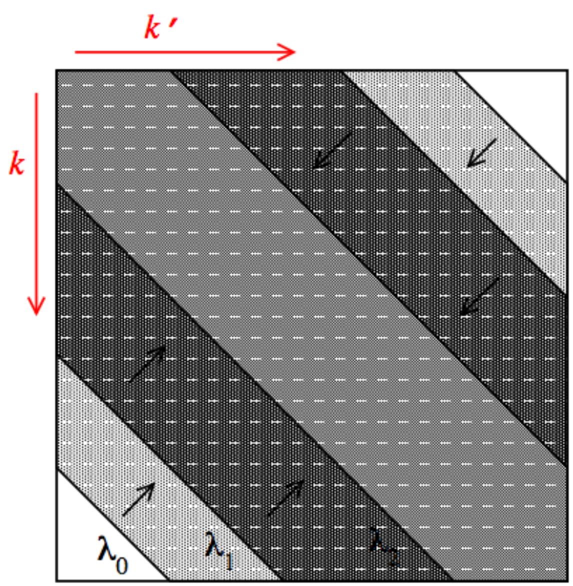
Chiral nuclear potentials naturally represented in **plane-wave basis**



- Finite set of single-particle basis states… but how to choose “L” and “a”?
- Lattice spacing defines resolution scale (develop consistent “low-momentum” chiral nuclear potentials)
- Formal description with “discrete variable representation” (DVR) basis

“Low-momentum” chiral nuclear potentials





- Traditionally constructed via **RG-evolution**
  [Bogner, Furnstahl, Kuo, Schwenk,…]

“Good”

Desirable convergence properties in **perturbation theory**

Desirable convergence properties in **finite model spaces**

“Bad”

Induced many-body forces and currents

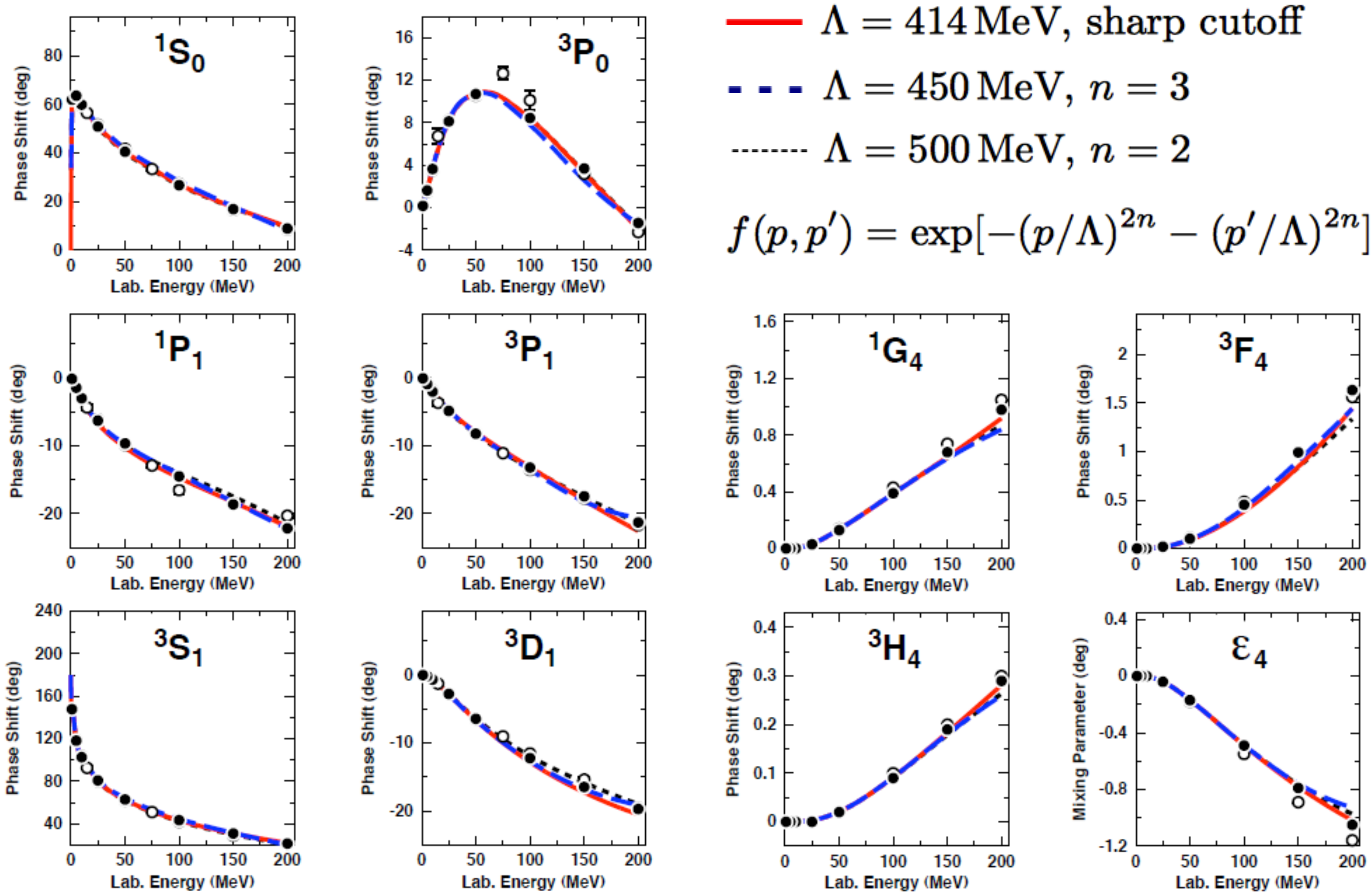
Analytical form of potential is lost

- Certain ab-initio many-body methods more convenient if analytical form of potential is known

- Construct nuclear potentials at different cutoff scales

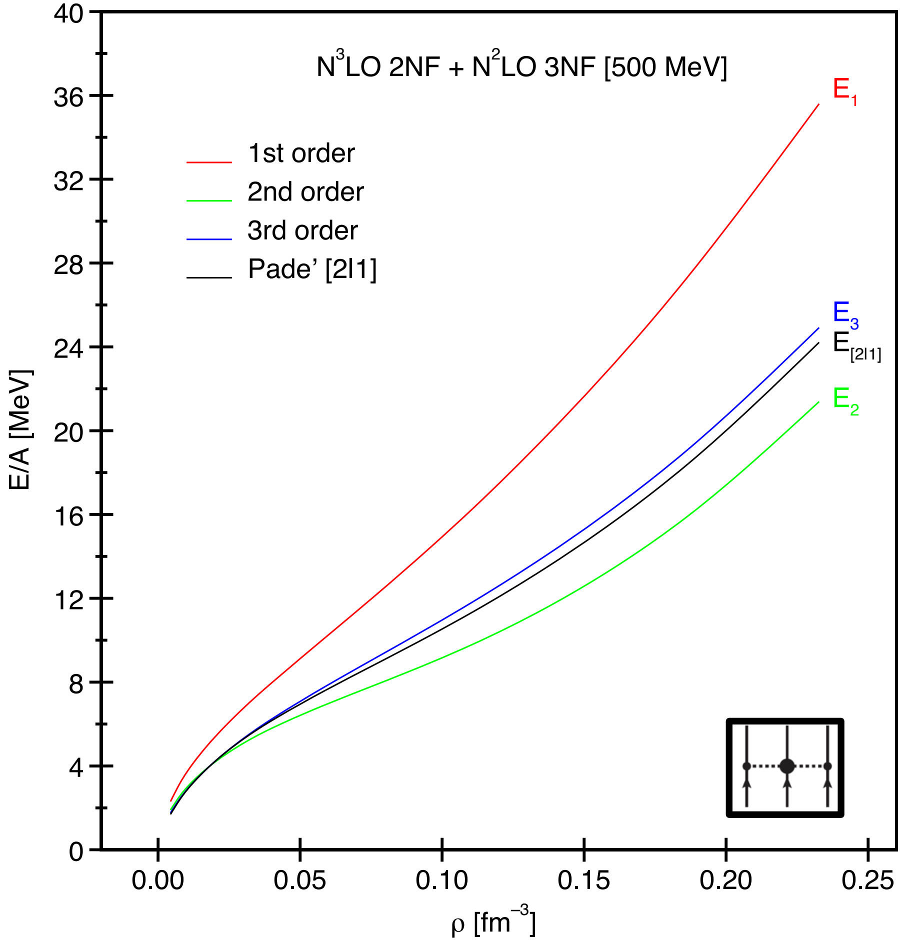
Fit c_i LEC's to peripheral NN phase shifts

Coraggio, Holt, Itaco, Machleidt, Sammarruca, PRC 2013

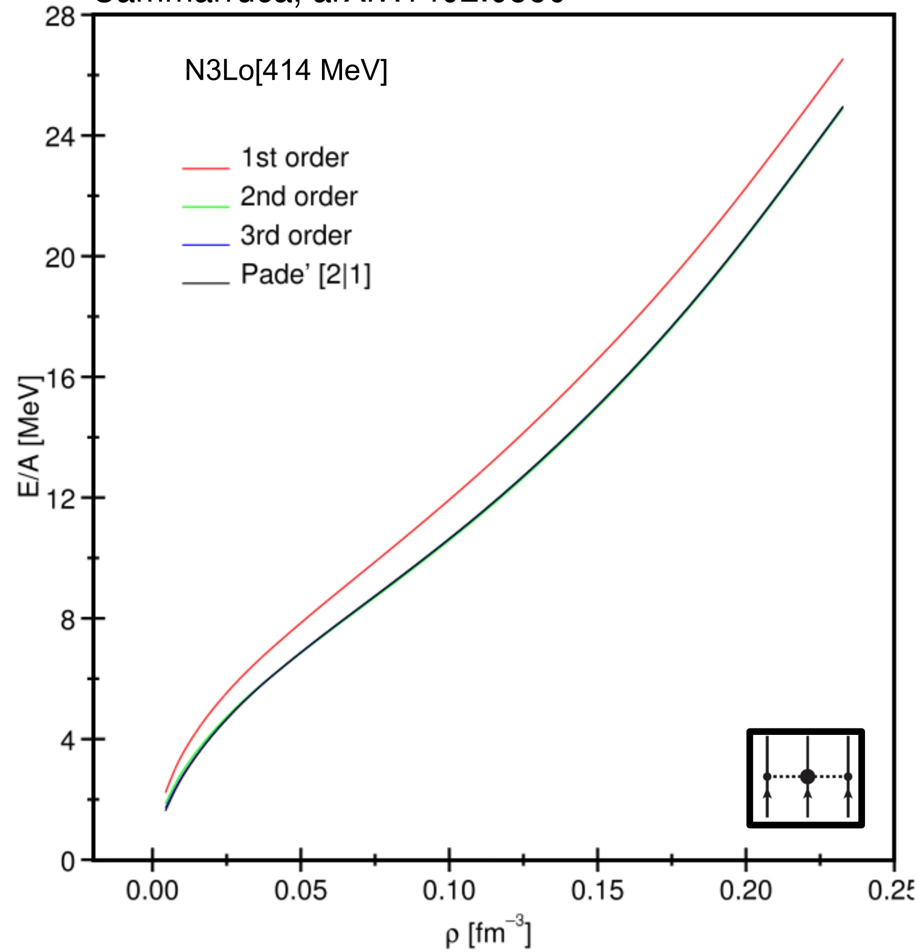


Perturbative features: neutron matter equation of state

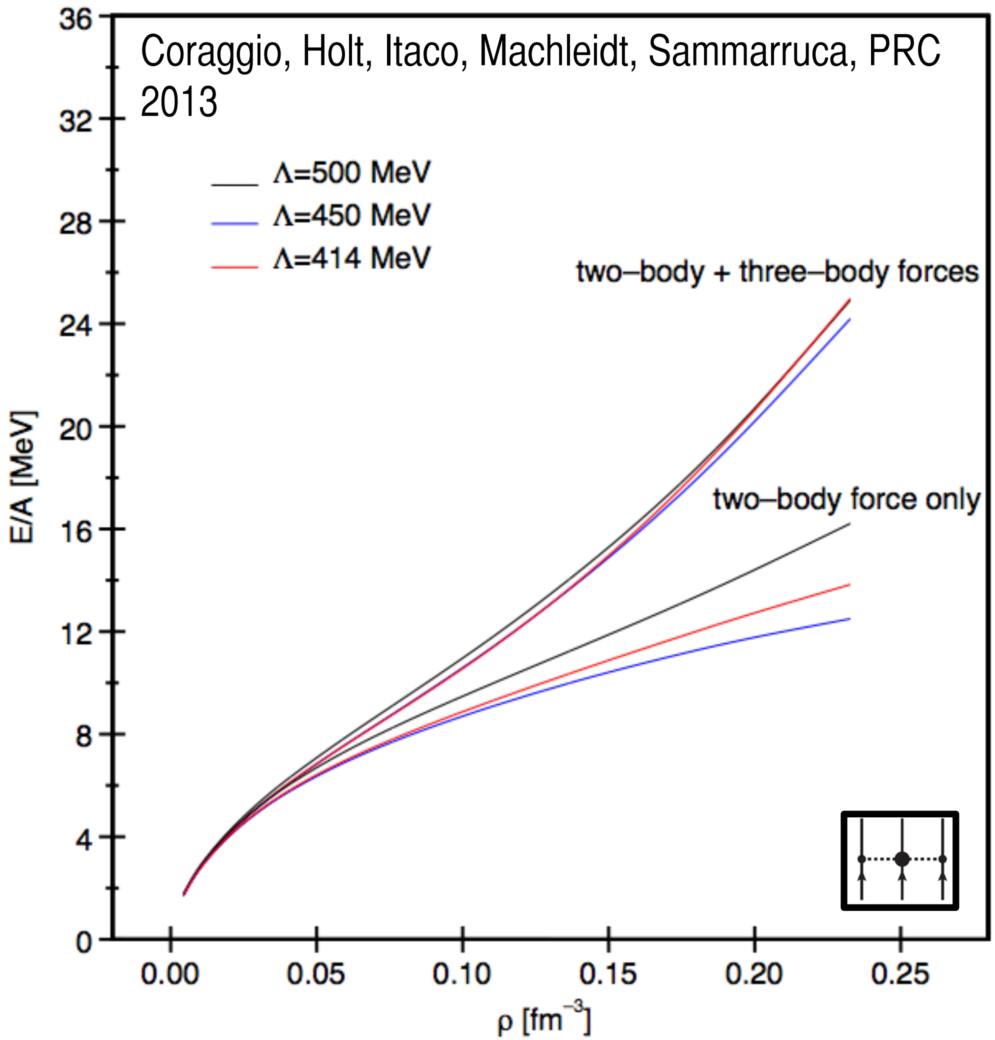
Coraggio, Holt, Itaco, Machleidt, Sammarruca, PRC 2013



Coraggio, Holt, Itaco, Machleidt, Marcucci, Sammarruca, arXiv:1402.0380

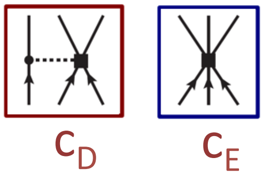


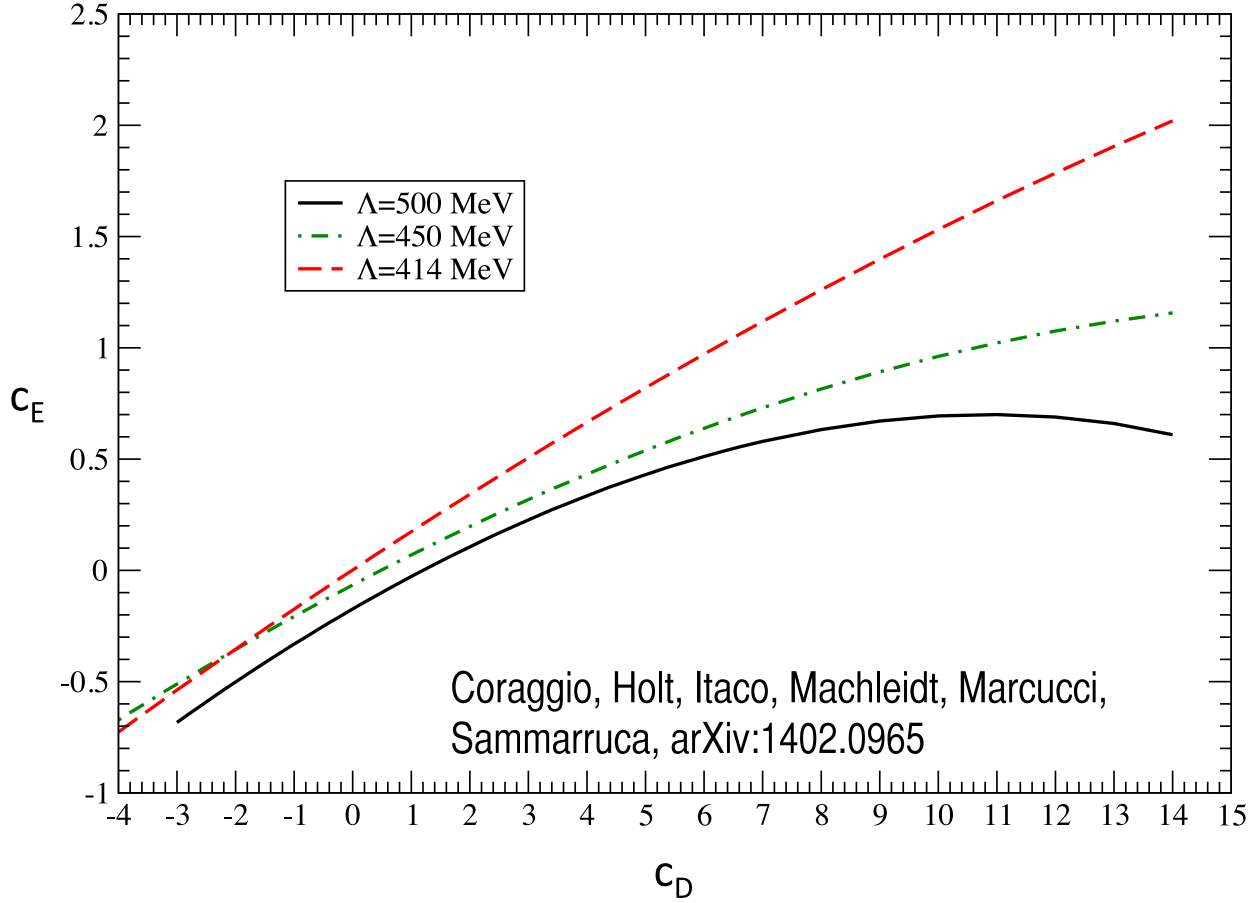
Scale dependence of neutron matter EOS



Determination of c_D and c_E low-energy constants

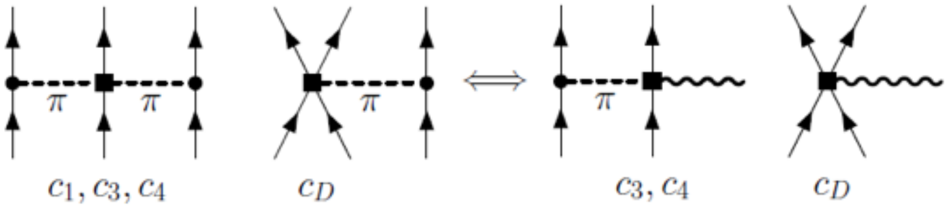
- **Optimized fit** to ^{3}H and ^{3}He binding energies

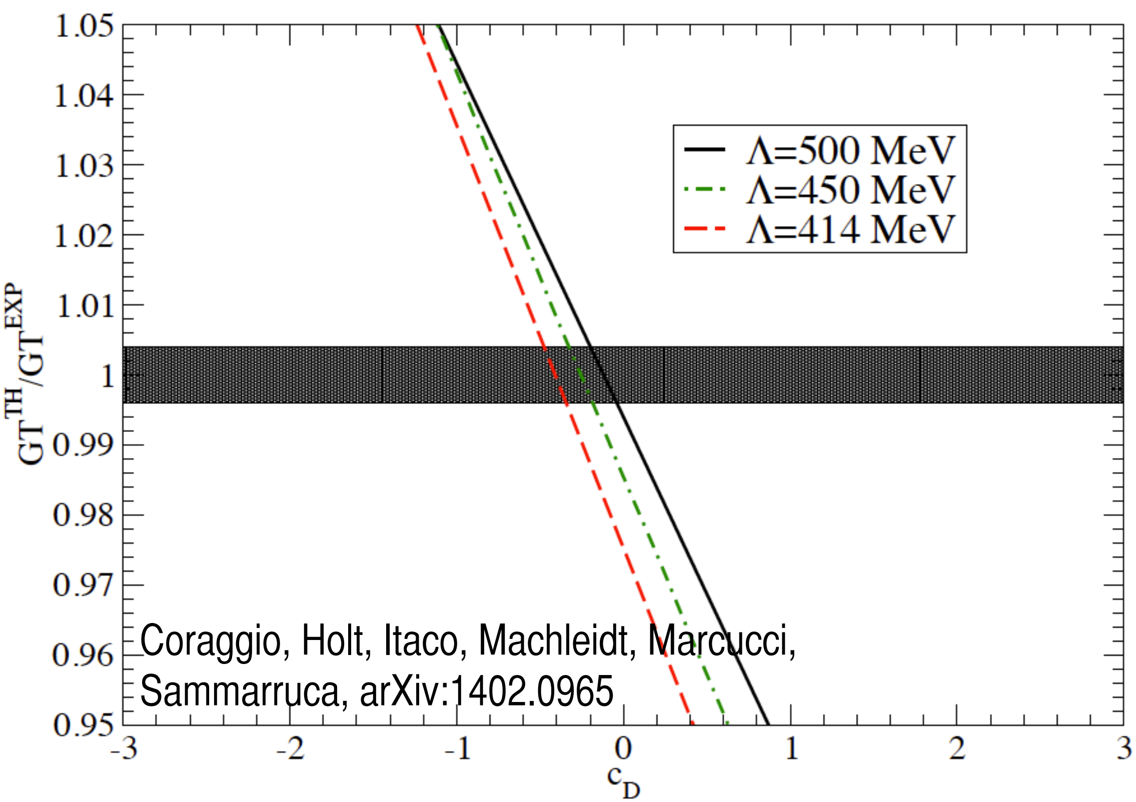




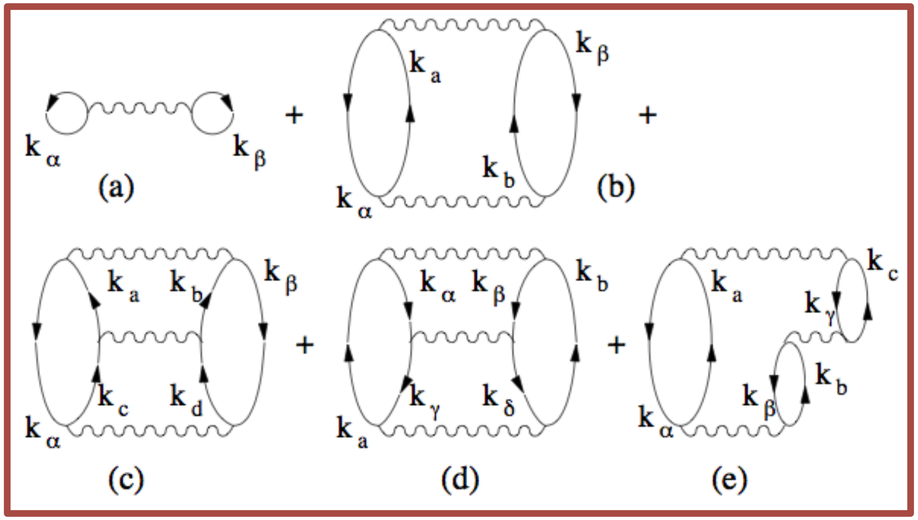
Symmetric nuclear matter: determination of c_D

- Fit c_D to triton lifetime [A Gårdestig and D R Phillips, PRL (2006); D. Gazit et al., PRL (2009)]





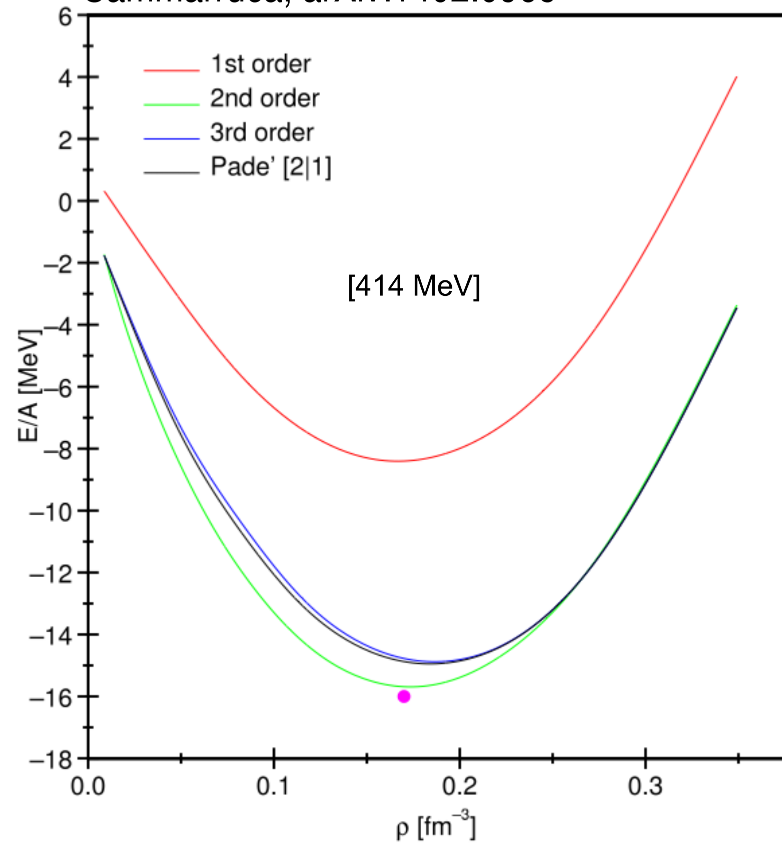
Nuclear matter equation of state



$K_f = 1.33\ fm^{-1}$	414	450	500
HF contribution	-28.792	-25.688	-19.503
2nd order *pp* diagram	-7.388	-11.273	-13.511
3rd order *pp* diagram	0.563	0.745	1.642
3rd order *hh* diagram	-0.010	-0.008	-0.008
3rd order *ph* diagram	0.581	0.152	-1.516

- Consistent 3rd-order calculation of equation of state

Coraggio, Holt, Itaco, Machleidt, Marcucci, Sammarruca, arXiv:1402.0965



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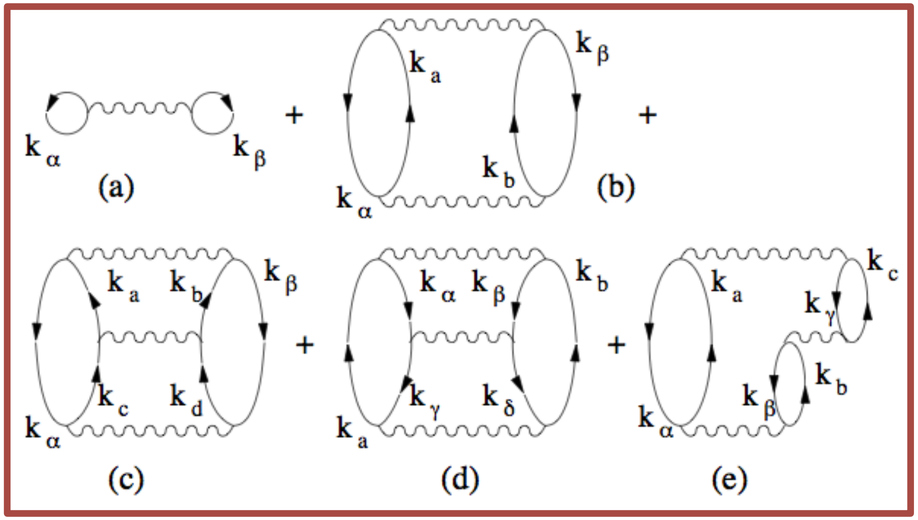

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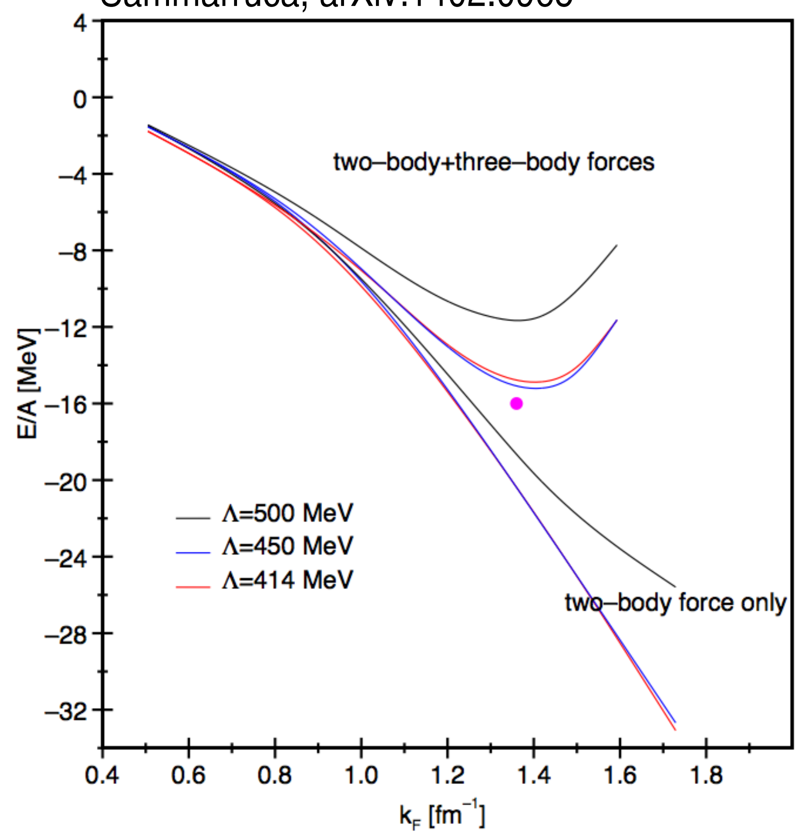


Discrete Variable Representation

Discrete variable representation (DVR) basis

- Widely used method for **discretizing** the Schrödinger equation
- Maintains the **locality of operators** (e.g., potential energy)
- **Rapid (exponential) convergence** for appropriate potentials and boundary conditions
- Direct-product DVR's typically lead to **sparse-matrix representation** of Hamiltonian in multidimensional problems
- Easily coupled to **iterative techniques** (e.g., Lanczos) to find lowest eigenvalues of the Hamiltonian matrix

Discrete variable representation (DVR) basis

- The DVR is a **quasi-local** (in coordinate space) but **discrete** representation
- Start with finite set of energy eigenstates defining projector $P = \sum_i |\phi_i\rangle\langle\phi_i|$

E.g., plane waves: $P = \sum_{|\vec{k}|<k_c} |\vec{k}\rangle\langle\vec{k}|$

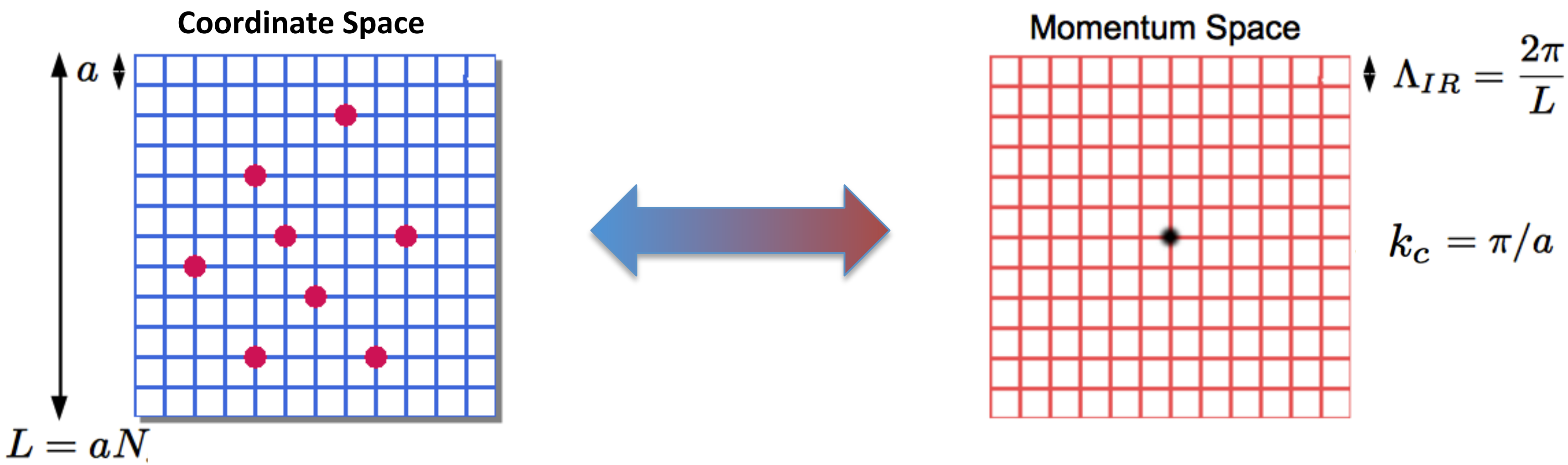
- Look for grid points $\{x_i\}$ such that $|\Delta_j\rangle \equiv P|x_j\rangle = \sum_i |\phi_i\rangle\phi_i^*(x_j)$ satisfy

$$\boxed{\langle\Delta_\alpha|\Delta_\beta\rangle = \langle x_\alpha|P|x_\beta\rangle = \Delta_\beta(x_\alpha) = N_\alpha\delta_{\alpha\beta}}$$

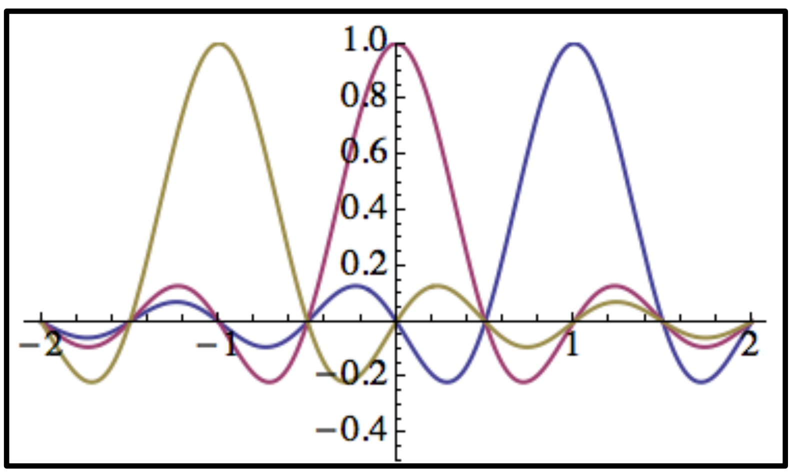
(nontrivial requirement)

- Basis functions have nodes at all other lattice points
- Quasi-locality: $\langle\Delta_i|V|\Delta_j\rangle \simeq \delta_{ij}N_iV(x_i)$

Plane-wave basis

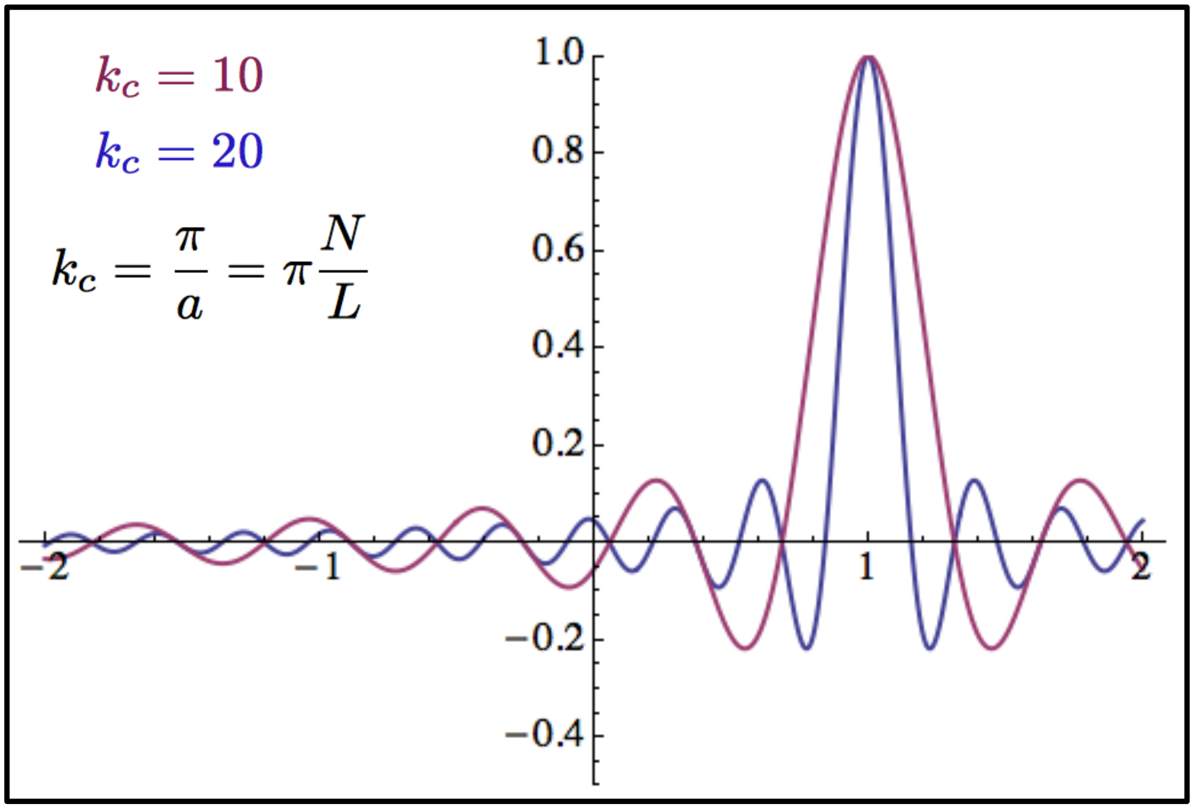


- Sinc function basis: $\frac{1}{\sqrt{N_i}}\Delta_i(x) = \mathrm{sinc}(k_c(x - x_i)) = \frac{\sin(k_c(x - x_i))}{k_c(x - x_i)}$



Dependence on lattice spacing

- Sinc function basis: $\frac{1}{\sqrt{N_i}}\Delta_i(x) = \mathrm{sinc}(k_c(x-x_i)) = \frac{\sin(k_c(x-x_i))}{k_c(x-x_i)}$

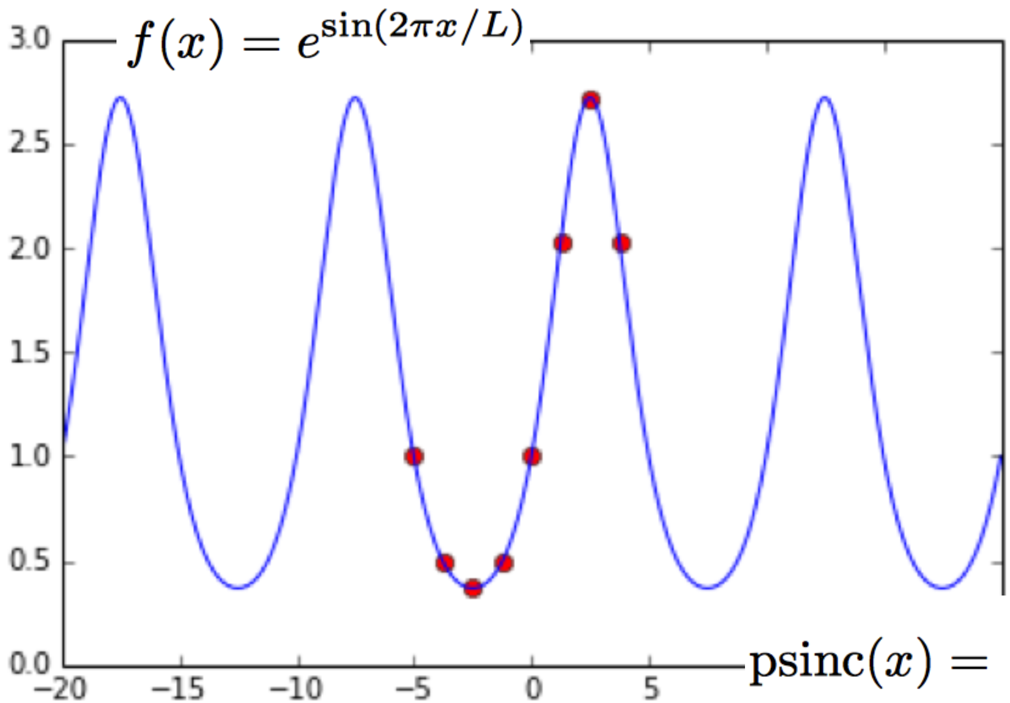


Function interpolation

- To express a function in the basis, simply evaluate it at the abscissa:

$$f(x) = \sum_i \frac{1}{N_i} f(x_i) \Delta_i(x)$$

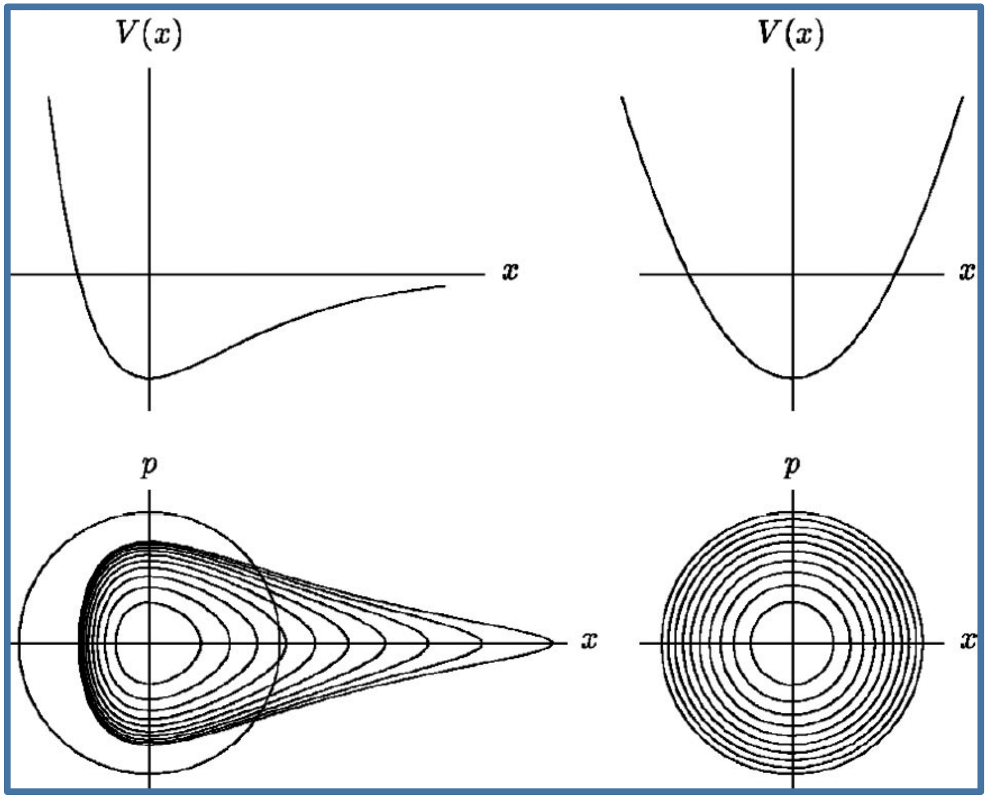
```
array([-5.  , -3.75, -2.5 , -1.25,  0.  ,  1.25,  2.5 ,  3.75])
```



$$\mathrm{psinc}(x) = \frac{\sin(x)}{N \sin(x/N)}$$

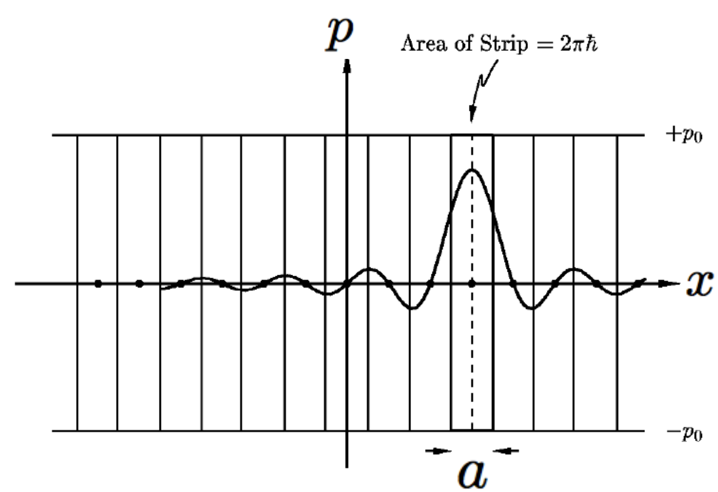
Phase-space coverage

- For convergence must at least cover the same semi-classical phase space

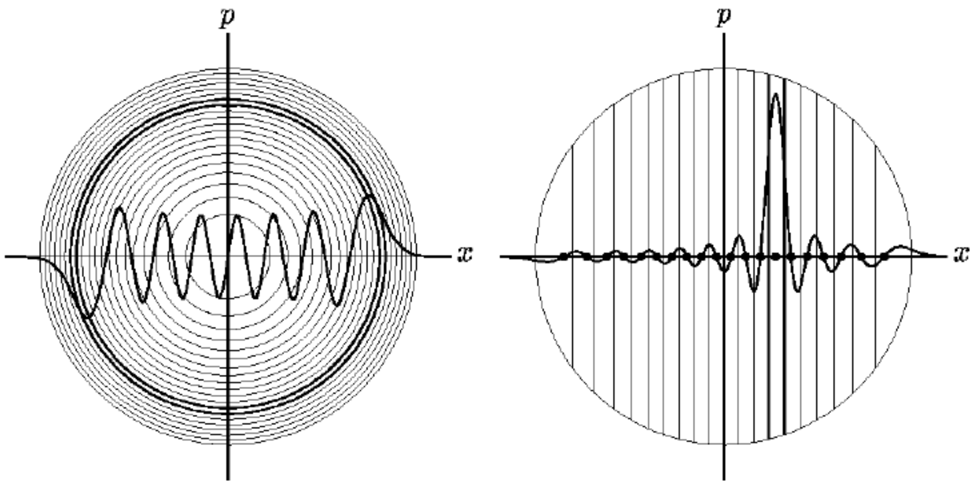


R. G. Littlejohn et al., J Chem Phys 2002

- DVR basis covers phase space with strips of area $2\pi\hbar$



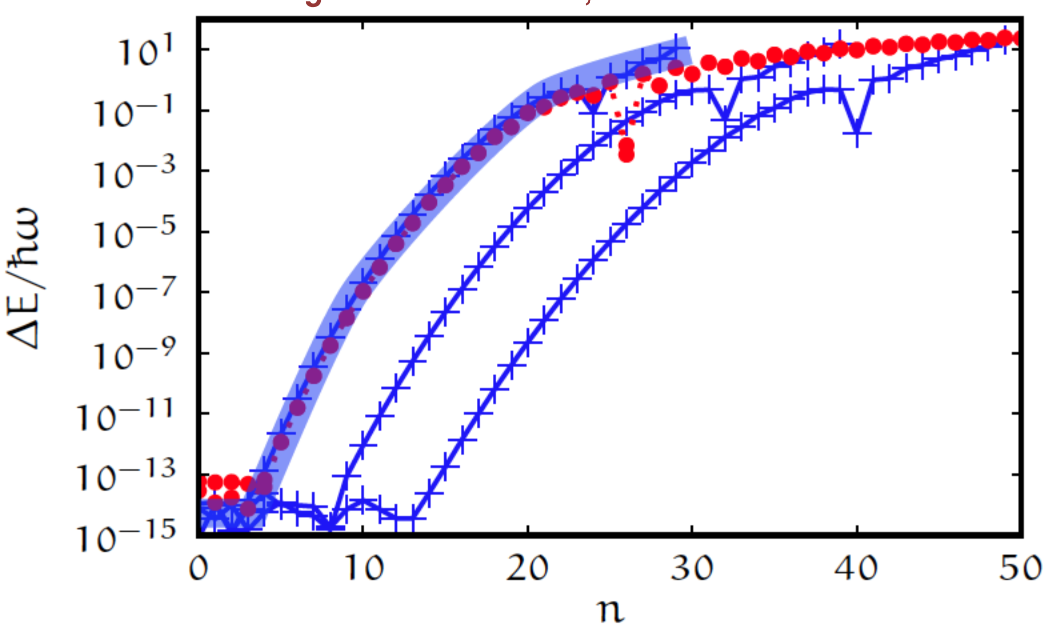
Convergence of 1D harmonic oscillator

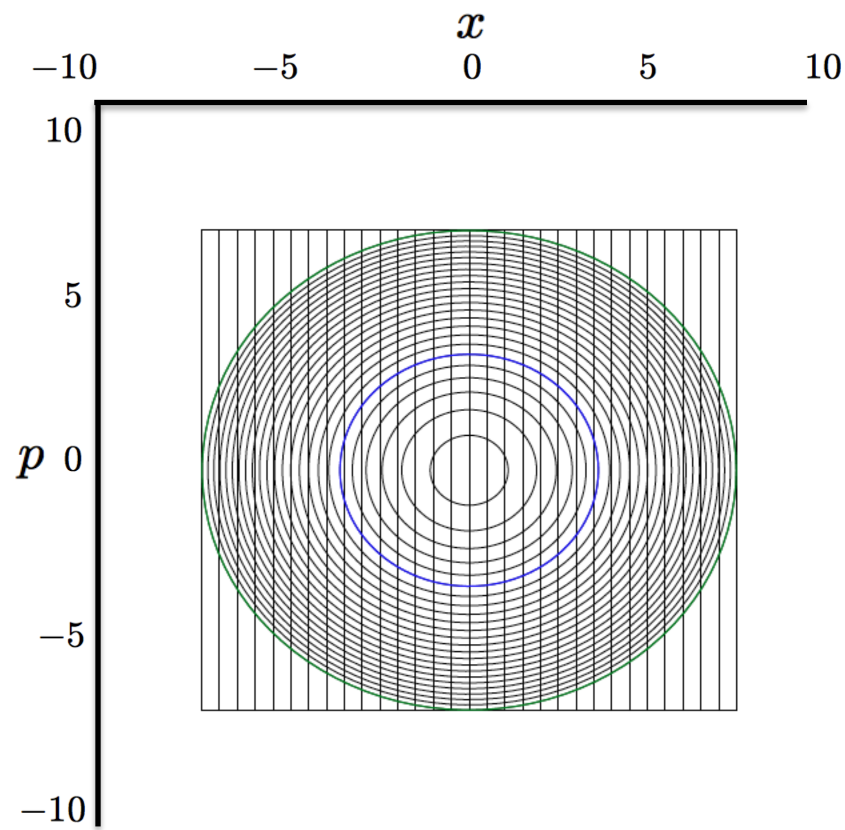


Harmonic oscillator eigenvalues

- 5 excellent (machine precision)
- 24 good (10% error)

A. Bulgac & M. M. Forbes, PRC 2013





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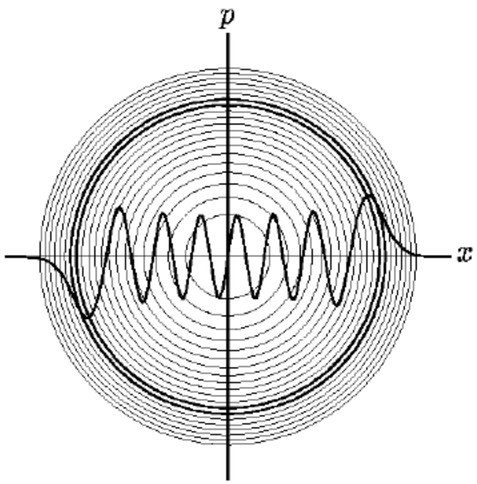
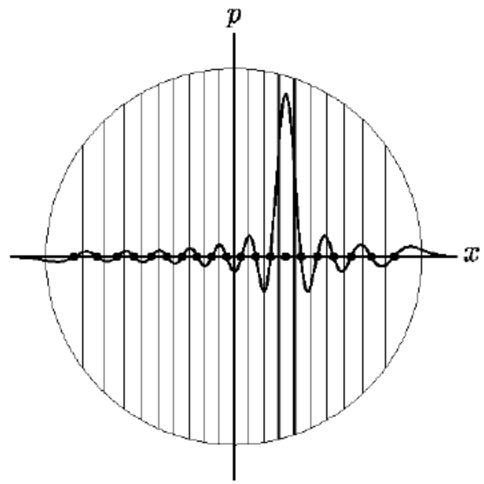
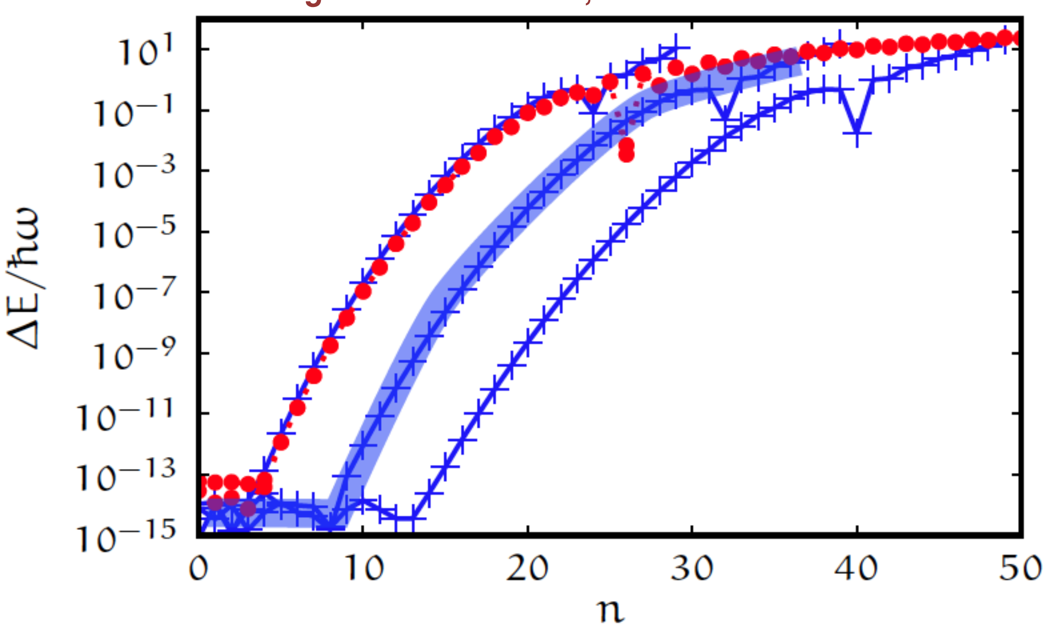


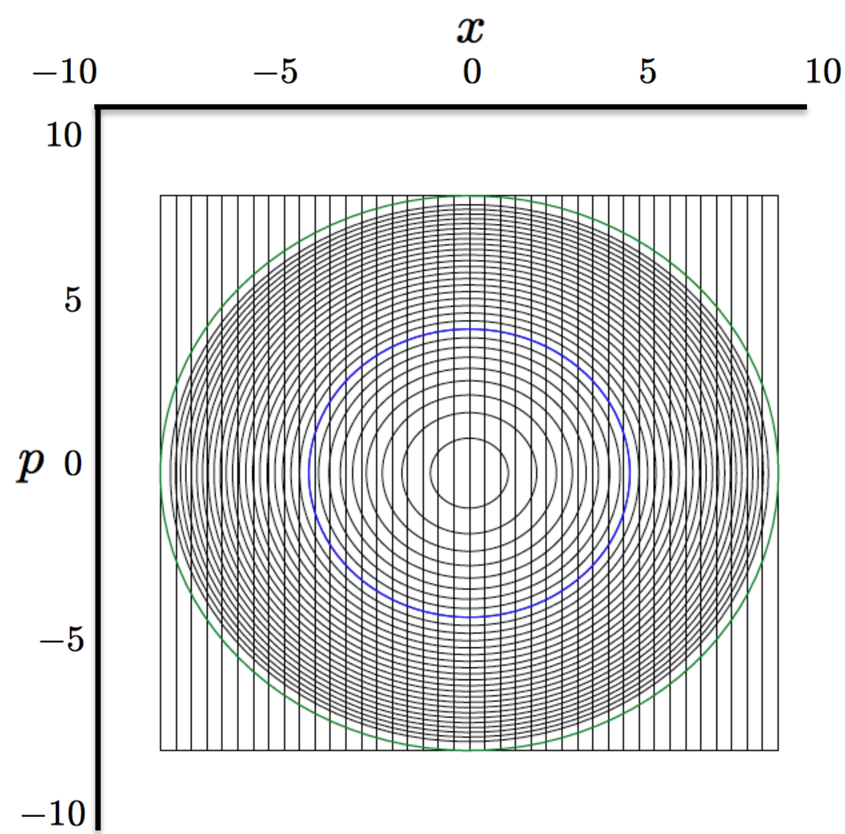


Harmonic oscillator eigenvalues

- 8 excellent (machine precision)
- 32 good (10% error)

A. Bulgac & M. M. Forbes, PRC 2013





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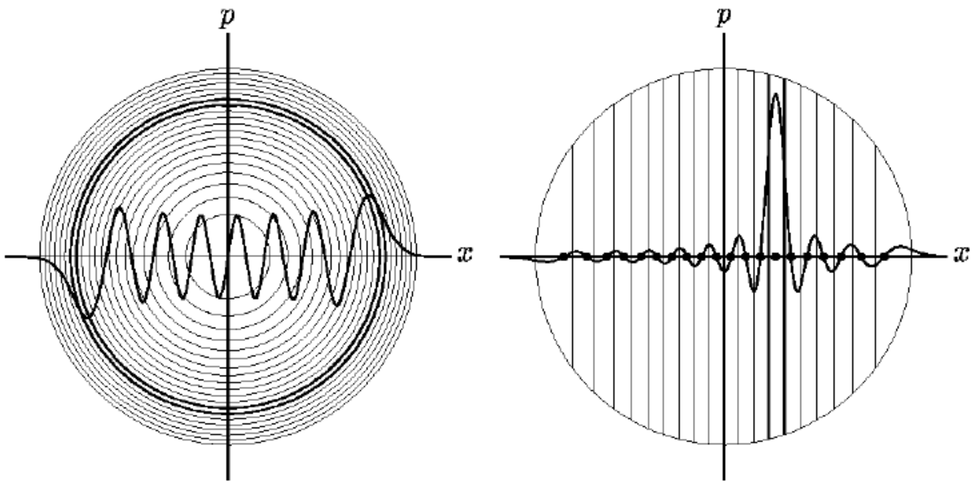

Harmonic oscillator eigenvalues

- 14 excellent (machine precision)
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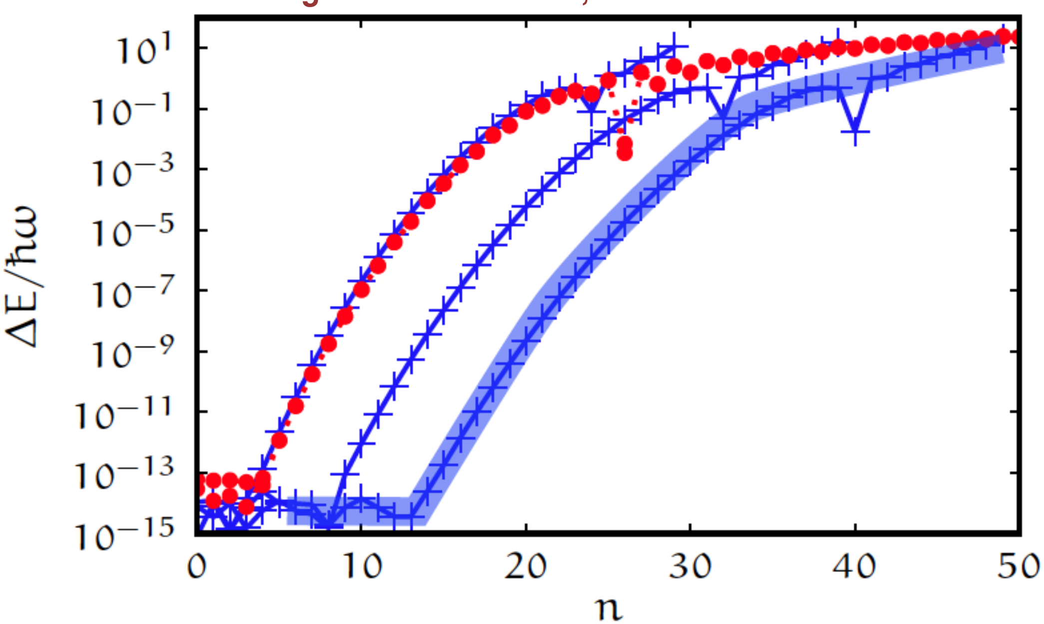
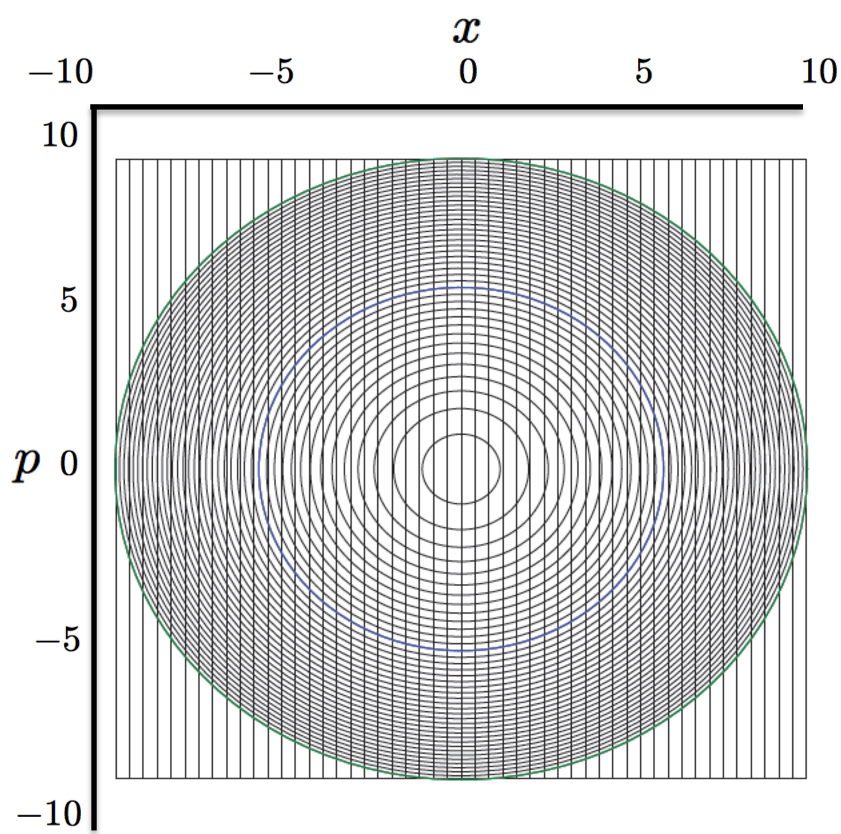
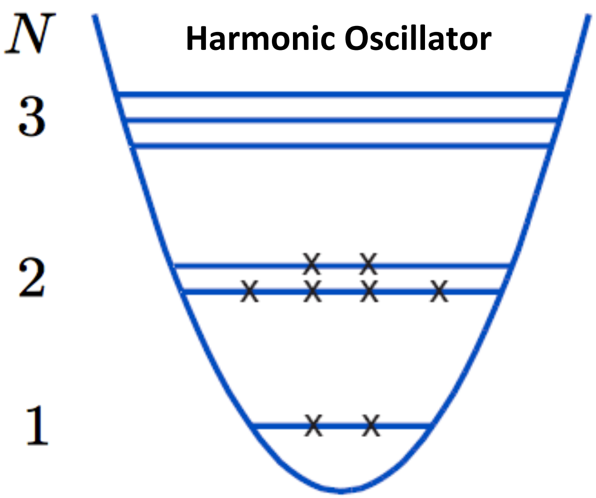
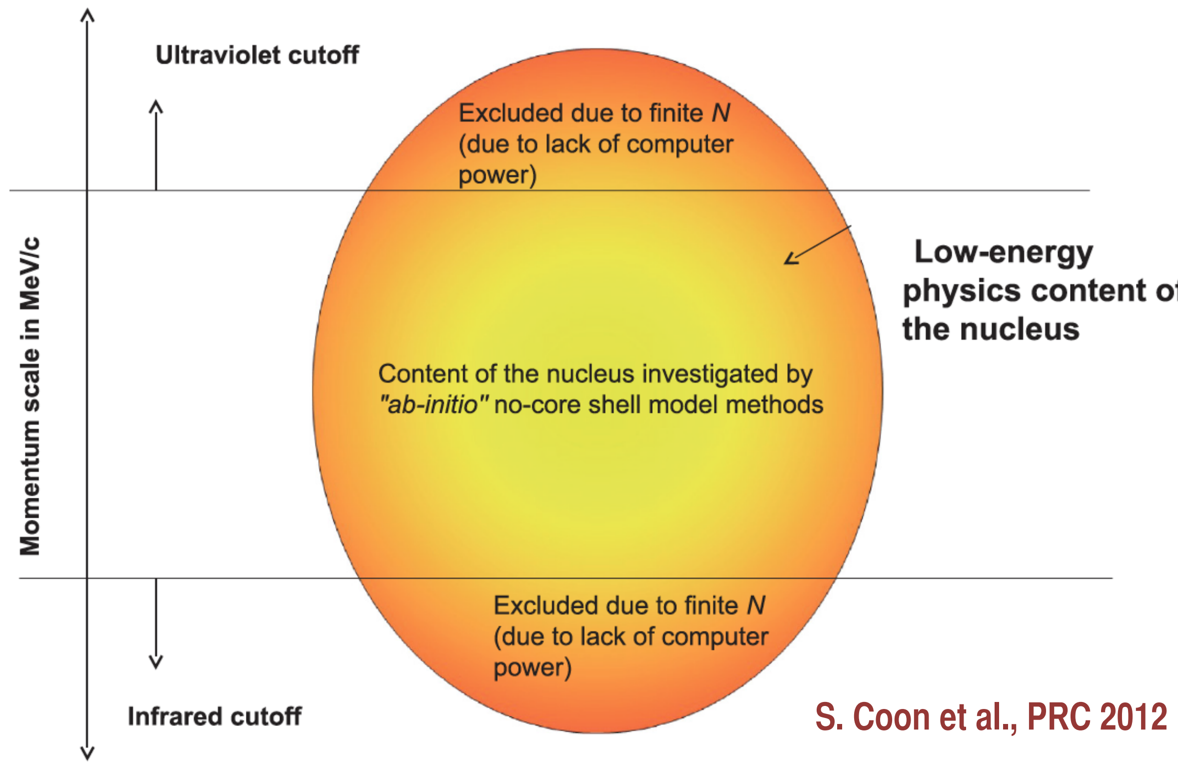
A. Bulgac & M. M. Forbes, PRC 2013





IR and UV convergence in shell model calculations





- Maximum momentum associated with filling the highest available single-particle state

$$\Lambda = \sqrt{m_N(N+3/2)\hbar\omega}$$

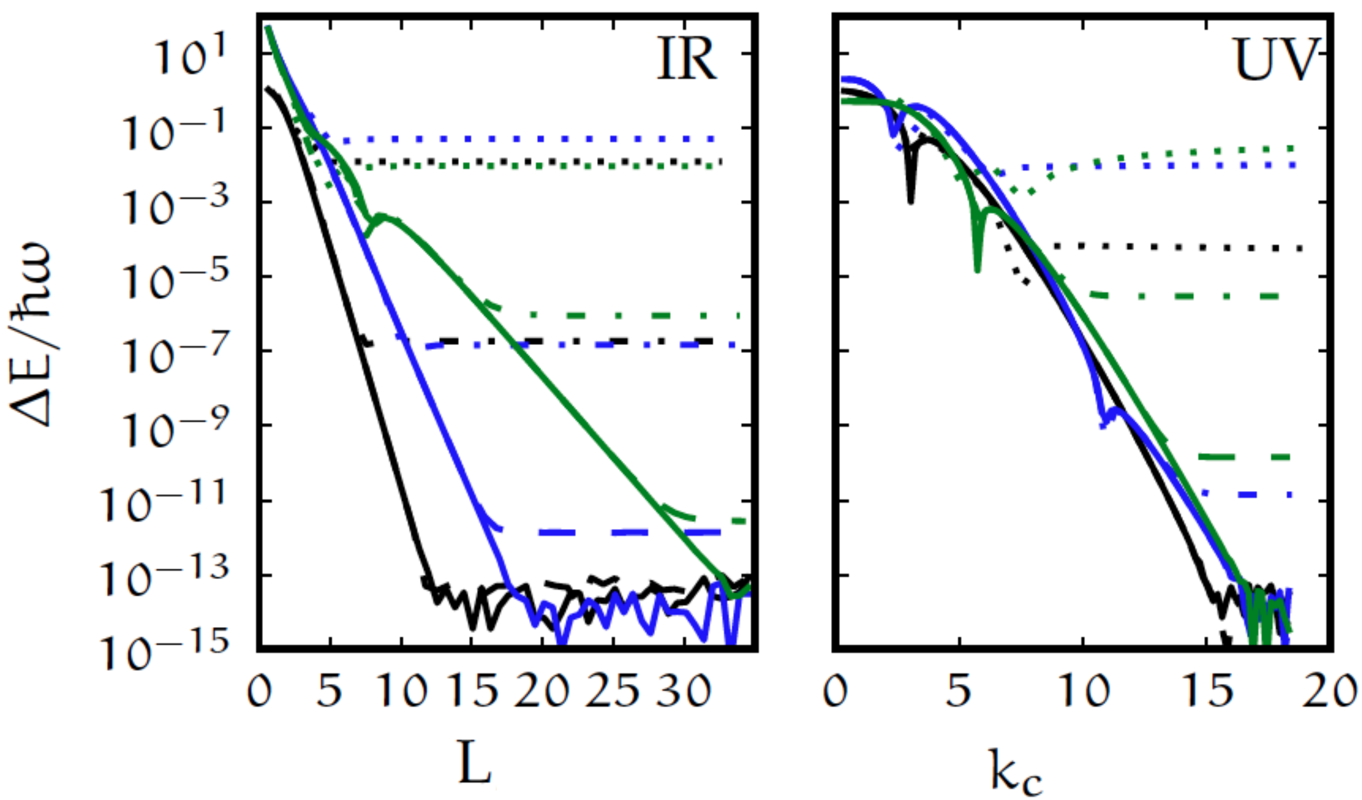
- Minimum momentum associated with inverse rms radius of highest single-particle state

$$\lambda_{sc} = \sqrt{m_N\hbar\omega/(N+3/2)}$$

Exponential convergence

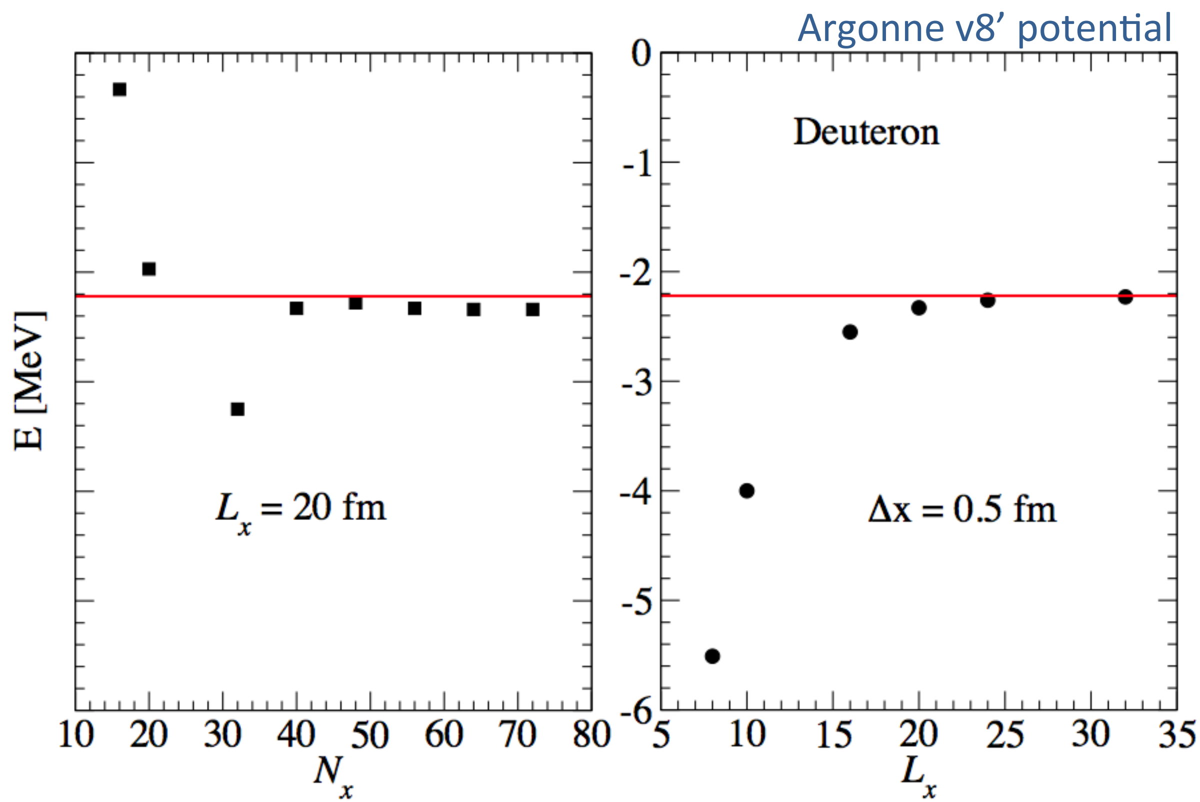
- For appropriate basis functions and boundary conditions
- Example (analytically solvable): $V(x) = \dfrac{a + b\sinh(x)}{\cosh^2(x)}$

A. Bulgac & M. M. Forbes, PRC 2013



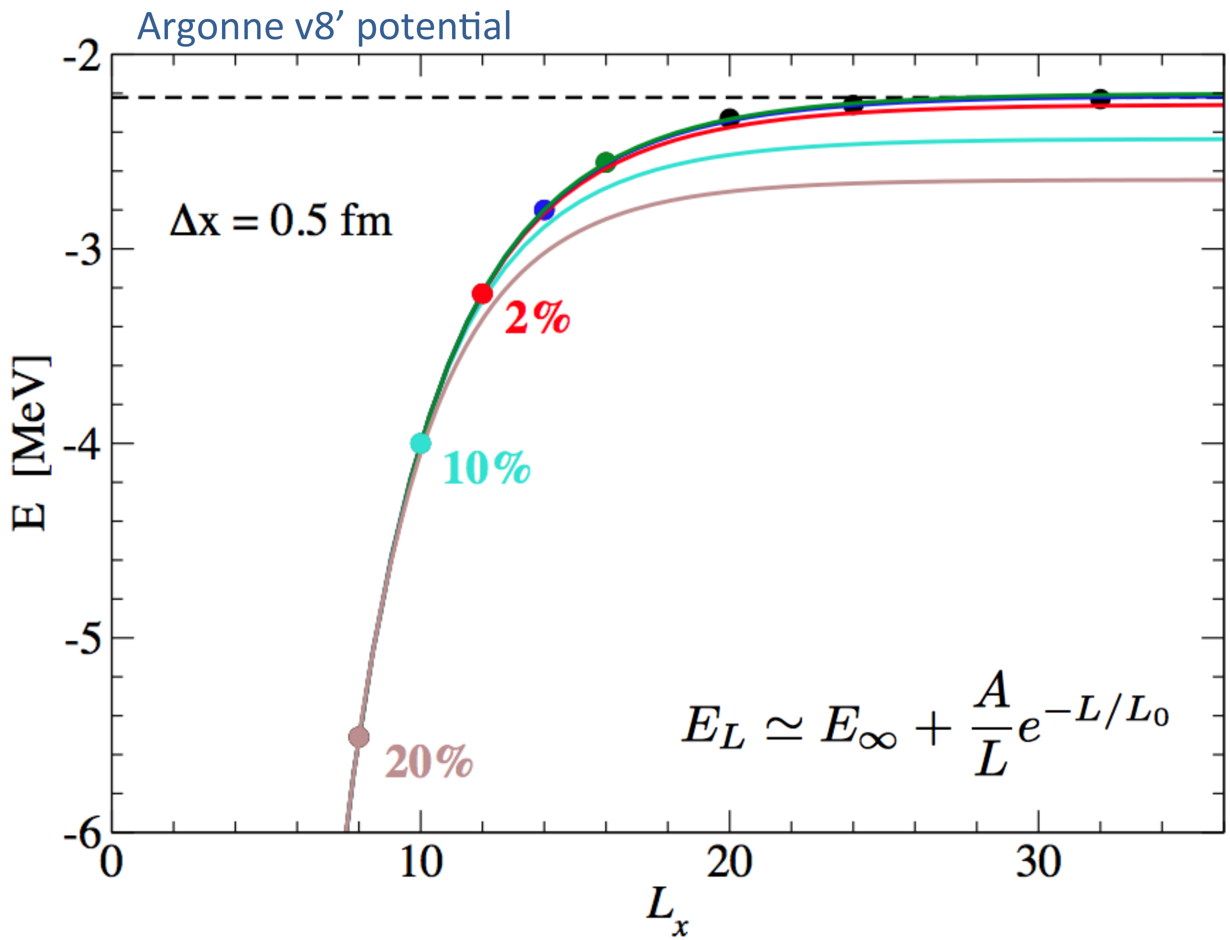
Convergence of deuteron (realistic NN potential)

- Solve Schrödinger equation in 3D (no partial-wave decomposition)



- Argonne potential requires resolution scale of $\Delta x = 0.5\ \mathrm{fm}$
- Chiral potentials should have significantly better UV convergence properties

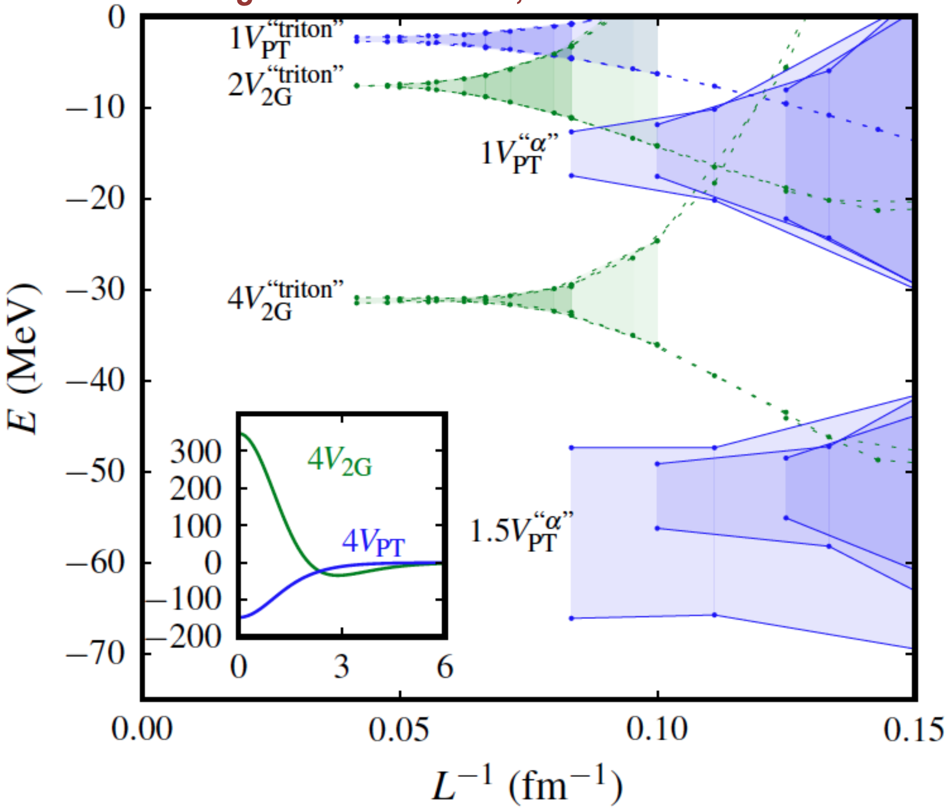
Finite-volume corrections to energy



- Exponential convergence [S. Beane et al., PLB 2004] [S. Kreuzer & H.-W. Hammer, PLB 2011]

Application to “light nuclei”

A. Bulgac & M. M. Forbes, PRC 2013



- Distinguishable spinless particles
- Lowest energies from Lanczos

$$a = 0.5 - 1.5\,\mathrm{fm}$$

$$\Lambda_{UV} = 400 - 1200\,\mathrm{MeV}$$

- “Triton”: $N^6 = 8^6 - 16^6$

  Up to 10^7 elements in Hilbert space

- “Alpha”: $N^9 = 4^9 - 8^9$

  Up to 10^8 elements in Hilbert space

Neutron matter from quantum Monte Carlo

Nuclear ground states

- **Consider an arbitrary trial wavefunction:**

$$\psi(x_1, x_2, \ldots, x_n) = \sum_i c_i \overbrace{\phi_i(x_1, x_2, \ldots, x_n)}^{\text{Energy eigenstates}}$$

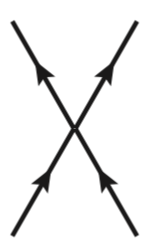
- **Propagate system in imaginary time:**

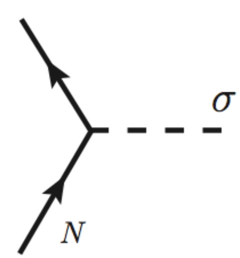
Hamiltonian $\hat{H} = \hat{T} + \hat{V}_{2N} + \cdots$

Imaginary-time evolution operator $\hat{U}(\tau) = e^{-\hat{H}\tau}$

(filter out ground state) $$e^{-\hat{H}\tau}|\psi\rangle = \sum_i c_i e^{-E_i \tau}|\phi_i\rangle \xrightarrow{\tau \to \infty} |\phi_0\rangle$$

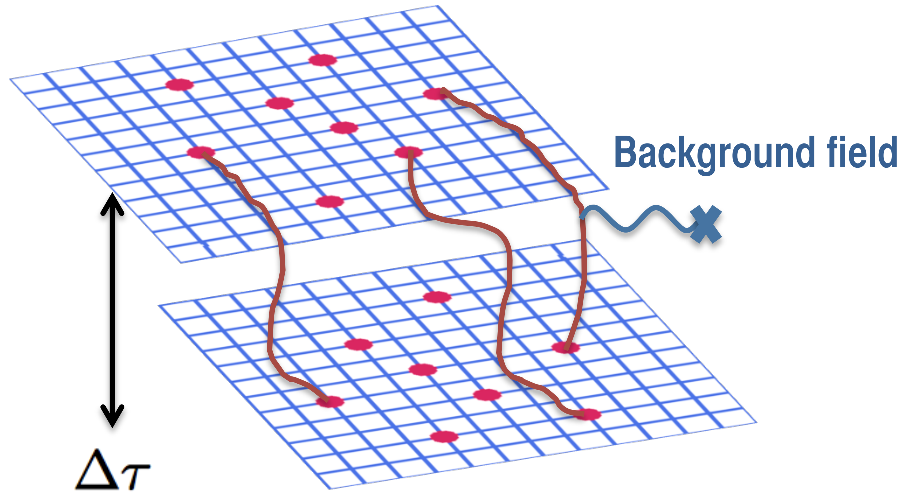
$$e^{-\frac{1}{2}A(\psi_N^\dagger \psi_N)^2} = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} d\sigma e^{-\frac{1}{2}\sigma^2 + \sqrt{-A}\sigma \psi_N^\dagger \psi_N}$$



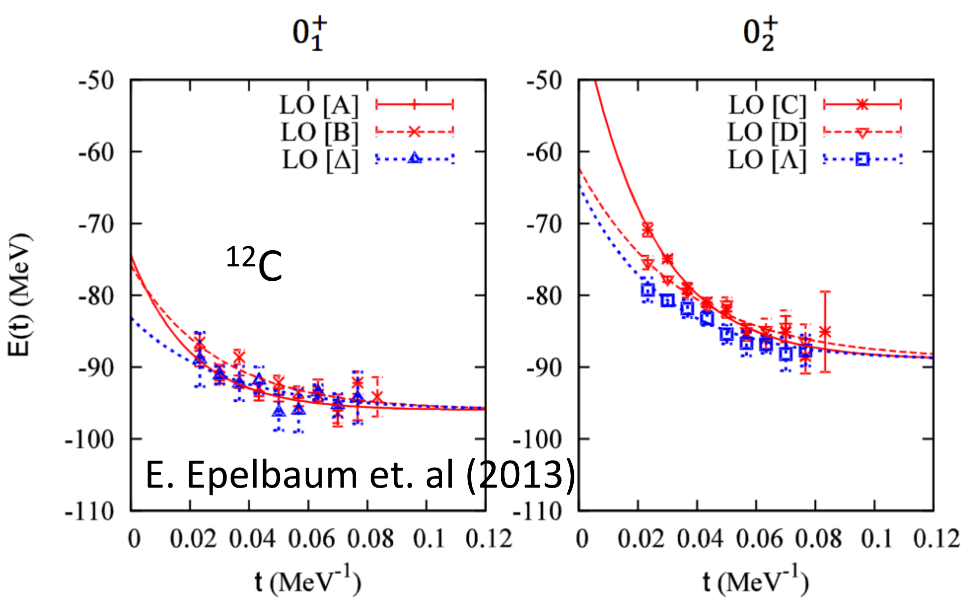


Monte Carlo evaluation

- Nucleons interact with **auxiliary background field**
- Propagate in small time steps
- Evaluate **stochastically** with **Monte Carlo methods**



- **Current implementations:** limited to light nuclei
- **But:** certain interactions exhibit **no sign problem**
- **Our (ambitious) goal:** simulate **several hundred nucleons**



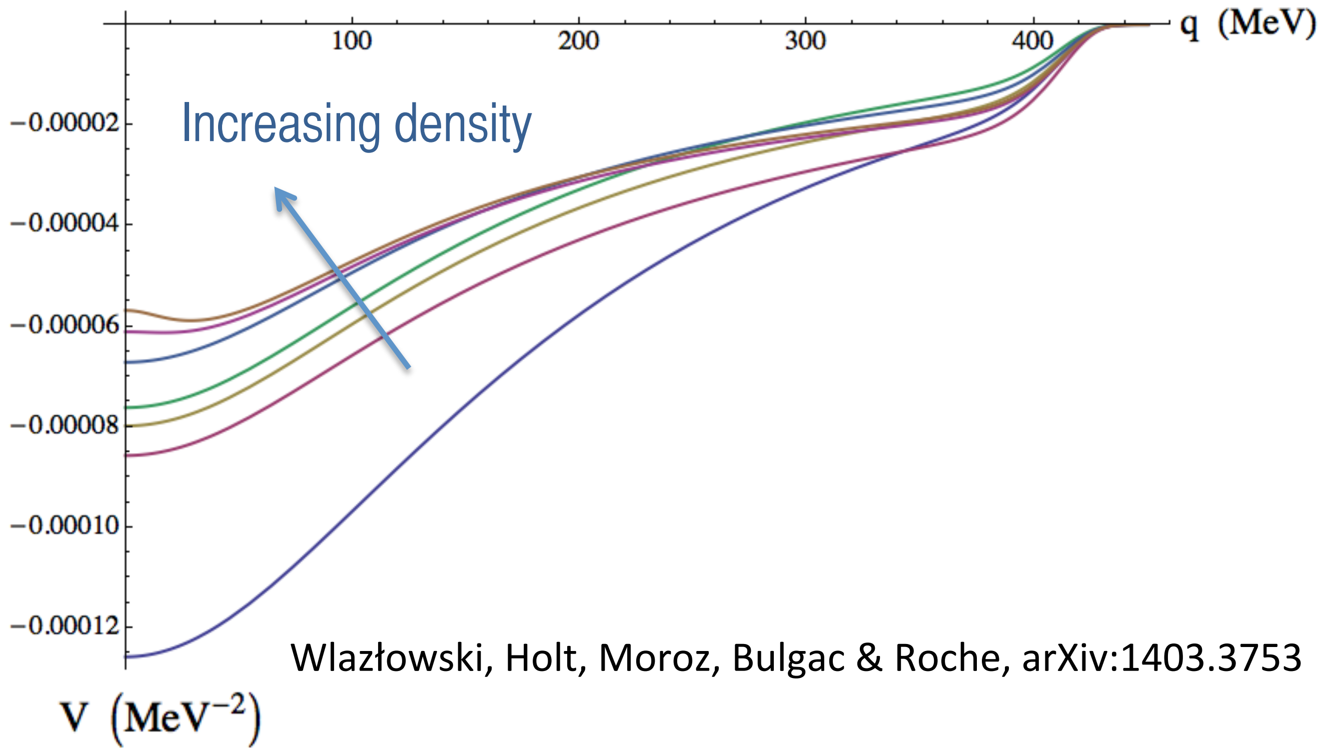
Evolution potential

Chiral N3LO 2N interaction + N2LO 3N interaction

$$H = T + V_\chi = (T + V_{\rm ev}) + (V_\chi - V_{\rm ev})$$

$$V_{\rm ev}(q^2) = \frac{V_\pi}{m_\pi^2 + q^2} + \boxed{\frac{V_\sigma}{m_\sigma^2 + q^2} + \frac{V_\omega}{m_\omega^2 + q^2}}$$

(Constrained by phase shifts and perturbative equation of state)



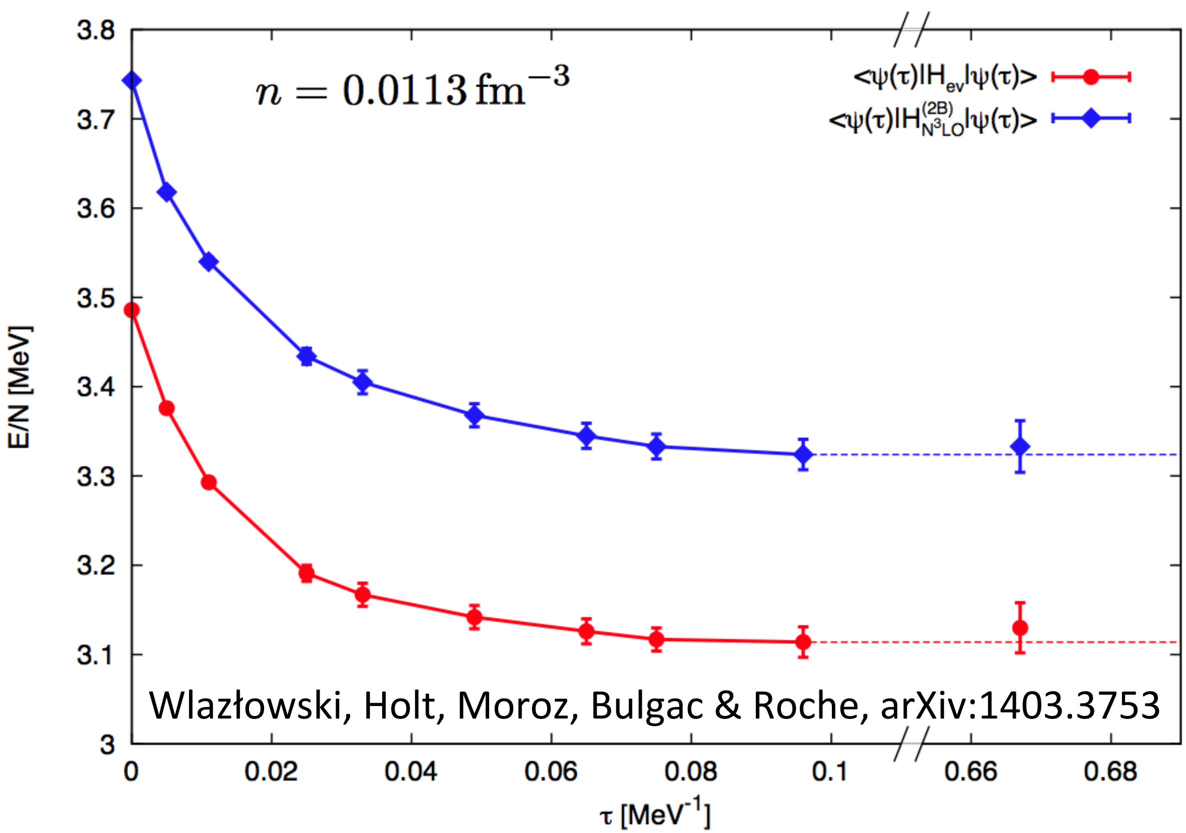
Wlazłowski, Holt, Moroz, Bulgac & Roche, arXiv:1403.3753

Imaginary-time evolution

\# Neutrons: **38 to 342**

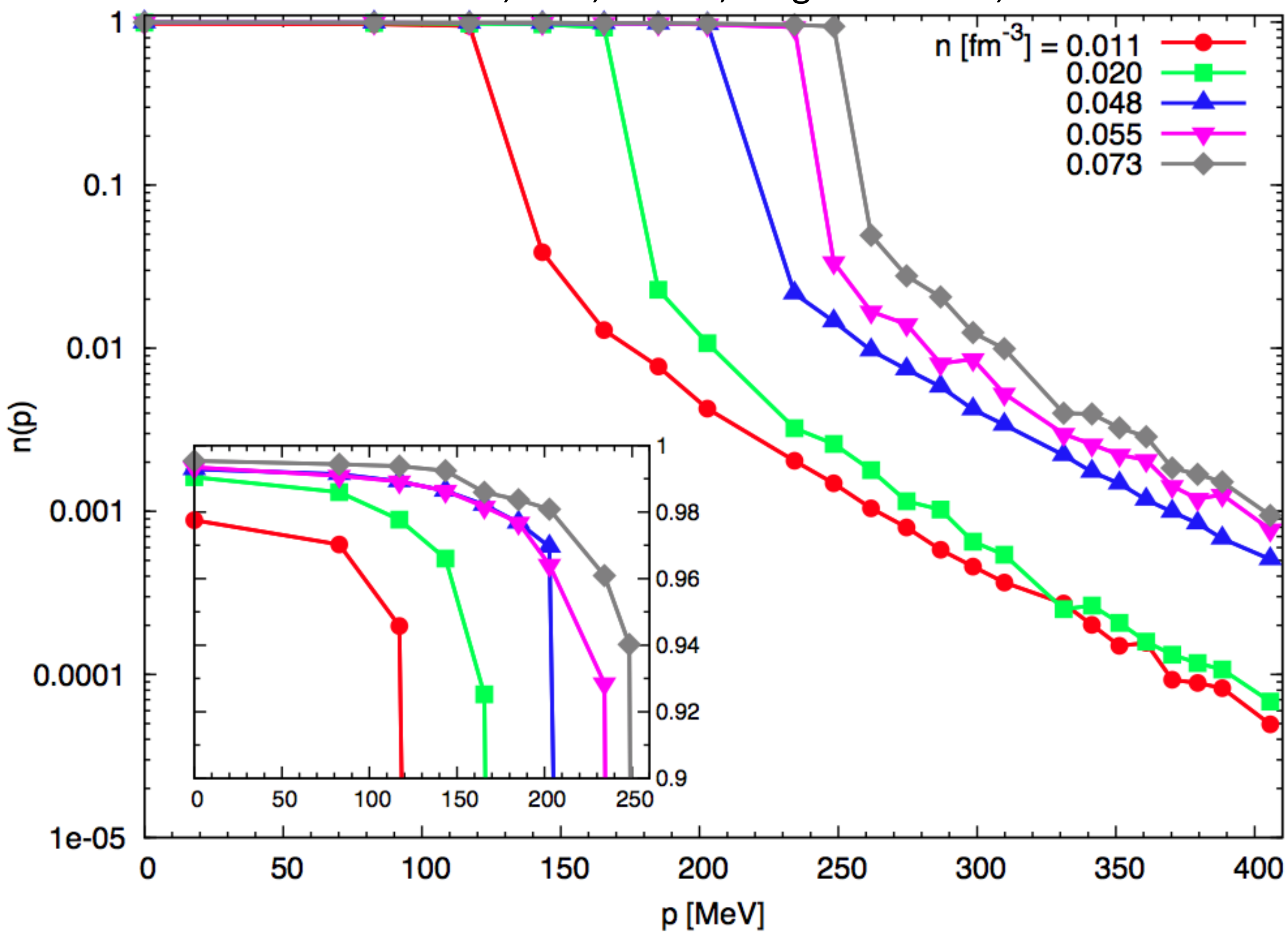
10^3 Lattice

$\Delta x = 1.5\,\mathrm{fm} \to \Lambda = 414\,\mathrm{MeV}$

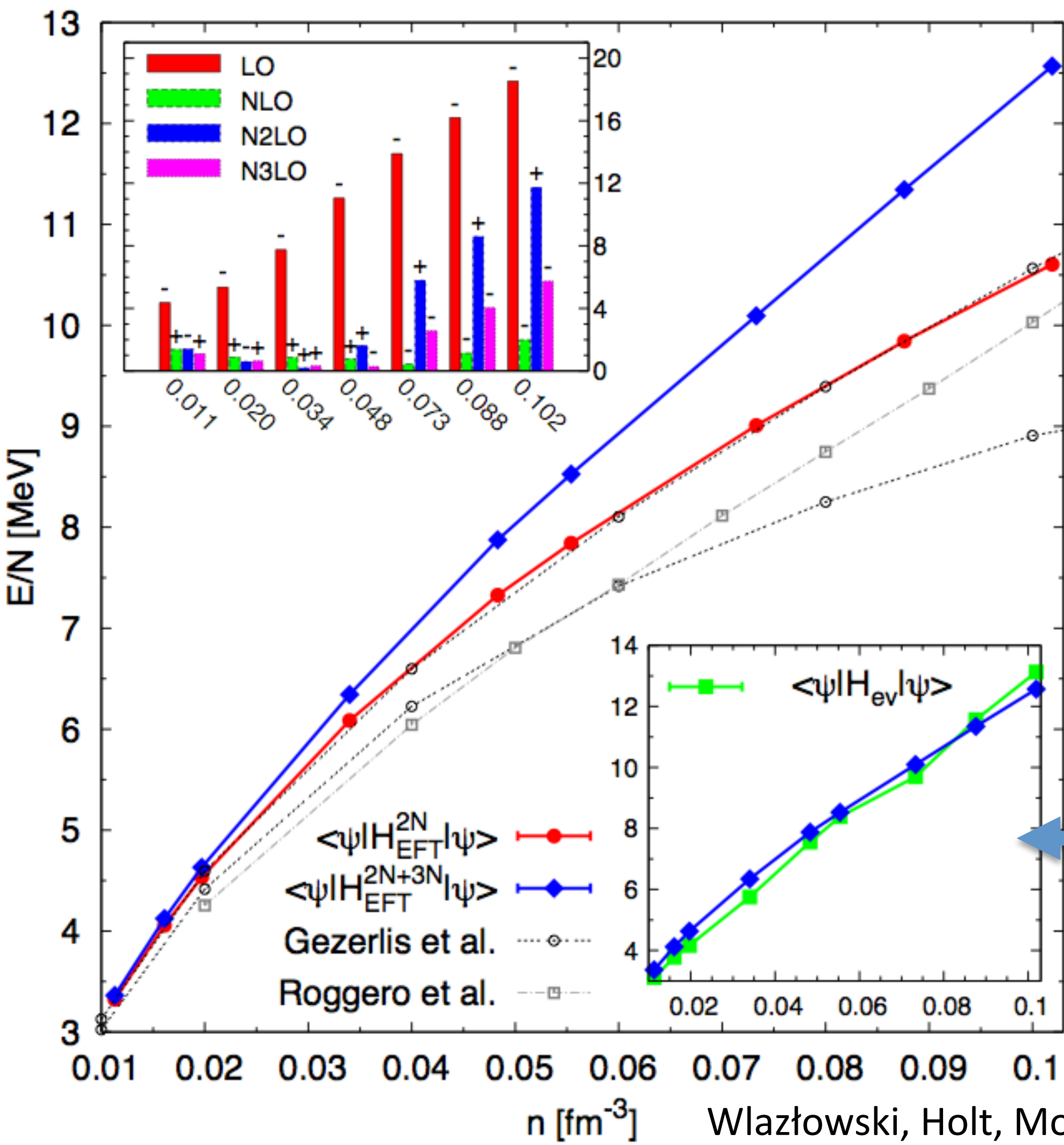


Occupation probabilities

Wlazłowski, Holt, Moroz, Bulgac & Roche, arXiv:1403.3753



Neutron matter equation of state



- Two-nucleon forces at N3LO
- Three-nucleon forces at N2LO *(still inconsistent, but N3LO next step)*
- **Compare:** *Gezerlis et al.*, *Roggero et al.* two-body forces at N2LO

Chiral EOS matches non-perturbative EOS of H_{ev}

Wlazłowski, Holt, Moroz, Bulgac & Roche, arXiv:1403.3753

Summary

Consistency at N3LO: three- and four-body forces currently a challenge

Lattice techniques a promising path forward: formally developed in the framework of the discrete variable representation (DVR) basis

Compatible low-momentum chiral NN interactions: Improved convergence in perturbation theory (and finite model-space calculations)

Simple IR and UV convergence properties

Light nuclei and nuclear matter:

(1) Direct diagonalization (Lanczos) for light nuclei

(2) Auxiliary-field quantum Monte Carlo for neutron matter and finite nuclei