Applications of Lattice Effective Field Theory to Nuclear Forces and Structure

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Nuclear Theory in the Supercomputing Era
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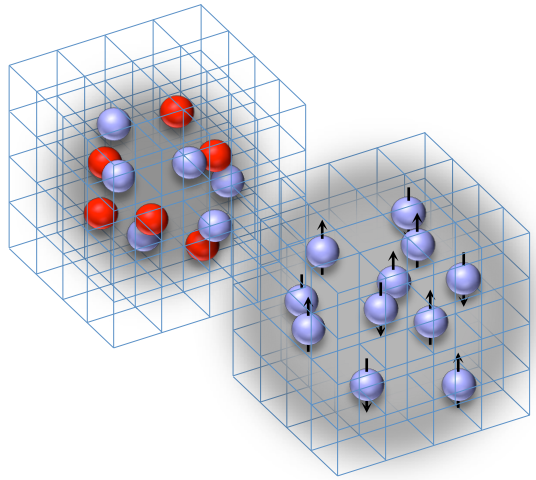

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Study of Strongly Interacting Matter HadronPhysics
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Outline

Lattice effective field theory

Improved short-range interactions

Nuclear forces and nuclear structure

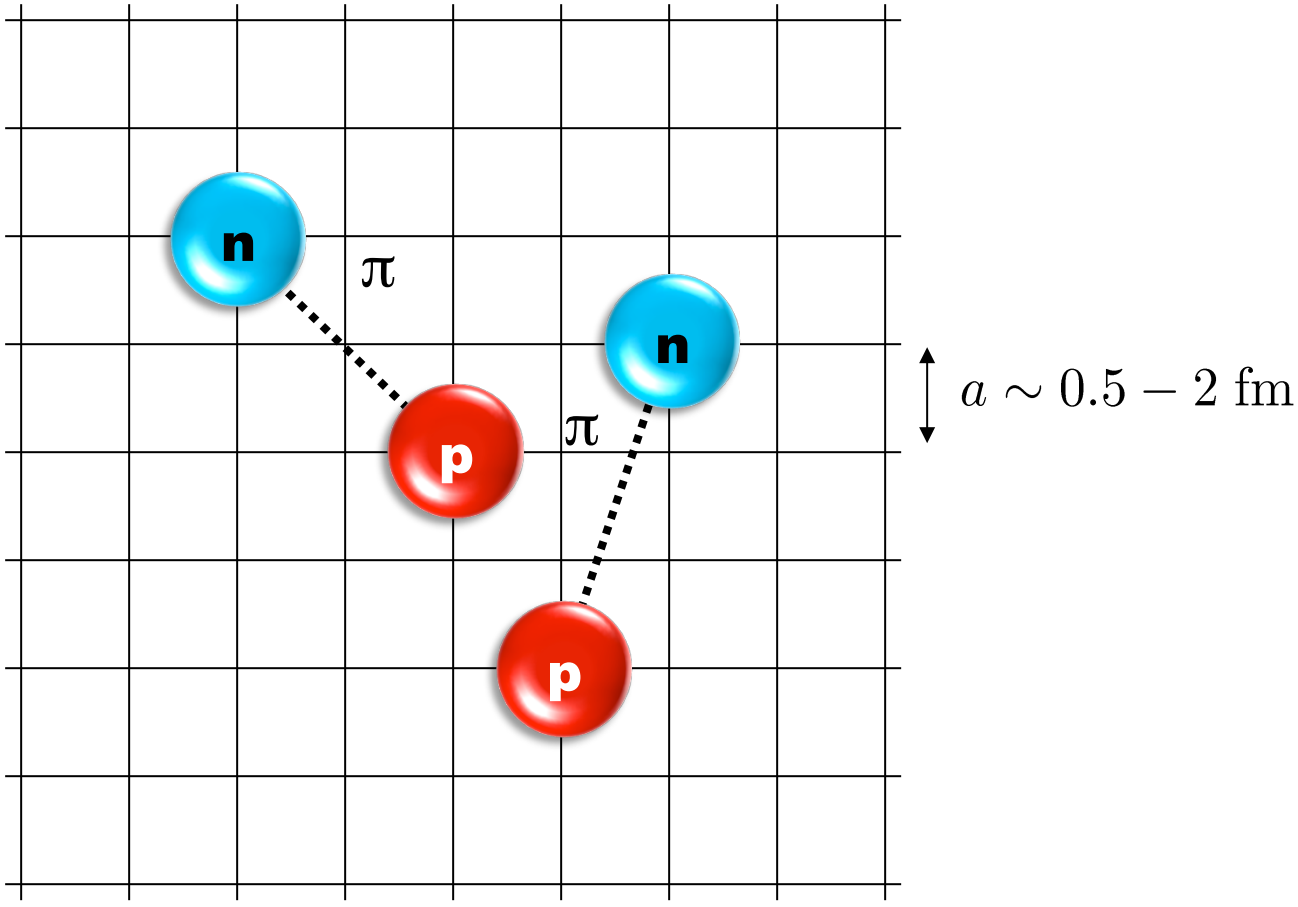
Nuclear thermodynamics using pinholes

Eigenvector continuation

Superfluidity and pairing correlations

Summary and outlook

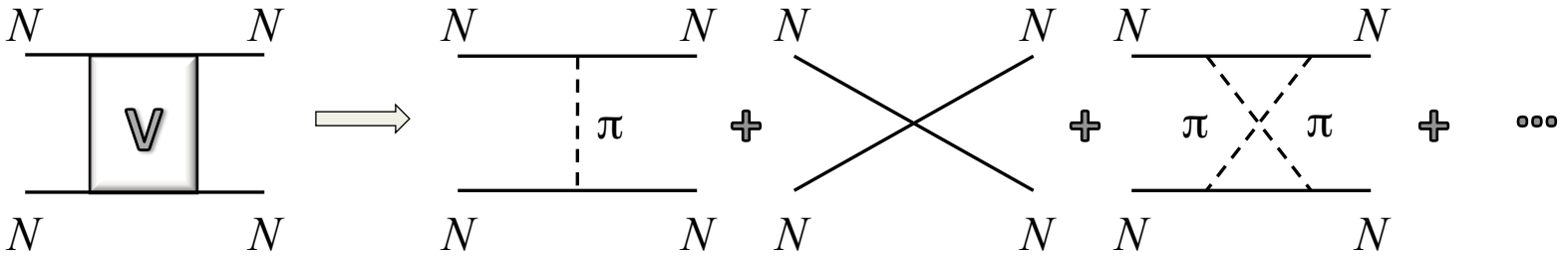
Lattice effective field theory



Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)
TALENT summer school lectures: qmc2016.wordpress.ncsu.edu

Chiral effective field theory

Construct the effective potential order by order



V^{OPEP} Contact interactions V^{TPEP}

Leading order (LO) Next-to-leading order (NLO)

Improved short-range lattice operators

We define the smeared annhilation and creation operators. This procedure gives us better rotational symmetry properties when taking spatial derivatives as finite differences.

$$a_{i,j}^{s_{\rm NL}}(\mathbf{n}) = a_{i,j}(\mathbf{n}) + s_{\rm NL} \sum_{|\mathbf{n}'|=1} a_{i,j}(\mathbf{n}+\mathbf{n}')$$

$$a_{i,j}^{s_{\rm NL}\dagger}(\mathbf{n}) = a_{i,j}^{\dagger}(\mathbf{n}) + s_{\rm NL} \sum_{|\mathbf{n}'|=1} a_{i,j}^{\dagger}(\mathbf{n}+\mathbf{n}')$$

Next we form bilinear functions of the annihilation operators with spin and isospin quantum numbers S, S_z, I, I_z.

$$[a(\mathbf{n})a(\mathbf{n}')]^{s_{\rm NL}}_{S,S_z,I,I_z} = \sum_{i,j,i',j'} a_{i,j}^{s_{\rm NL}}(\mathbf{n}) M_{ii'}(S,S_z) M_{jj'}(I,I_z) a_{i',j'}^{s_{\rm NL}}(\mathbf{n}')$$

Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

We put in orbital angular momentum using solid spherical harmonics

$$R_{L,L_z}(\mathbf{r}) = \sqrt{\frac{4\pi}{2L+1}} r^L Y_{L,L_z}(\theta,\phi),$$

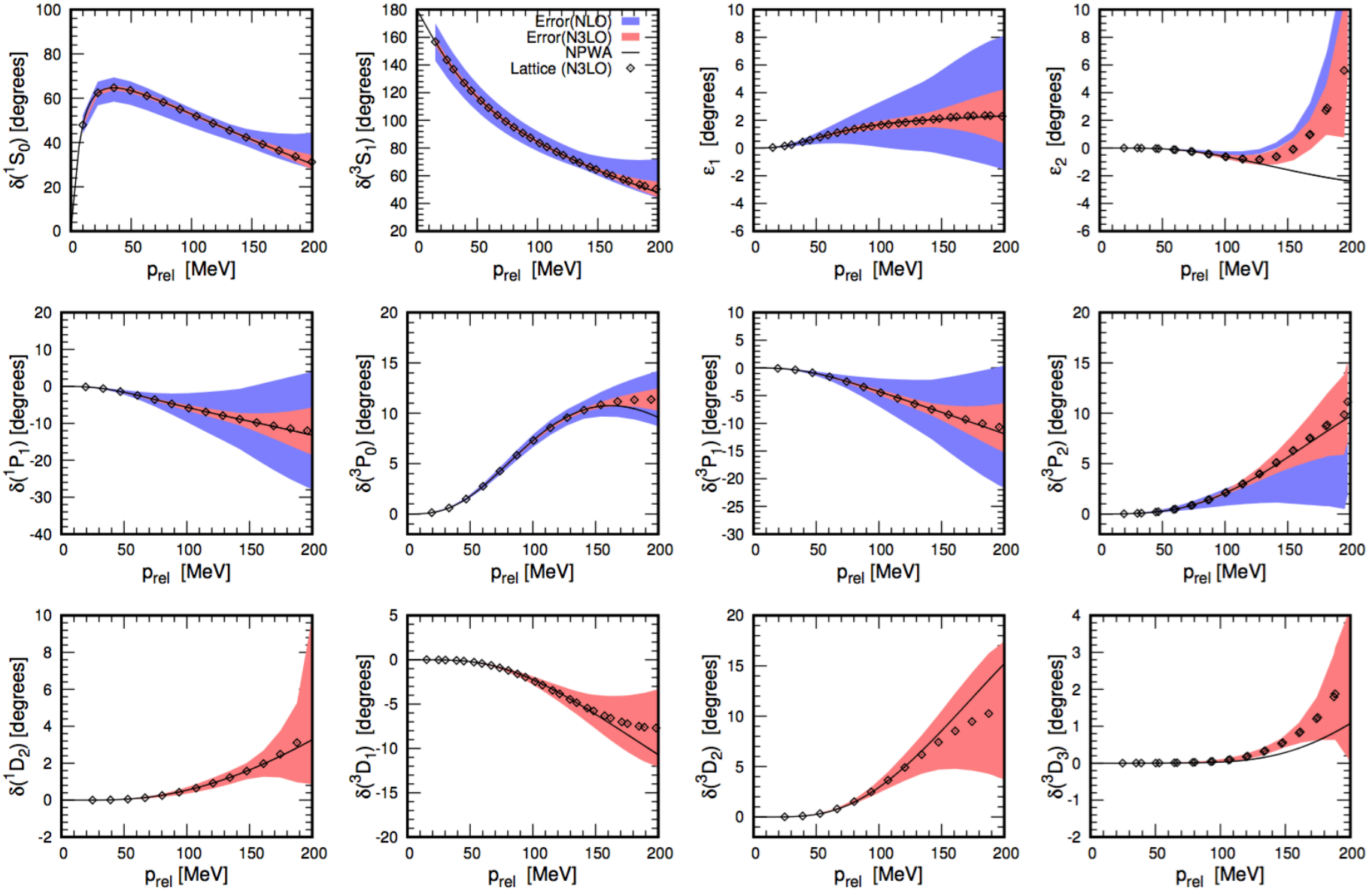
that are written as functions of the lattice derivatives on one of the annihilation operators

$$P^{2M,s_{\rm NL}}_{S,S_z,L,L_z,I,I_z}(\mathbf{n}) = [a(\mathbf{n})\nabla^{2M}_{1/2} R^*_{L,L_z}(\nabla) a(\mathbf{n})]^{s_{\rm NL}}_{S,S_z,I,I_z}$$

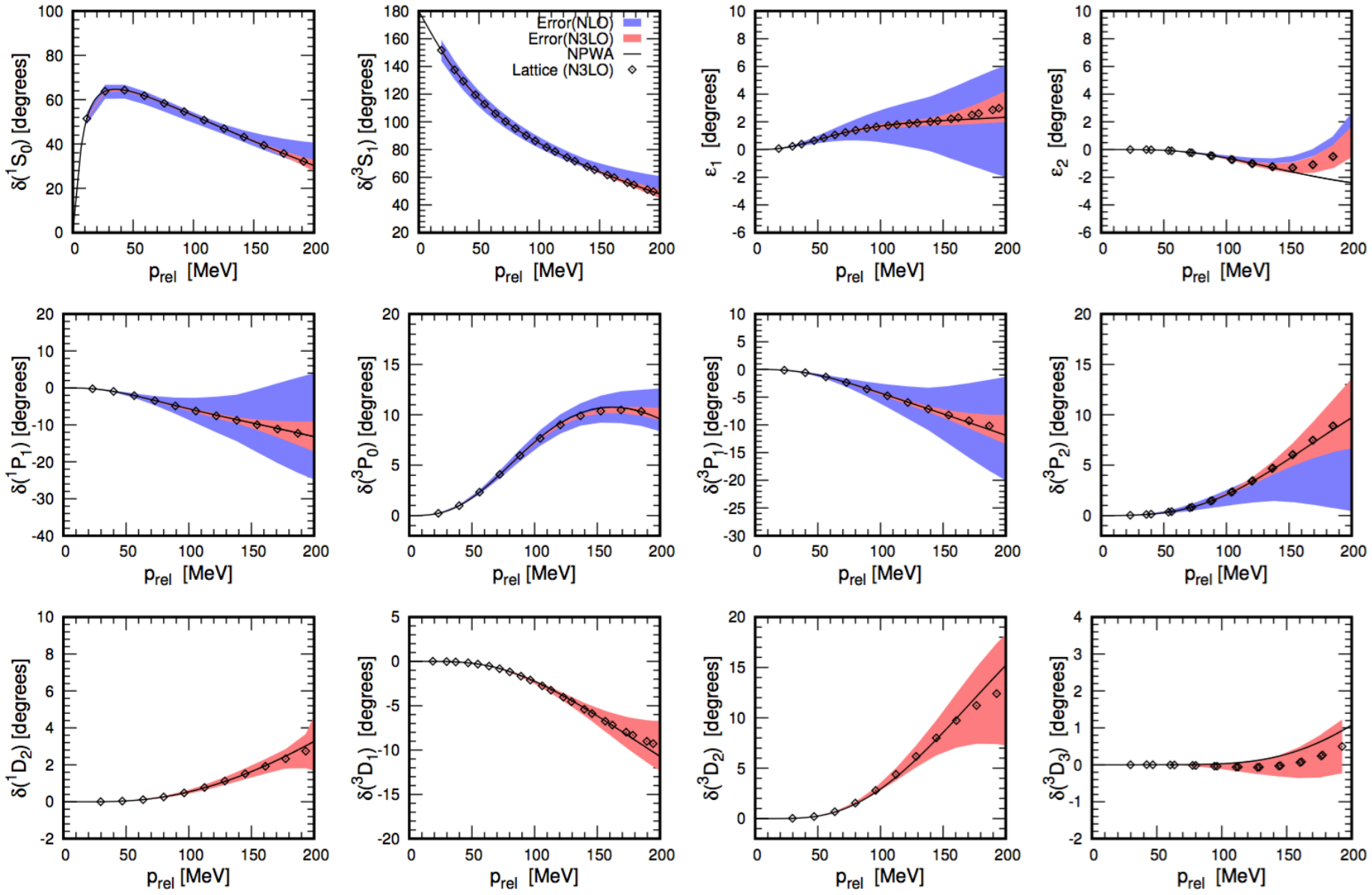
We then project onto the selected spin and orbital angular momentum using Clebsch-Gordan coefficients

$$O^{2M,s_{NL}}_{S,L,J,J_z,I,I_z}(\mathbf{n}) = \sum_{S_z,L_z} \langle SS_z LL_z | JJ_z \rangle P^{2M,s_{NL}}_{S,S_z,L,L_z,I,I_z}(\mathbf{n})$$

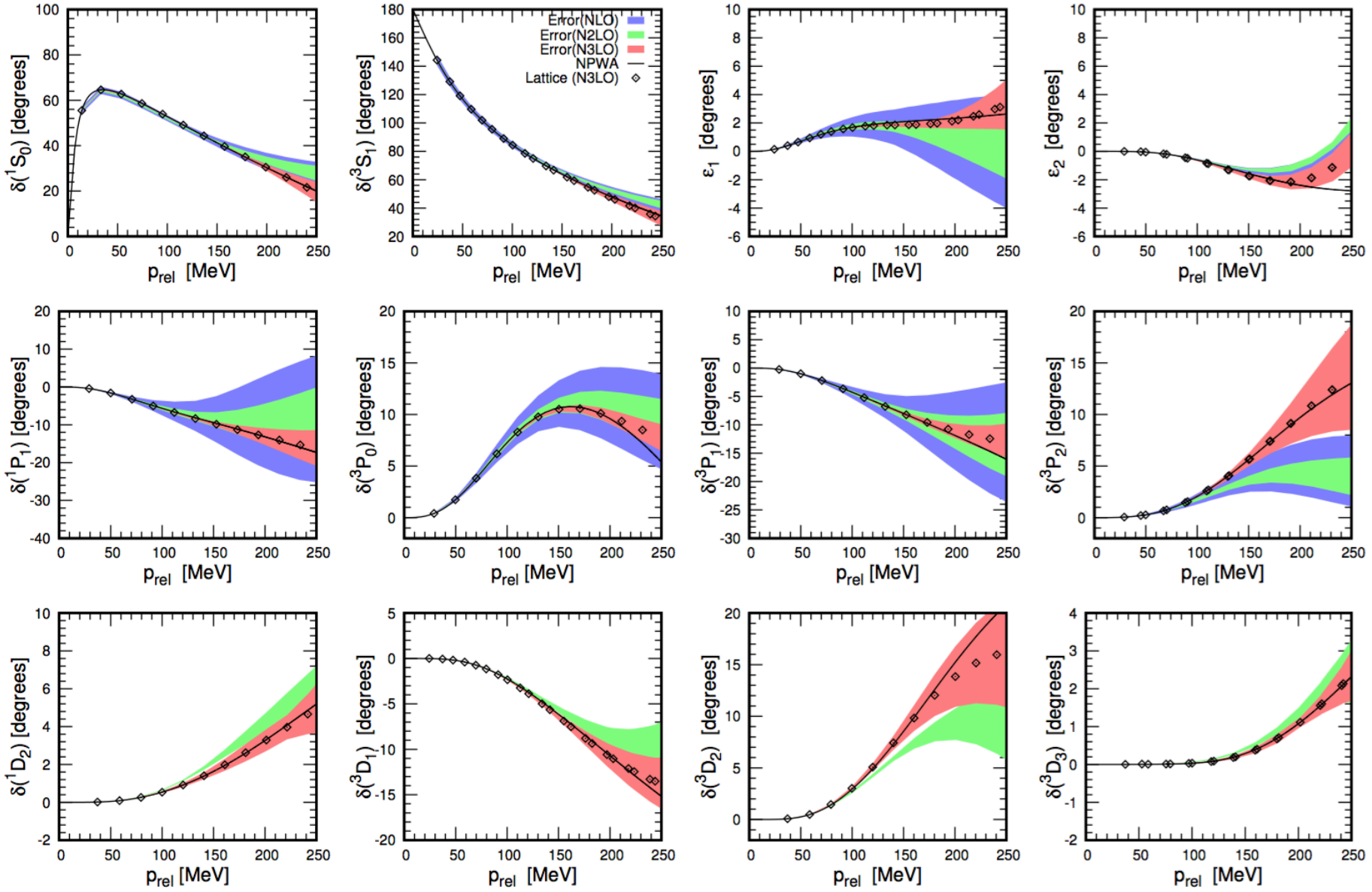
$a = 1.973\,\mathrm{fm}$



$a = 1.644\,\mathrm{fm}$



$a = 1.315\,\mathrm{fm}$



$a = 0.987\,\mathrm{fm}$

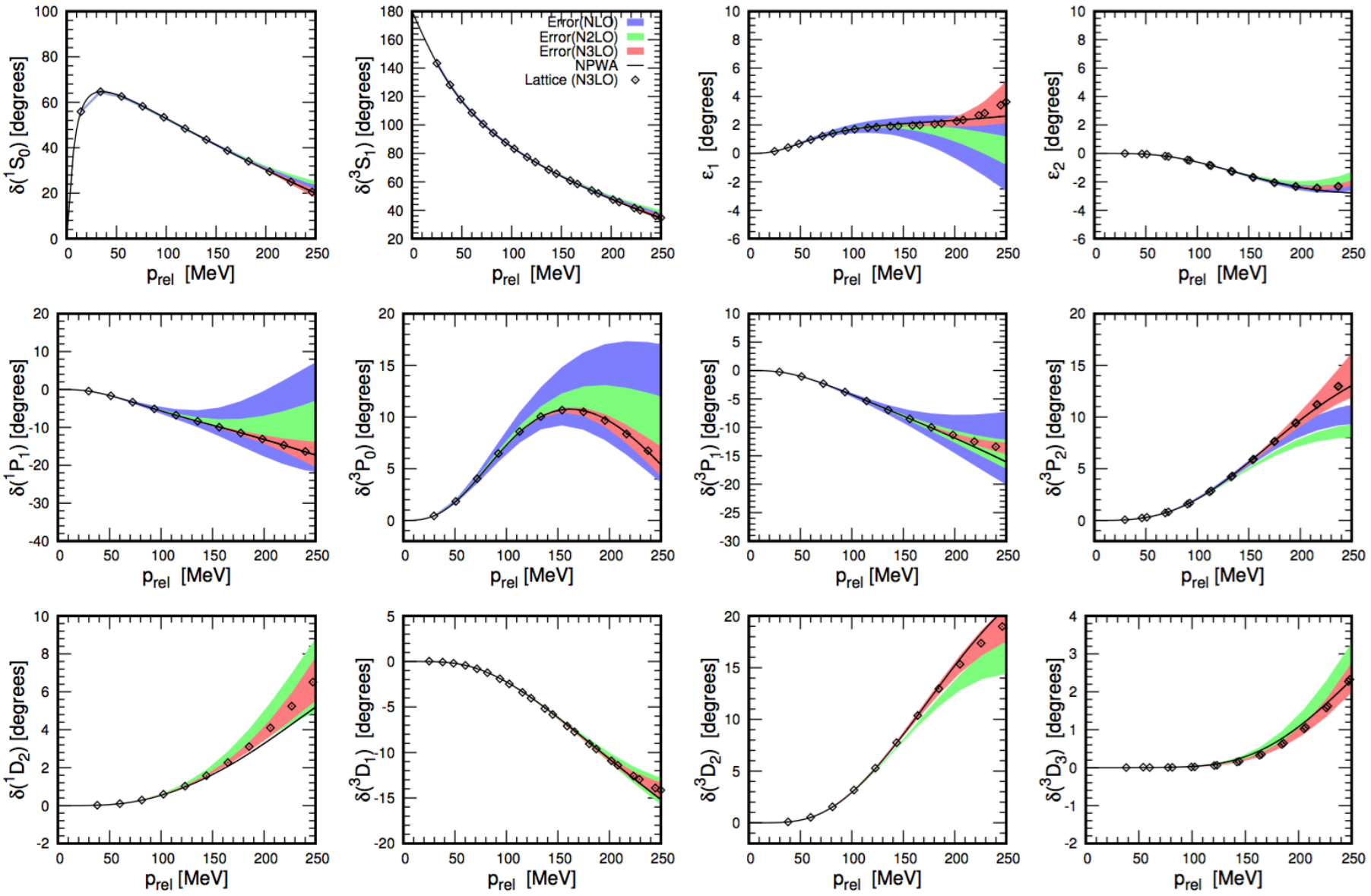
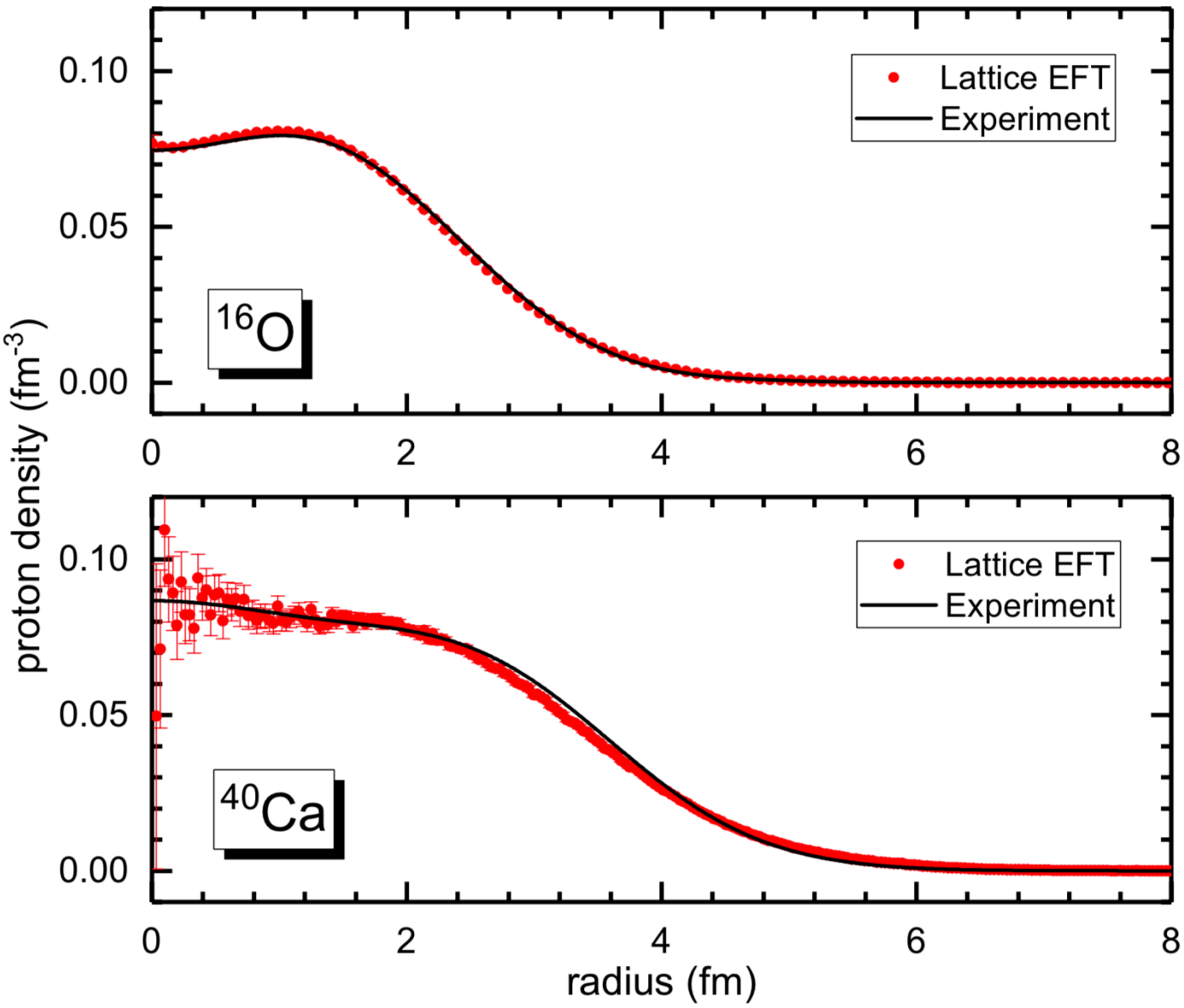


TABLE II. The deuteron properties and S-wave parameters calculated with the full NN interaction up to chiral order $O(Q^4)$ using $a = 0.99$ fm. The error bars we quote in this table indicate uncertainties from the fitting procedure only.

	LO	NLO	N^{2}LO	N^{3}LO	Empirical
E_d (MeV)	2.2246 ± 0.0002	2.224575 ± 0.000016	2.224575 ± 0.000025	2.224575 ± 0.000011	2.224575(9)[24]
$A_s(\mathrm{fm}^{-1/2})$	0.8662 ± 0.0007	0.8772 ± 0.0003	0.8777 ± 0.0004	0.8785 ± 0.0004	0.8846(9)[25]
η	0.0212 ± 0.0000	0.0258 ± 0.0001	0.0257 ± 0.0002	0.0254 ± 0.0001	0.0256(4) [26]
$Q_d(\mathrm{fm}^2)$	0.2134 ± 0.00000	0.2641 ± 0.0016	0.2623 ± 0.0023	0.2597 ± 0.0013	0.2859(3) [27]
r_d (fm)	1.9660 ± 0.0001	1.9548 ± 0.0005	1.9555 ± 0.0008	1.9545 ± 0.0005	1.97535(85) [28]
$a_{^3S_1}$	5.461 ± 0.000	5.415 ± 0.001	5.421 ± 0.002	5.417 ± 0.001	5.424(4) [29]
$r_{^3S_1}$	1.831 ± 0.0003	1.759 ± 0.002	1.760 ± 0.003	1.758 ± 0.002	1.759(5)[29]
$a_{^1S_0}$	-23.8 ± 0.1	-23.69 ± 0.05	-23.8 ± 0.2	-23.678 ± 0.038	−23.748(10)[29]
$r_{^1S_0}$	2.666 ± 0.001	2.647 ± 0.003	2.69 ± 0.02	2.647 ± 0.004	2.75(5) [29]

Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

	E (MeV)	exp.	R_{ch} (fm)	exp.
^{3}H	−8.47	−8.48	1.90	1.76
^{4}He	−28.3	−28.3	1.72	1.68
^{16}O	−118.4	−127.6	2.74	2.70
^{20}Ne	−157.5	−160.6	2.95	3.01
^{24}Mg	−194.7	−198.3	3.13	3.06
^{28}Si	−231.1	−236.5	3.26	3.12
^{40}Ca	−334.9	−342.1	3.42	3.48



Courtesy: Bing-nan Lu

Nuclear thermodynamics using pinholes

In order to compute thermodynamic properties of finite nuclei, nuclear matter, and neutron matter, we need to compute the partition function

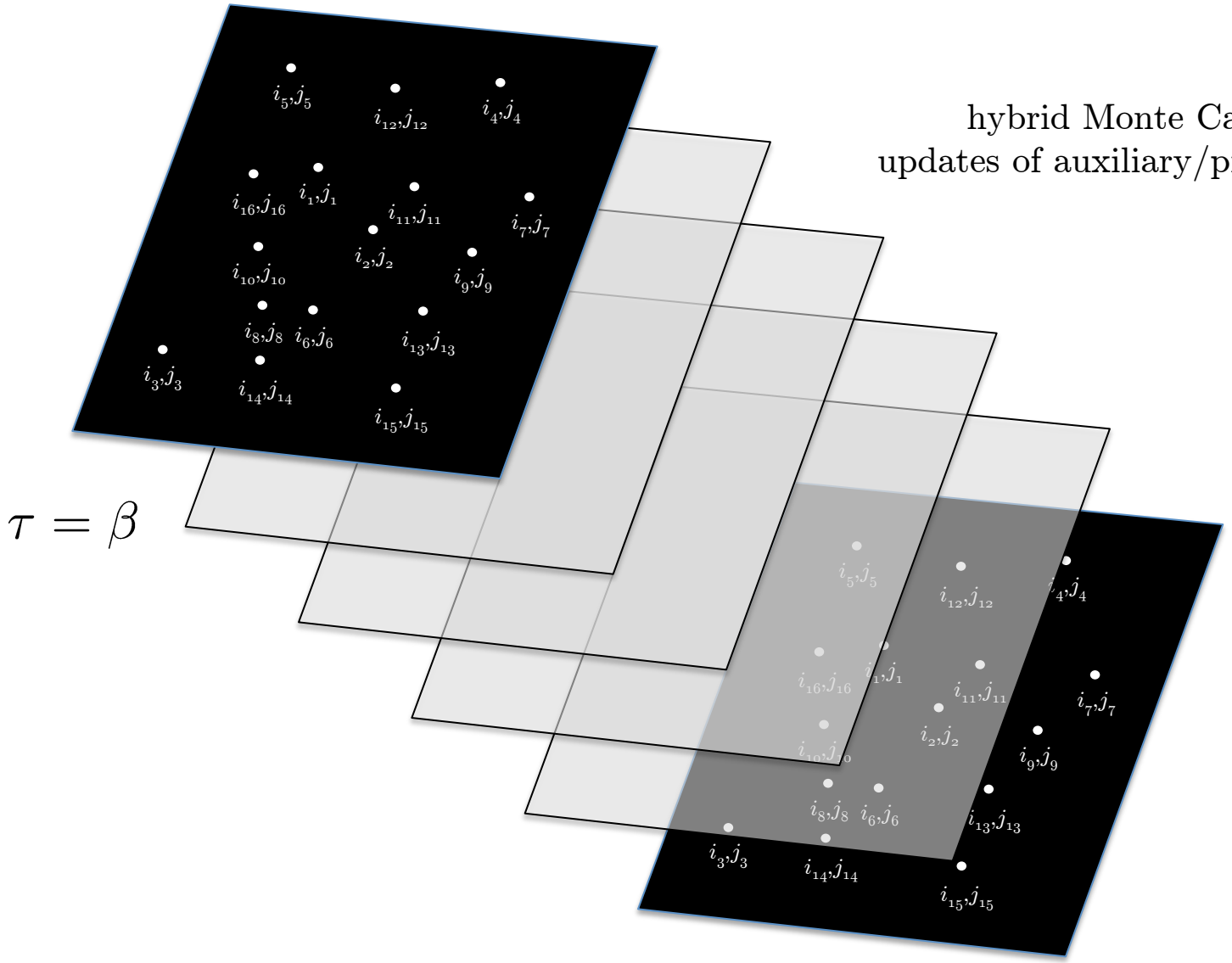
$$\mathrm{Tr}\exp(-\beta H)$$

We compute the quantum mechanical trace over A-nucleon states by summing over pinholes (position eigenstates) for the initial and final states

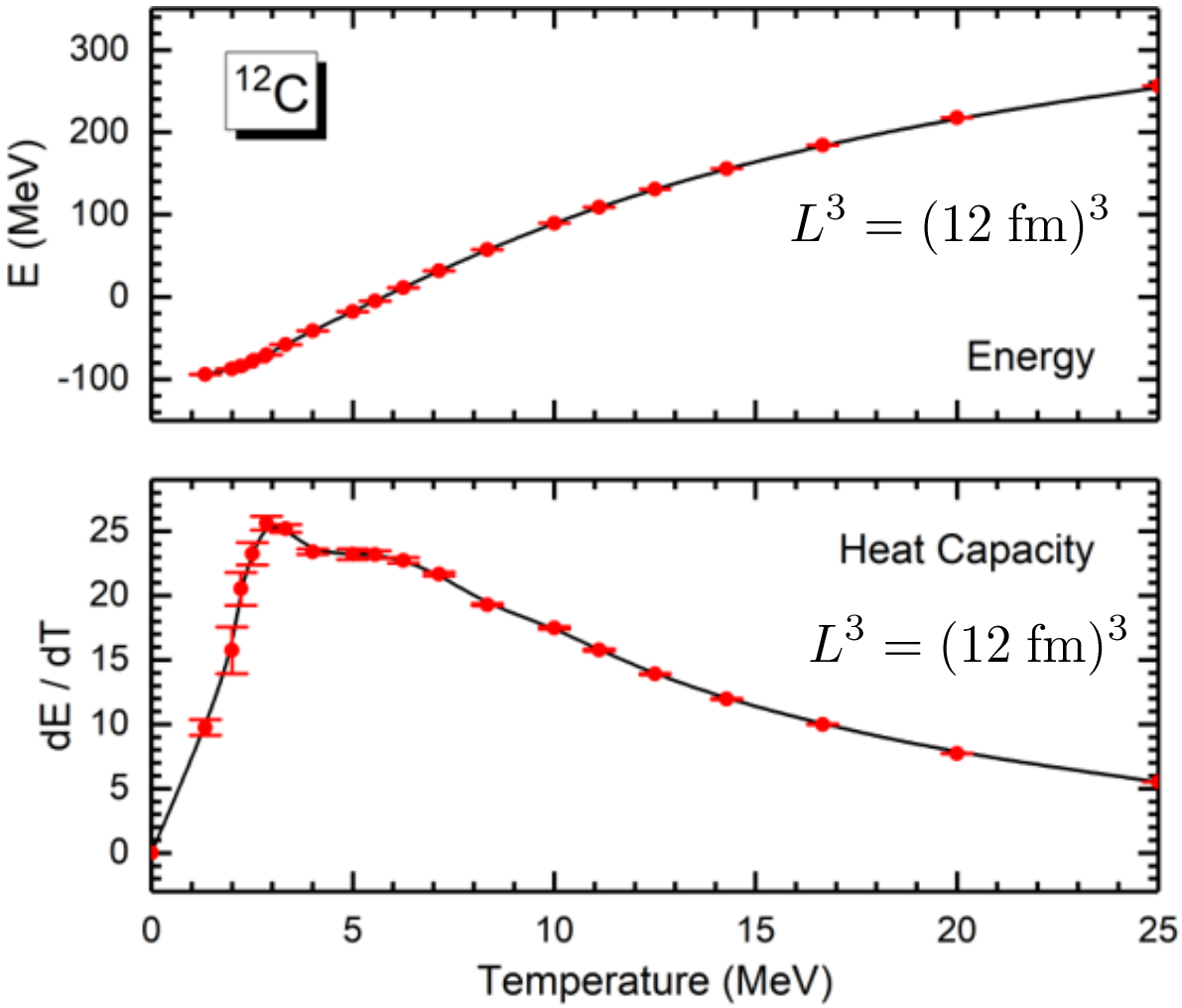
$$\mathrm{Tr}\, O = \frac{1}{A!}\sum_{i_1\cdots i_A, j_1\cdots j_A, \mathbf{n}_1\cdots\mathbf{n}_A} \langle 0|a_{i_A,j_A}(\mathbf{n}_A)\cdots a_{i_1,j_1}(\mathbf{n}_1)\, O\, a^\dagger_{i_1,j_1}(\mathbf{n}_1)\cdots a^\dagger_{i_A,j_A}(\mathbf{n}_A)|0\rangle$$

This can be used to calculate the partition function in the canonical ensemble.

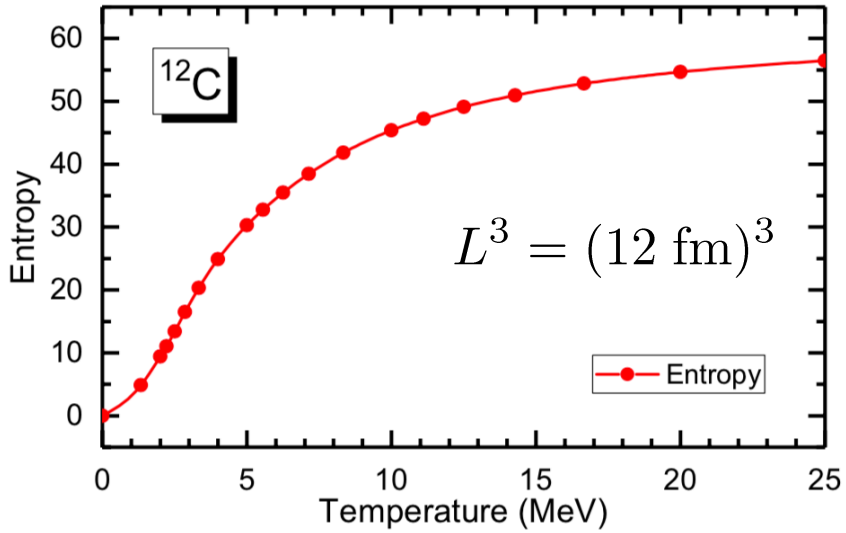
Metropolis updates of pinholes



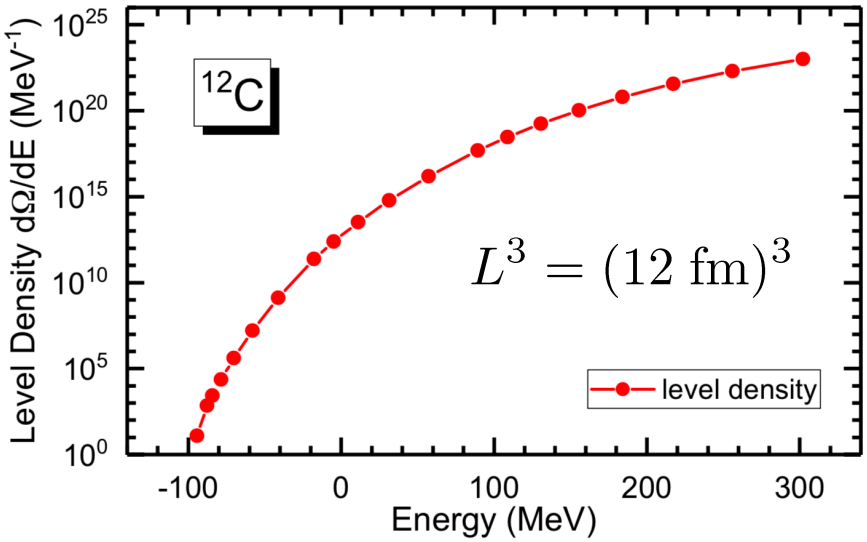
hybrid Monte Carlo
updates of auxiliary/pion fields



Courtesy: Bing-Nan Lu

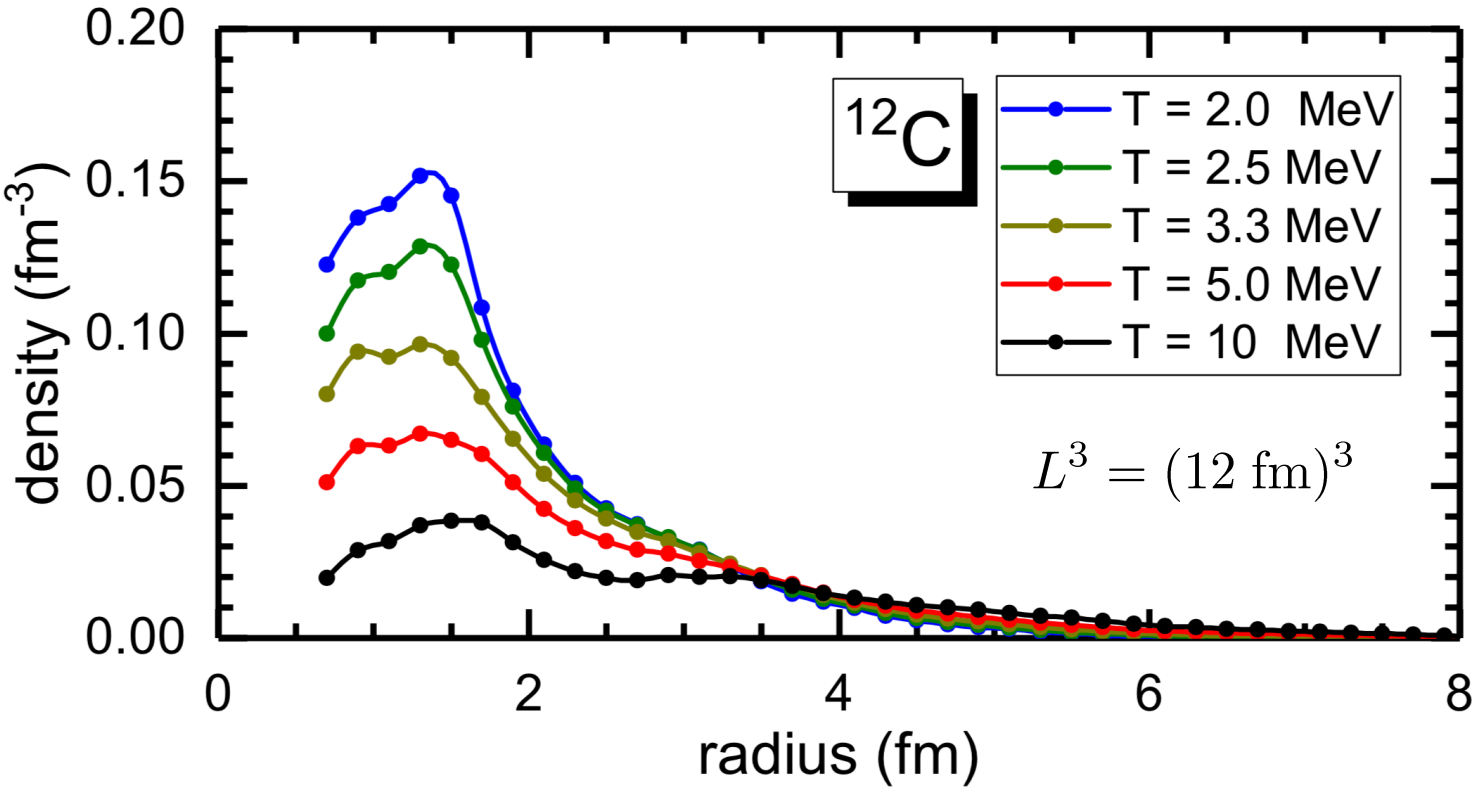


$$\text{Entropy} \quad S(T_0) = \int_0^{T_0} \frac{1}{T} dU$$

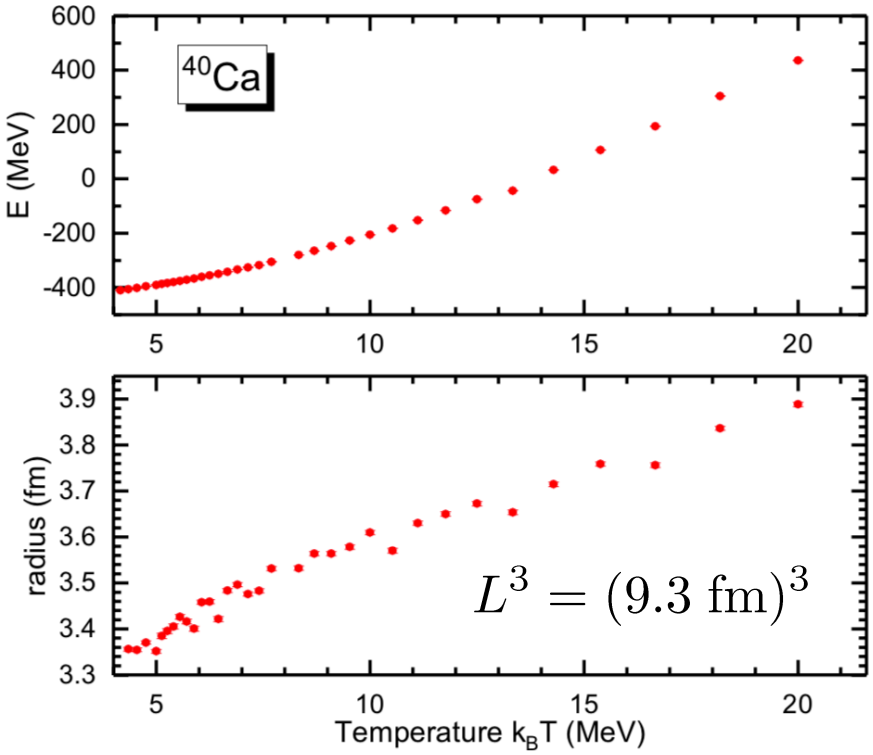


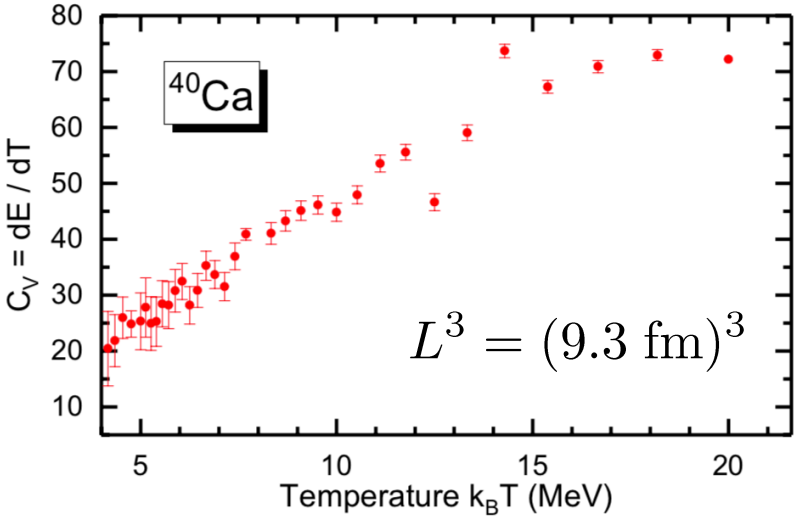
$$\text{Level Density} \quad \rho(E) = \frac{e^S}{\sqrt{2\pi C_V T}}$$

Courtesy: Bing-Nan Lu



Courtesy: Bing-Nan Lu





Courtesy: Bing-Nan Lu

Eigenvector continuation

We demonstrate that when a control parameter in the Hamiltonian matrix is varied smoothly, the extremal eigenvectors do not explore the large dimensionality of the linear space. Instead they trace out trajectories with significant displacements in only a small number of linearly-independent directions.

We prove this empirical observation using analytic function theory and the principles of analytic continuation.

Since the eigenvector trajectory is a low-dimensional manifold embedded in a very large space, we can find the desired eigenvector using methods similar to image recognition in machine learning.

D. Frame, R. He, I. Ipsen, Da. Lee, De. Lee, E. Rrapaj, PRL 121, 032501 (2018)

Consider a one-parameter family of Hamiltonian matrices of the form

$$H(c) = H_0 + cH_1$$

where H_0 and H_1 are Hermitian. Let the eigenvalues and eigenvectors be

$$H(c)|\psi_j(c)\rangle = E_j(c)|\psi_j(c)\rangle$$

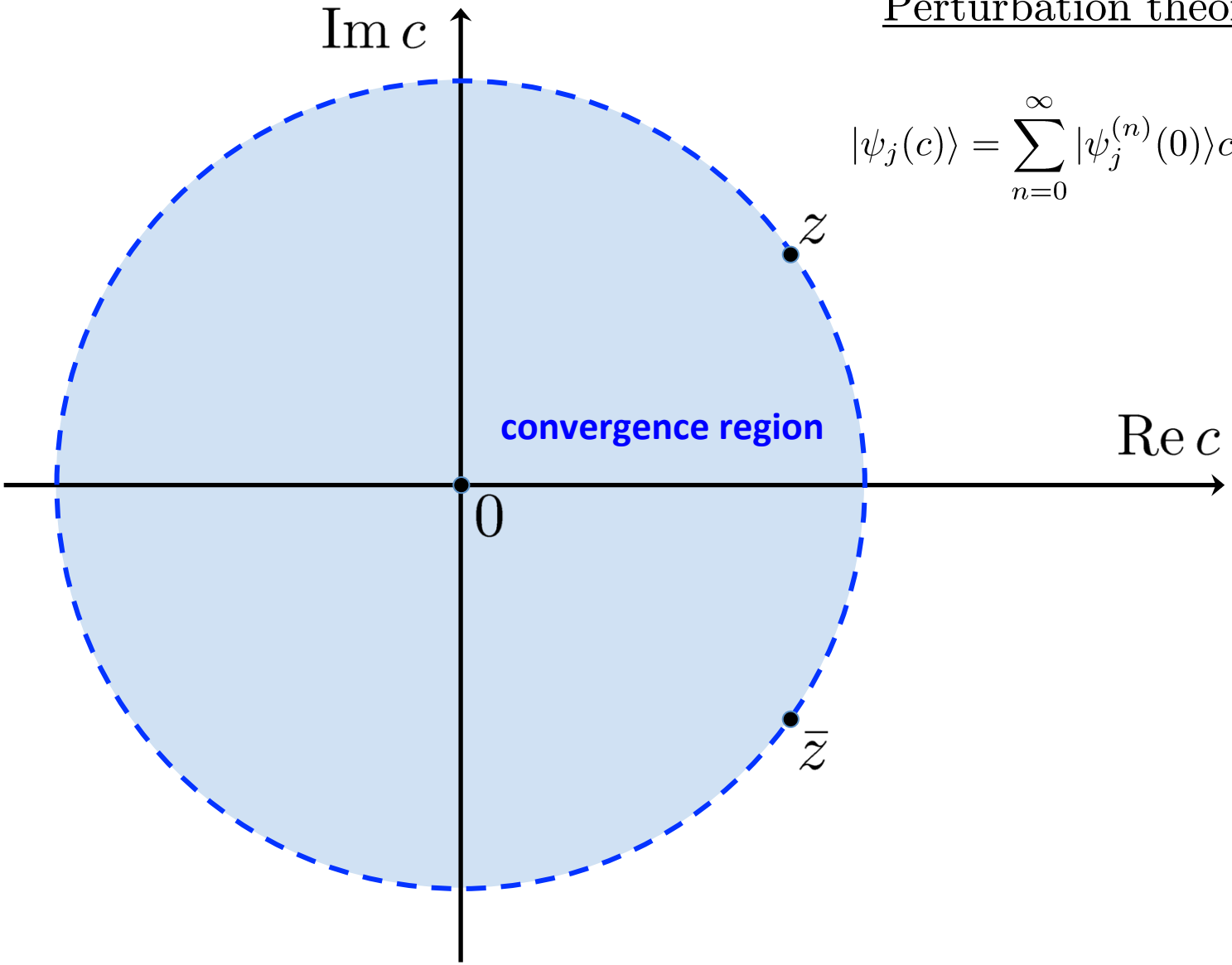
We can perform series expansions around the point $c = 0$.

$$E_j(c) = \sum_{n=0}^{\infty} E_j^{(n)}(0)c^n/n!$$
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

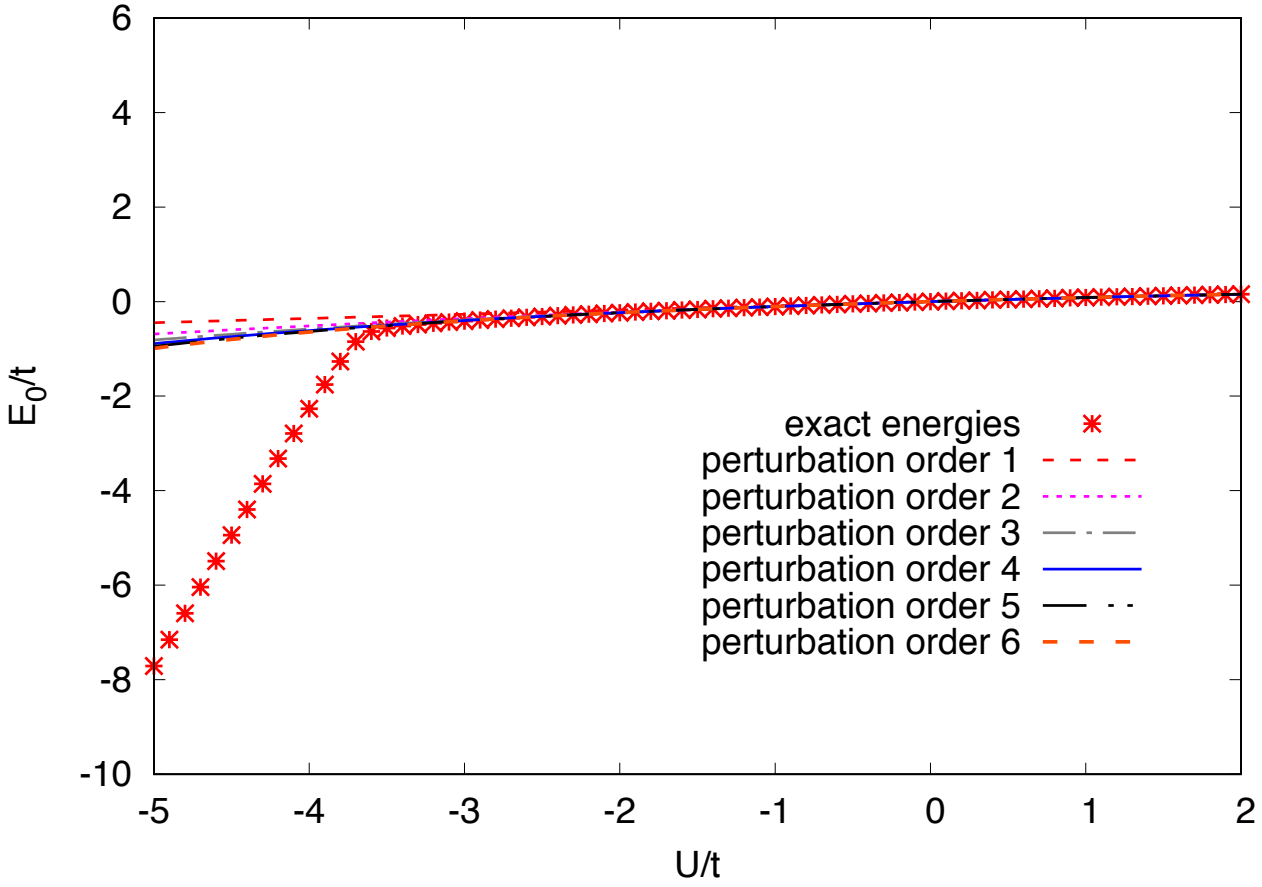
This is the strategy of perturbation theory. We can compute each term in the series when the eigenvalues and eigenvectors of H_0 are known or computable.

Perturbation theory

$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

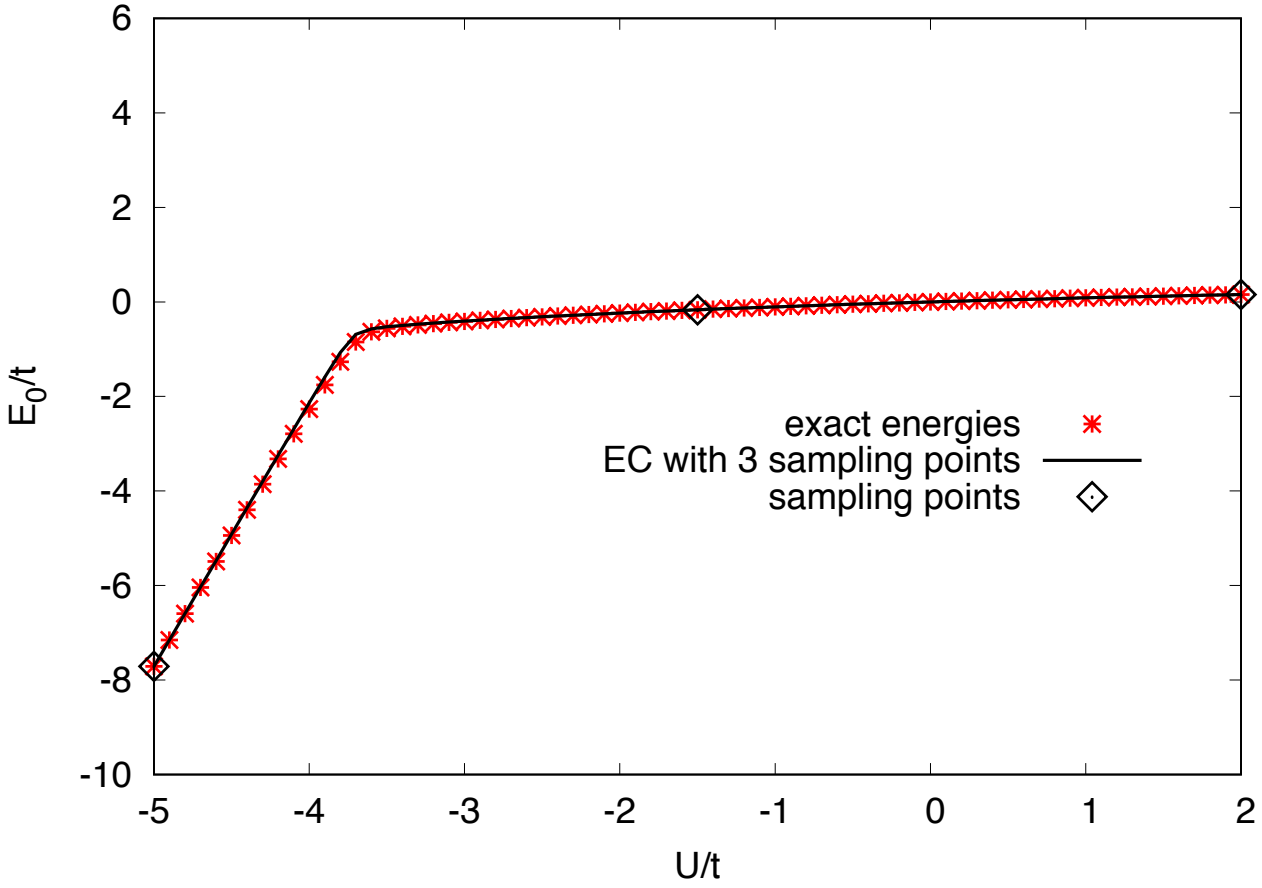


Bose-Hubbard model

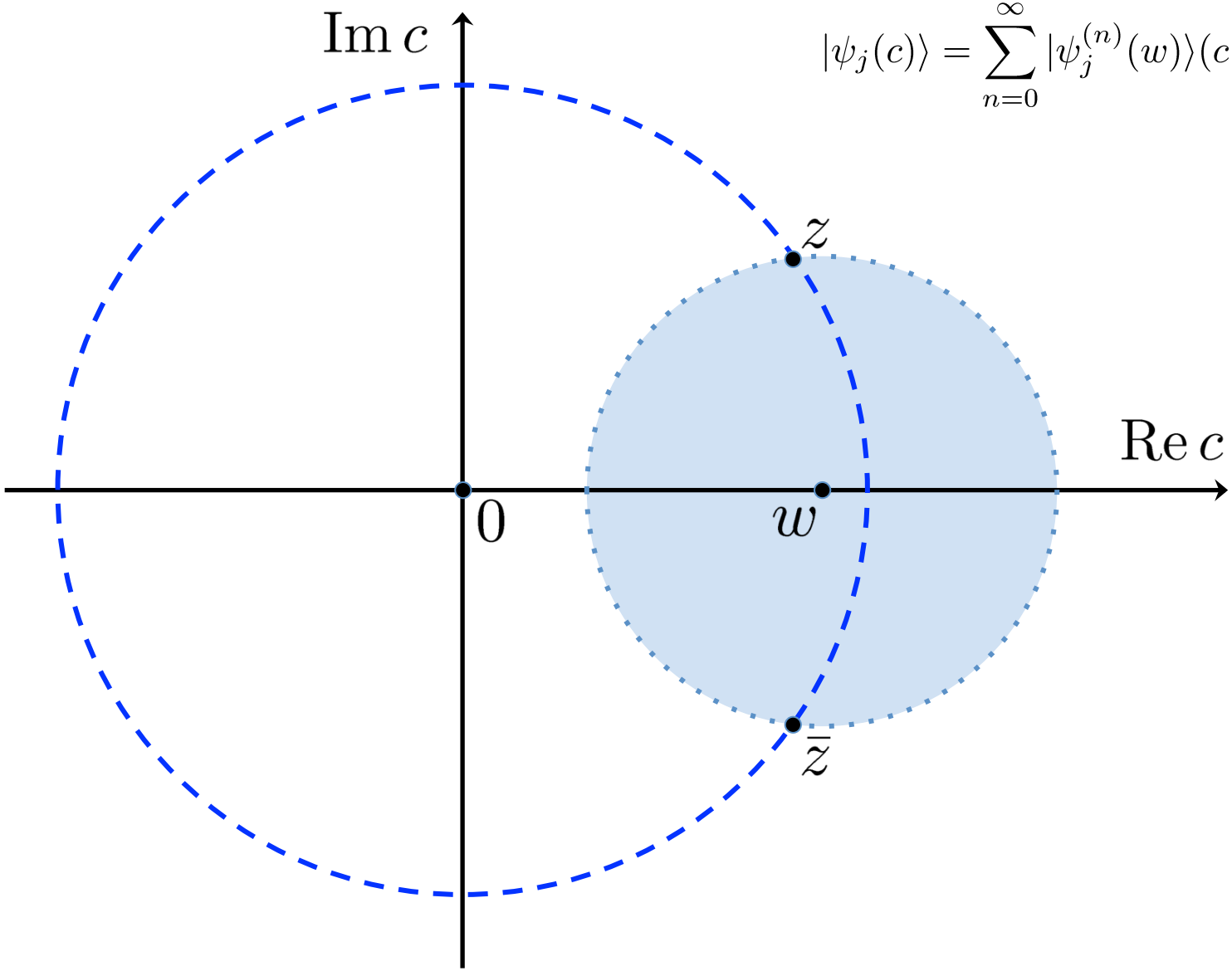


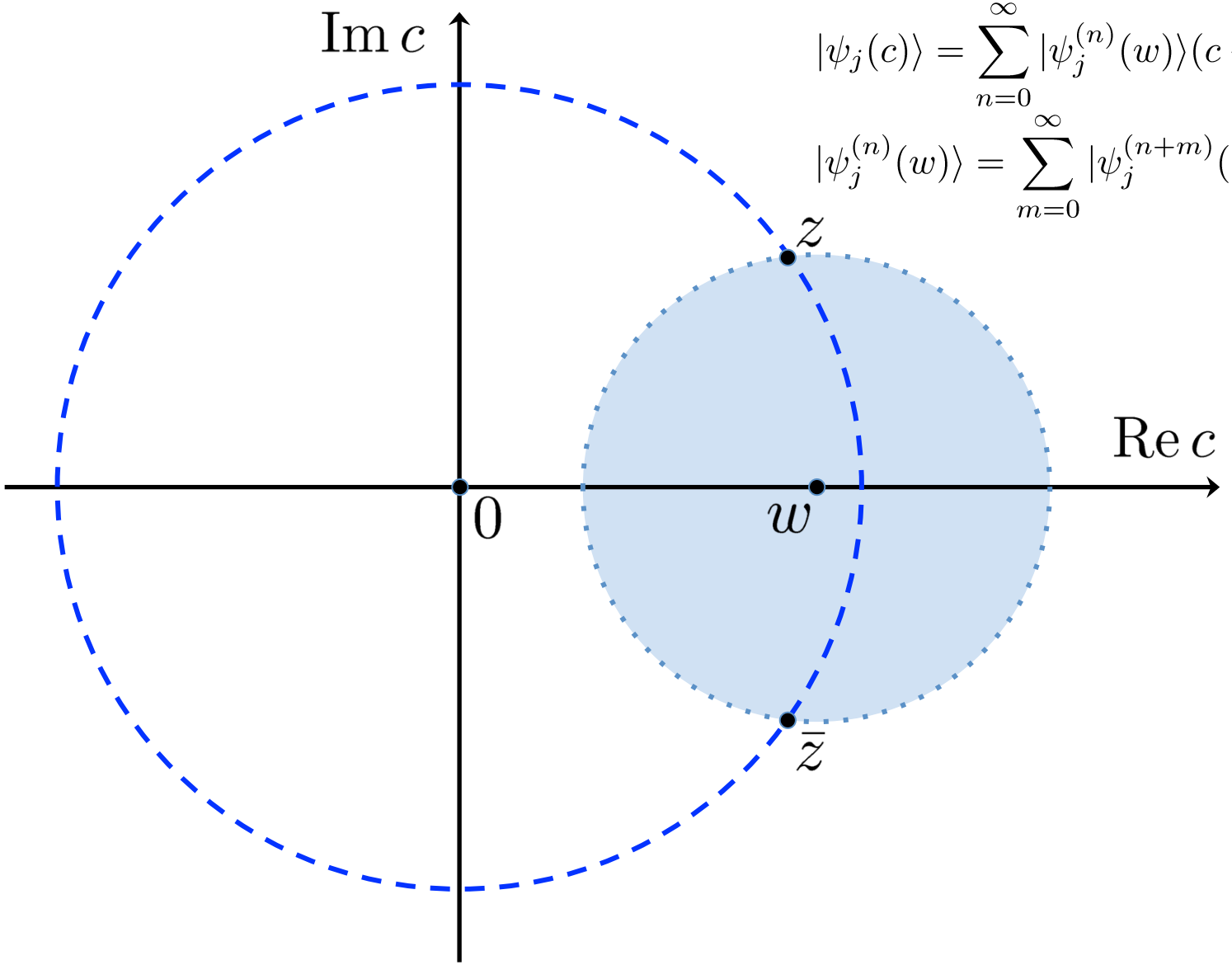
Perturbation theory fails at strong attractive coupling

Restrict the linear space to the span of three vectors



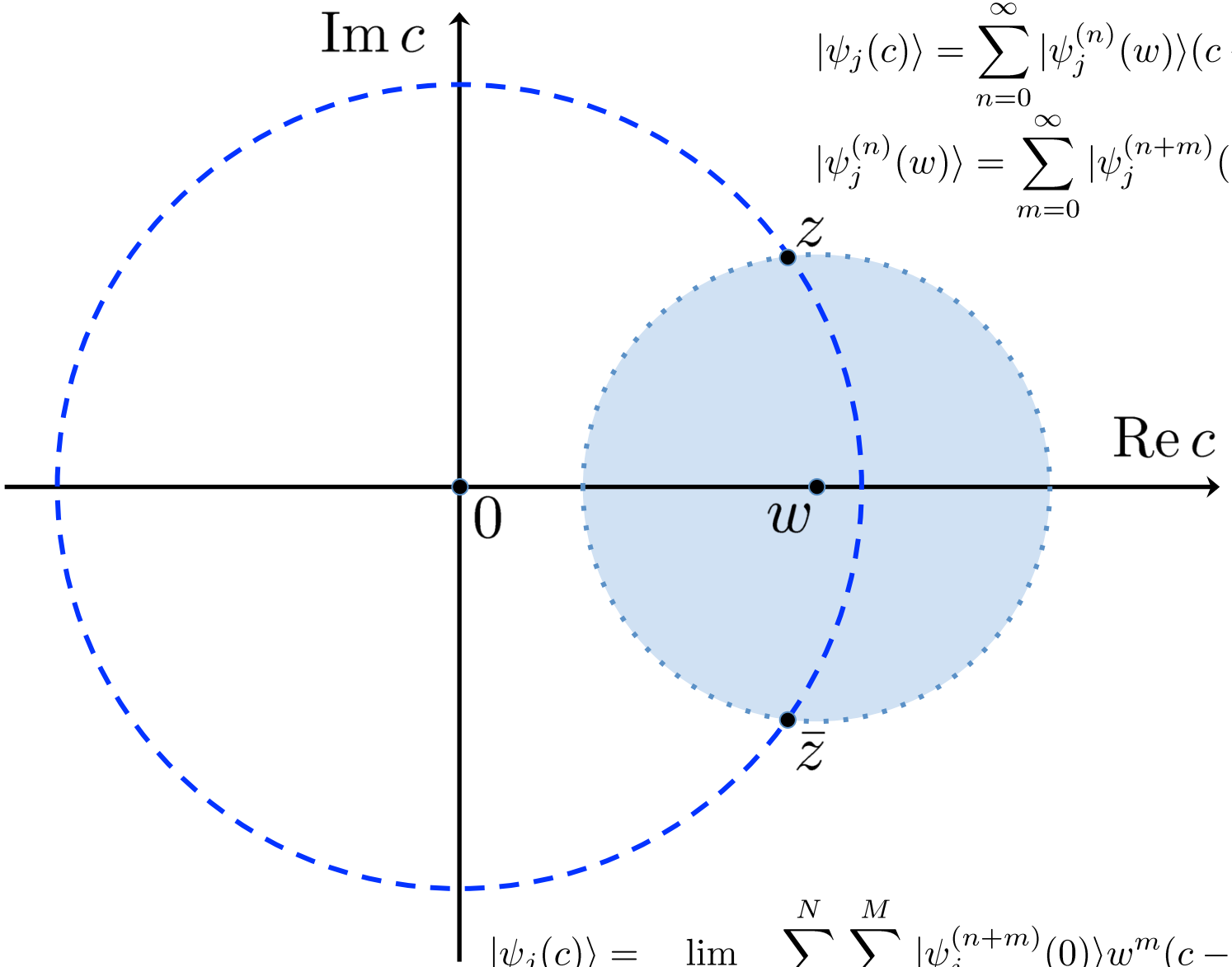
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$





$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$

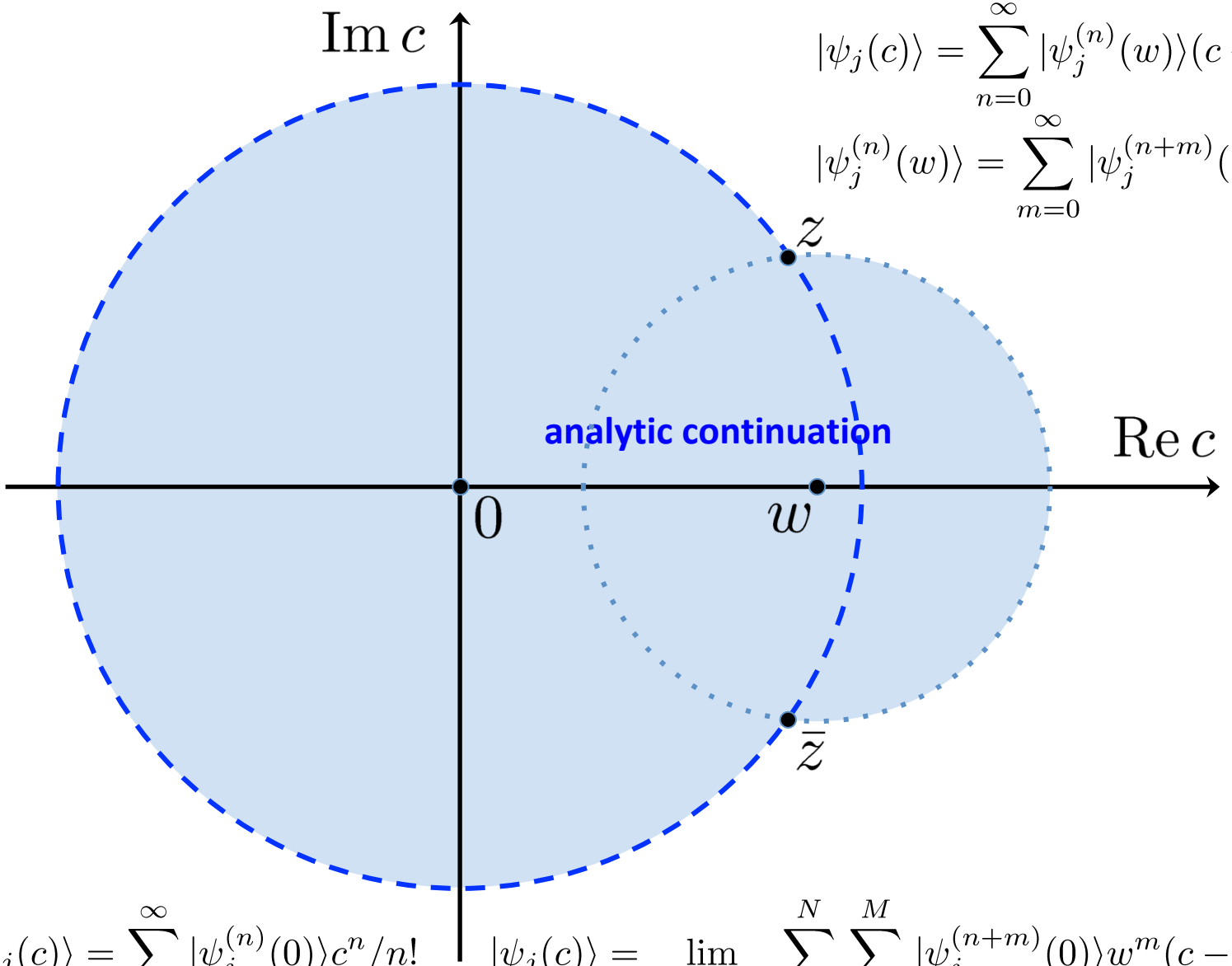
$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$



$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$

$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$

$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N}\sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$



$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$

$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$

$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

The eigenvector can be well approximated as a linear combination of a few vectors, using either the original series expansion

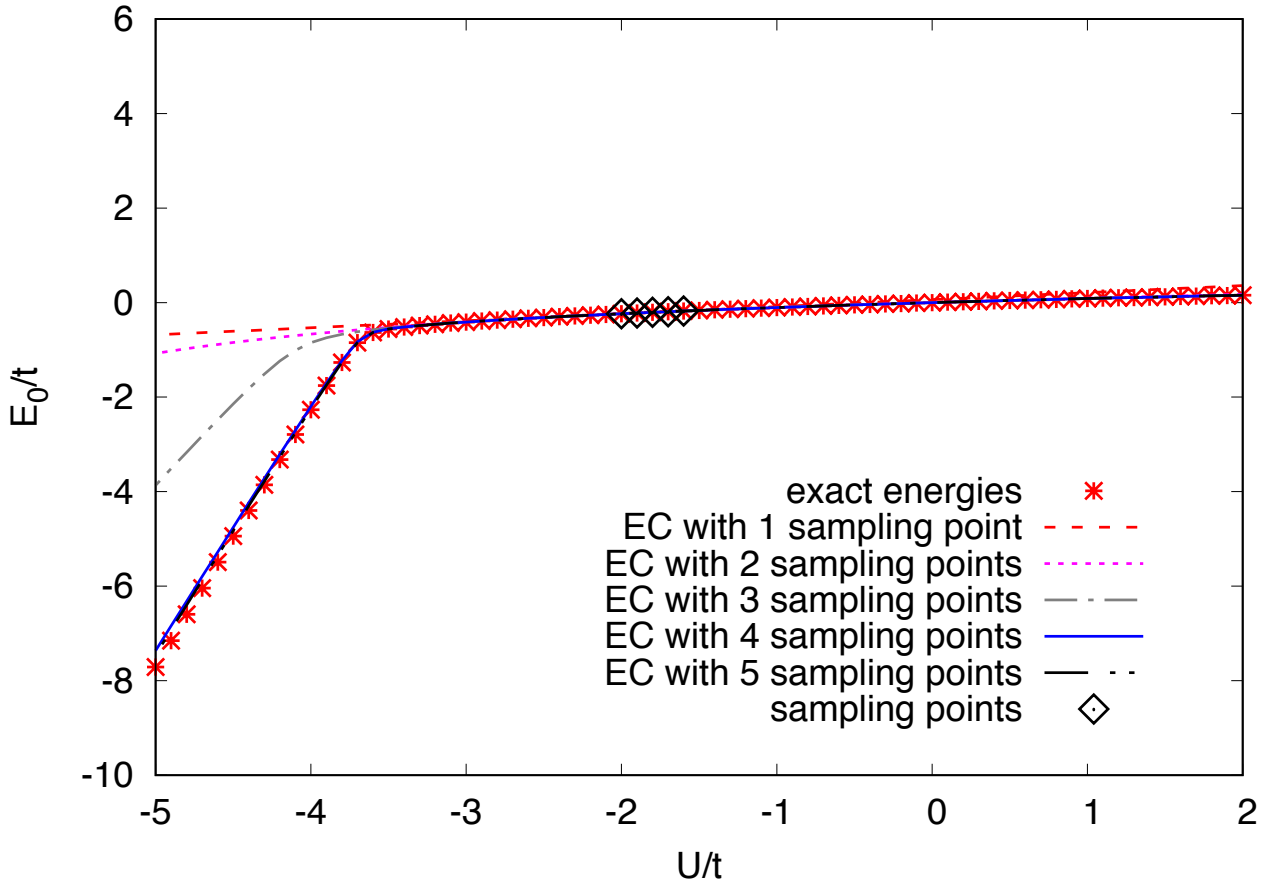
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

or the rearranged multi-series expansion we obtained through analytic continuation

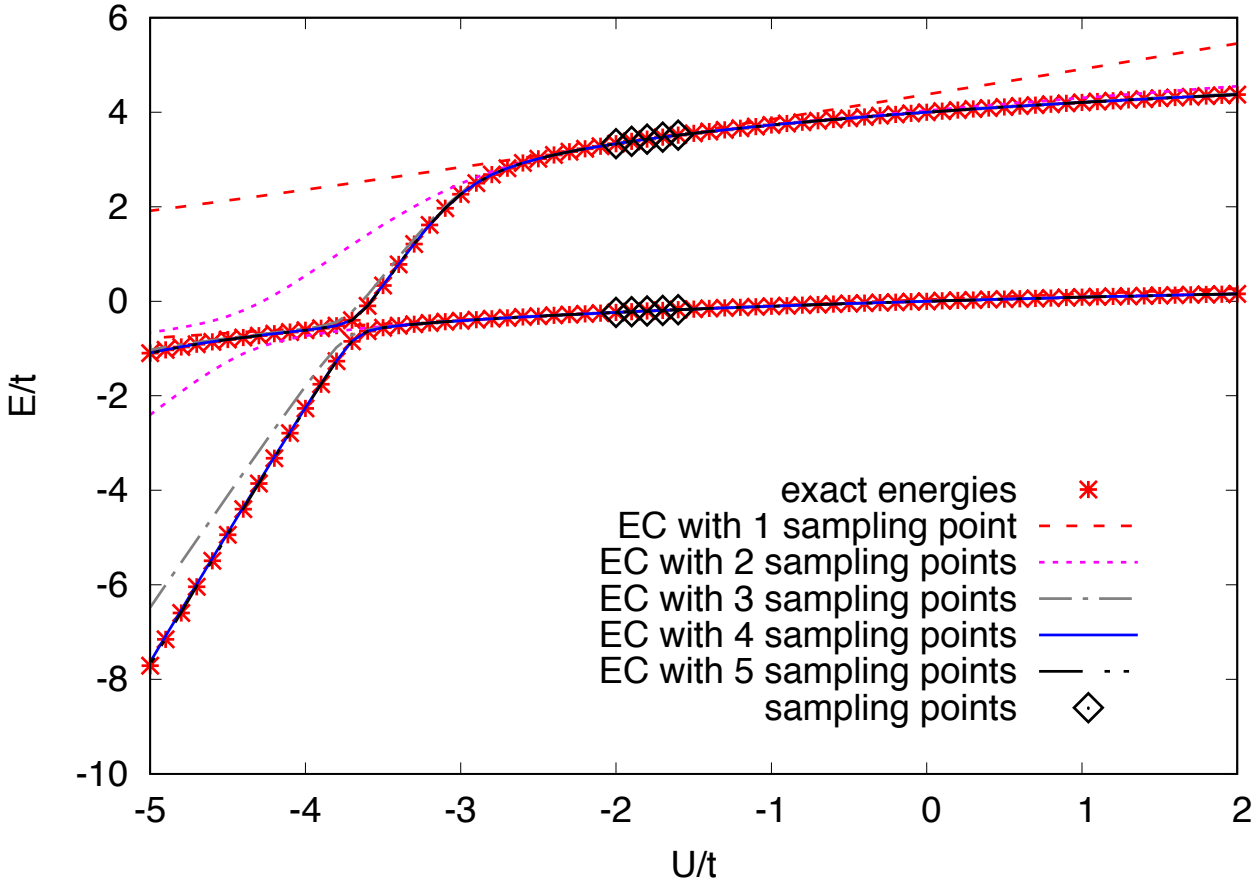
$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N} \sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

As c is varied the eigenvector does not explore the large dimensionality of the linear space, but is instead well approximated by a low-dimension manifold.

We can "learn" the eigenvector trajectory in one region and perform eigenvector continuation to another region



Applying eigenvector continuation to more than one eigenvector at a time accelerates convergence near avoided level crossings.



D. Frame, R. He, I. Ipsen, Da. Lee, De. Lee, E. Rrapaj, PRL 121, 032501 (2018)

Superfluidity and pairing correlations

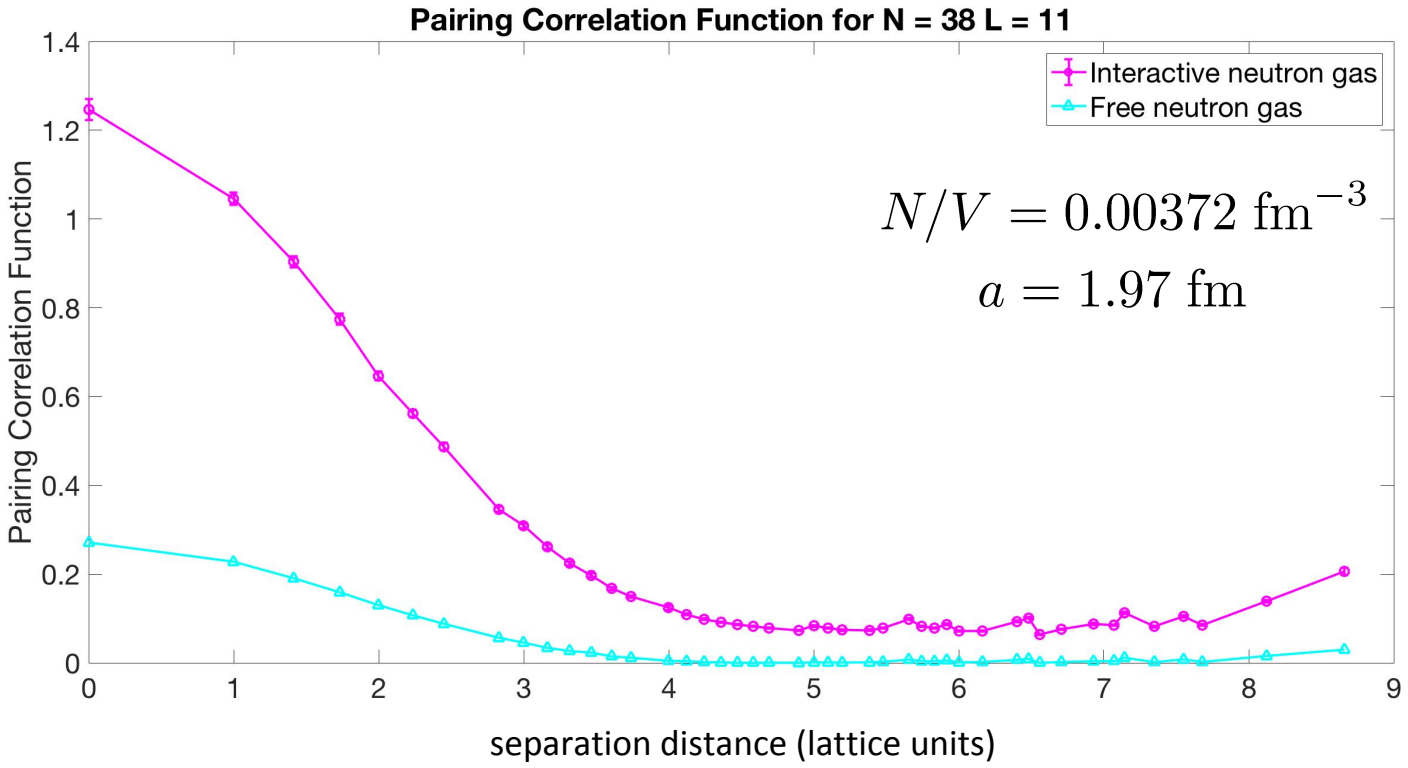
The two-body density matrix is defined as

$$\rho_2(\vec{r}\,'_1, \vec{r}\,'_2, \vec{r}_1, \vec{r}_2) = \left\langle \psi^\dagger_\downarrow(\vec{r}\,'_2)\psi^\dagger_\uparrow(\vec{r}\,'_1)\psi_\uparrow(\vec{r}_1)\psi_\downarrow(\vec{r}_2) \right\rangle$$

Long-range correlations in the two-body density matrix is a signature for pair superfluidity:

$$\rho_2(\vec{r}\,'_1, \vec{r}\,'_2, \vec{r}_1, \vec{r}_2) \to \alpha N/2 \cdot \phi^*(|\vec{r}\,'_1 - \vec{r}\,'_2|)\phi(|\vec{r}_1 - \vec{r}_2|)$$
$$|\vec{r}_1 - \vec{r}\,'_1|, |\vec{r}_2 - \vec{r}\,'_2| \to \infty$$

Yang, RMP 34, 694 (1962)



Courtesy: Rongzheng He

Summary and Outlook

These are exciting times for the nuclear theory community. In lattice EFT, we have new projects in motion which are pushing the current frontiers.

Currently working to improve our understanding of the detailed connection between bare nuclear forces and nuclear structure for light and medium-mass nuclei.

Applying the adiabatic projection method to low-energy nucleon-nucleus and alpha-nucleus scattering and reactions.

Using the pinhole algorithm to study the detailed structure of nuclei and thermodynamics of finite nuclei, nuclear matter, and neutron matter.

Implementing eigenvector continuation to treat all higher-order interactions in chiral effective field theory and other applications.

Calculating the two-body density matrix to measure pairing correlations in neutron matter and finite nuclei.