Nuclear Lattice Simulations
Lecture 4: Nuclear Reactions and Thermodynamics

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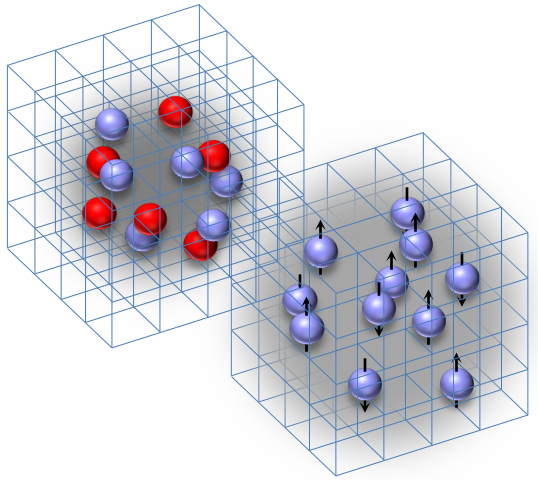


ACPTP Nuclear Physics School 2020
June 22-26, 2020

Outline

Adiabatic projection method

Alpha-alpha scattering

Pinhole trace algorithm

Nuclear thermodynamics

Phase diagram of symmetric nuclear matter

Inelastic reactions

Science objectives

Abinitio calculations of scattering and reactions relevant to alpha processes in stellar evolution and Type Ia supernovae

$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$

$^4\mathrm{He} + {}^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^{12}\mathrm{C} + \gamma$

$^{12}\mathrm{C} + {}^4\mathrm{He} \rightarrow {}^{16}\mathrm{O} + \gamma$

$^{16}\mathrm{O} + {}^4\mathrm{He} \rightarrow {}^{20}\mathrm{Ne} + \gamma$

$^{20}\mathrm{Ne} + {}^4\mathrm{He} \rightarrow {}^{24}\mathrm{Mg} + \gamma$

$^{24}\mathrm{Mg} + {}^4\mathrm{He} \rightarrow {}^{28}\mathrm{Si} + \gamma$

$^{12}\mathrm{C} + {}^{12}\mathrm{C} \rightarrow {}^{20}\mathrm{Ne} + {}^4\mathrm{He}$

$^{16}\mathrm{O} + {}^{16}\mathrm{O} \rightarrow {}^{28}\mathrm{Si} + {}^4\mathrm{He}$

Challenges

How to reduce computational scaling with number of nucleons in participating nuclei? Can we provide useful *abinitio* input for halo or cluster EFT calculations?

Adiabatic projection method

Development inspired by progress using no-core shell model with resonating group method to describe *abinitio*scattering and reactions in light nuclei.

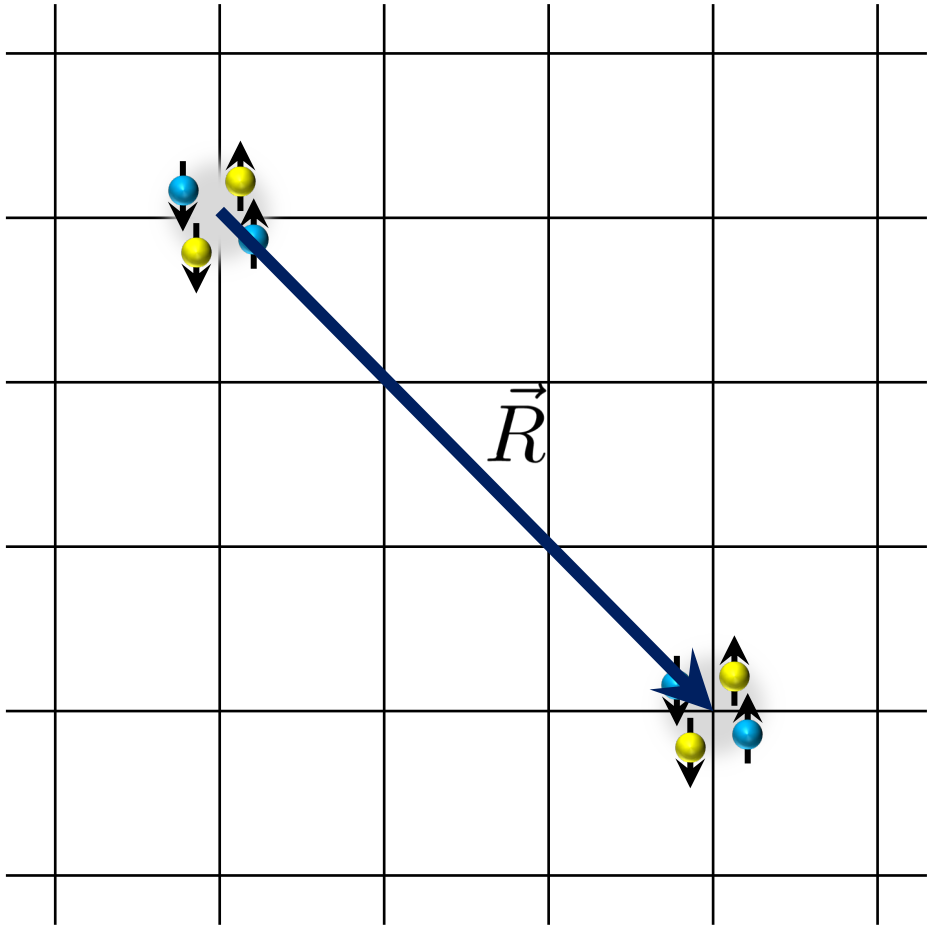
Navratil, Roth, Quaglioni, PRC 82 034609 (2010); Navratil, Quaglioni, PRC 83 044609 (2011); etc.

Strategy is to divide the problem into two parts. In the first part, we use Euclidean time projection and lattice Monte Carlo to derive an *ab initio*low-energy cluster Hamiltonian, called the adiabatic Hamiltonian (adiabatic transfer matrix for nonzero temporal lattice spacing).

In the second part, we use the adiabatic Hamiltonian to compute scattering phase shifts or reaction amplitudes.

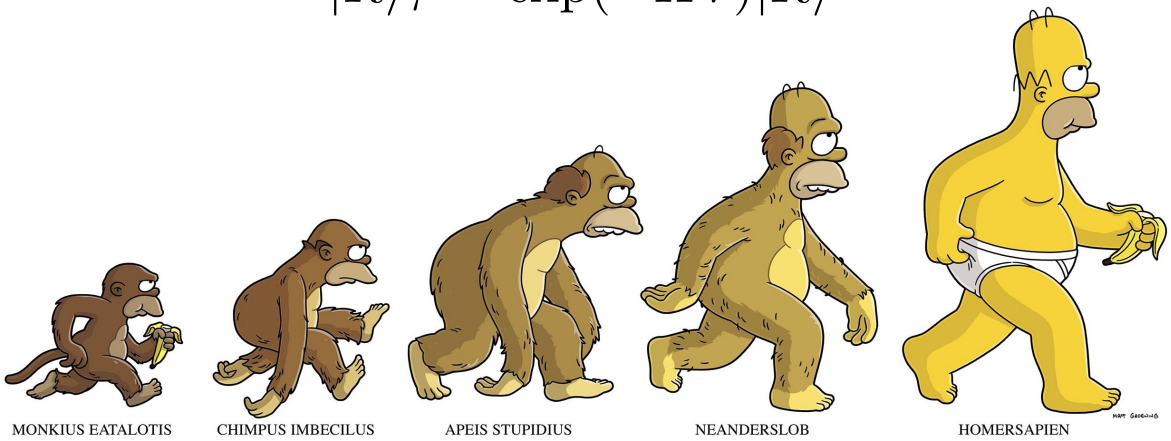
Start with localized cluster states for all possible separation vectors $\vec{R}$

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r}+\vec{R}\rangle_1 \otimes |\vec{r}\rangle_2$$



Cluster evolution with Euclidean time.

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$



For notational simplicity we use the language of continuous time evolution. The actual calculations use normal-ordered transfer matrices.

$$|\vec{R}\rangle_\tau = [: \exp(-H\alpha_t) :]^{L_t} \, |\vec{R}\rangle$$

M. Groening

Use projection Monte Carlo to propagate cluster wavefunctions in Euclidean time to form dressed cluster states

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$

Evaluate matrix elements of the full microscopic Hamiltonian with respect to the dressed cluster states,

$$[H_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau$$

Since the dressed cluster states are in general not orthogonal, we construct a norm matrix given by the inner product

$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

The adiabatic Hamiltonian is defined by the matrix product

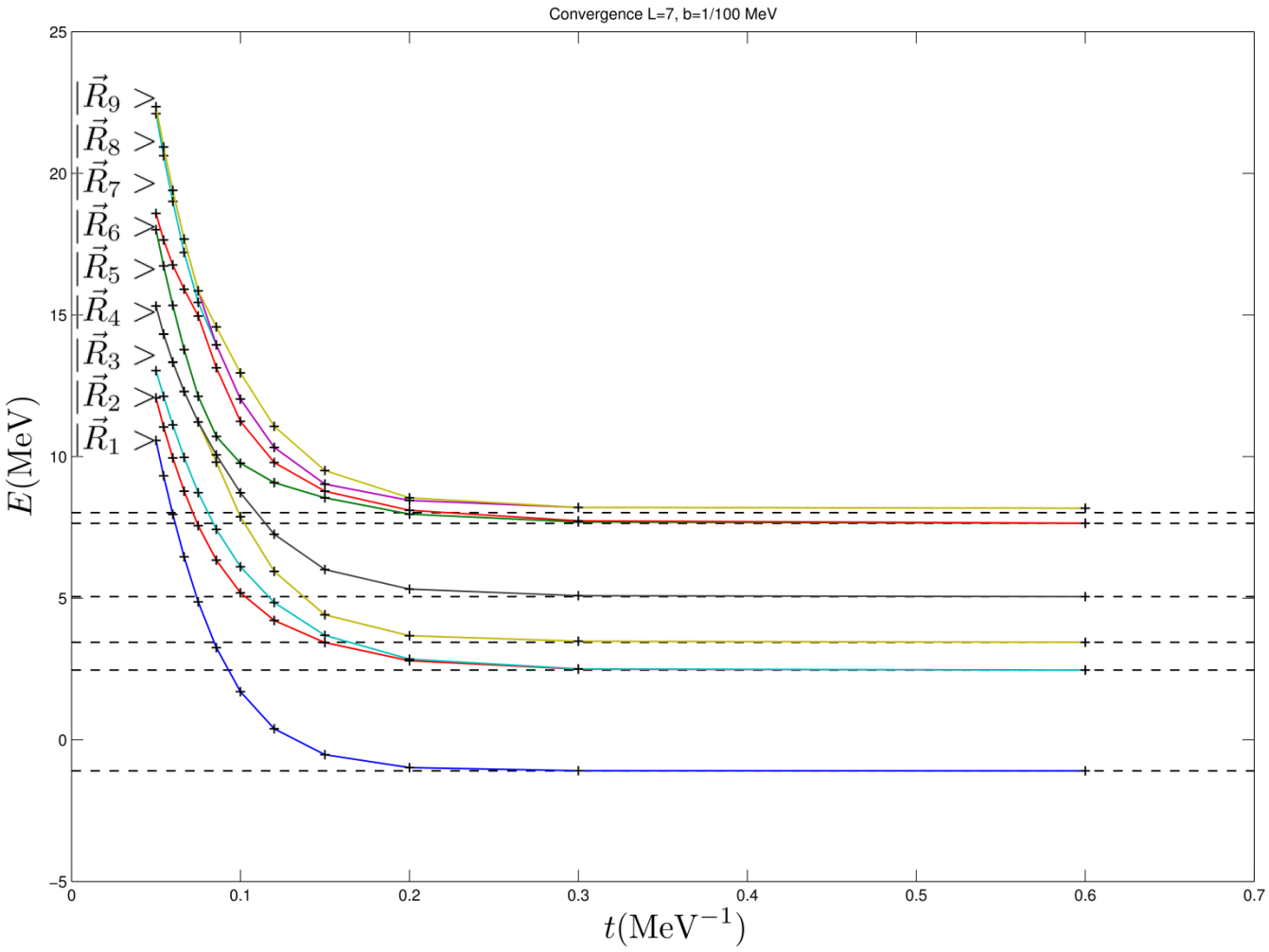
$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

One can see the similarity to no-core shell model with resonating group method. But in the adiabatic projection method we don't need to include excitations of the participating nuclei unless the energy is above the corresponding inelastic threshold.

Distortion and polarization of the nuclear wave functions are automatically produced by the Euclidean time projection.

As we increase the projection time, the adiabatic Hamiltonian exactly reproduces the low-energy spectrum of the full microscopic Hamiltonian.

Spin-quartet neutron-deuteron scattering



Pine, D.L., Rupak, EPJA 49 (2013)

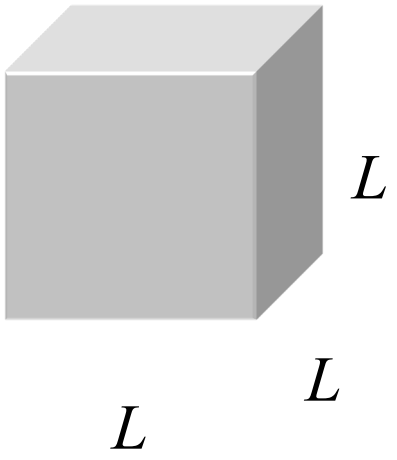
Lüscher's finite-volume formula

Lüscher, Comm. Math. Phys. 105 (1986) 153; NPB 354 (1991) 531

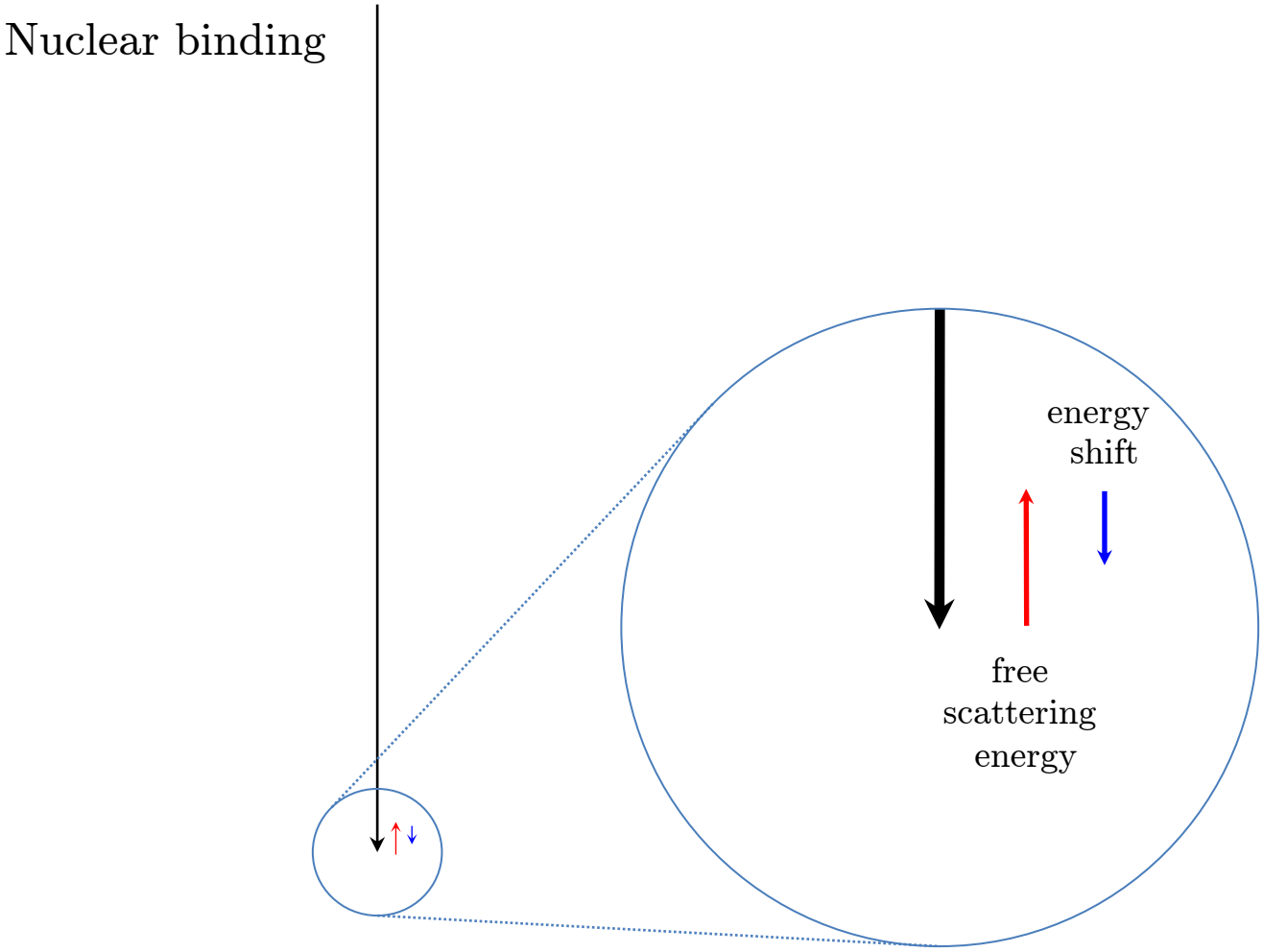
Two-particle energy levels near threshold in a periodic cube are related to the elastic phase shifts

$$p \cot \delta_0(p) = \frac{1}{\pi L} S(\eta), \qquad \eta = \left(\frac{Lp}{2\pi}\right)^2$$

$$S(\eta) = \lim_{\Lambda \to \infty} \left[\sum_{\vec{n}} \frac{\theta(\Lambda^2 - \vec{n}^2)}{\vec{n}^2 - \eta} - 4\pi\Lambda \right]$$



Signal-to-noise problems for finite-volume energy extraction



Asymptotic cluster scattering wave functions

In the far asymptotic region where our dressed clusters are widely separated, they interact only through infinite-range forces such as the Coulomb interaction.

Therefore we can describe everything with an effective cluster Hamiltonian $H^{\rm eff}$ that is nothing more than a free lattice Hamiltonian for two point particles plus any infinite-range interactions inherited from the full microscopic Hamiltonian. So in the asymptotic region we have

$$[N_\tau]_{\vec{R},\vec{R}'} = c \cdot \left[e^{-2H^{\rm eff}\tau} \right]_{\vec{R},\vec{R}'} ,$$

$$[H_\tau]_{\vec{R},\vec{R}'} = c \cdot \left[e^{-H^{\rm eff}\tau} H^{\rm eff} e^{-H^{\rm eff}\tau} \right]_{\vec{R},\vec{R}'} ,$$

Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, PRC 92 (2015) 054612

Since

$$\left[N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'} = c^{-1/2} \cdot \left[e^{H^{\text{eff}}\tau}\right]_{\vec{R},\vec{R}'}$$

we conclude that the adiabatic Hamiltonian coincides with the effective cluster Hamiltonian in the asymptotic region

$$[H_\tau^a]_{\vec{R},\vec{R}'} = \left[H^{\text{eff}}\right]_{\vec{R},\vec{R}'}$$

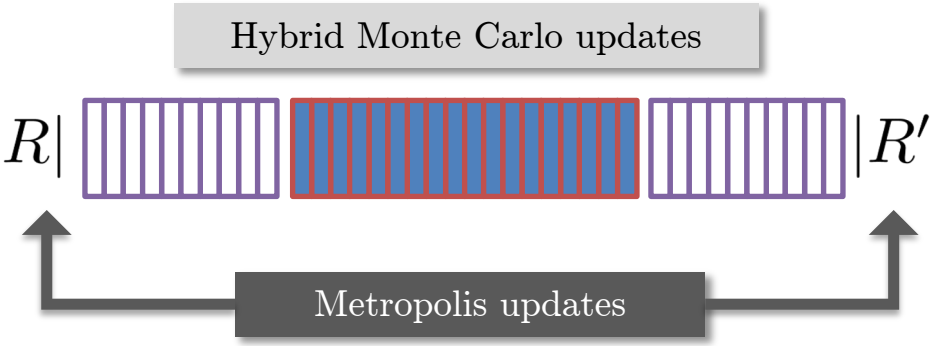
In the asymptotic region, we are inverting the diffusion process when computing the adiabatic Hamiltonian and are left with an effective cluster Hamiltonian in position space basis.

We use projections onto spherical harmonics defined on sets of lattice points with approximately the same distance from the origin.

$$|R\rangle^{L,L_z} = \sum_{||\vec{R}'|-R|<\Delta R} Y_{L,L_z}(\hat{R}')|\vec{R}'\rangle$$

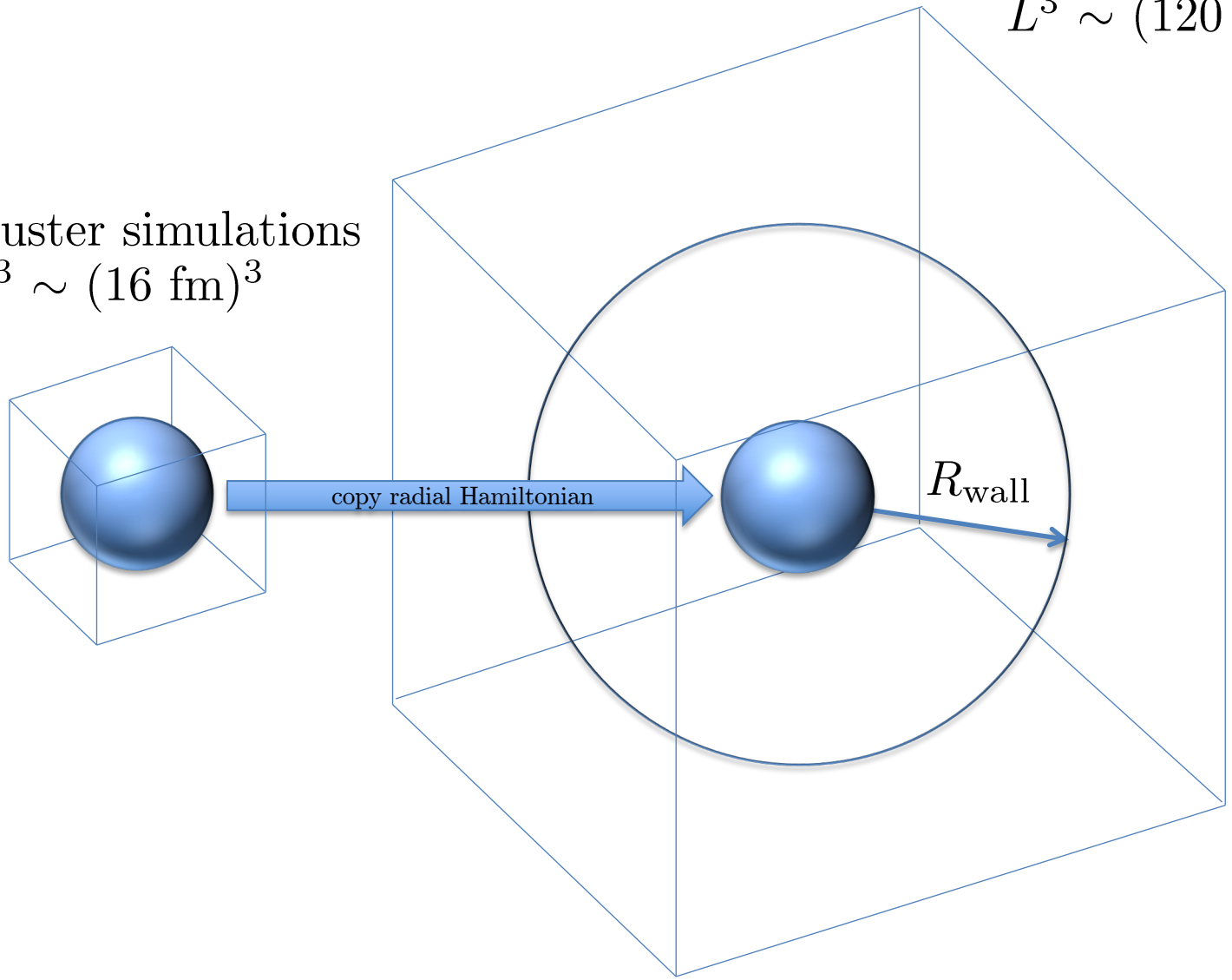
New algorithm developed for auxiliary field updates and initial/final state updates

$$[Z_{n_t,\mathrm{LO}}]^{L,L_z}_{R,R'} = {}^{L,L_z}\langle R| \quad |R'\rangle^{L,L_z}$$



single cluster simulations
$L^3 \sim (120 \text{ fm})^3$

two cluster simulations
$L^3 \sim (16 \text{ fm})^3$

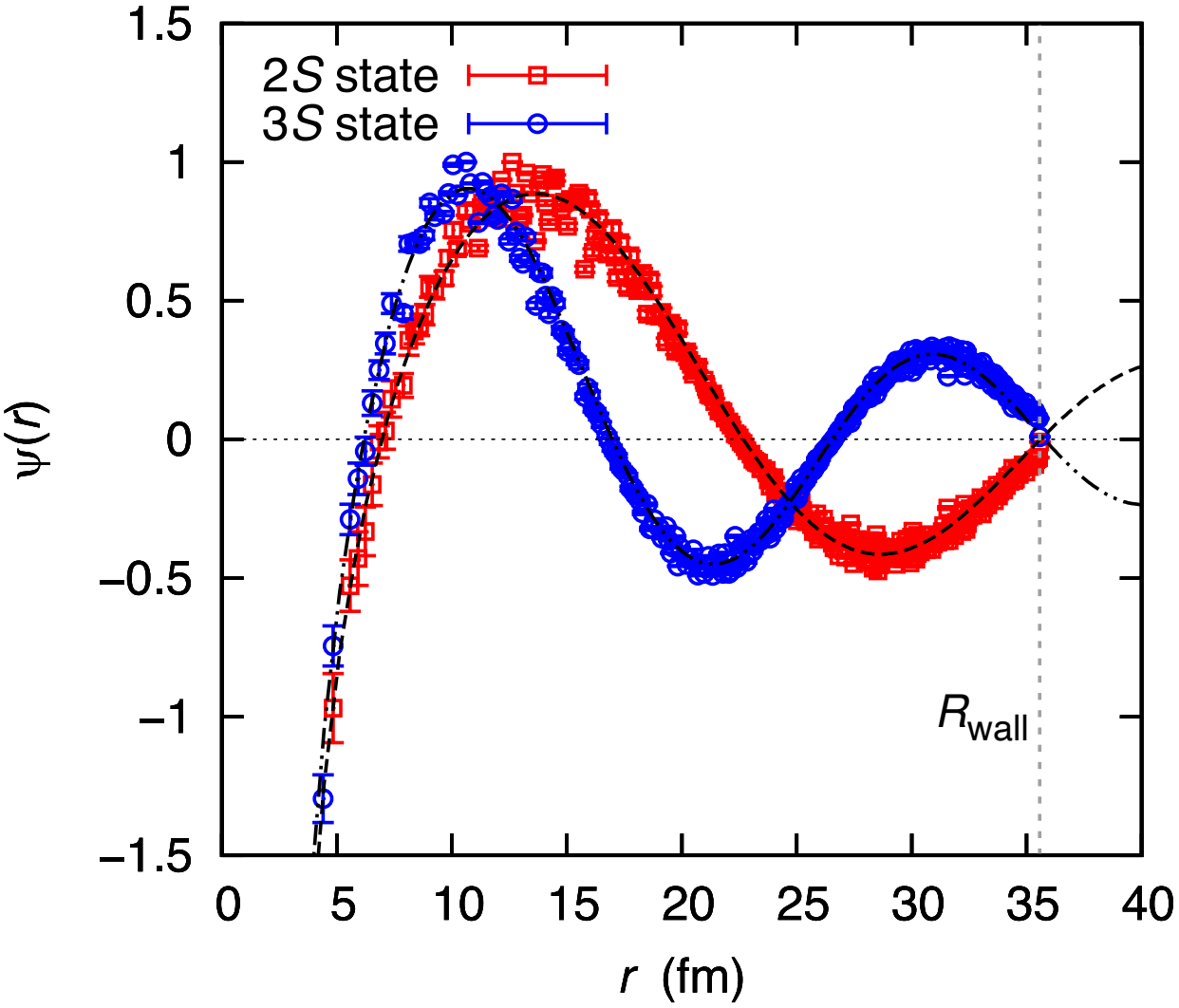


$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$

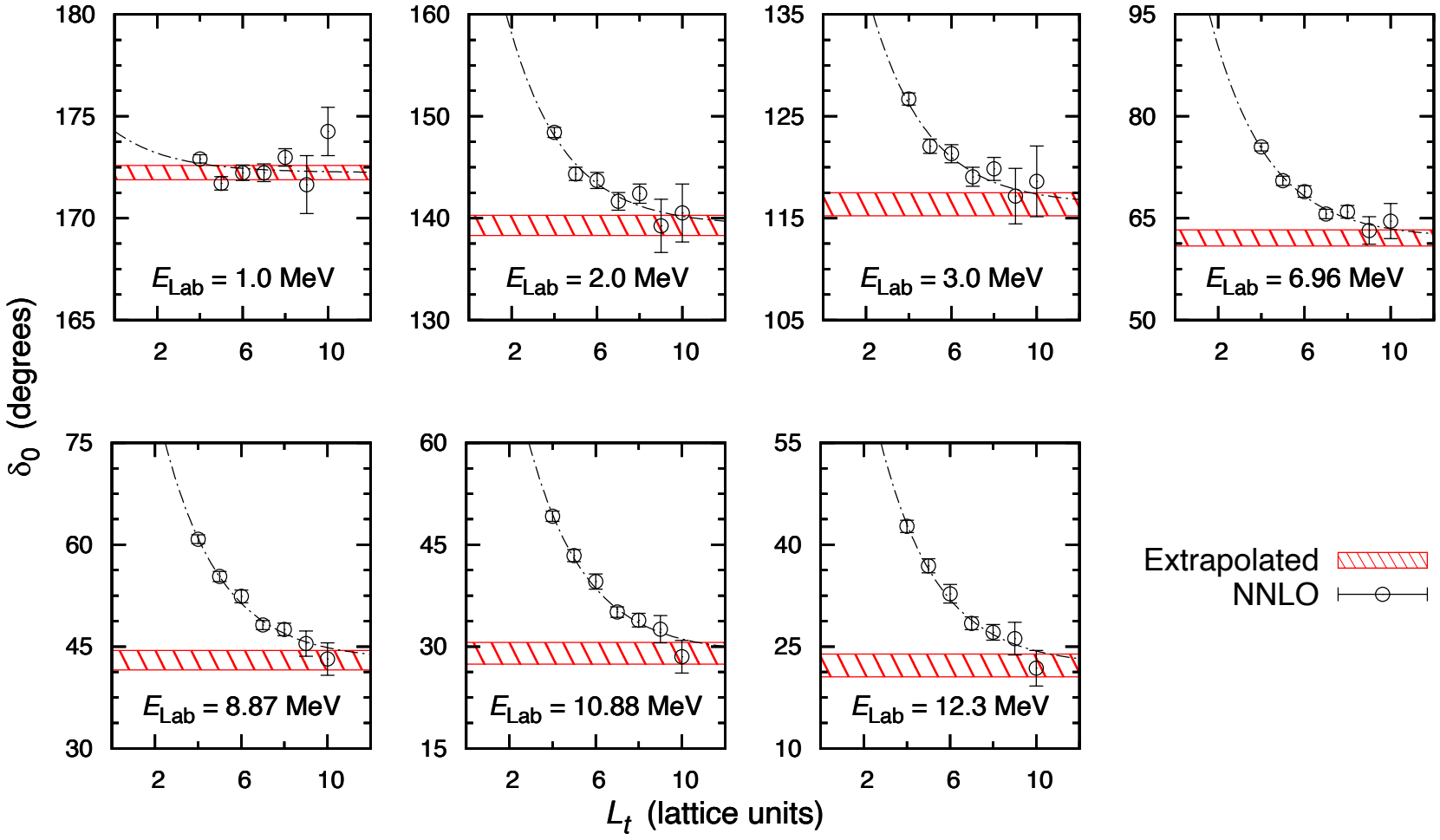
We now present *abinitio* results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.

Using the adiabatic projection method, we performed lattice simulations for the S-wave and D-wave channels.

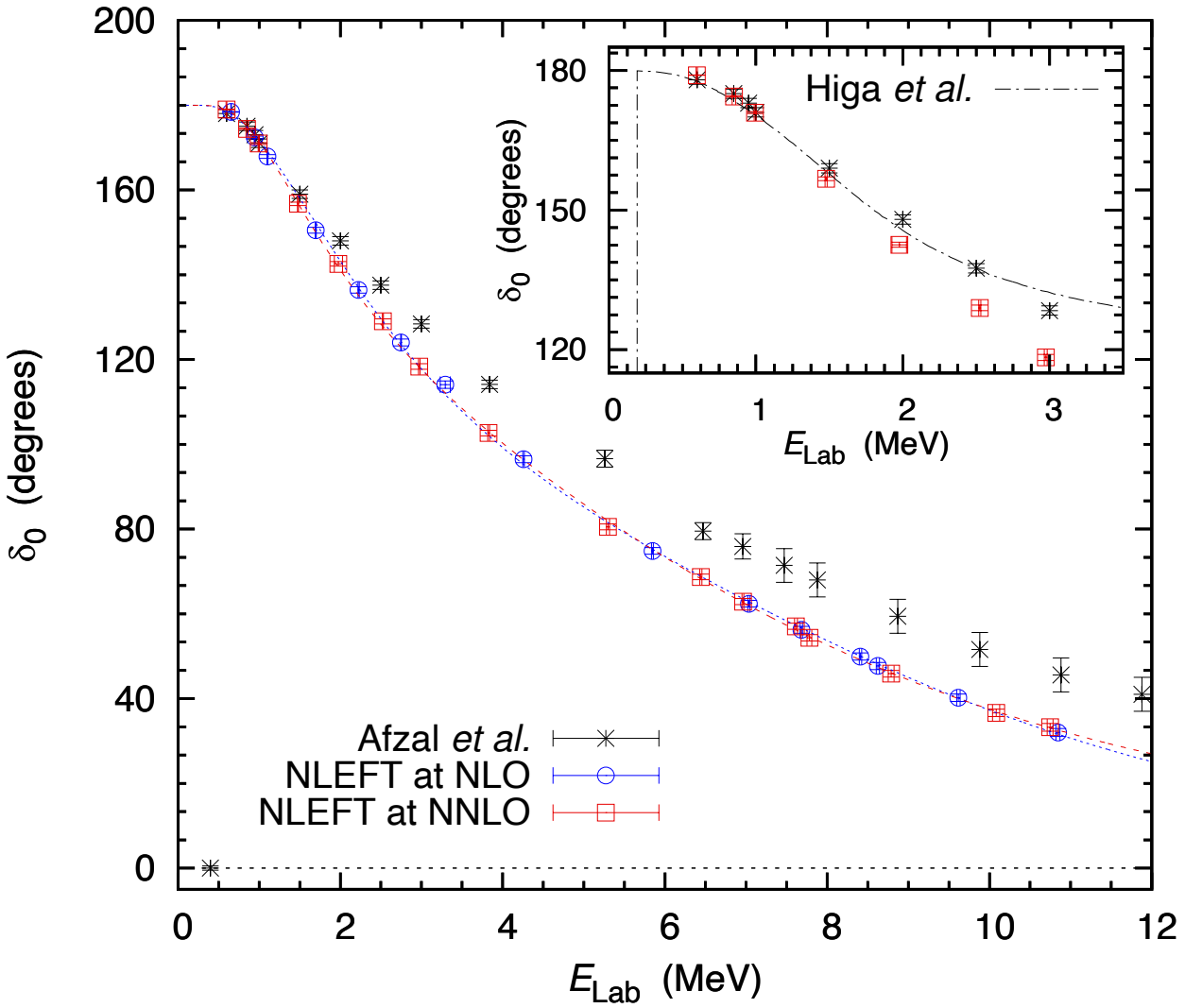
Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)


2S state
3S state
1.5
1
0.5
0
−0.5
−1
−1.5
ψ(r)
0
5
10
15
20
25
30
35
40
r (fm)
R_wall

S-wave scattering



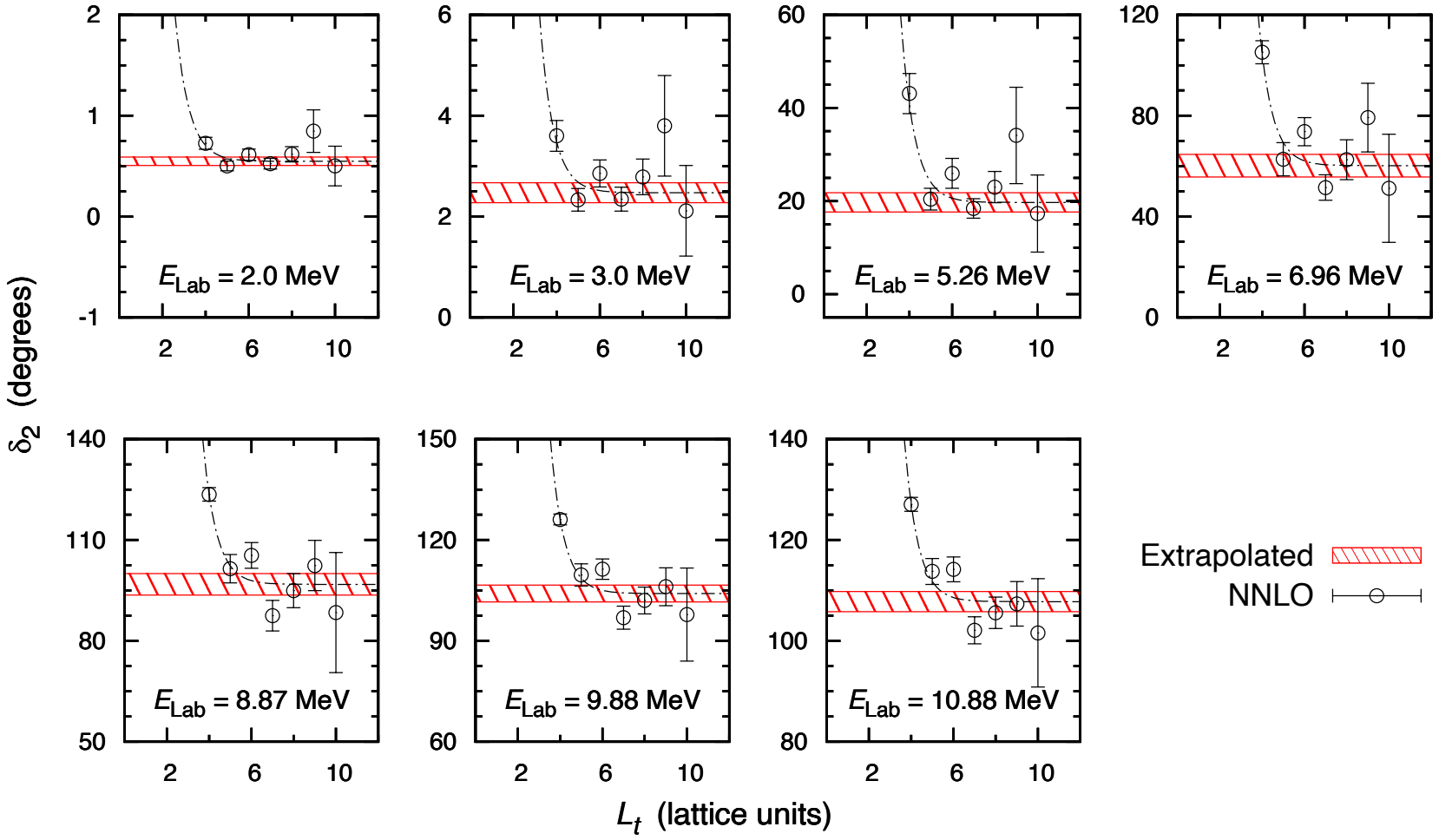
S-wave scattering



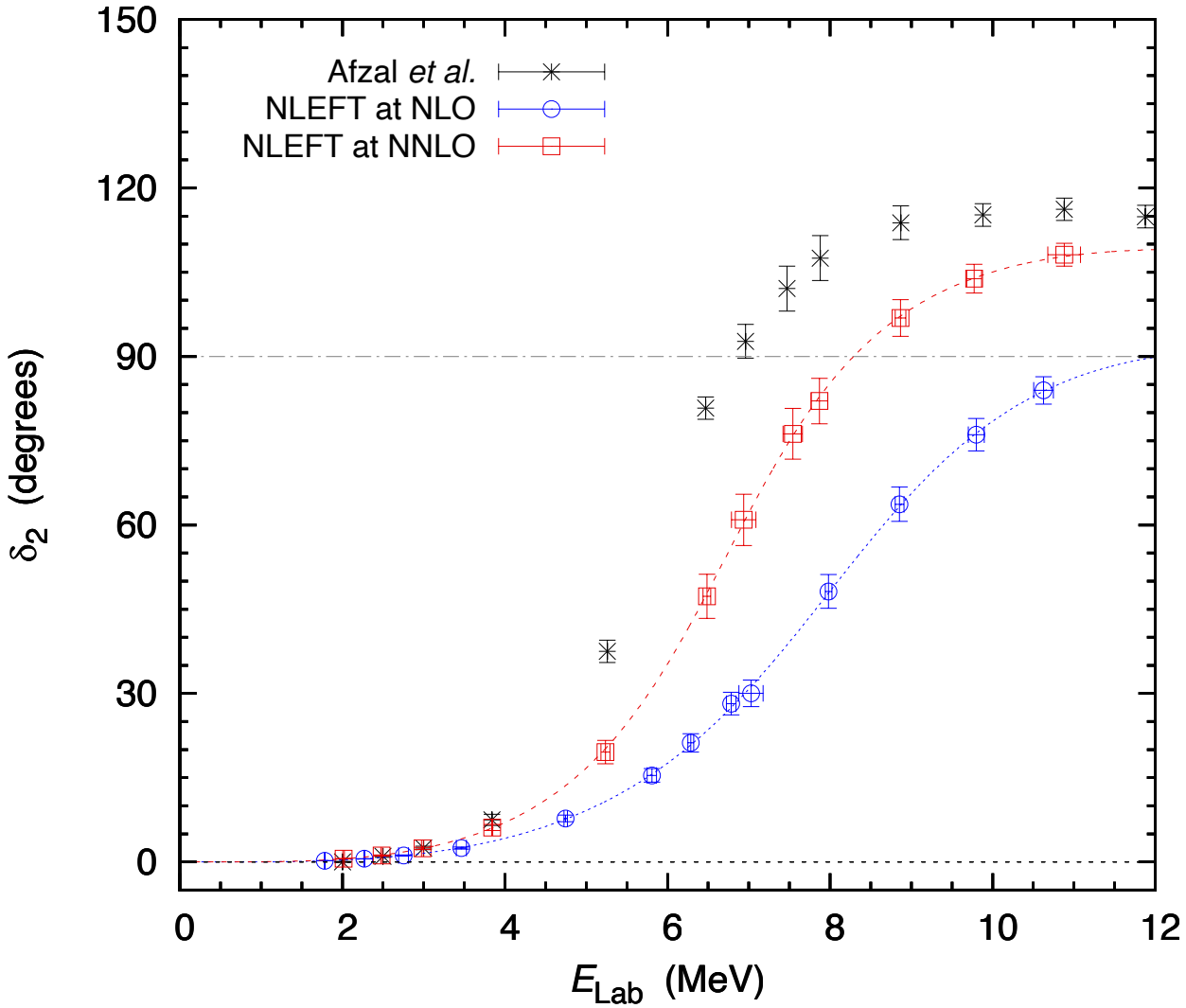
Afzal, Ahmad, Ali, RMP 41 247 (1969)

Higa, Hammer, van Kolck, NPA 809 171(2008)

D-wave scattering



D-wave scattering



Nuclear thermodynamics

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

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

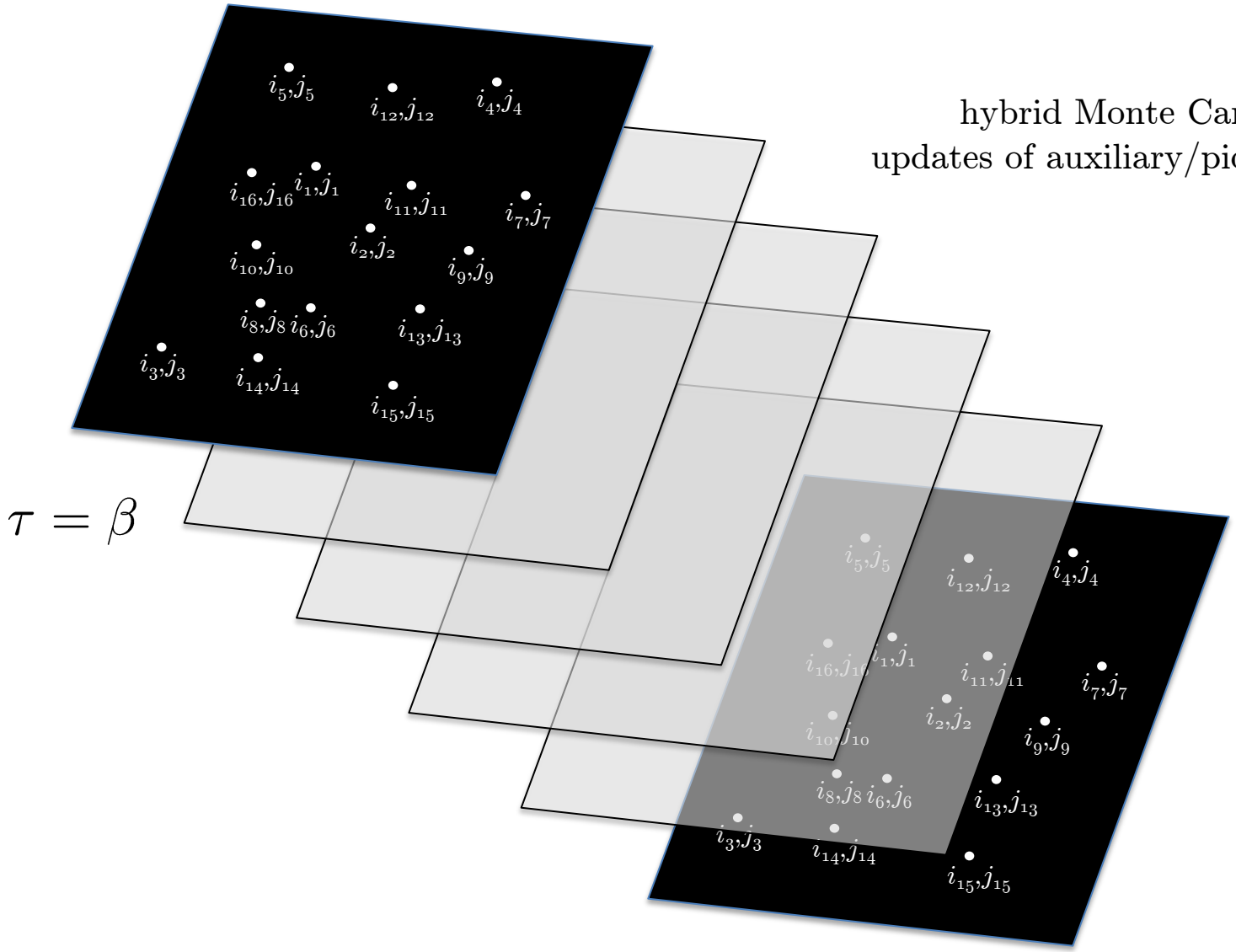
We compute the quantum mechanical trace over A-nucleon states by summing over pinholes (position eigenstates) for the initial and final states

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

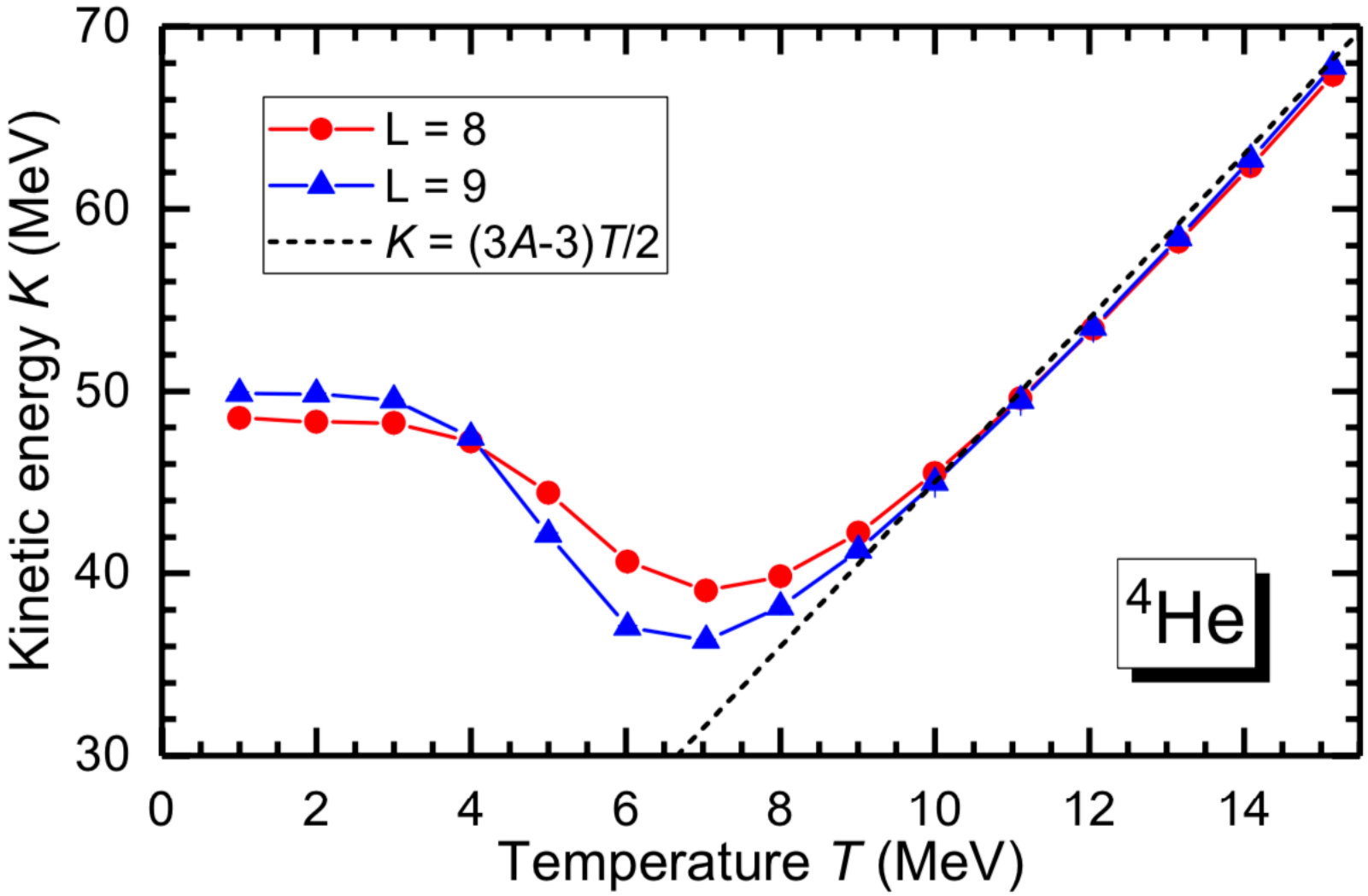
This can be used to calculate the partition function in the canonical ensemble.

Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, work in progress

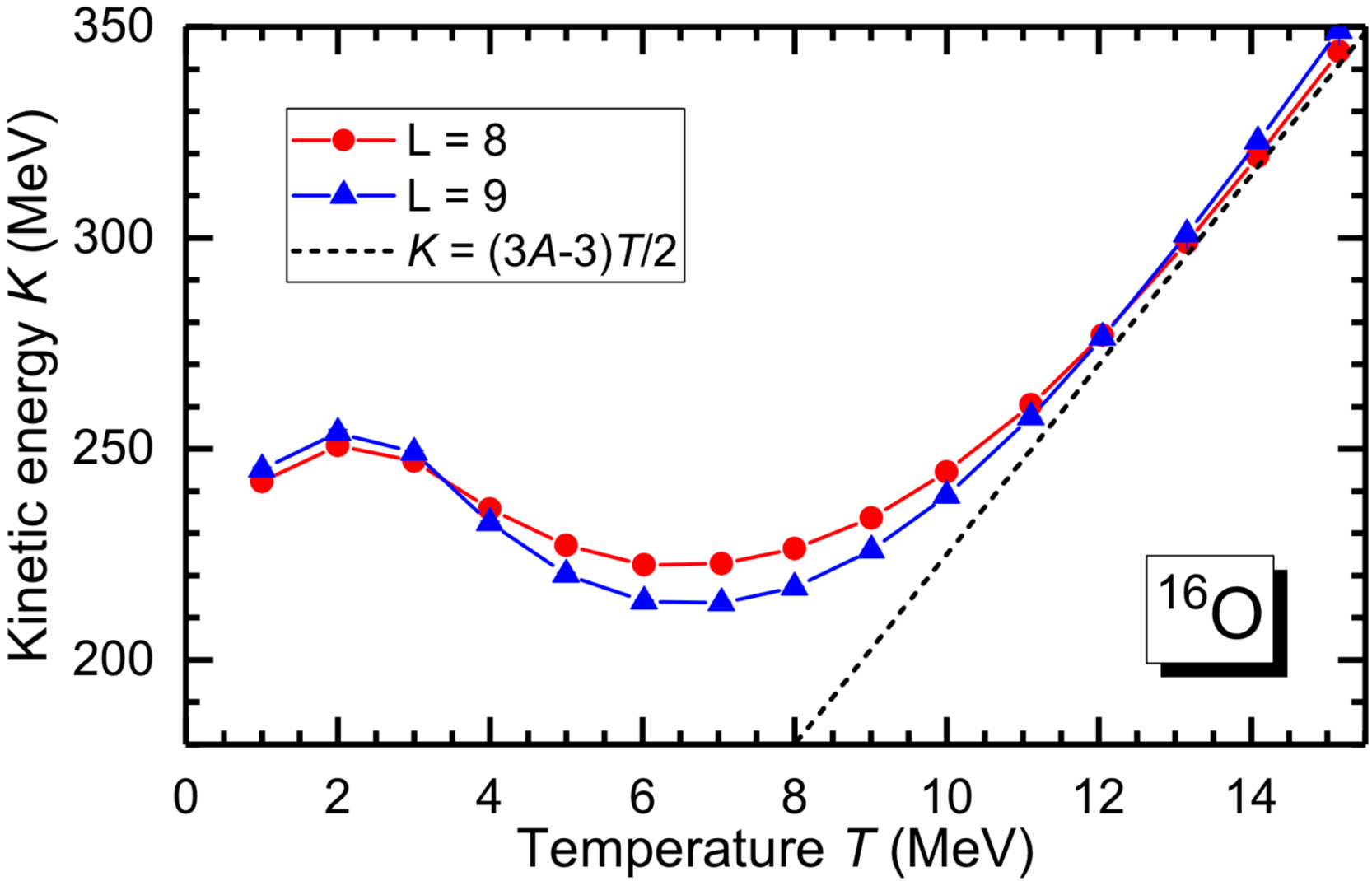
Metropolis updates of pinholes

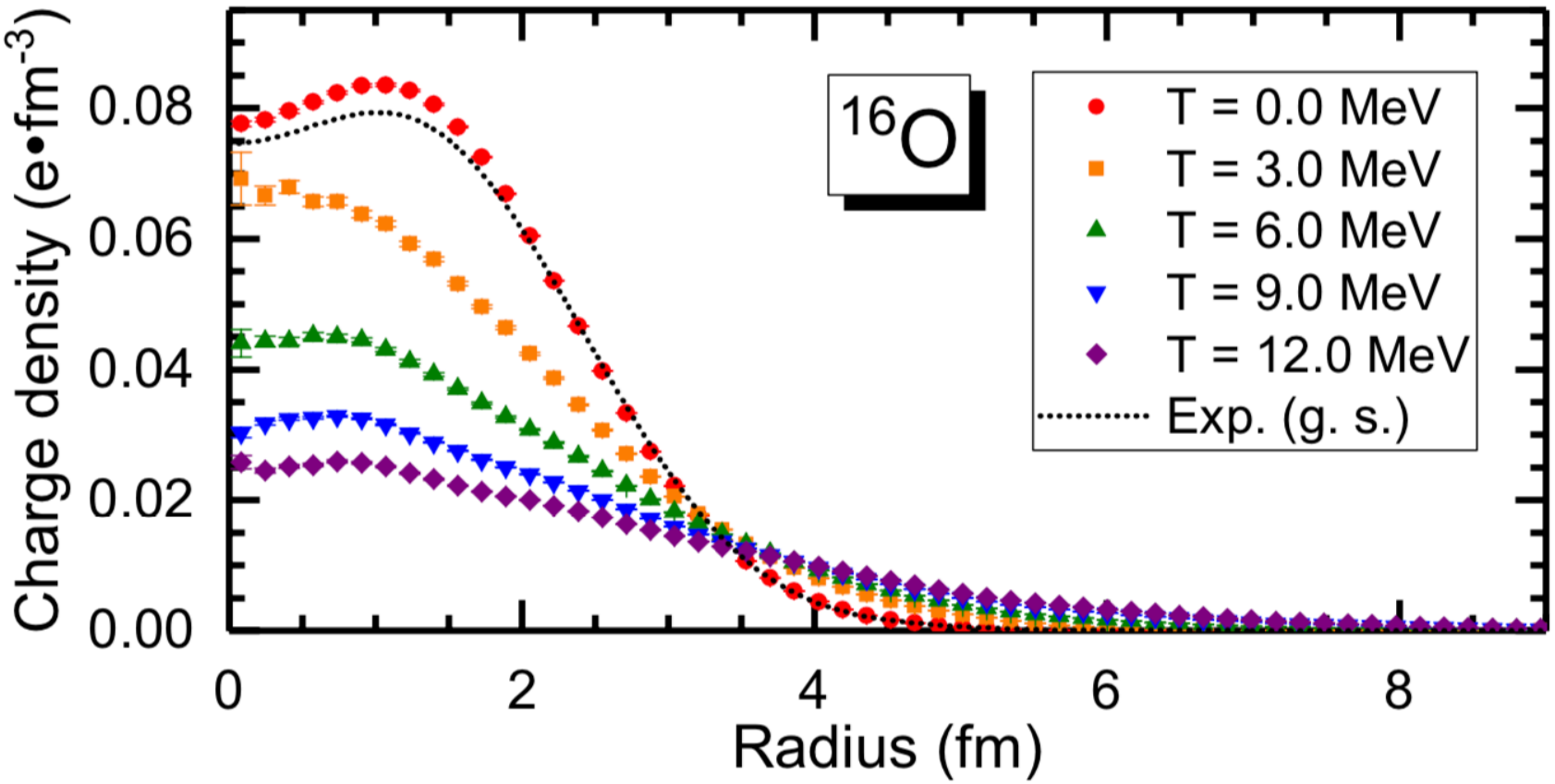


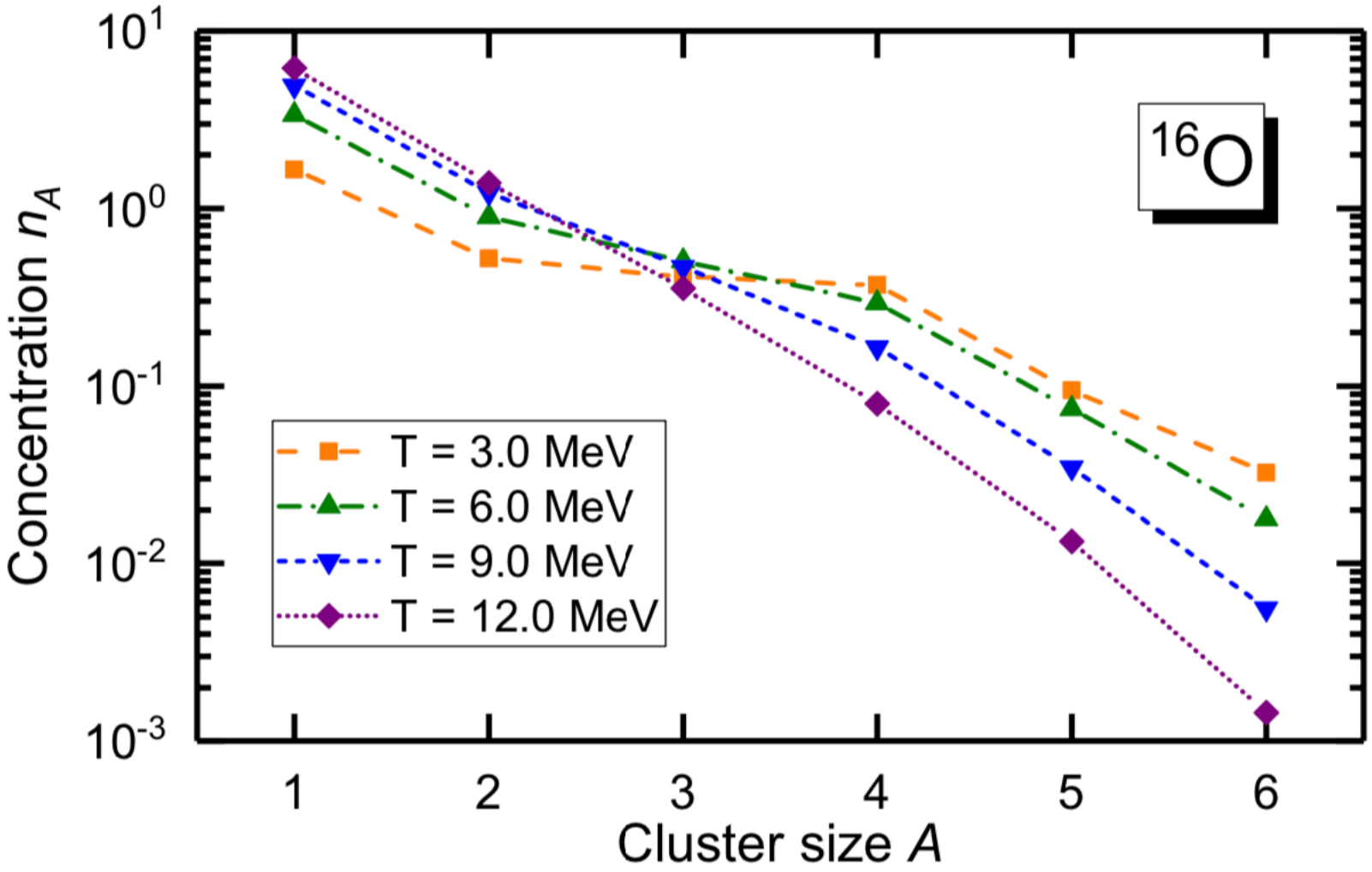
hybrid Monte Carlo
updates of auxiliary/pion fields

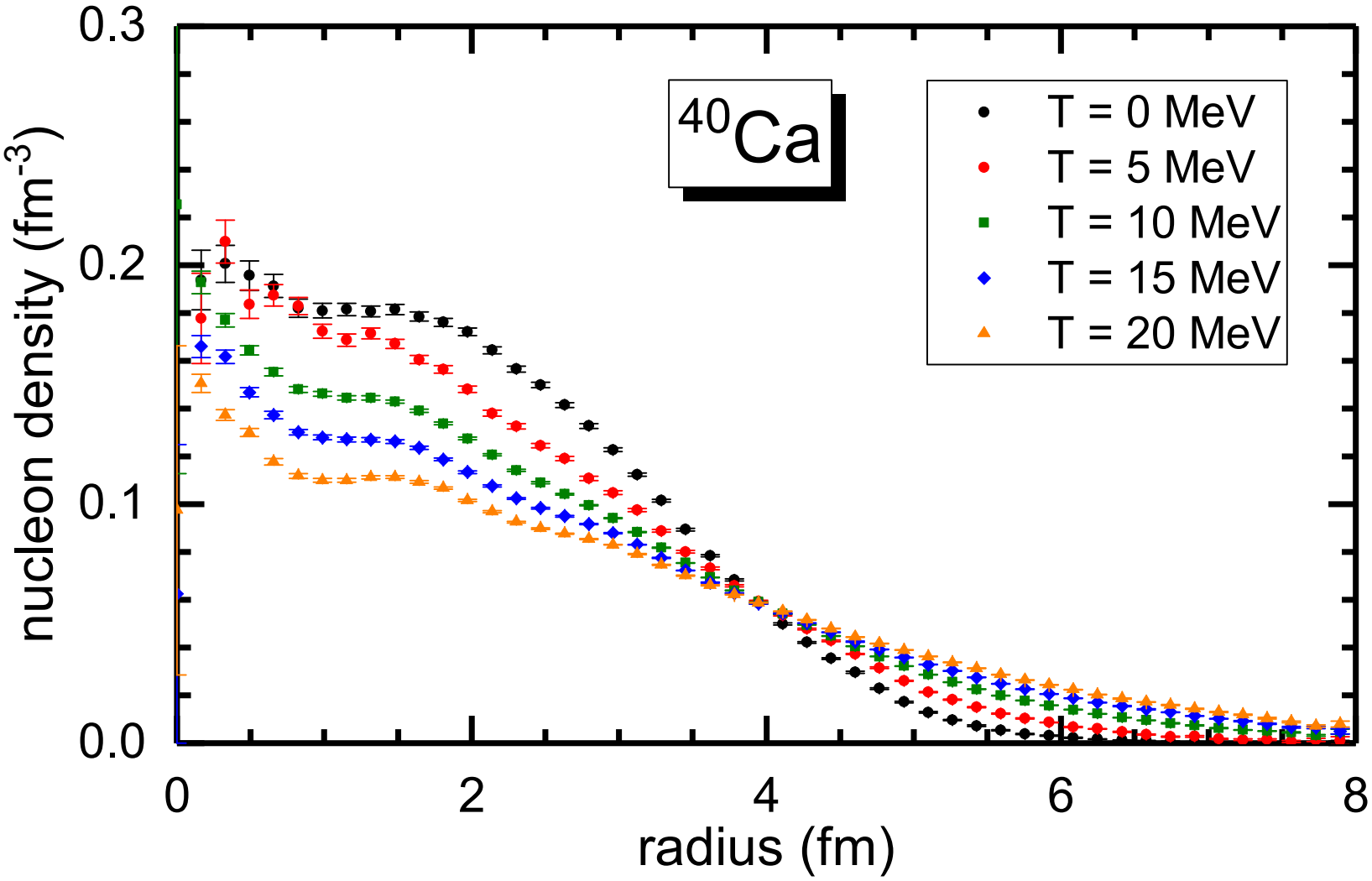


Figures by Bing-Nan Lu

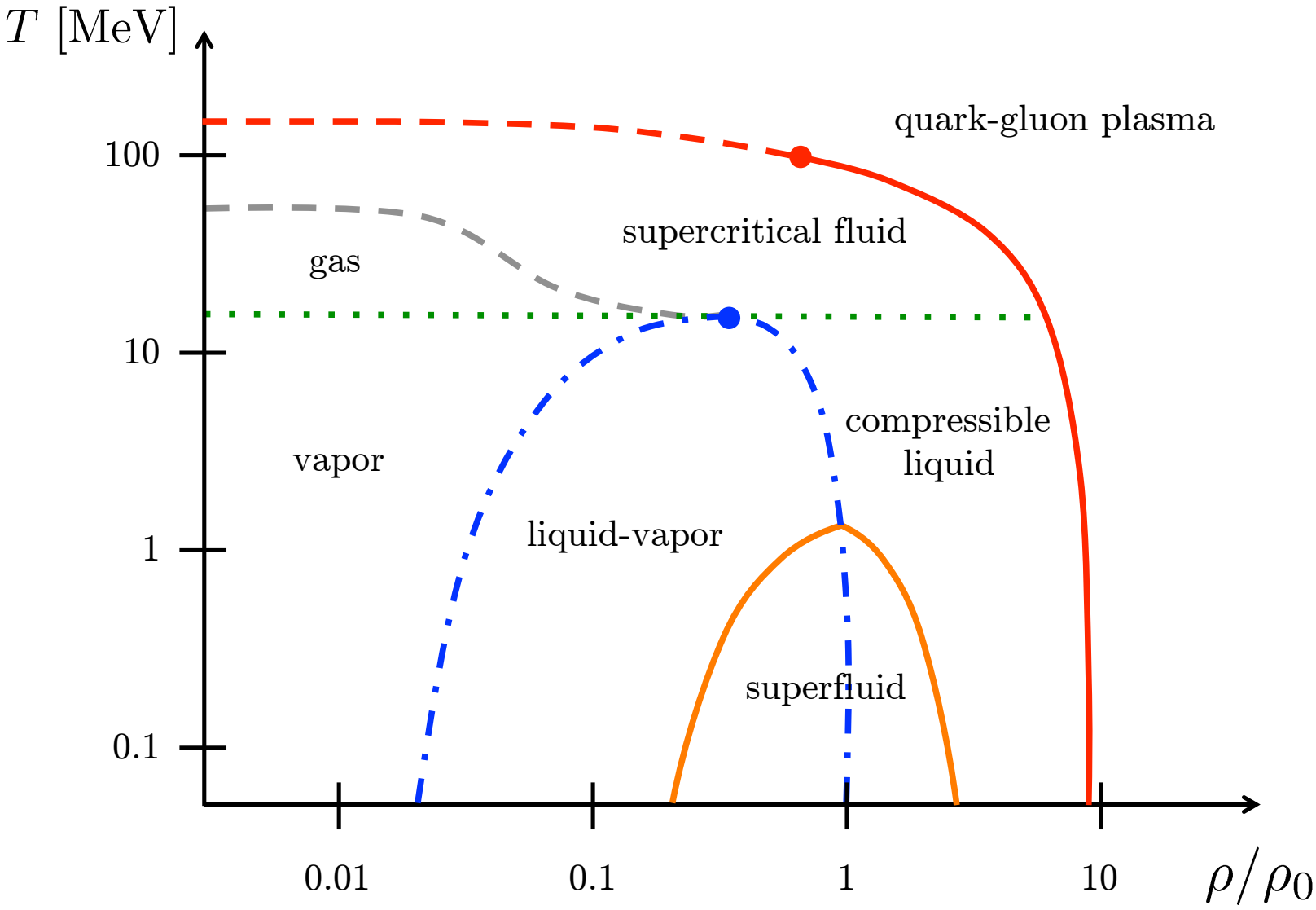

350
300
250
200
Kinetic energy K (MeV)
0
2
4
6
8
10
12
14
Temperature T (MeV)
L = 8
L = 9
$K = (3A\text{-}3)T/2$
^{16}O

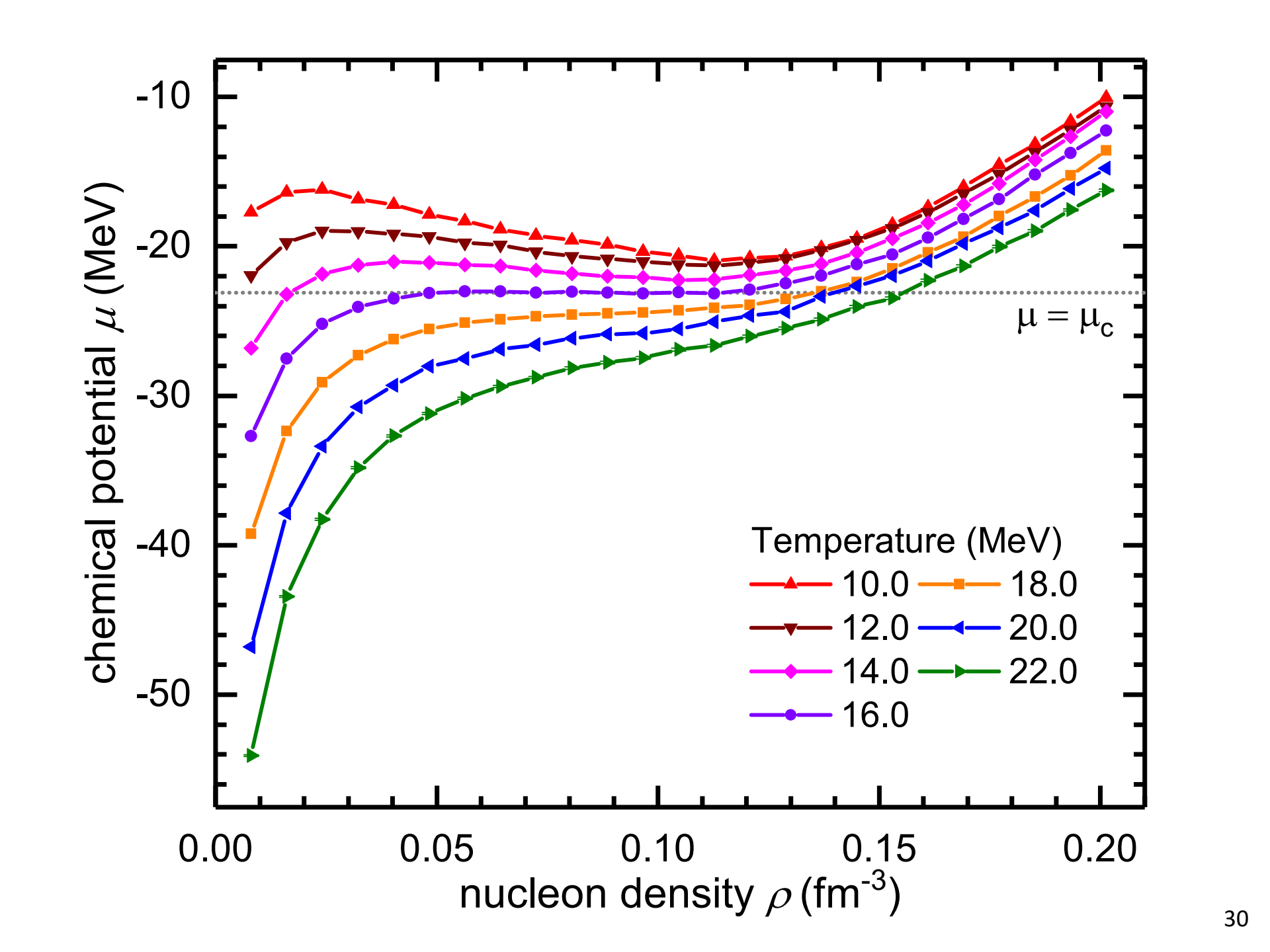

Charge density (e•fm^{-3})
0.00
0.02
0.04
0.06
0.08
0
2
4
6
8
Radius (fm)
^{16}O
T = 0.0 MeV
T = 3.0 MeV
T = 6.0 MeV
T = 9.0 MeV
T = 12.0 MeV
Exp. (g. s.)


Concentration n_A
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
1
2
3
4
5
6
Cluster size A
^{16}O
T = 3.0 MeV
T = 6.0 MeV
T = 9.0 MeV
T = 12.0 MeV

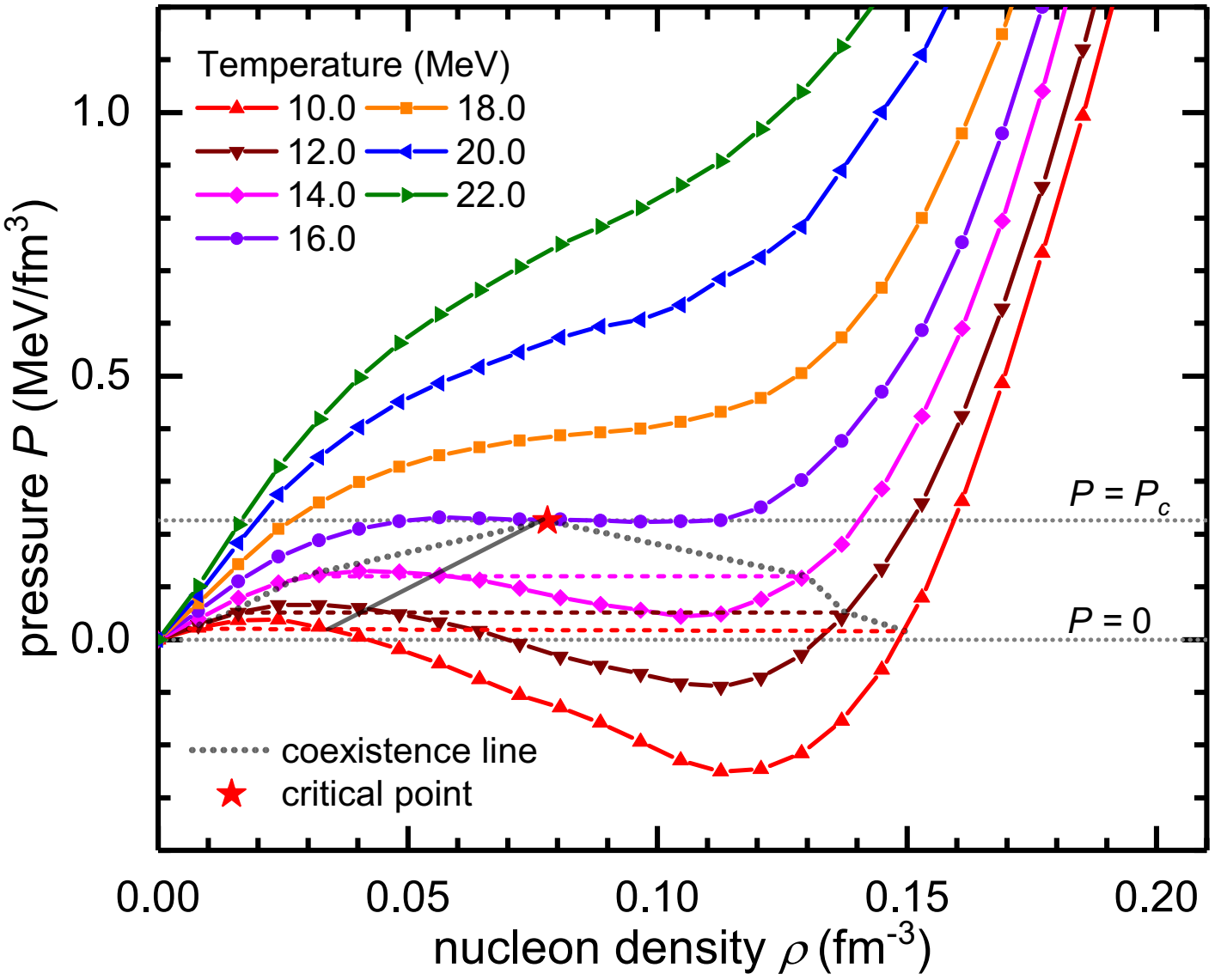

^{40}Ca
T = 0 MeV
T = 5 MeV
T = 10 MeV
T = 15 MeV
T = 20 MeV
nucleon density (fm^{-3})
radius (fm)
0.0
0.1
0.2
0.3
0
2
4
6
8

Phase diagram of symmetric nuclear matter

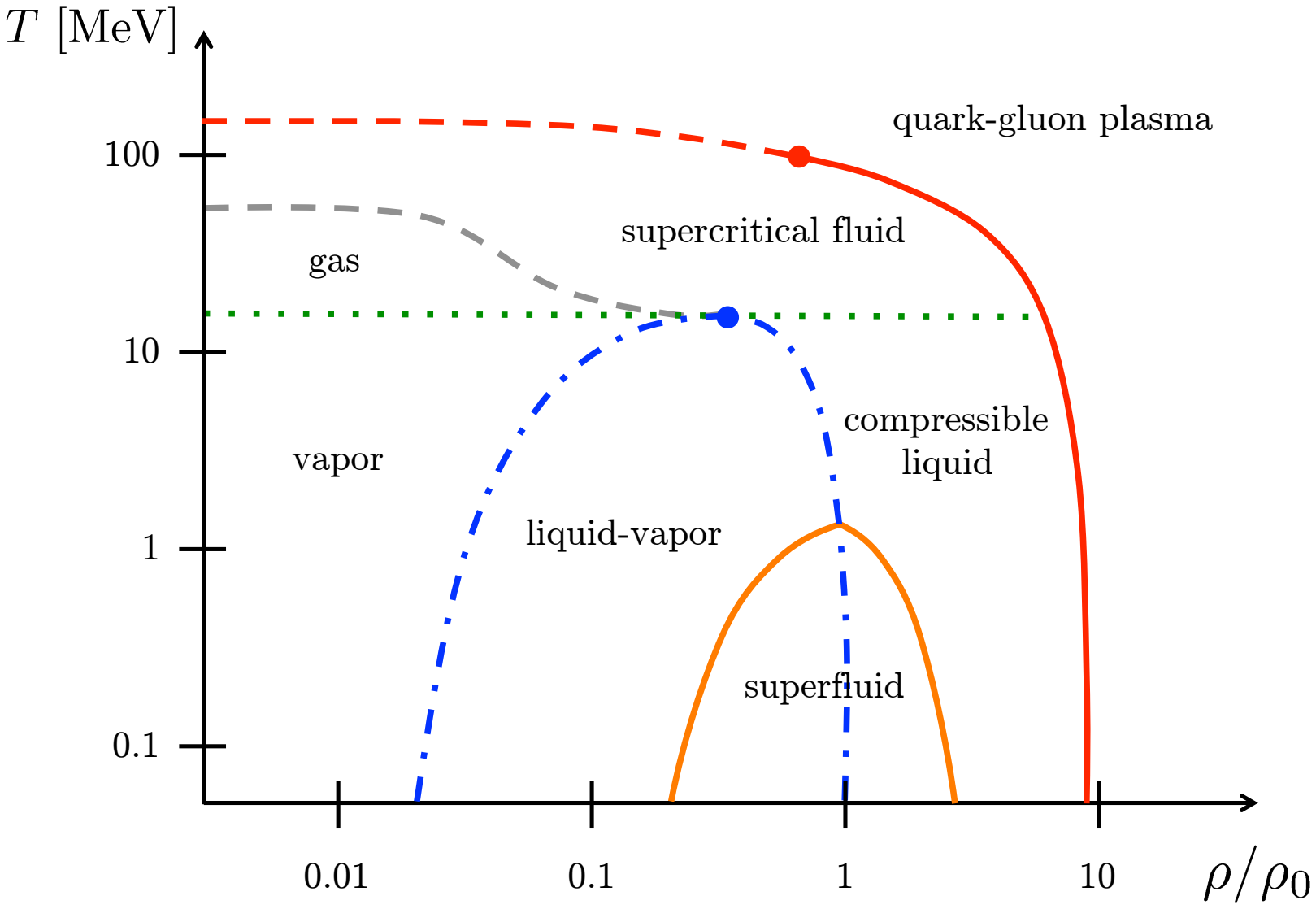



-10
-20
-30
-40
-50
chemical potential μ (MeV)
0.00
0.05
0.10
0.15
0.20
nucleon density ρ (fm^{-3})
$\mu = \mu_c$
Temperature (MeV)
10.0
18.0
12.0
20.0
14.0
22.0
16.0

Experiment: $T_c = 15.0(3)\,\mathrm{MeV}, P_c = 0.31(7)\,\mathrm{MeV/fm^{-3}}, \rho_c = 0.06(2)\,\mathrm{fm^{-3}}$



Phase diagram of symmetric nuclear matter



Inelastic reactions

We would like to develop a first principles approach to compute inelastic reactions. We envision a typical scattering experiment where the initial state is two colliding clusters but we are well above the inelastic threshold and the outgoing state can have many separate clusters.

If our detector only counts outgoing states with two clusters, the same as our two initial clusters, then we can generalize the notion of elastic scattering above the inelastic threshold by considering complex phase shifts which record the loss of probability into other unmeasured outgoing states.

This non-unitary time evolution can be exactly reproduced in an effective Hamiltonian with a non-Hermitian interaction. The interactions of this effective Hamiltonian is called an optical potential.

Work in progress: Hicks, Elhatisari, Rupak, Epelbaum, Krebs, D.L., Li, Lu, Meißner, Rusetsky

We can compute the effective Hamiltonian in the following manner:

Feshbach, Annals of Physics 5, 357 (1958)

We consider a projection operator P that projects onto the space that contains all of our asymptotic two-cluster states. Let Q be the projection operator onto the rest of the Hilbert space.

$$P + Q = 1$$

Eigenstates of the Hamiltonian H can be broken into two parts

$$\begin{bmatrix} PHP & PHQ \\ QHP & QHQ \end{bmatrix} \begin{bmatrix} P\psi \\ Q\psi \end{bmatrix} = E \begin{bmatrix} P\psi \\ Q\psi \end{bmatrix}$$

$$\begin{bmatrix} PHP & PHQ \\ QHP & QHQ \end{bmatrix} \begin{bmatrix} P\psi \\ Q\psi \end{bmatrix} = E \begin{bmatrix} P\psi \\ Q\psi \end{bmatrix}$$

$$PHP\psi + PHQ\psi = EP\psi$$
$$QHP\psi + QHQ\psi = EQ\psi$$

We can rearrange the last equation as

$$Q\psi = (E - QHQ + i\epsilon)^{-1} QHP\psi$$

This can used to define the effective Hamiltonian

$$H_{\text{eff}} P\psi = EP\psi$$
$$H_{\text{eff}} = PHP + PHQ(E - QHQ + i\epsilon)^{-1} QHP$$

See also

D. Agadjanov, Döring, Mai, Meißner, Rusetsky, JHEP 43, 2016 (2016)

Model #1

Consider a field theory in one spatial dimension where two particles of type A can scatter at a point vertex and convert in two particles of type B and vice versa. The masses of all the particles are equal.

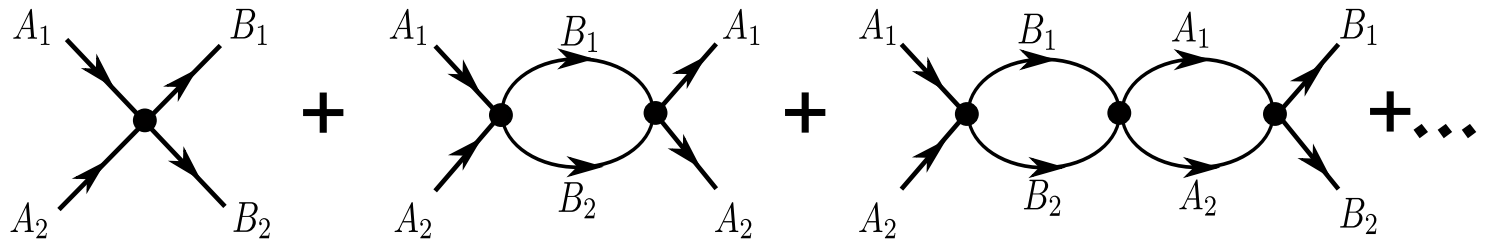


Diagram courtesy of S. Elhatisari

Let the coefficient of the point interaction be C.

1. Green's function method in full space

We compute the T-matrix using the LSZ formula

$$\lim_{\epsilon\to 0^+} \langle \vec{p}' | \, T(E_{\vec{p}} + i\epsilon) \, | \vec{p} \rangle = \lim_{\epsilon\to 0^+} \left[\langle \vec{p}' | \, G(E_{\vec{p}} + i\epsilon) \, | \vec{p} \rangle \, (i\epsilon)^2 - \delta^{(d)}(\vec{p}' - \vec{p})(i\epsilon) \right],$$

$$\delta^{(d)}(\vec{0}) \to L^d/(2\pi)^d$$

See, for example,

Rupak, D.L., PRL 111, 032502 (2013)

2. Green's function method using effective Hamiltonian

Same Green's function method, but this time we apply it to the effective Hamiltonian that contains our optical potential.

$$\lim_{\epsilon\to 0^+} \langle \vec{p}' | \, T_{\rm eff}(E_{\vec{p}} + i\epsilon) \, | \vec{p} \rangle = \lim_{\epsilon\to 0^+} \langle \vec{p}' | \, G_{\rm eff}(E_{\vec{p}} + i\epsilon) \, | \vec{p} \rangle \, (i\epsilon)^2 - \delta^{(d)}(\vec{p}' - \vec{p})(i\epsilon),$$

3. Applying Lüscher's method to effective Hamiltonian

We apply Lüscher's method to the effective Hamiltonian. Because the energy is complex, the corresponding momenta and phase shifts will be complex also.

4. Applying hardwall boundaries to effective Hamiltonian

We apply hardwall boundary conditions to the effective Hamiltonian.

5. Optical potential projection method

Instead of using the entire Q space to compute the interaction

$$PHQ(E - QHQ + i\epsilon)^{-1}QHP$$

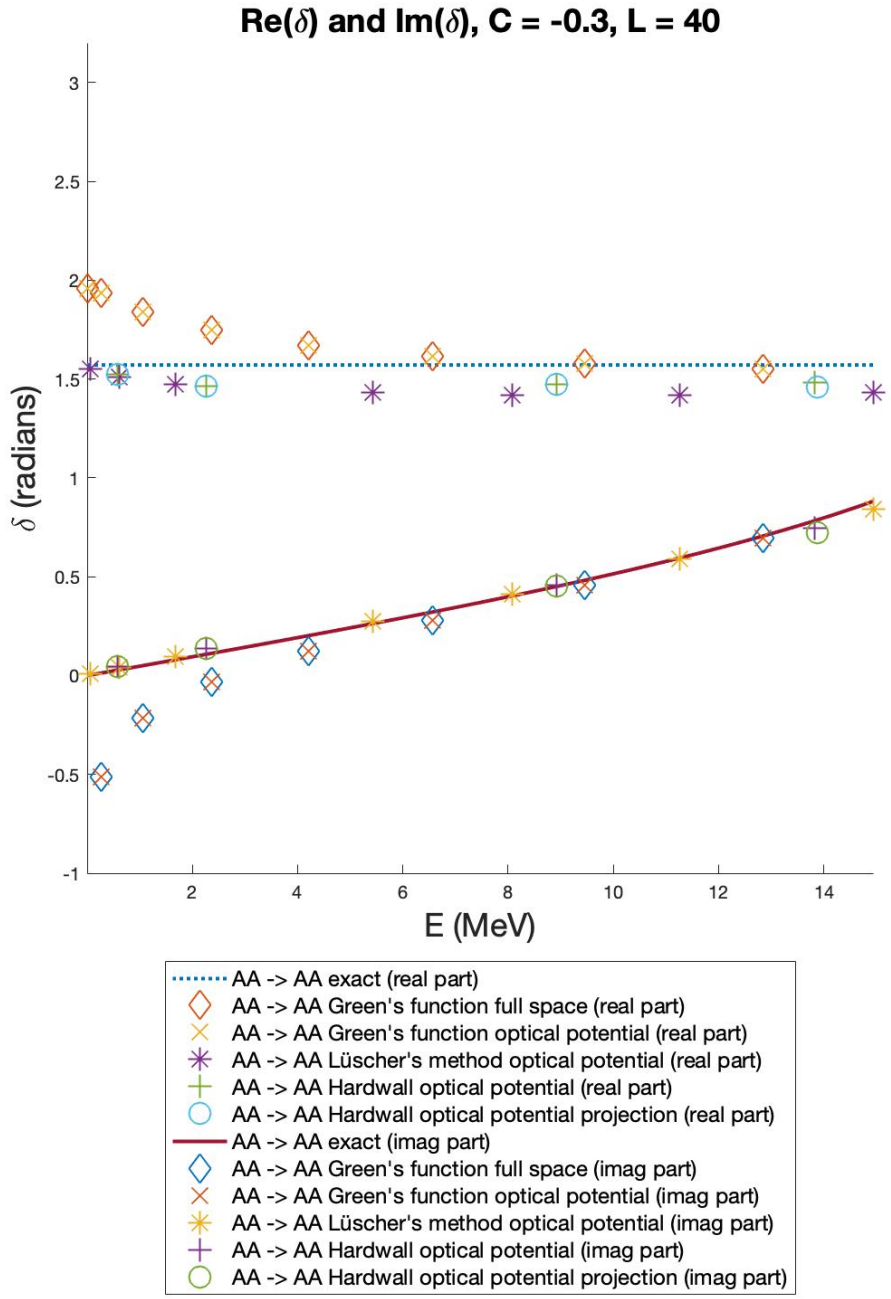
For each pair of vectors v_P and w_P in the P space, we use

$$w_P^\dagger HR(E - RHR + i\epsilon)^{-1} RHv_P \approx w_P^\dagger HQ(E - QHQ + i\epsilon)^{-1} QHv_P$$

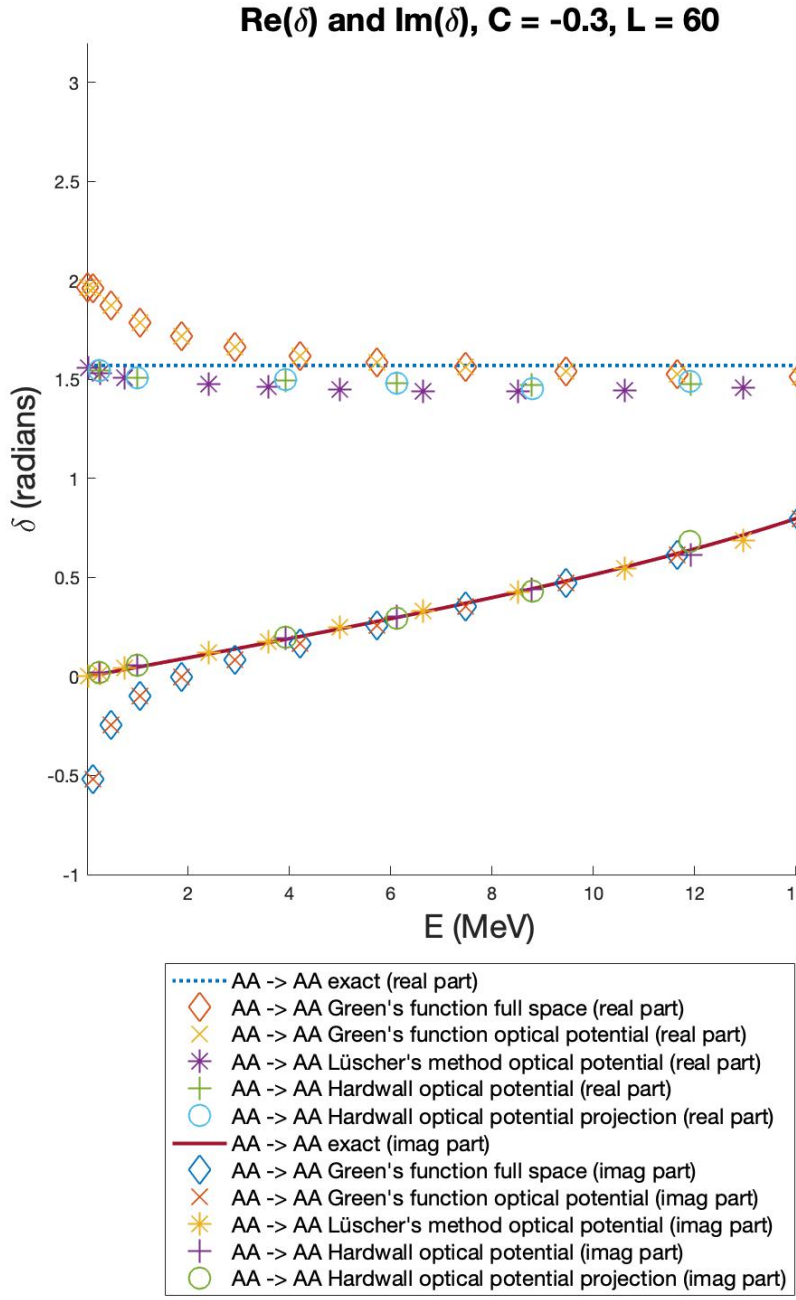
where R is a projection operator onto a much smaller space of vectors generated by Euclidean time evolution from vectors v_P and w_P. These vectors have the form

$$\exp(-Ht)v_P, \exp(-2Ht)v_P, \exp(-3Ht)v_P, \cdots$$

$$\exp(-Ht)w_P, \exp(-2Ht)w_P, \exp(-3Ht)w_P, \cdots$$



preliminary



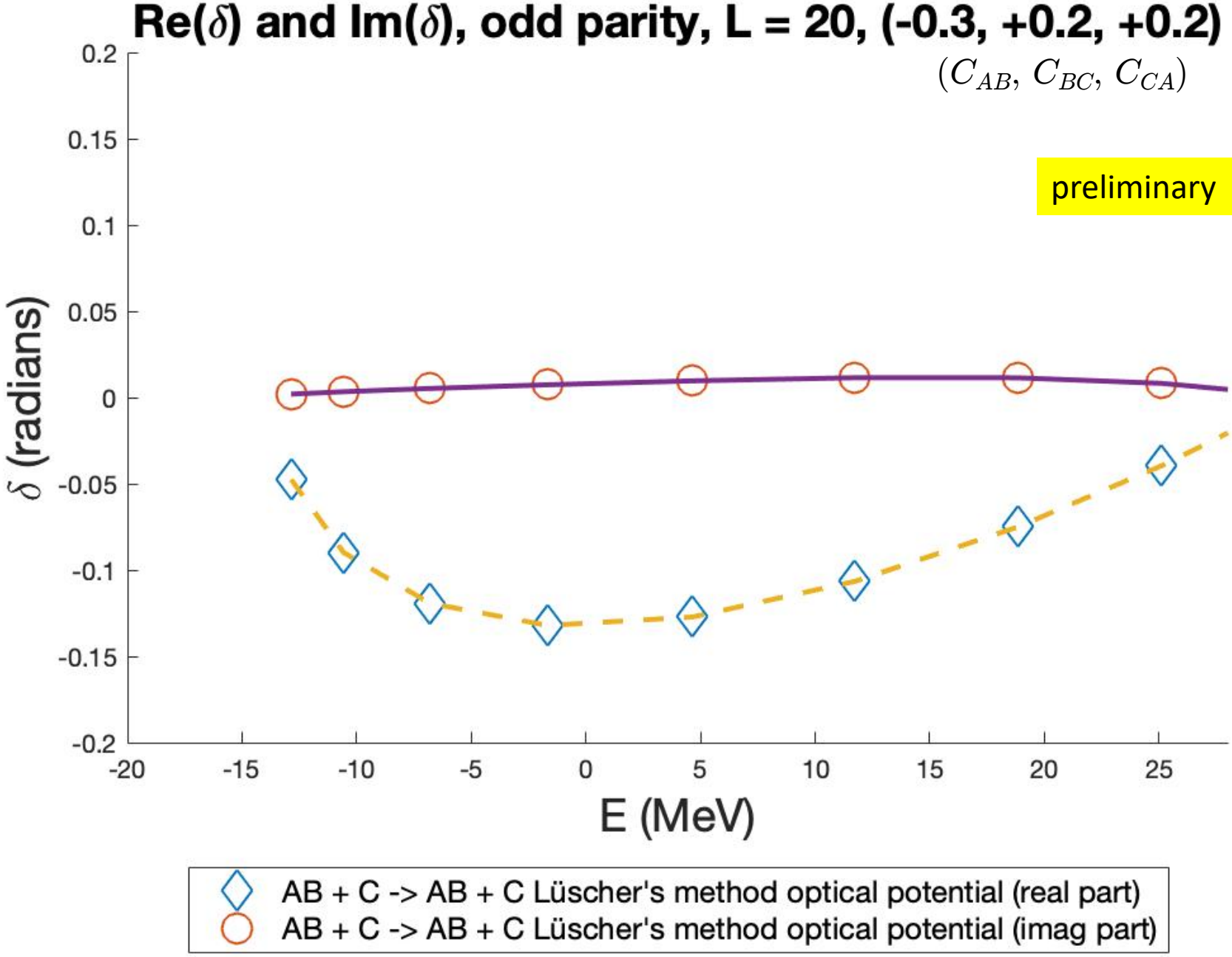
preliminary

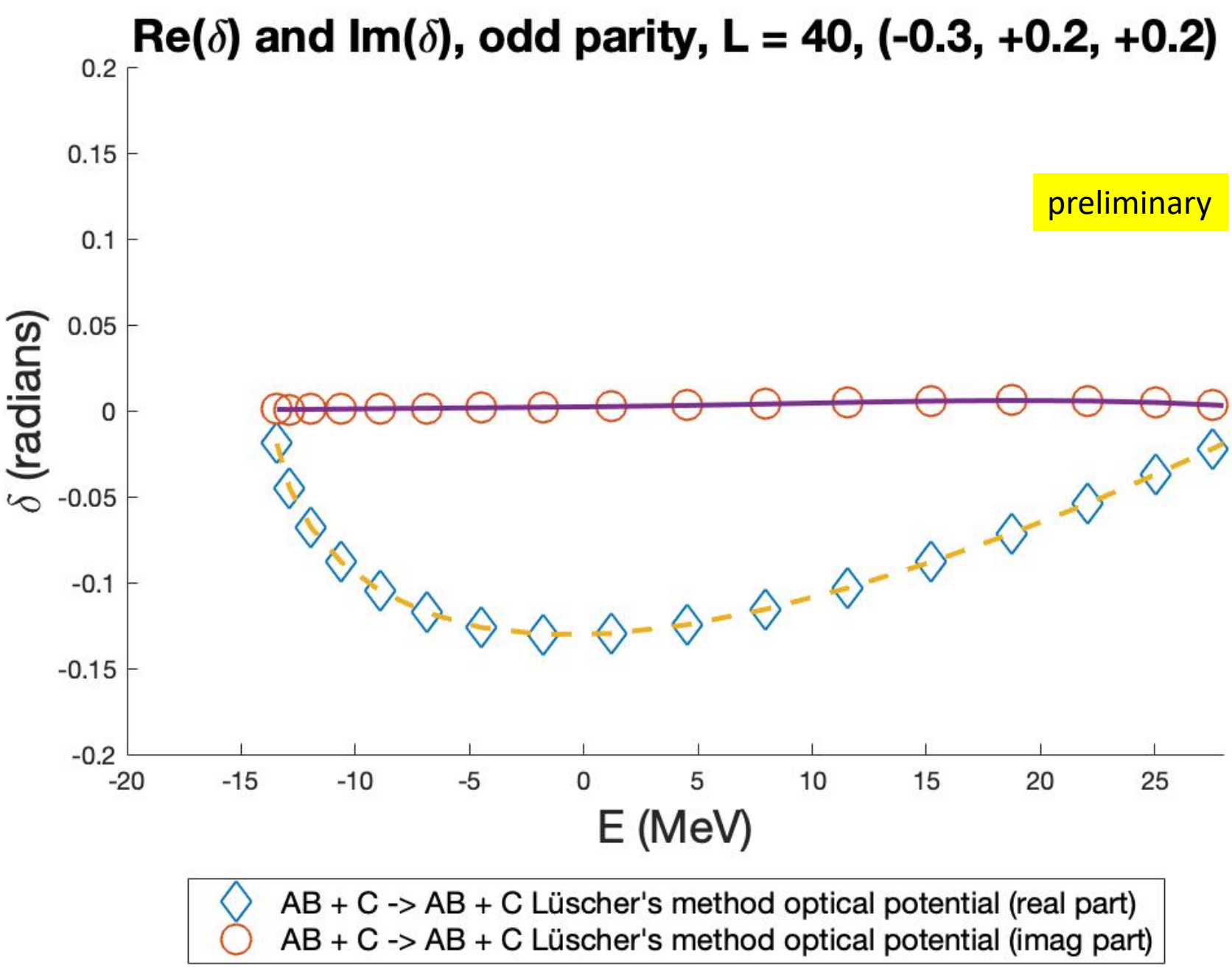
Model #2

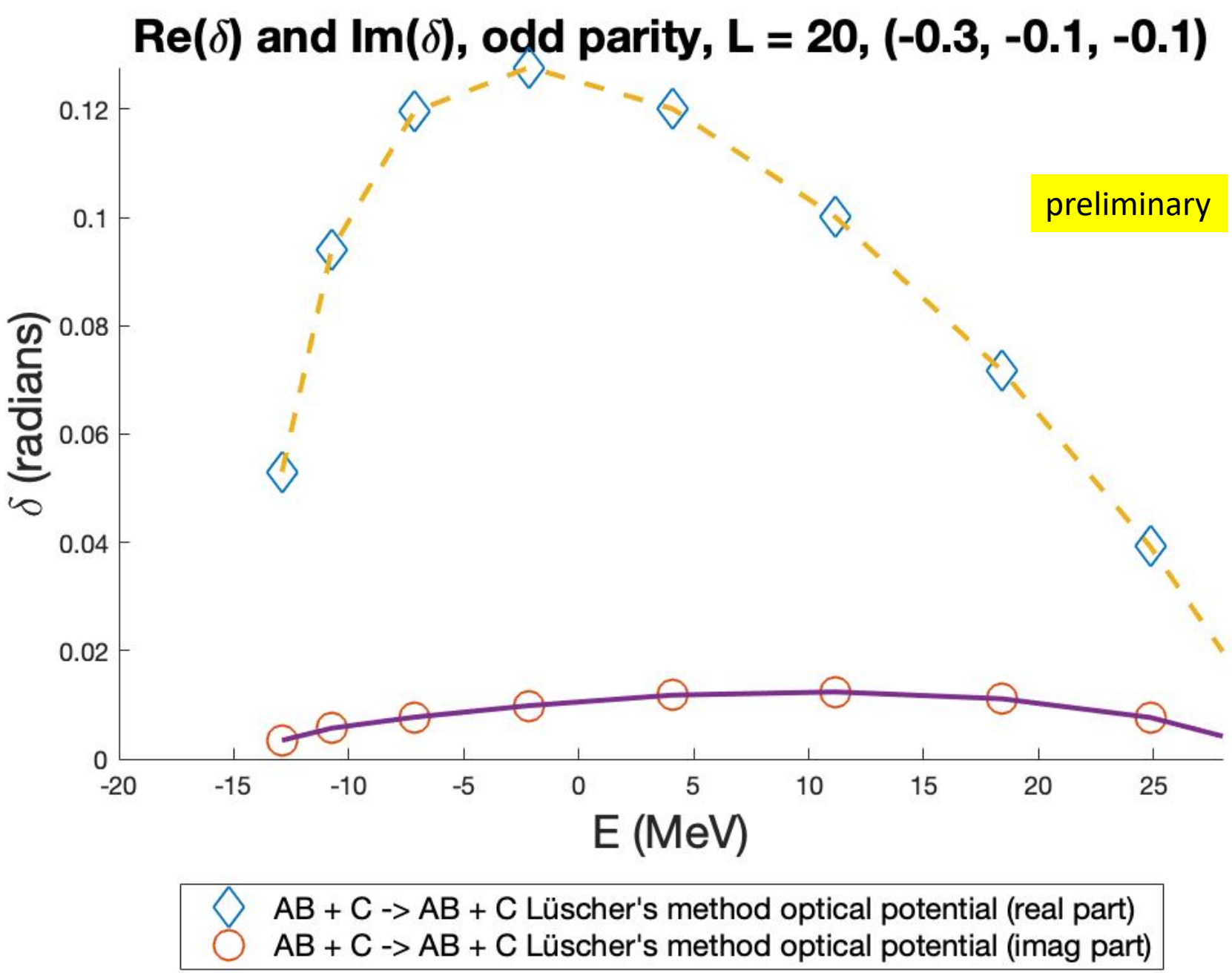
Consider a field theory in one spatial dimension with three particles A, B,C with pairwise point-like contact interactions of strength C_{AB}, C_{BC}, C_{CA}. The masses of all particles are equal.

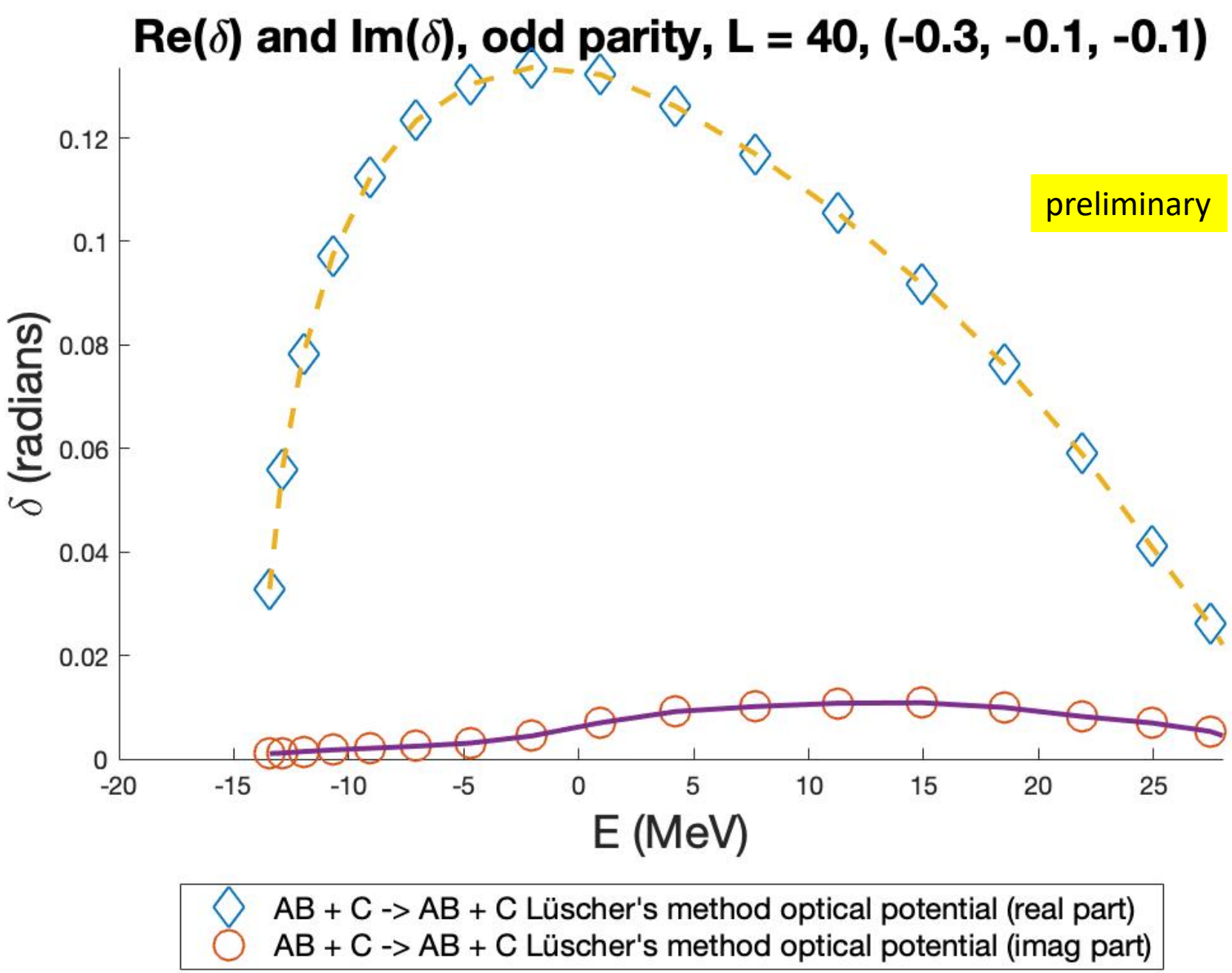
We now compute the optical potential for the scattering of

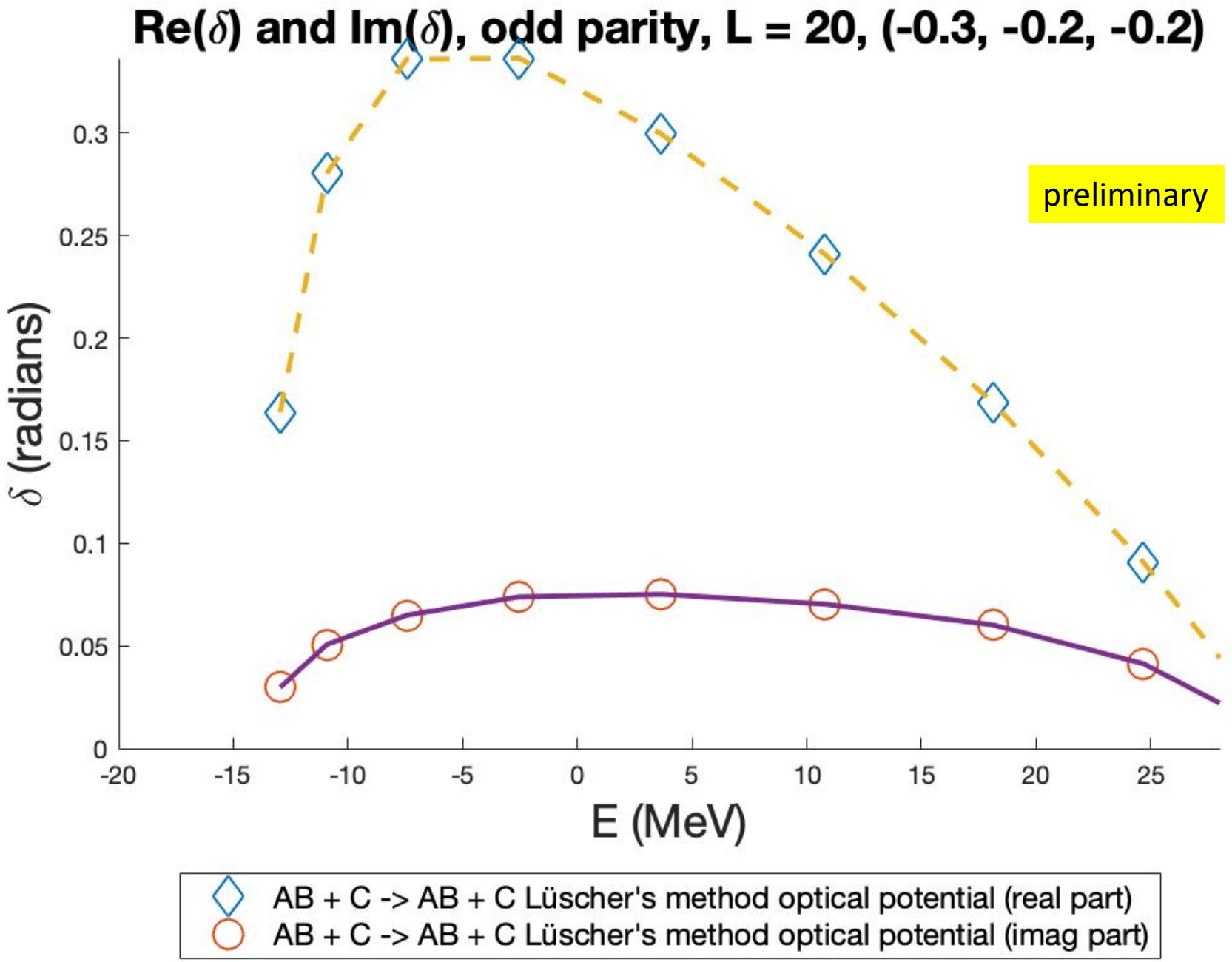
dimer AB + particle C

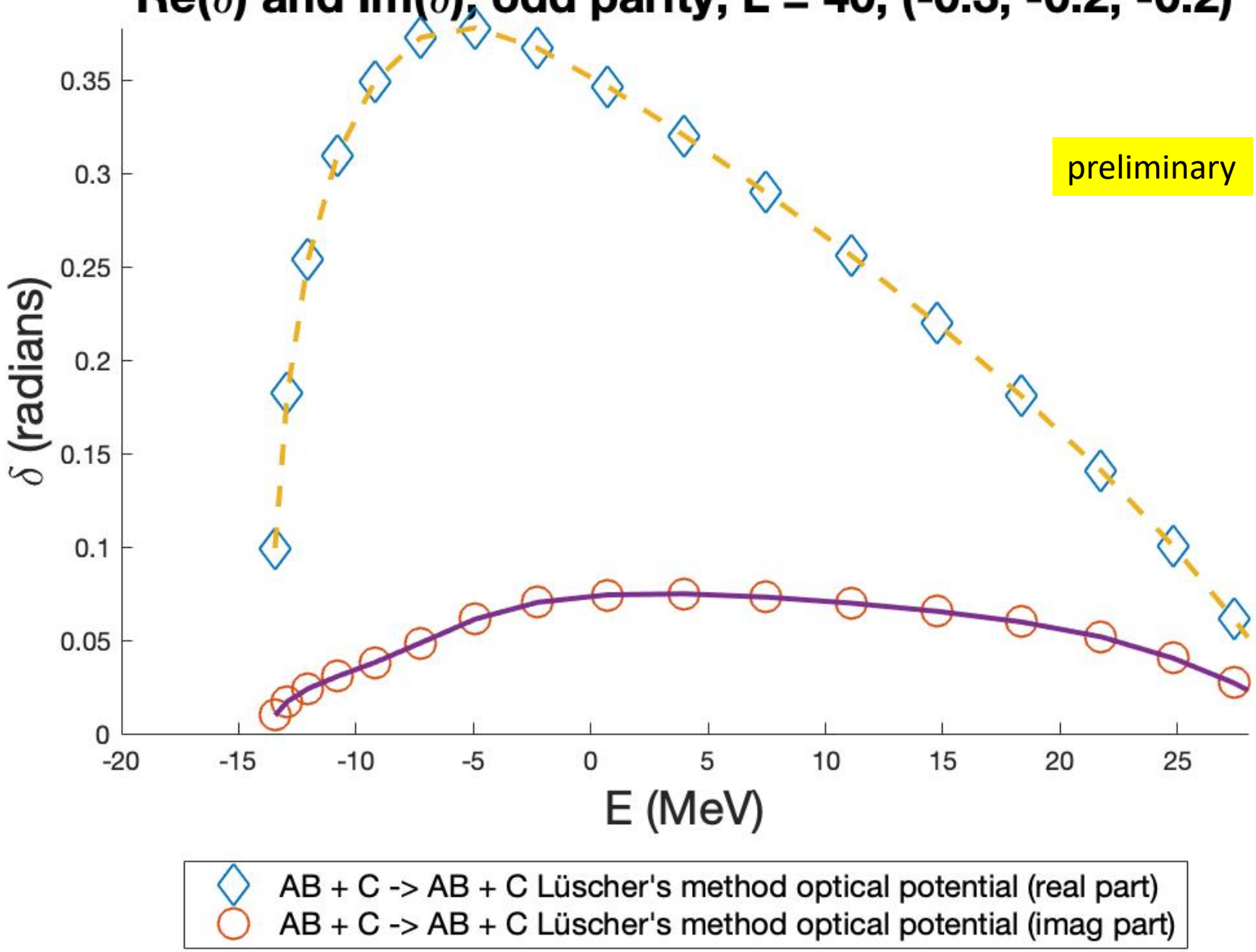

Re(δ) and Im(δ), odd parity, L = 20, (-0.3, +0.2, +0.2)
(C_{AB}, C_{BC}, C_{CA})
preliminary
δ (radians)
E (MeV)
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-20
-15
-10
-5
0
5
10
15
20
25
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)

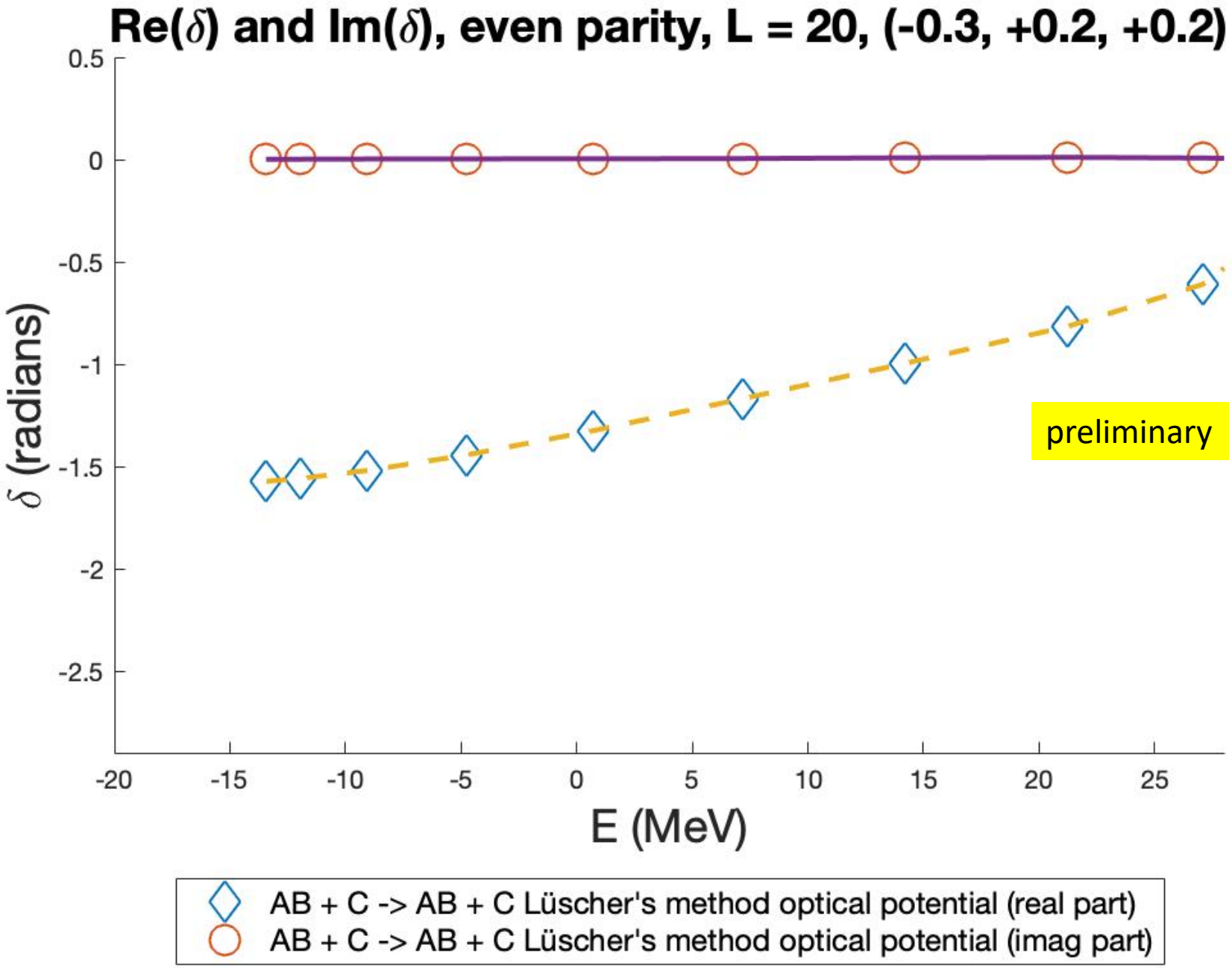

Re(δ) and Im(δ), odd parity, L = 40, (-0.3, +0.2, +0.2)
preliminary
δ (radians)
E (MeV)
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-20
-15
-10
-5
0
5
10
15
20
25
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)

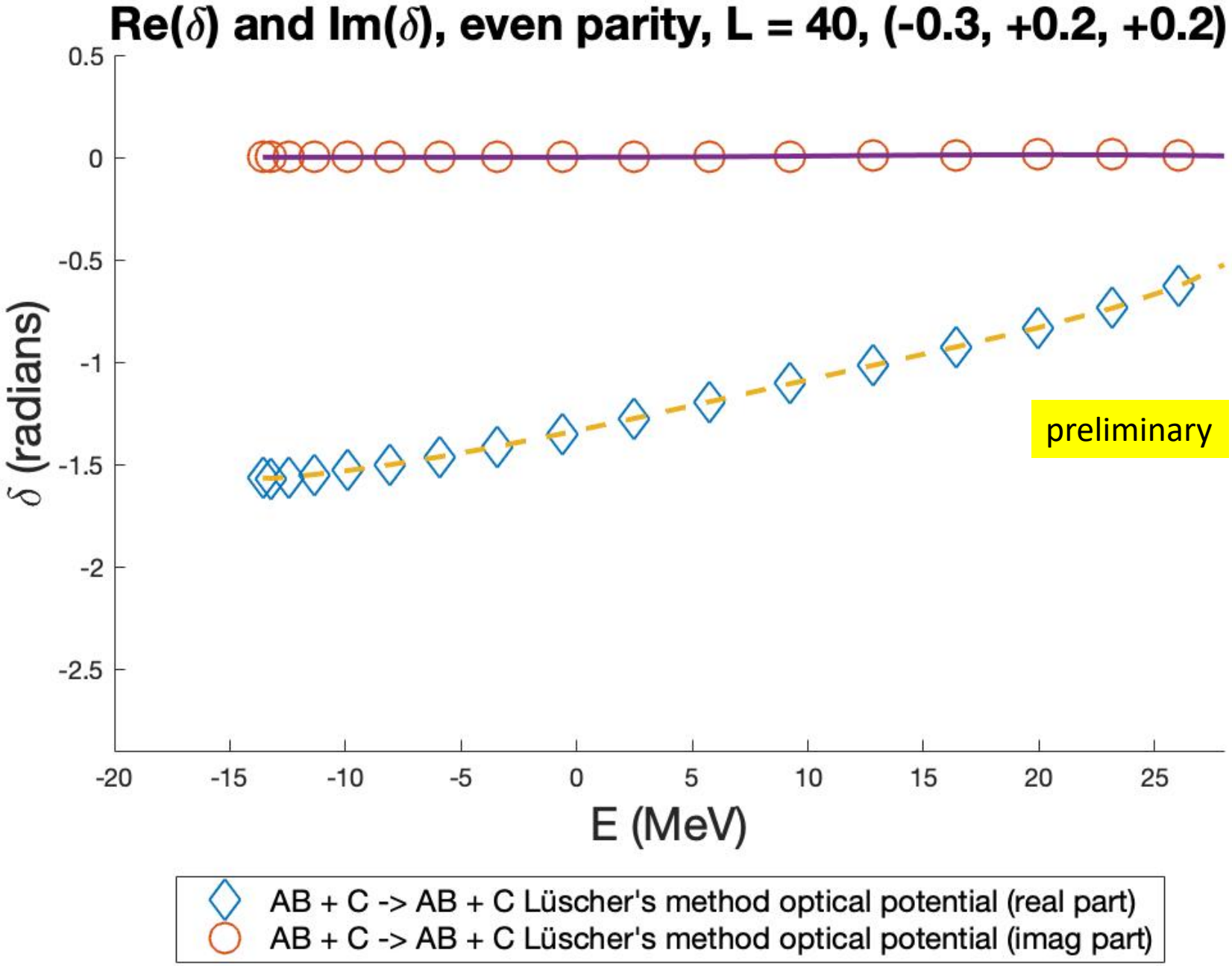

Re(δ) and Im(δ), odd parity, L = 20, (-0.3, -0.1, -0.1)
preliminary
δ (radians)
0.12
0.1
0.08
0.06
0.04
0.02
0
-20
-15
-10
-5
0
5
10
15
20
25
E (MeV)
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)

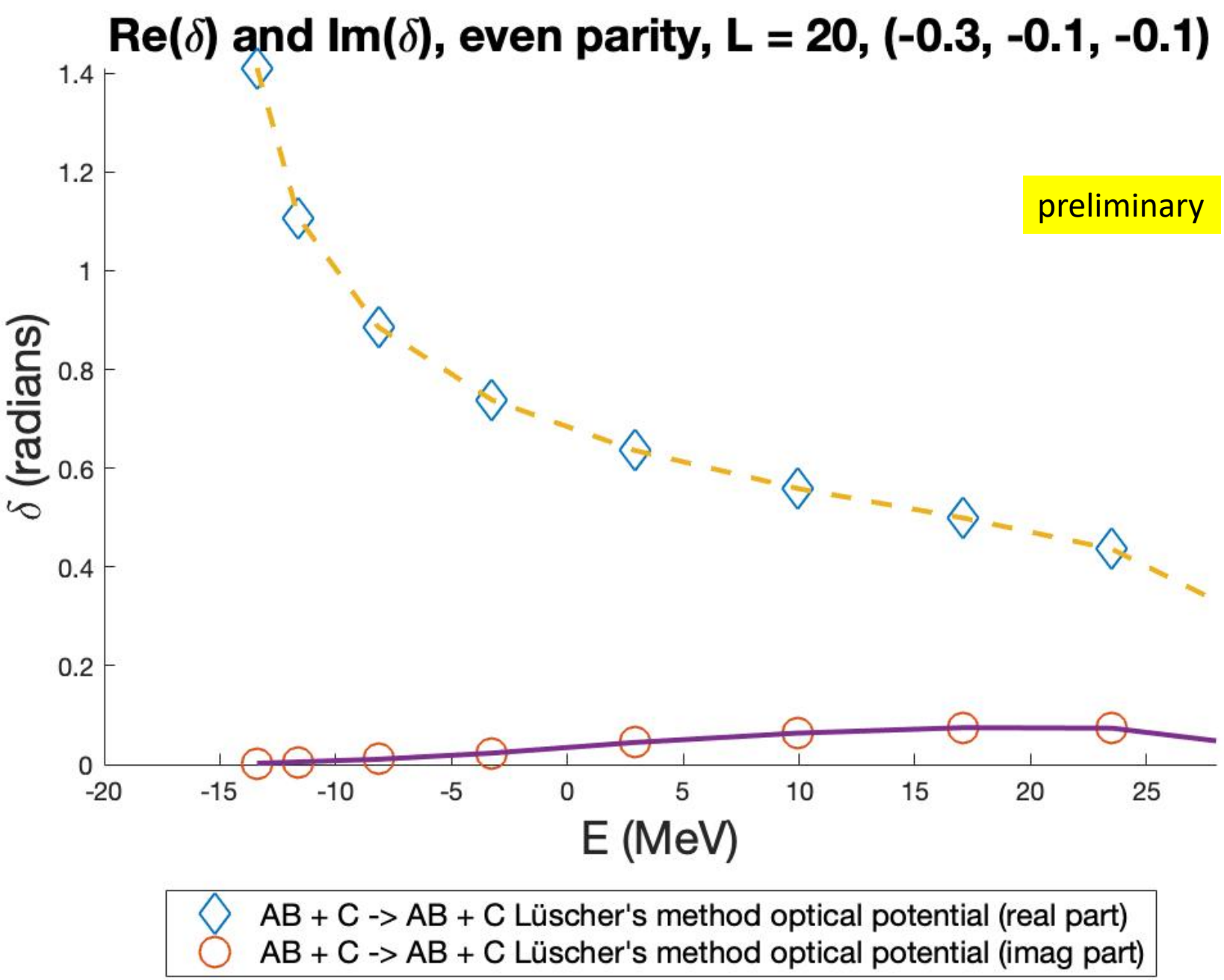

Re(δ) and Im(δ), odd parity, L = 40, (-0.3, -0.1, -0.1)
preliminary
δ (radians)
0.12
0.1
0.08
0.06
0.04
0.02
0
-20
-15
-10
-5
0
5
10
15
20
25
E (MeV)
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)

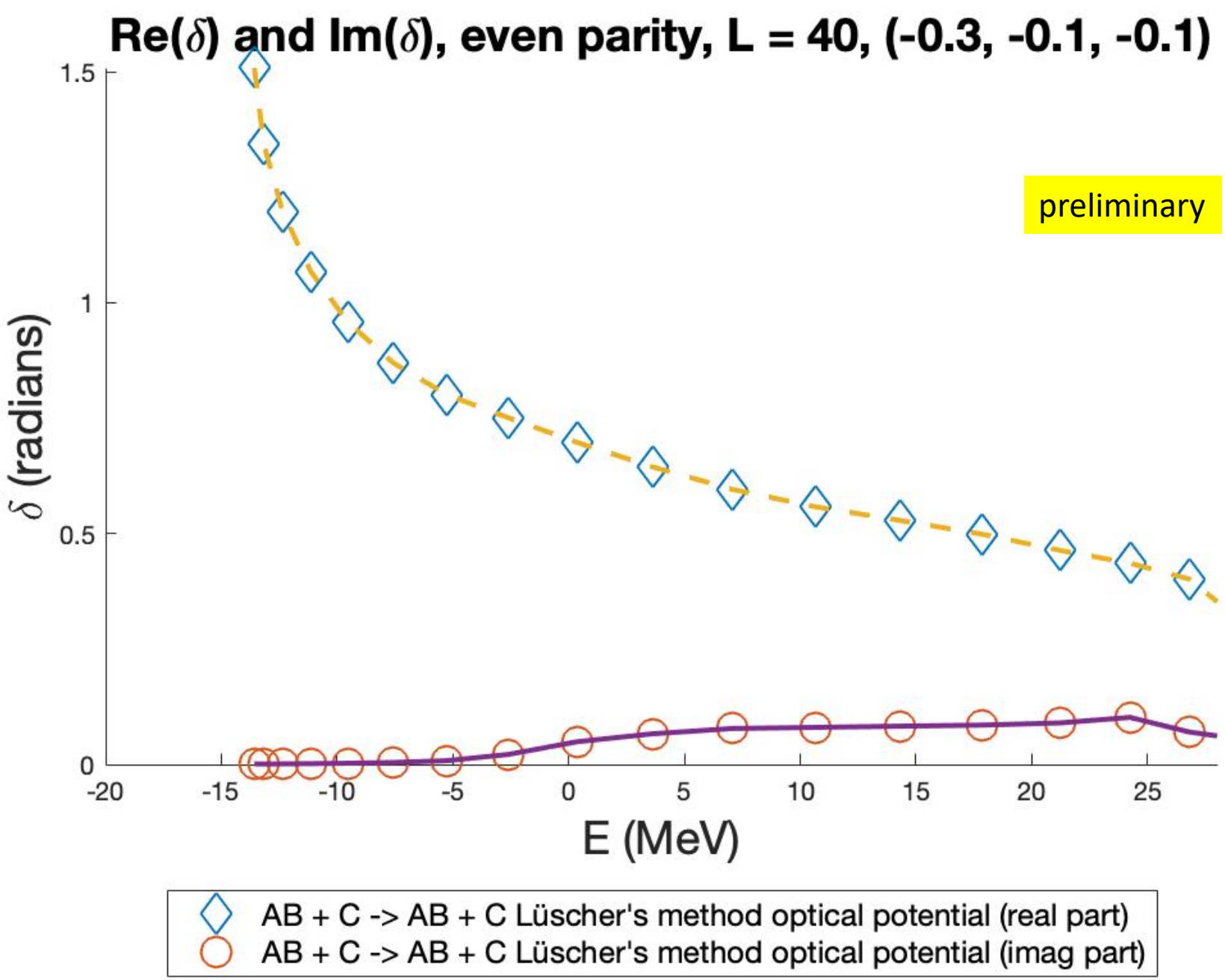

Re(δ) and Im(δ), odd parity, L = 20, (-0.3, -0.2, -0.2)
preliminary
δ (radians)
0
0.05
0.1
0.15
0.2
0.25
0.3
-20
-15
-10
-5
0
5
10
15
20
25
E (MeV)
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)

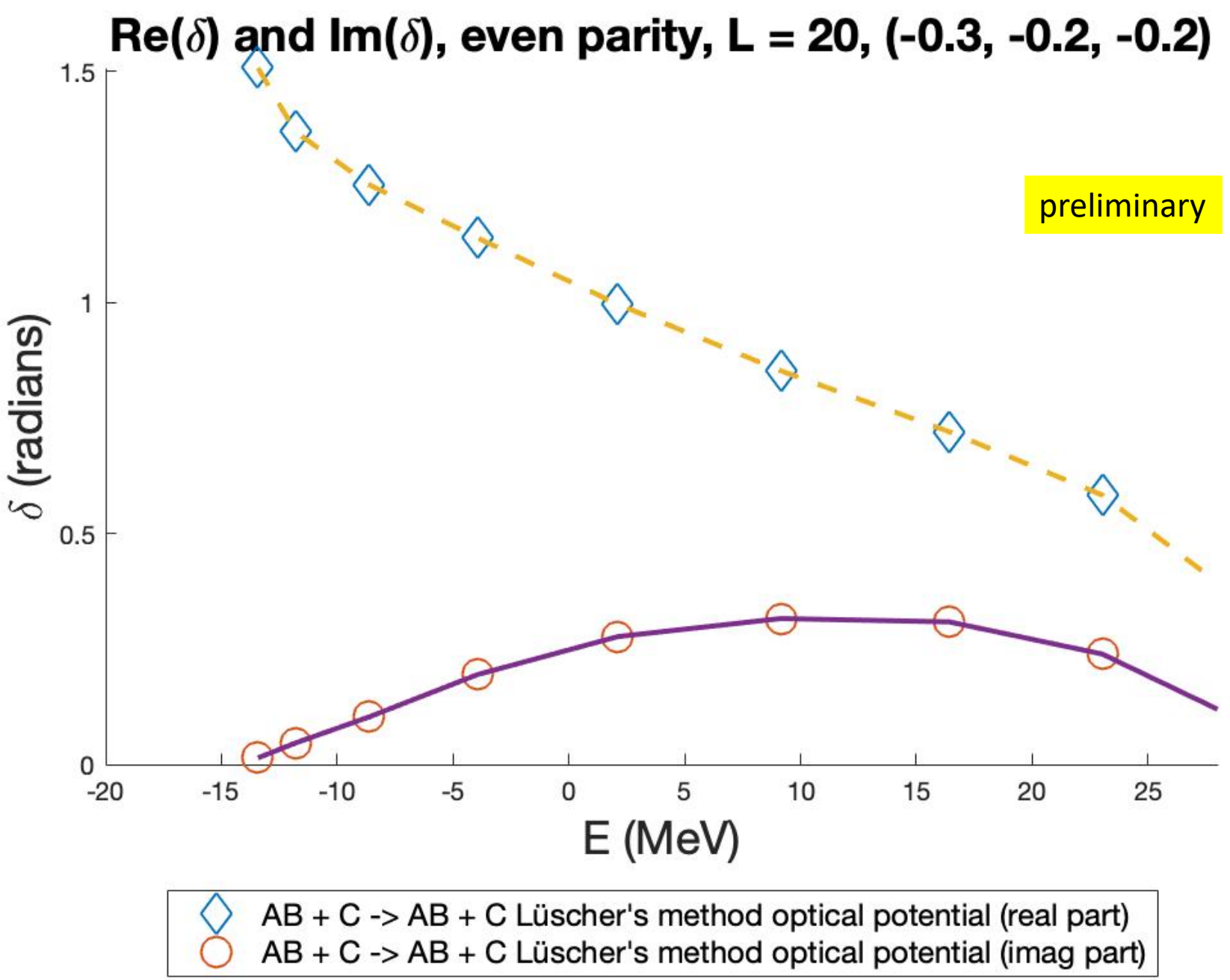

Re(δ) and Im(δ), odd parity, L = 40, (-0.3, -0.2, -0.2)
preliminary
δ (radians)
E (MeV)
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-20
-15
-10
-5
0
5
10
15
20
25
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)

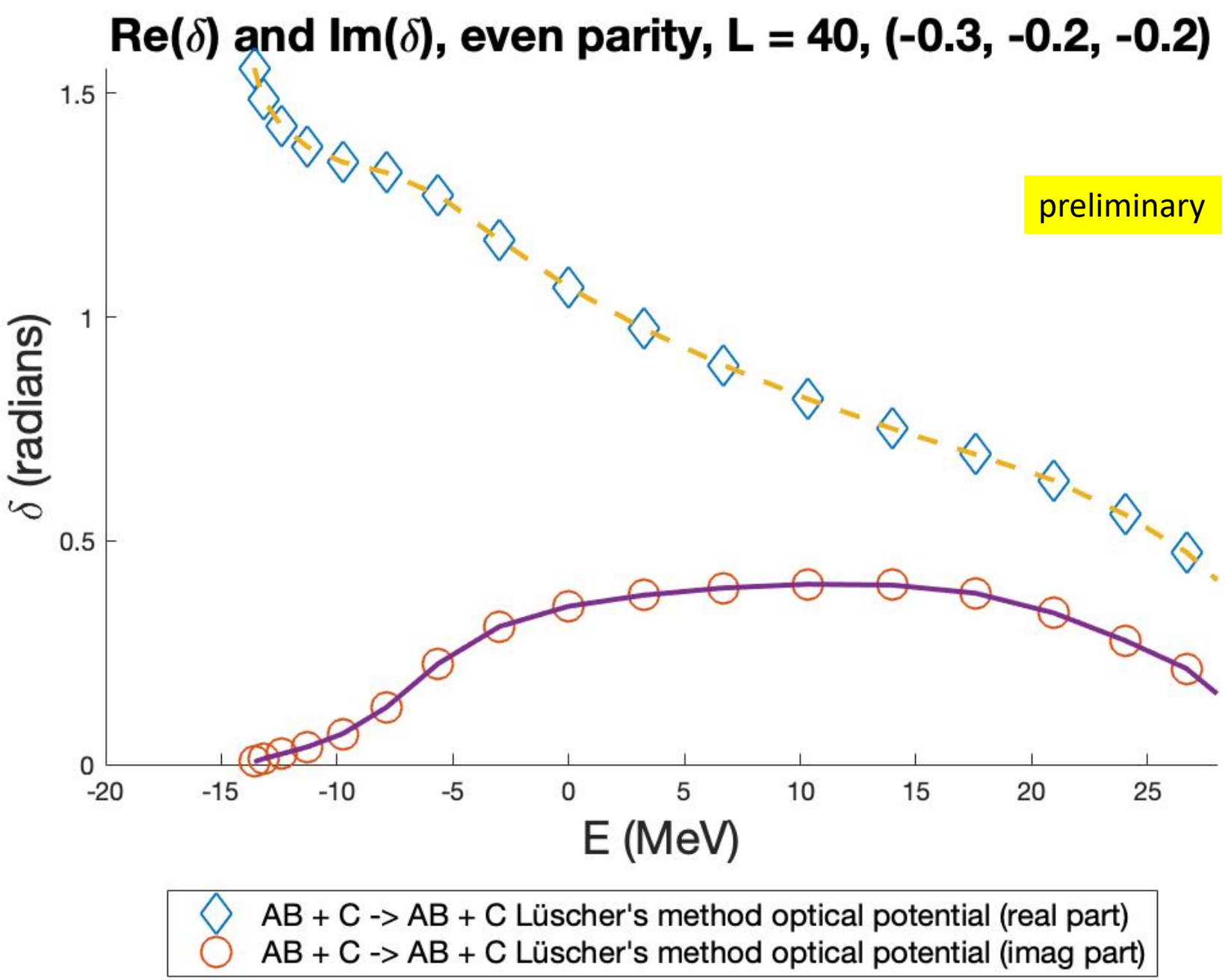

Re(δ) and Im(δ), even parity, L = 20, (-0.3, +0.2, +0.2)
δ (radians)
E (MeV)
0.5
0
-0.5
-1
-1.5
-2
-2.5
-20
-15
-10
-5
0
5
10
15
20
25
preliminary
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)


Re(δ) and Im(δ), even parity, L = 40, (-0.3, +0.2, +0.2)
0.5
0
-0.5
-1
-1.5
-2
-2.5
δ (radians)
-20
-15
-10
-5
0
5
10
15
20
25
E (MeV)
preliminary
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)


Re(δ) and Im(δ), even parity, L = 20, (-0.3, -0.1, -0.1)
preliminary
δ (radians)
E (MeV)
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-20
-15
-10
-5
0
5
10
15
20
25
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)


Re(δ) and Im(δ), even parity, L = 40, (-0.3, -0.1, -0.1)
preliminary
δ (radians)
E (MeV)
1.5
1
0.5
0
-20
-15
-10
-5
0
5
10
15
20
25
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)


Re(δ) and Im(δ), even parity, L = 20, (-0.3, -0.2, -0.2)
preliminary
δ (radians)
E (MeV)
1.5
1
0.5
0
-20
-15
-10
-5
0
5
10
15
20
25
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)


Re(δ) and Im(δ), even parity, L = 40, (-0.3, -0.2, -0.2)
preliminary
δ (radians)
1.5
1
0.5
0
-20
-15
-10
-5
0
5
10
15
20
25
E (MeV)
AB + C -> AB + C Lüscher's method optical potential (real part)
AB + C -> AB + C Lüscher's method optical potential (imag part)

Review of topics

Adiabatic projection method

Alpha-alpha scattering

Pinhole trace algorithm

Nuclear thermodynamics

Phase diagram of symmetric nuclear matter

Inelastic reactions