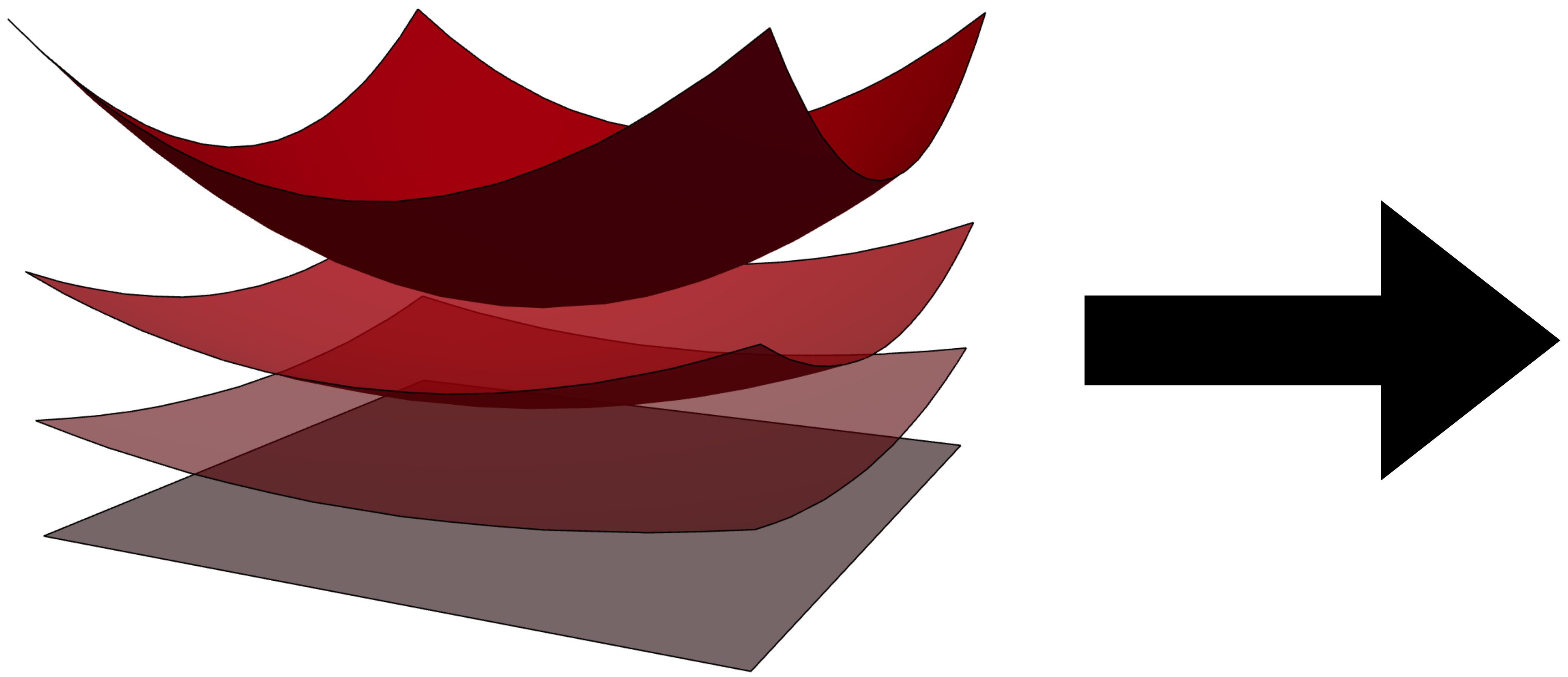
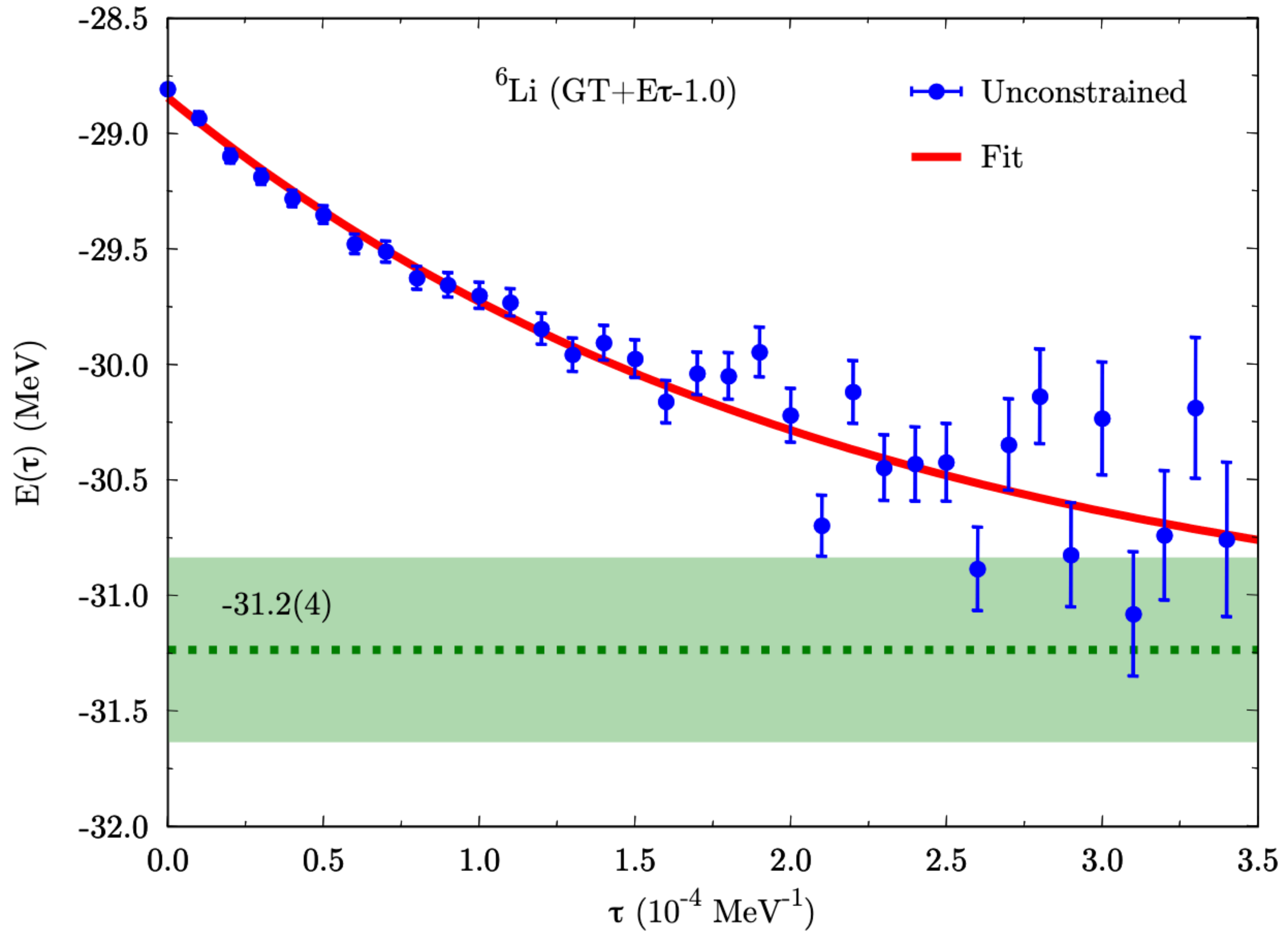
Mitigating noise in Green's function Monte Carlo using contour deformations





Gurtej Kanwar

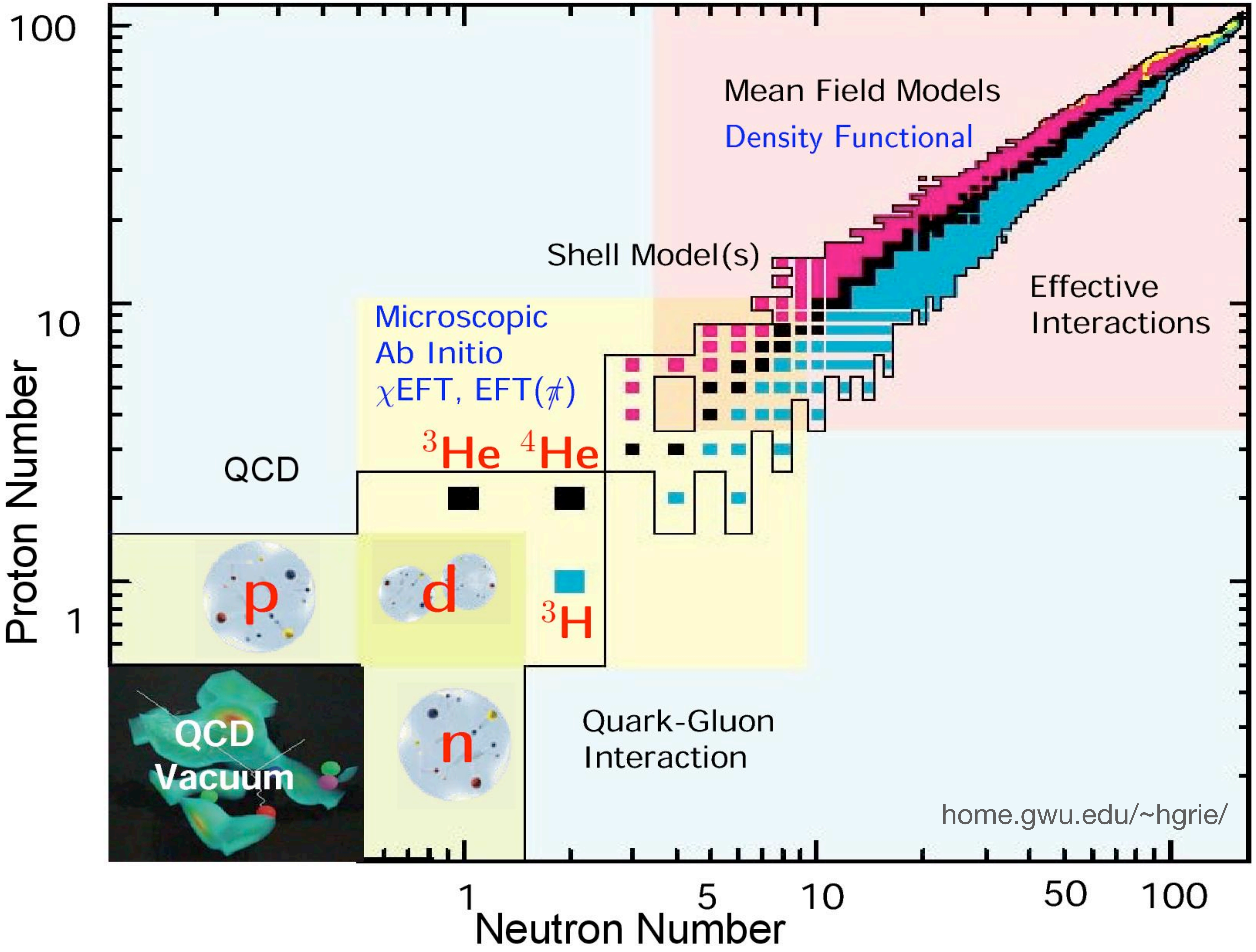
University of Bern

In collaboration with: A. Lovato, N. Rocco, M. L. Wagman

[GK, Lovato, Rocco, Wagman **2304.03229**]

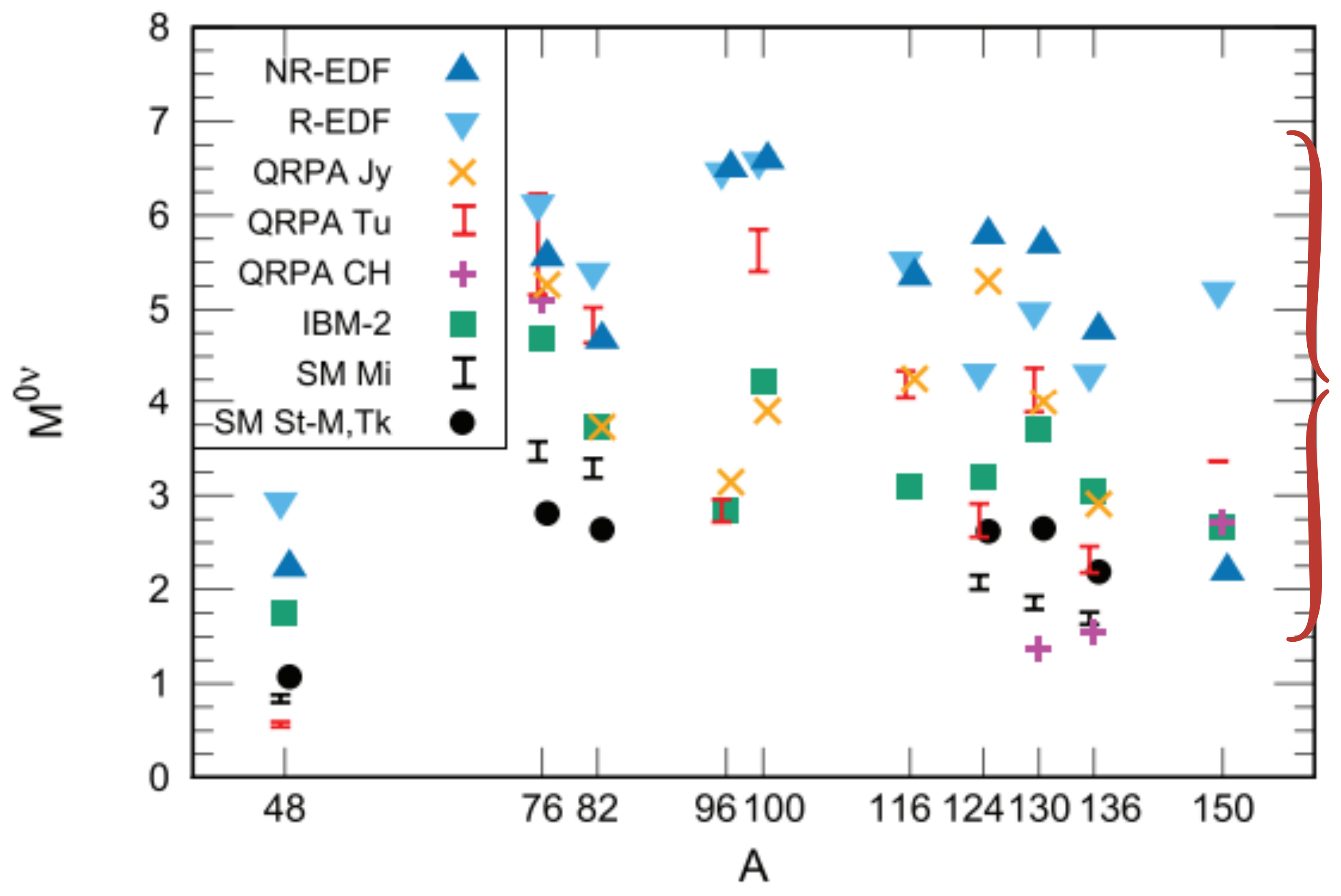
RBRC seminar | June 8, 2023

The rich nuclear landscape

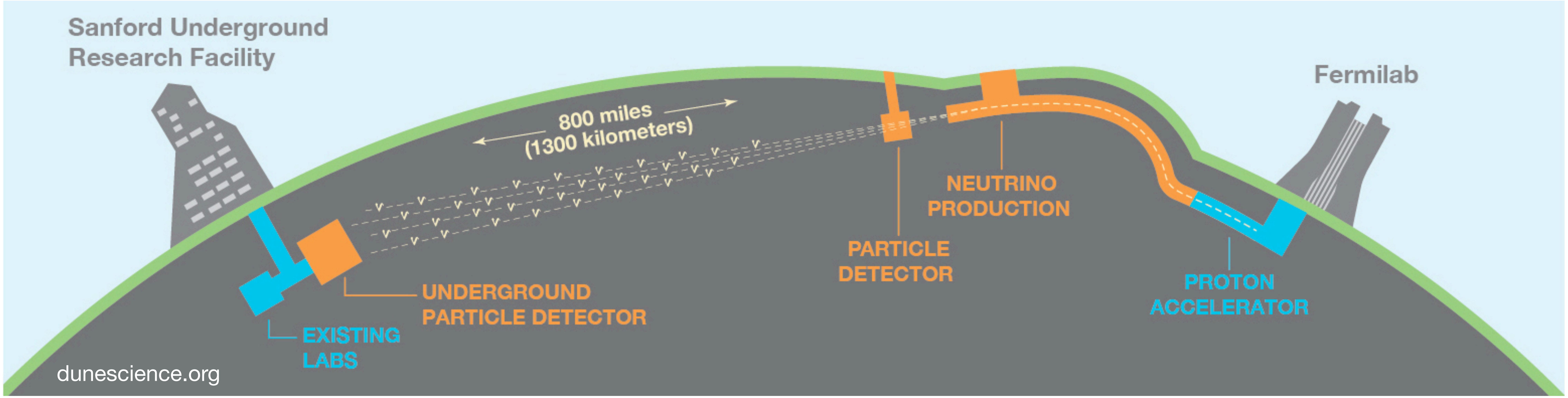


Nuclei as targets

[Engel & Menéndez, Rep Prog Phys 2017, 046301]



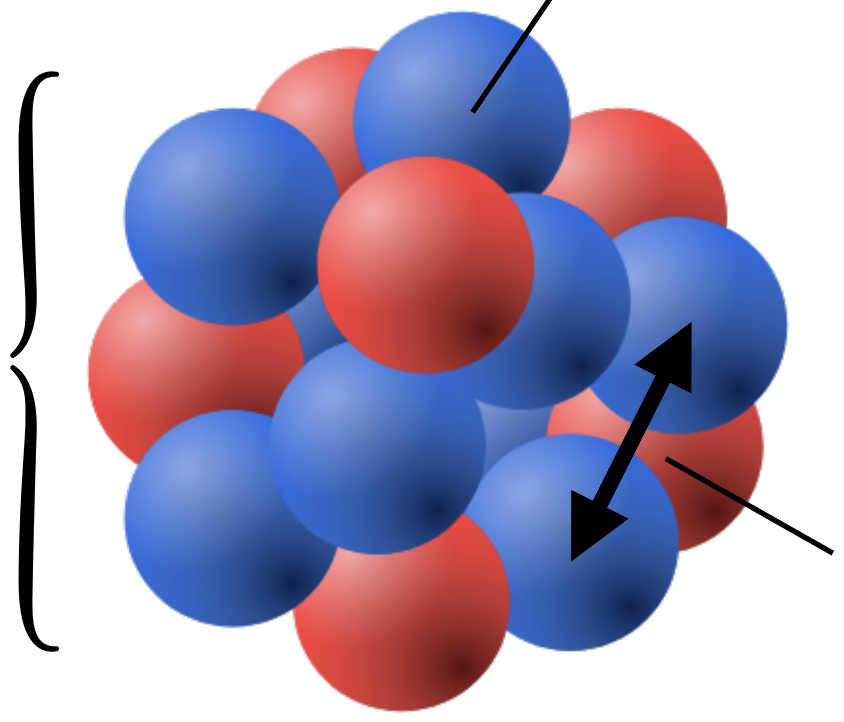
Model uncertainties restrict the efficiency of studies using nuclear targets!



Nuclear effective Hamiltonian

Non-relativistic two-body Hamiltonian:

$$H = \sum_{i=1}^{A} \frac{\boldsymbol{p}_i^2}{2M_N} + \sum_{i<j} v_{ij}(\boldsymbol{r}_{ij})$$



Argonne v_{18} (AV18) potential:

[Wiringa, Stoks, Schiavilla PRC51 (1995)]

- Nijmegen *pp* and *np* scattering data
- Low-energy *nn* scattering
- Deuteron binding energy

$$v_{ij}(\boldsymbol{r}_{ij}) = \sum_p v_p(|\boldsymbol{r}_{ij}|) O_{ij}^p(\boldsymbol{r}_{ij})$$

$O_{ij}^1 = 1,$ $\quad O_{ij}^2 = \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$

$O_{ij}^3 = \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j,$ $\quad O_{ij}^4 = (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)$

$O_{ij}^5 = S_{ij}(\vec{r}_{ij}),$ $\quad O_{ij}^6 = (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)\, S_{ij}(\vec{r}_{ij})$

$\dots$ $\quad \dots$

$[\, S_{ij}(\boldsymbol{r}_{ij}) \equiv 3(\boldsymbol{\sigma}_i \cdot \hat{r}_{ij})(\boldsymbol{\sigma}_j \cdot \hat{r}_{ij}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \,]$

Green's function Monte Carlo

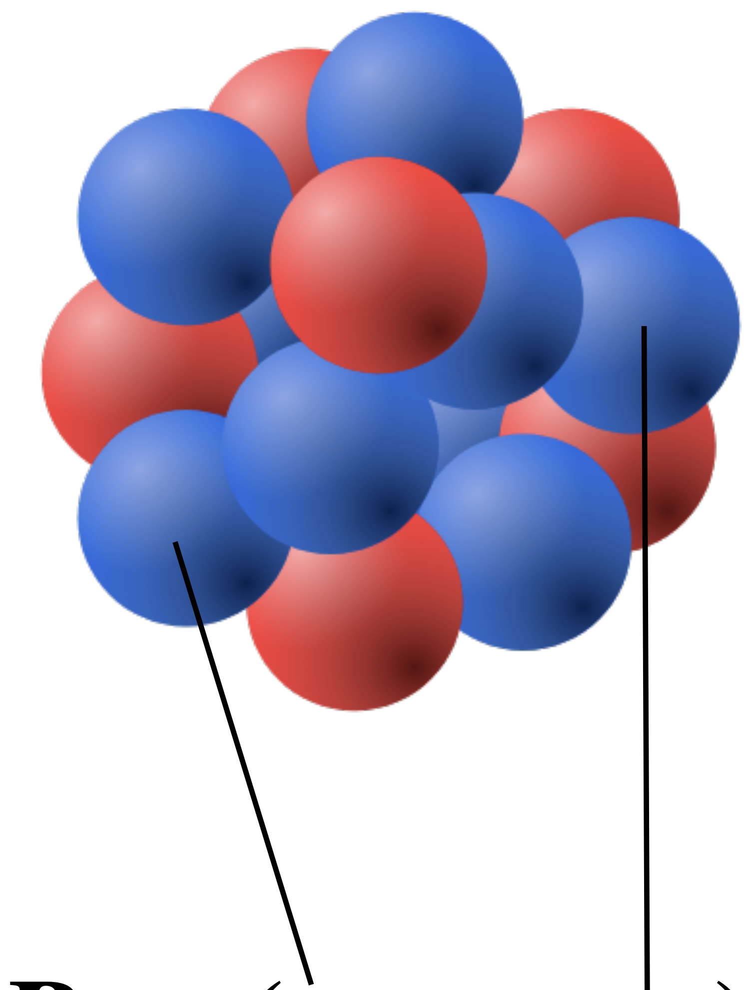
Variational ansatz $|\Phi\rangle$ $\xrightarrow{e^{-H\tau},\ \tau \gg 0}$ Ground state $|\Psi_0\rangle$

Lie-Trotter-Suzuki

$$\begin{cases} e^{-H\delta\tau} = e^{-V\delta\tau/2} e^{-T\delta\tau} e^{-V\delta\tau/2} + \mathcal{O}(\delta\tau^3) \\ T = \sum_i \boldsymbol{p}_i^2/2M_N \text{ and } V = \sum_{i<j} v_{ij}(\boldsymbol{r}_{ij}) \end{cases}$$

Short-time propagator / Green's function

$$\begin{cases} G_{\delta\tau}(\boldsymbol{R}', \boldsymbol{R}) \equiv \langle \boldsymbol{R}' | e^{-H\delta\tau} | \boldsymbol{R} \rangle \\ \qquad \approx S_{\frac{1}{2}\delta\tau}(\boldsymbol{R}') G^0_{\delta\tau}(\boldsymbol{R}', \boldsymbol{R}) S_{\frac{1}{2}\delta\tau}(\boldsymbol{R}) \\ S_{\frac{1}{2}\delta\tau} \sim e^{-V\delta\tau/2} \end{cases}$$



$\boldsymbol{R} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$,
$\boldsymbol{R} \in \mathbb{R}^{3A}$

Green's function Monte Carlo

$$G_{\delta\tau}(\boldsymbol{R}', \boldsymbol{R}) \equiv \langle \boldsymbol{R}' | e^{-H\delta\tau} | \boldsymbol{R} \rangle \approx S_{\frac{1}{2}\delta\tau}(\boldsymbol{R}') G^0_{\delta\tau}(\boldsymbol{R}', \boldsymbol{R}) S_{\frac{1}{2}\delta\tau}(\boldsymbol{R})$$

Wavefunction $\Psi(\boldsymbol{R}) \equiv \langle \boldsymbol{R} | \Psi \rangle$ is a spin-isospin vector with dim $2^A \binom{A}{Z}$

$S_{\frac{1}{2}\delta\tau}$ are matrices in this space

Free propagator is a simple Gaussian

$$G^0_{\delta\tau}(\boldsymbol{R}', \boldsymbol{R}) \sim \exp\left[-\frac{(\boldsymbol{R}' - \boldsymbol{R})^2}{2\delta\tau / M_N}\right]$$

GFMC approach:

Sample $\boldsymbol{R}$, explicitly track $\Psi(\boldsymbol{R})$

Green's function Monte Carlo

Path integral definition of $\Psi(\tau)$:

$$\Psi(\tau, \boldsymbol{R}^N) = \int \prod_{n=0}^{N-1} [d\boldsymbol{R}^n G^0_{\delta\tau}(\boldsymbol{R}^{n+1}, \boldsymbol{R}^n)] \times \prod_{n=0}^{N-1} \left[S_{\frac{1}{2}\delta\tau}(\boldsymbol{R}^{n+1}) S_{\frac{1}{2}\delta\tau}(\boldsymbol{R}^n) \right] \Phi(\boldsymbol{R}^0)$$

1. Sample $\boldsymbol{R}^0 \sim \Phi(\boldsymbol{R}^0)$
2. Draw $\boldsymbol{R}^n \sim I(\boldsymbol{R}^n \,|\, \boldsymbol{R}^{n-1}, \ldots, \boldsymbol{R}^0)$, where

$$I(\boldsymbol{R}^n \,|\, \ldots) \equiv G^0_{\delta\tau}(\boldsymbol{R}^n, \boldsymbol{R}^{n-1}) \frac{\Phi^\dagger(\boldsymbol{R}^n)\, S(\boldsymbol{R}^n, \ldots, \boldsymbol{R}^0)\, \Phi(\boldsymbol{R}^0)}{\Phi^\dagger(\boldsymbol{R}^{n-1})\, S(\boldsymbol{R}^{n-1}, \ldots, \boldsymbol{R}^0)\, \Phi(\boldsymbol{R}^0)}$$

Typically: "Diffuse" according to $G^0_{\delta\tau}$, then apply population sampling and heatbath to account for full importance weight

3. Use samples to compute $\langle O \rangle = \dfrac{\langle \Phi \,|\, O \exp(-H\tau) \,|\, \Phi \rangle}{\langle \Phi \,|\, \exp(-H\tau) \,|\, \Phi \rangle}$

Fermionic sign problem in GFMC

$$I(\boldsymbol{R}^n\,|\,\ldots) \equiv G^0_{\delta\tau}(\boldsymbol{R}^n, \boldsymbol{R}^{n-1}) \frac{\Phi^\dagger(\boldsymbol{R}^n)\, S(\boldsymbol{R}^n, \ldots, \boldsymbol{R}^0)\, \Phi(\boldsymbol{R}^0)}{\Phi^\dagger(\boldsymbol{R}^{n-1})\, S(\boldsymbol{R}^{n-1}, \ldots, \boldsymbol{R}^0)\, \Phi(\boldsymbol{R}^0)}$$

Not guaranteed to be positive!

$$v_{ij}(\boldsymbol{r}_{ij}) = \sum_p v_p(|\boldsymbol{r}_{ij}|) O^p_{ij}(\boldsymbol{r}_{ij})$$

$O^1_{ij} = 1,$ $\quad O^2_{ij} = \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$

$O^3_{ij} = \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j,$ $\quad O^4_{ij} = (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)$

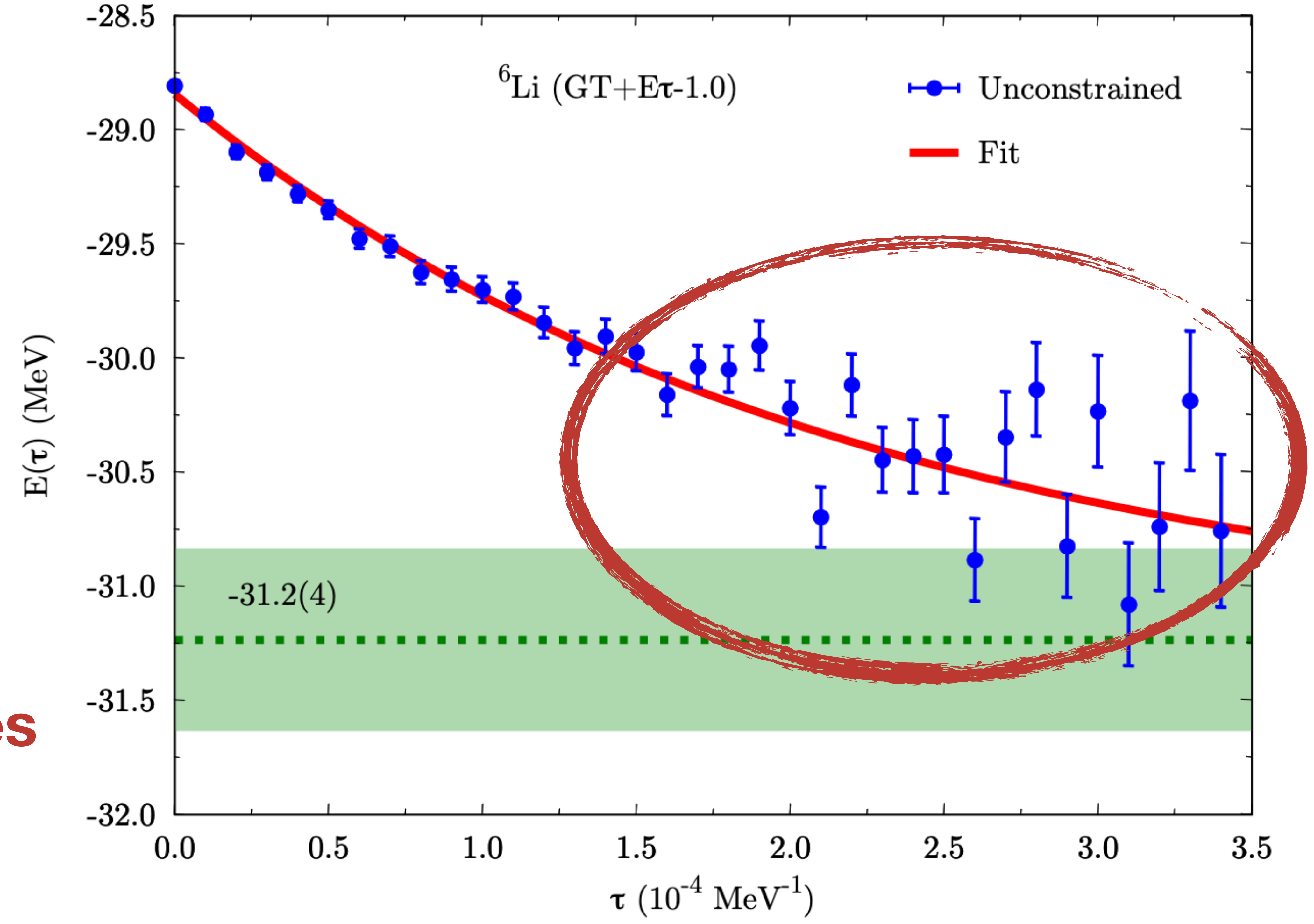
$O^5_{ij} = S_{ij}(\vec{r}_{ij}),$ $\quad O^6_{ij} = (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)\, S_{ij}(\vec{r}_{ij})$

$\cdots \qquad \cdots$

$[\, S_{ij}(\boldsymbol{r}_{ij}) \equiv 3(\boldsymbol{\sigma}_i \cdot \hat{r}_{ij})(\boldsymbol{\sigma}_j \cdot \hat{r}_{ij}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \,]$

E.g. tensor operator gives non-trivial phases

[Gandolfi+ 2001.01374]

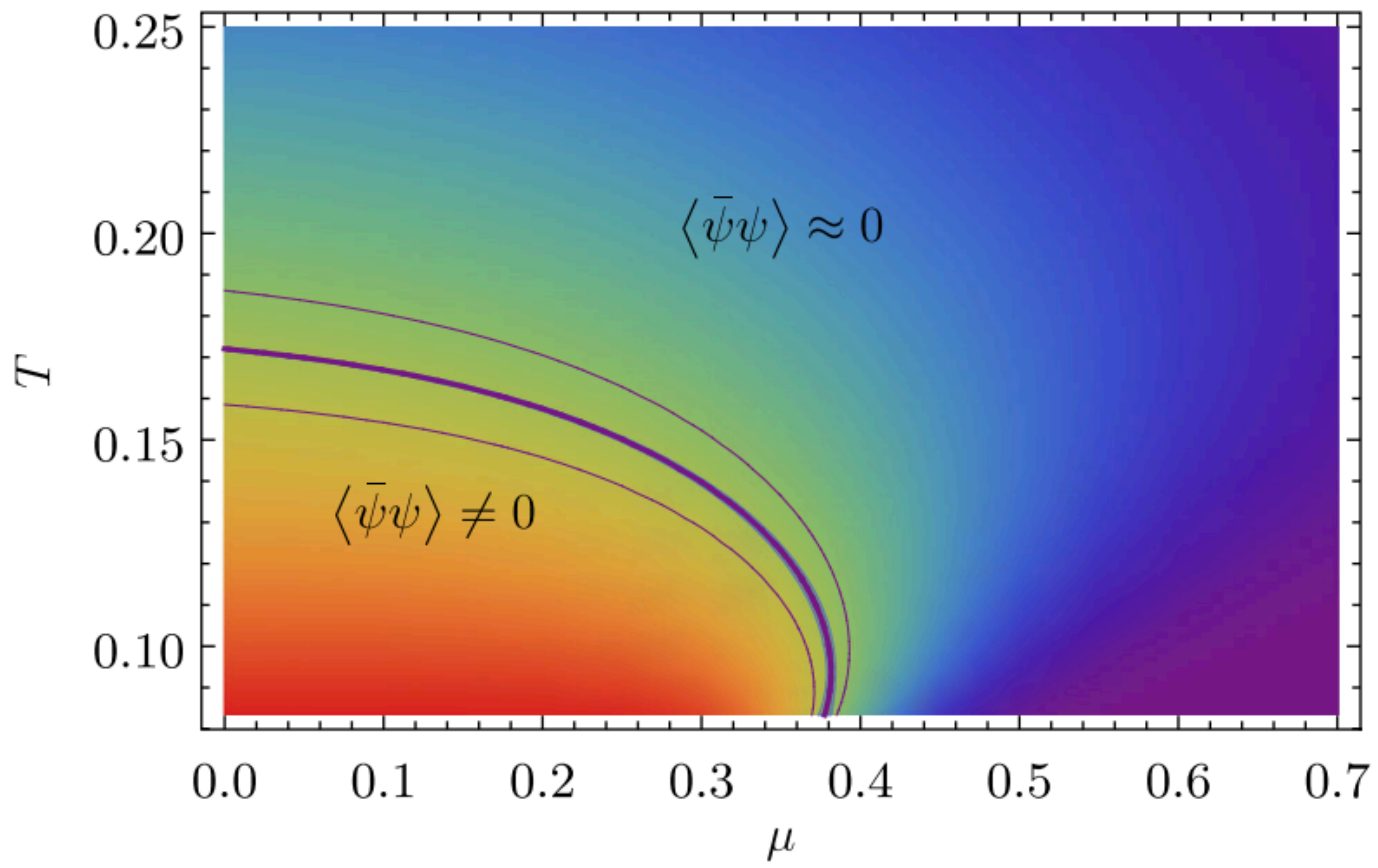


Contour deformations for sign problems

Sign problems solved in some lattice field theories with **complex actions**

Non-zero density
- **Cristoforetti+** PRD86(074506), PRD88(051501), PRD89(114505)
- **Aarts** PRD88(094501)
- **Alexandru+** PRD93(014504), JHEP05(053), PRD96(094505), PRD98(054514), PRD98(034506), PRD97(094510), PRL121(191602)
- **Fujii+** JHEP12(125)
- **Tanizaki+** NJP18(033002)
- **Mori+** PTEP2018(023B04), PRD99(014033)
- ...

Real-time evolution
- **Alexandru+** PRL117(081602), PRD95(114501)
- **Mou+** JHEP11(135)
- **GK & Wagman** PRD104(014513)



2+1D Thirring model [Alexandru+ PRL121(191602)]

Non-relativistic nuclear path integral quite different, but similar inspirations!

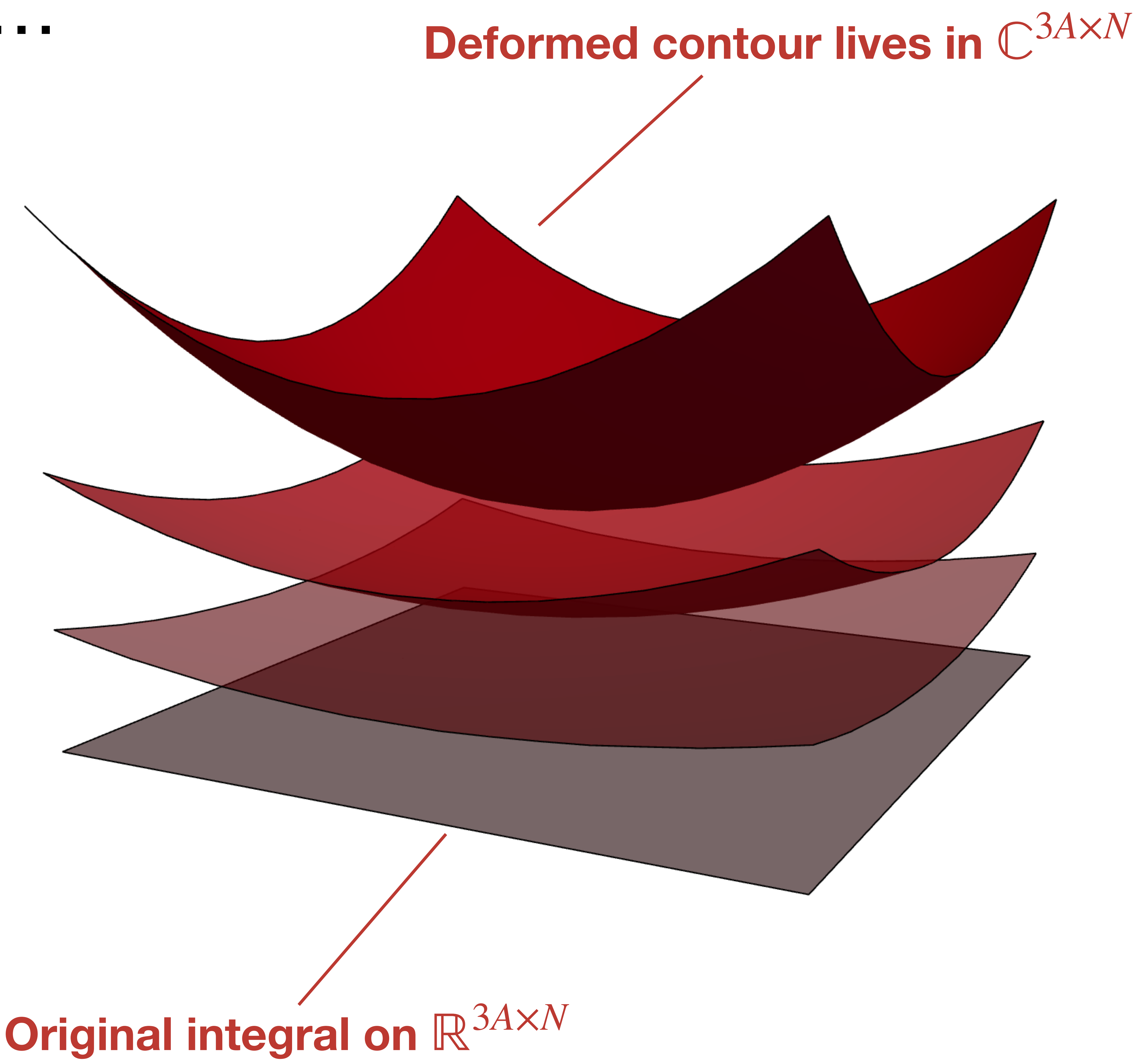
Deforming the GFMC path integral

Just contour deformation in $3A \times N$ dimensions…

$$\Psi(\tau, \boldsymbol{R}^N) = \int \prod_{n=0}^{N-1} [d\boldsymbol{R}^n G^0_{\delta\tau}(\boldsymbol{R}^{n+1}, \boldsymbol{R}^n)]$$

$$\times \prod_{n=0}^{N-1} \left[S_{\frac{1}{2}\delta\tau}(\boldsymbol{R}^{n+1}) S_{\frac{1}{2}\delta\tau}(\boldsymbol{R}^n) \right] \Phi(\boldsymbol{R}^0)$$

$$= \int \prod_{n=0}^{N-1} [d\tilde{\boldsymbol{R}}^n G^0_{\delta\tau}(\tilde{\boldsymbol{R}}^{n+1}, \tilde{\boldsymbol{R}}^n)] \times \ldots$$



Cauchy's theorem guarantees **exact equality** as long as integrand is *holomorphic*

[Image credit: Neill Warrington]

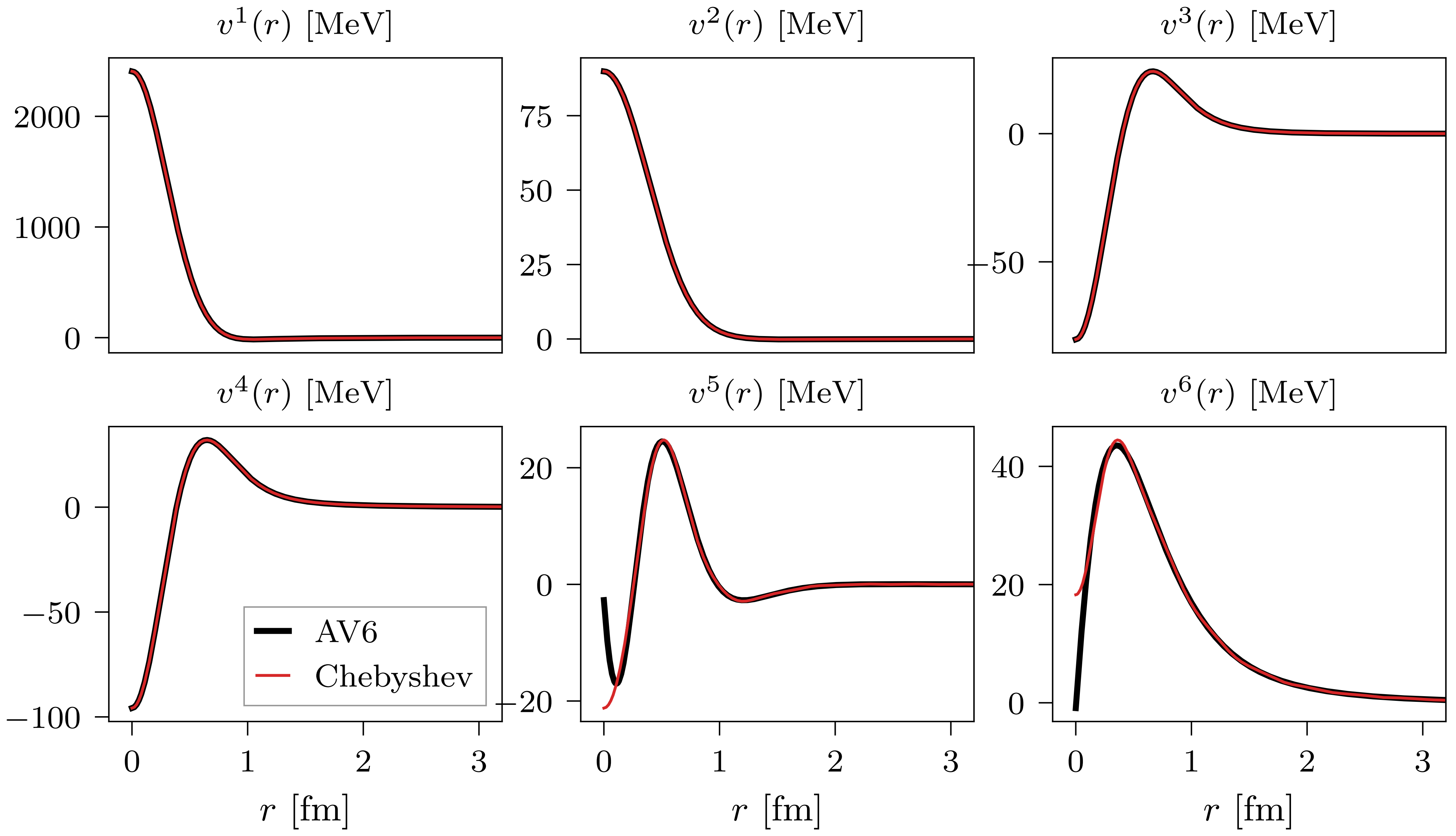
Analytic continuation

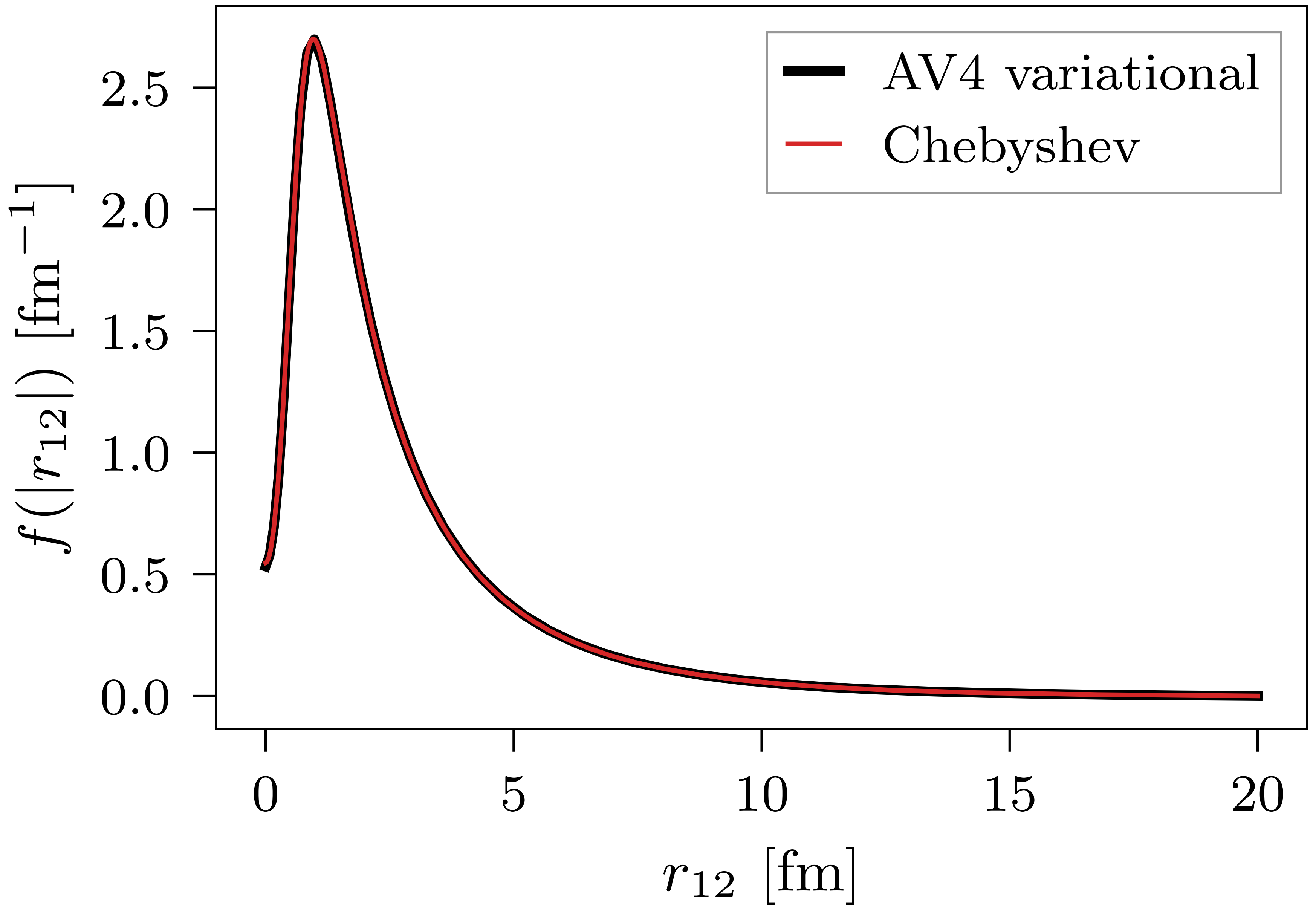
1. Replace $v_{ij}(|\boldsymbol{r}_{ij}|) \longrightarrow v_{ij}^{H}(\rho_{ij})$, with $\rho_{ij} \equiv \boldsymbol{r}_{ij} \cdot \boldsymbol{r}_{ij}$

Chebyshev fits

2. Replace $\Phi(\{|\boldsymbol{r}_{ij}|\}_{i<j}) \longrightarrow \Phi^{H}(\{\rho_{ij}\}_{i<j})$

3. Rewrite $\boldsymbol{p}_i \Psi(\boldsymbol{R}) \longrightarrow i \frac{\partial}{\partial \boldsymbol{r}_i} \Psi(\boldsymbol{R})$ and apply derivatives

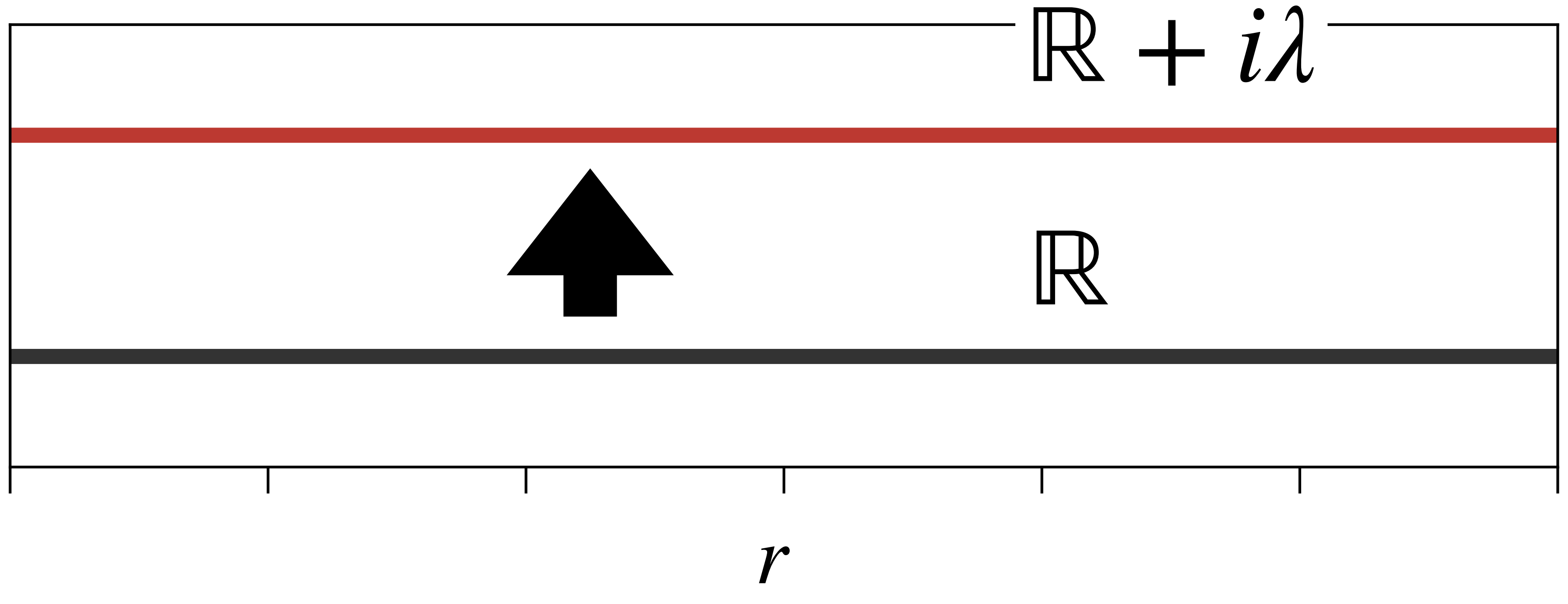




Cartesian contour deformations

Simple choice: Constant shift per coordinate

$$\tilde{\boldsymbol{r}}_i^n = \boldsymbol{r}_i^n + i\boldsymbol{\lambda}_i^n$$



- No Jacobian factor
- $3A \times N$ free parameters $\boldsymbol{\lambda}_i^n = (\lambda_{1,i}^n, \lambda_{2,i}^n, \lambda_{3,i}^n)$

More generally: Additional coordinate dependence $\boldsymbol{\lambda}_i^n(\boldsymbol{R}^n)$

- Jacobian factor must be kept tractable!
- Behavior at infinity

Spherical contour deformations

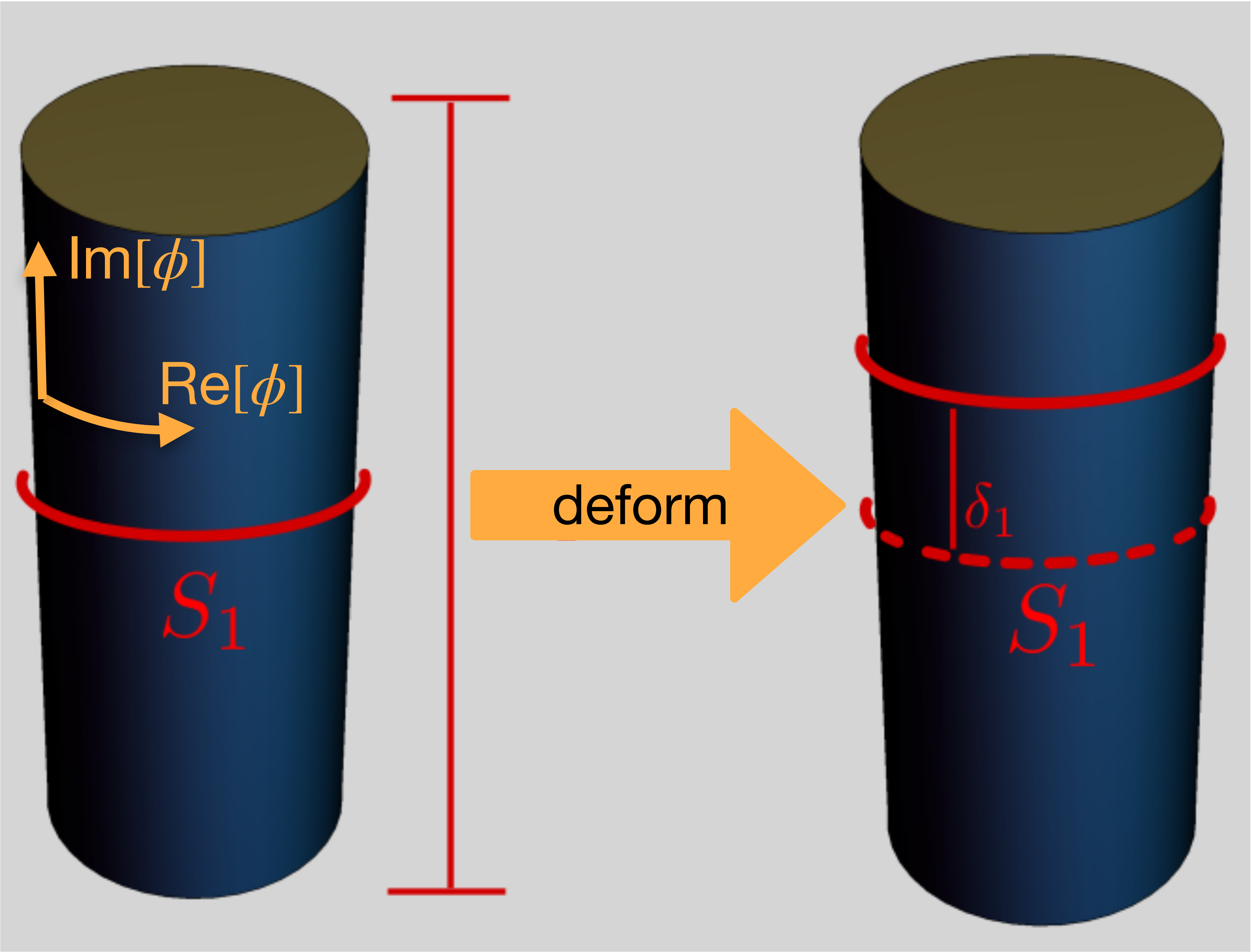
Simple choice: Constant shift in polar angle

$$(\tilde{r}_i^n, \tilde{\theta}_i^n, \tilde{\phi}_i^n) = (r_i^n, \theta_i^n, \phi_i^n + i\lambda_i^n)$$

- No Jacobian factor
- $A \times N$ free parameters λ_i^n

More generally: Deform r, θ and/or additional coordinate dependence

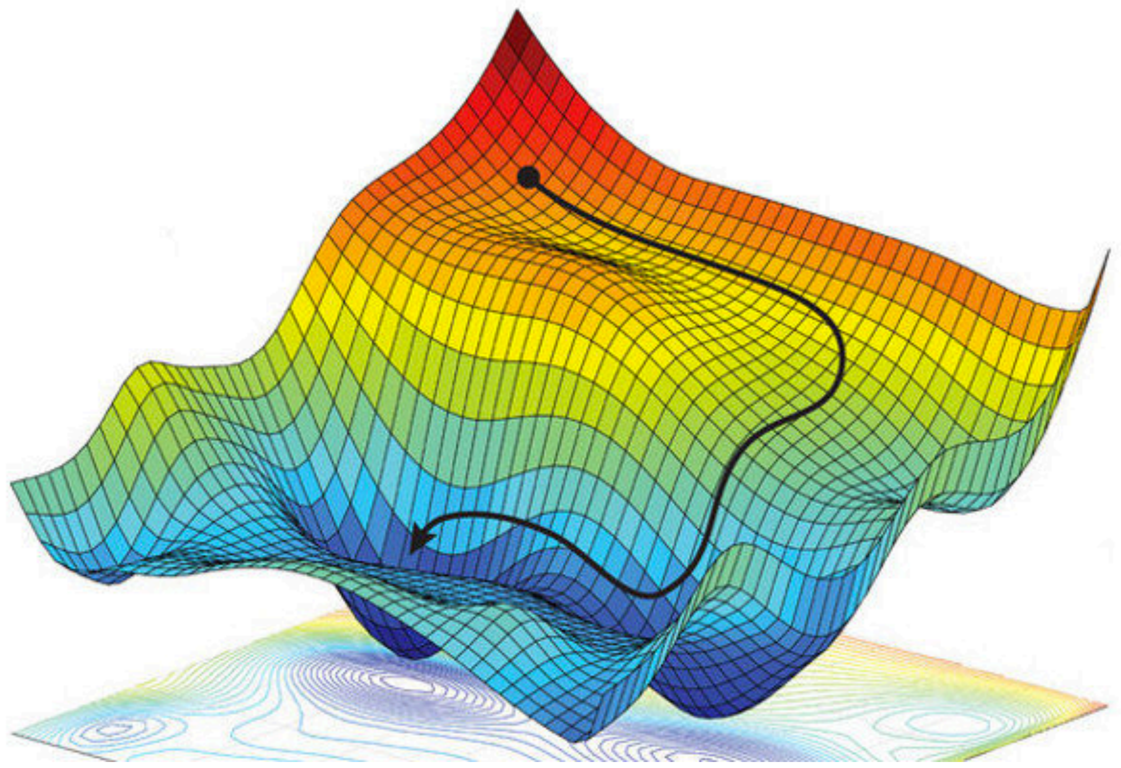
- Endpoints $r \to 0,\infty$ and $\theta \to 0,\pi$ fixed
- 2π-Periodicity of ϕ in the real direction



[Image credit: Neill Warrington]

Optimizing the contour

Choice of $\tilde{\boldsymbol{R}}$ defines new GFMC procedure and generally modifies the variance.



[Image credit: 1805.04829]

We optimize parameters by numerically minimizing variance per observable studied.

Gradients of (log) variance using Monte Carlo estimates:

Importance sampling using deformed weights $\tilde{I}(\boldsymbol{R}^n | \dots)$

$$\mathscr{L}_O(\alpha) \equiv (1-\alpha)\log\left\langle \left| \tilde{W}(\boldsymbol{R}^N, \dots, \boldsymbol{R}^0) \right|^2 \right\rangle_{\tilde{P}}$$

$$+\alpha \log\left\langle \left| \tilde{W}(\boldsymbol{R}^N, \dots, \boldsymbol{R}^0) \frac{\Phi^\dagger(\tilde{\boldsymbol{R}}^N) O S(\tilde{\boldsymbol{R}}^N, \dots, \tilde{\boldsymbol{R}}^0)\Phi(\tilde{\boldsymbol{R}}^0)}{\Phi^\dagger(\tilde{\boldsymbol{R}}^N) S(\tilde{\boldsymbol{R}}^N, \dots, \tilde{\boldsymbol{R}}^0)\Phi(\tilde{\boldsymbol{R}}^0)} \right|^2 \right\rangle_{\tilde{P}}.$$

Reweighting factors under deformed importance sampling

Deuteron binding energy: setup

Variational wavefunction optimized for **AV4**, evolved with **AV6** to induce a sign problem analogous to nuclei with larger A

$$\Phi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{1}{\sqrt{2}}(|p \uparrow n \uparrow\rangle - |n \uparrow p \uparrow\rangle) \times f(|\boldsymbol{r}_{12}|)$$

- Eigenstate of spin and isospin operators
- Tensor operator introduces a sign problem

$$\hat{S}_{12}(\boldsymbol{r}_{12}) = (\boldsymbol{\sigma}_1 \cdot \hat{r}_{12})(\boldsymbol{\sigma}_2 \cdot \hat{r}_{12})$$

Center-of-mass, spherical coordinates

$$\hat{S}_{12}(r, \theta, \phi) = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \otimes \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}$$

Deuteron binding energy: sign problem

Sign problem inspires contour deformation of ϕ in spherical coordinates

One timestep: $\tilde{\phi} = \phi + i\lambda$

$$\hat{S}_{12}(r, \theta, \tilde{\phi}) = X^{-1}(\lambda)\ \hat{S}_{12}(r, \theta, \phi)\ X(\lambda)$$

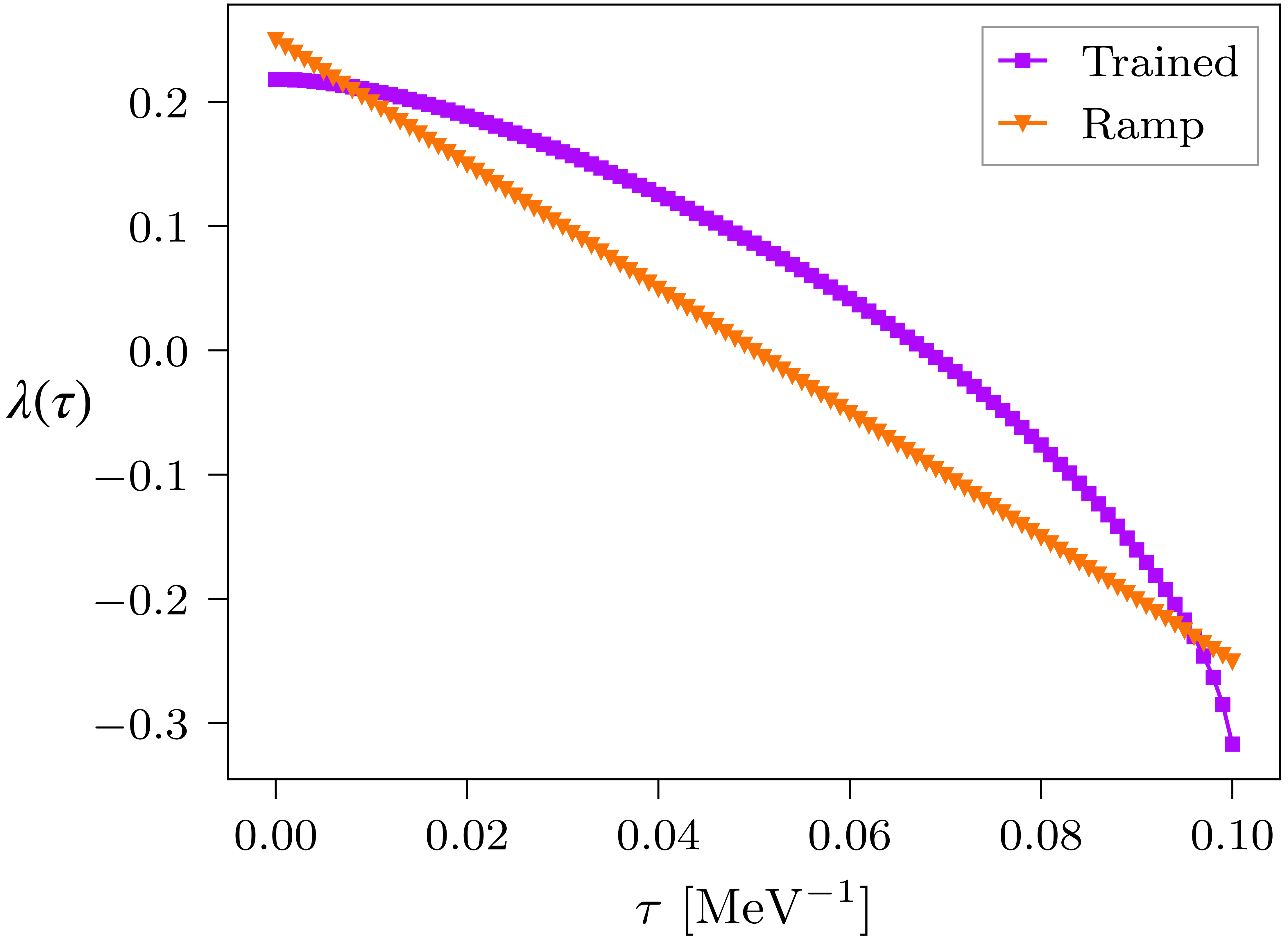
$$\text{where } X(\lambda) \equiv \begin{pmatrix} e^{-\lambda/2} & 0 \\ 0 & e^{\lambda/2} \end{pmatrix} \otimes \begin{pmatrix} e^{-\lambda/2} & 0 \\ 0 & e^{\lambda/2} \end{pmatrix}$$

Multiple timesteps: $\tilde{\phi}(\tau) = \phi(\tau) + i\lambda(\tau)$ can achieve similar effect using a "ramp"

$$\lambda(\tau) = (\tau - N\delta\tau/2)\ell$$

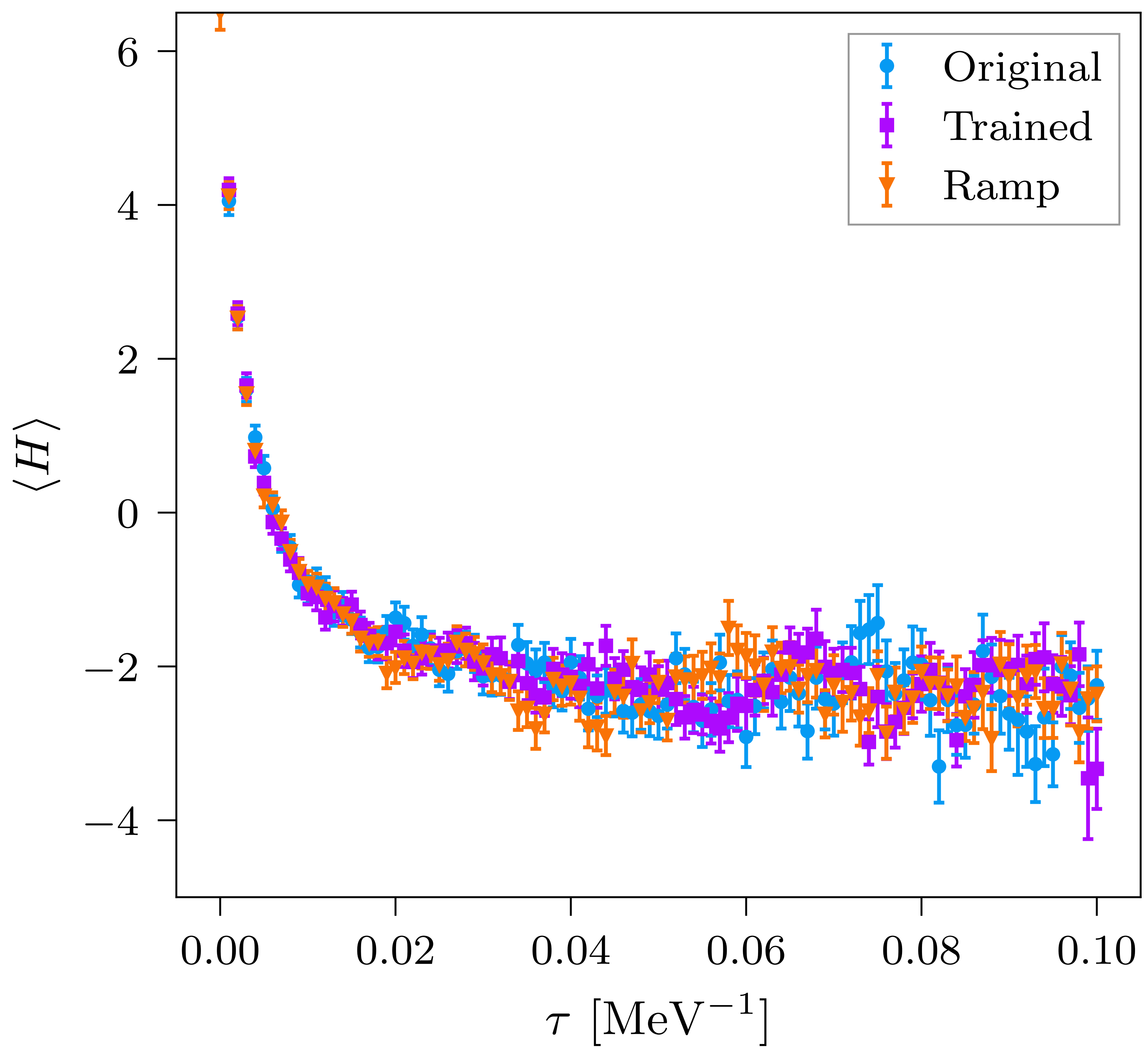
Deuteron binding energy: contour

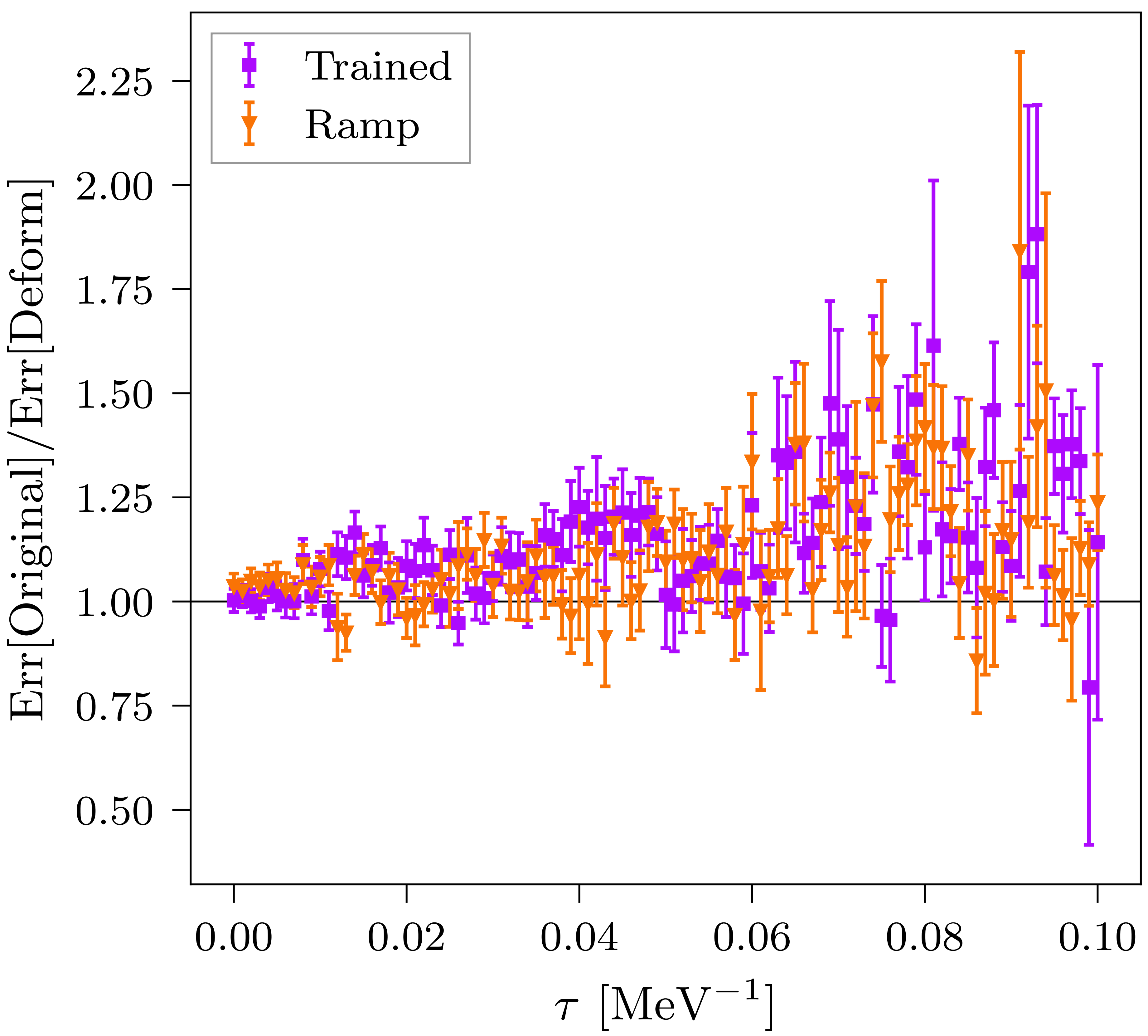
Ramp $\lambda(\tau)$ with optimal magnitude compared vs trained $\lambda(\tau)$



Deuteron binding energy: results

Unbiased result confirmed, but improvement is a small factor.





Deuteron Euclidean response: setup

Response functions:

$$\mathscr{R}_{J'J}(\boldsymbol{q},\tau) = \frac{\langle \Phi \,|\, J'^{\dagger}(\boldsymbol{q}) e^{-H\tau} J(\boldsymbol{q}) \,|\, \Phi \rangle}{\langle \Phi \,|\, e^{-H\tau} \,|\, \Phi \rangle}$$

- Response of nuclei to external (electromagnetic, axial, etc.) currents

Euclidean density response function:

$$\hat{N}_i(\boldsymbol{q}) = \int d^3r\, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \psi_i^{\dagger}(\boldsymbol{r}) \psi_i(\boldsymbol{r})$$

$$\rho_{ij}(\boldsymbol{q},\tau) \equiv \mathscr{R}_{N_i,N_j}(\boldsymbol{q},\tau) = \frac{1}{Z} \int \prod_{n=0}^{N} d\boldsymbol{R}^n \left[e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_i^N - \boldsymbol{r}_j^0)} \right] I(\boldsymbol{R}^N, \ldots, \boldsymbol{R}^0)$$

- Large sign problem already from observable
- Variational wavefunction optimized and evolved with AV6

Deuteron Euclidean response: sign problem

Expectation value of $\rho(\boldsymbol{q},\tau) = \sum_{i,j} \rho_{ij}(\boldsymbol{q},\tau) \sim e^{-\tau \boldsymbol{q}^2/4M_N}$

[Carlson+ PRC65 (2002), nucl-th/0106047]

Exponentially severe phase cancellation required for GFMC estimate of mean value!

Average magnitude of sample estimate of $\rho(\boldsymbol{q},\tau)$ is $\mathcal{O}(1)$

Form of the observable inspires Cartesian-coordinates deformation:

$$\tilde{\boldsymbol{r}}_1(\tau) = \boldsymbol{r}_1 + i\boldsymbol{\lambda}(\boldsymbol{q},\tau) \text{ and } \tilde{\boldsymbol{r}}_2(\tau) = \boldsymbol{r}_2 - i\boldsymbol{\lambda}(\boldsymbol{q},\tau)$$ [C.o.M. frame]

For $\rho_{11}(\boldsymbol{q},\tau) = \langle e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_1^N - \boldsymbol{r}_1^0)} \rangle$, for example:

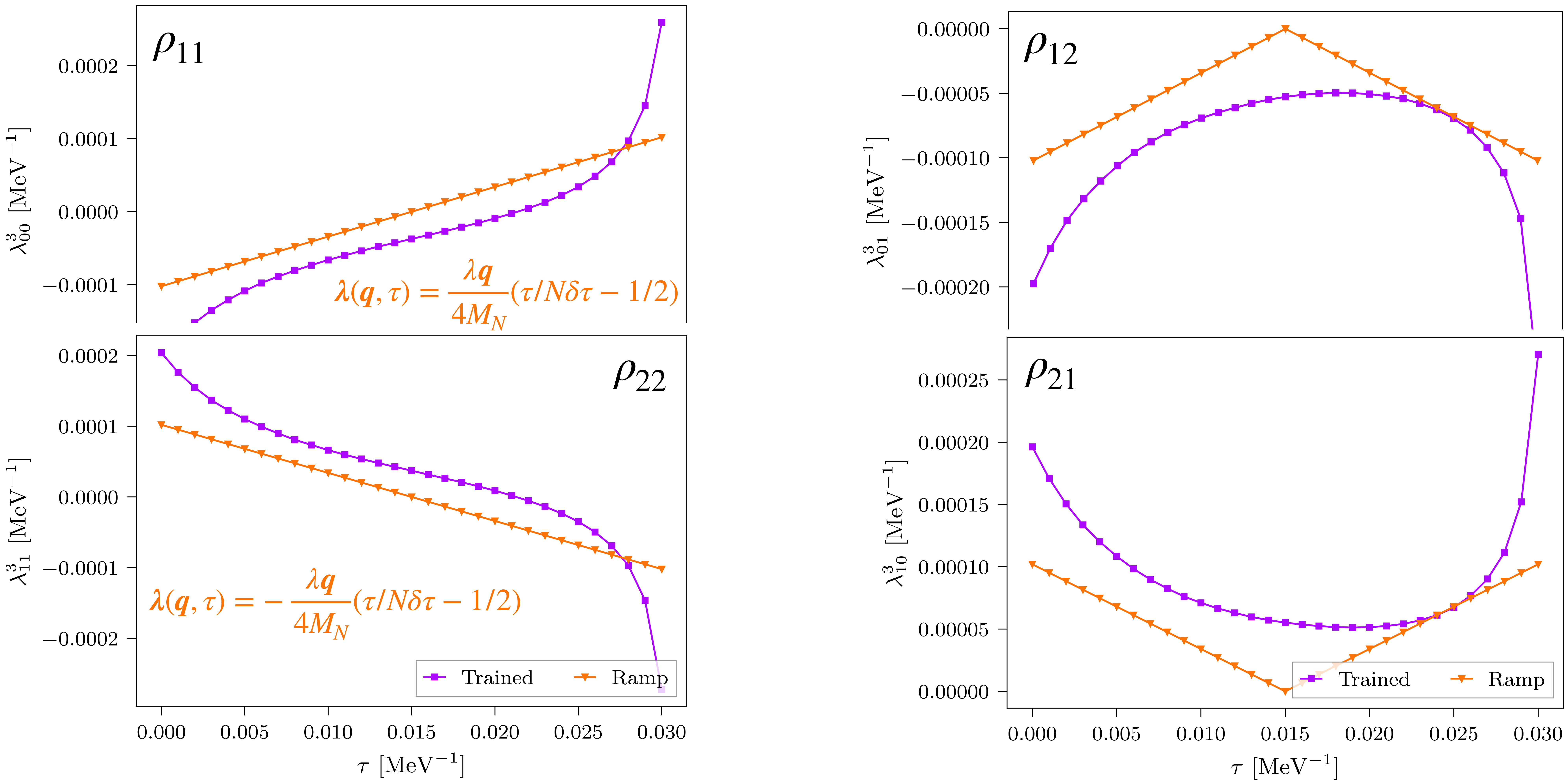
$$\boxed{\lambda(0) = -\,\boldsymbol{q}N\delta\tau/4M_N \text{ and } \lambda(N\delta\tau) = \boldsymbol{q}N\delta\tau/4M_N}$$

$$e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_1^N - \boldsymbol{r}_1^0)} \longrightarrow e^{-\tau\boldsymbol{q}^2/4M_N} e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_1^N - \boldsymbol{r}_1^0)}$$ ✅

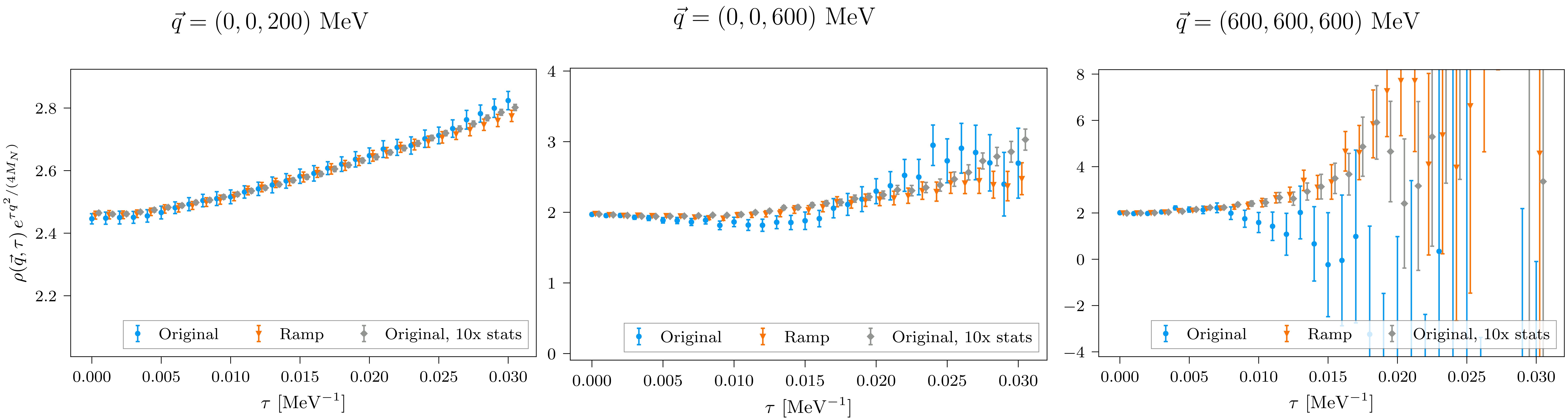
Note: Different deformation needed for each (i,j)

Deuteron Euclidean response: contours

Hand-selected “ramp” parameterizations compared against trained results.



Deuteron Euclidean response: results

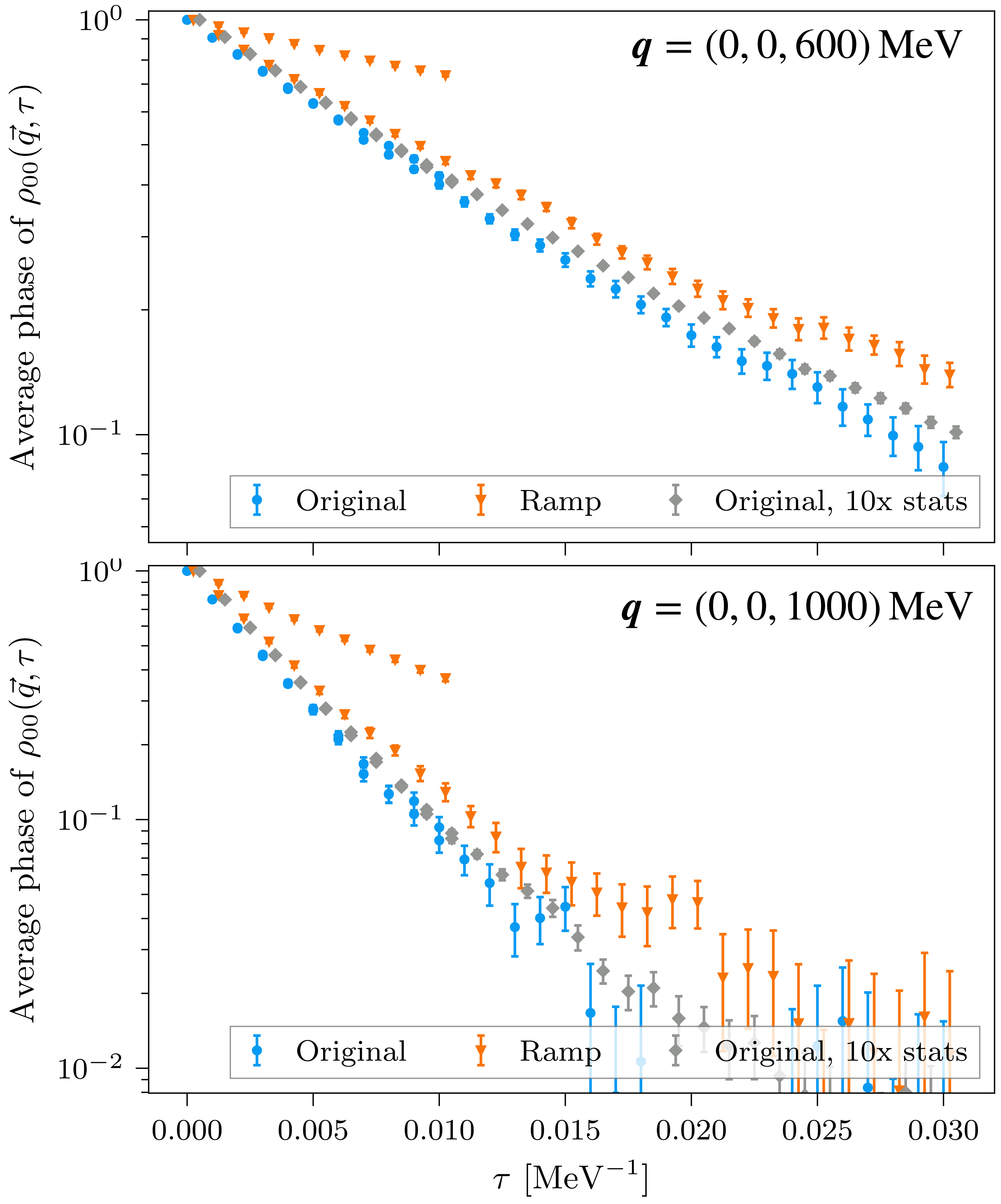


Deuteron Euclidean response: results

Average phase is improved, in some cases exponentially.

Strange dependence on total GFMC evolution time $N\delta\tau$?

- Numerically: $\lambda \approx 0.64\text{MeV}^{-1}$ roughly independent of $N\delta\tau$
- Analytical argument: $\lambda \sim N\delta\tau$
- Optimal deformation for $\tau < N\delta\tau$ extends continuously to remaining GFMC timesteps, adding noise?



Summary

This is proof-of-principle work, but already implements / demonstrates:

- **Analytic continuation** of nuclear potentials and variational wavefunctions
- **Deformed GFMC with $R \to \tilde{R}$**, guaranteed exact by Cauchy's thm
- **Numerical variance optimization**
- **Significant improvement** in deuteron Euclidean density response functions, although only modest improvement in the binding energy

Future work:

- Applications to larger nuclei
- More sophisticated / modern nuclear Hamiltonians
- Extension to Auxiliary Field Diffusion Monte Carlo (AFDMC)

Thanks!
Questions?