Nuclear ab initio studies for neutrino oscillations

Joanna Sobczyk

Hirschegg, 17 January 2023

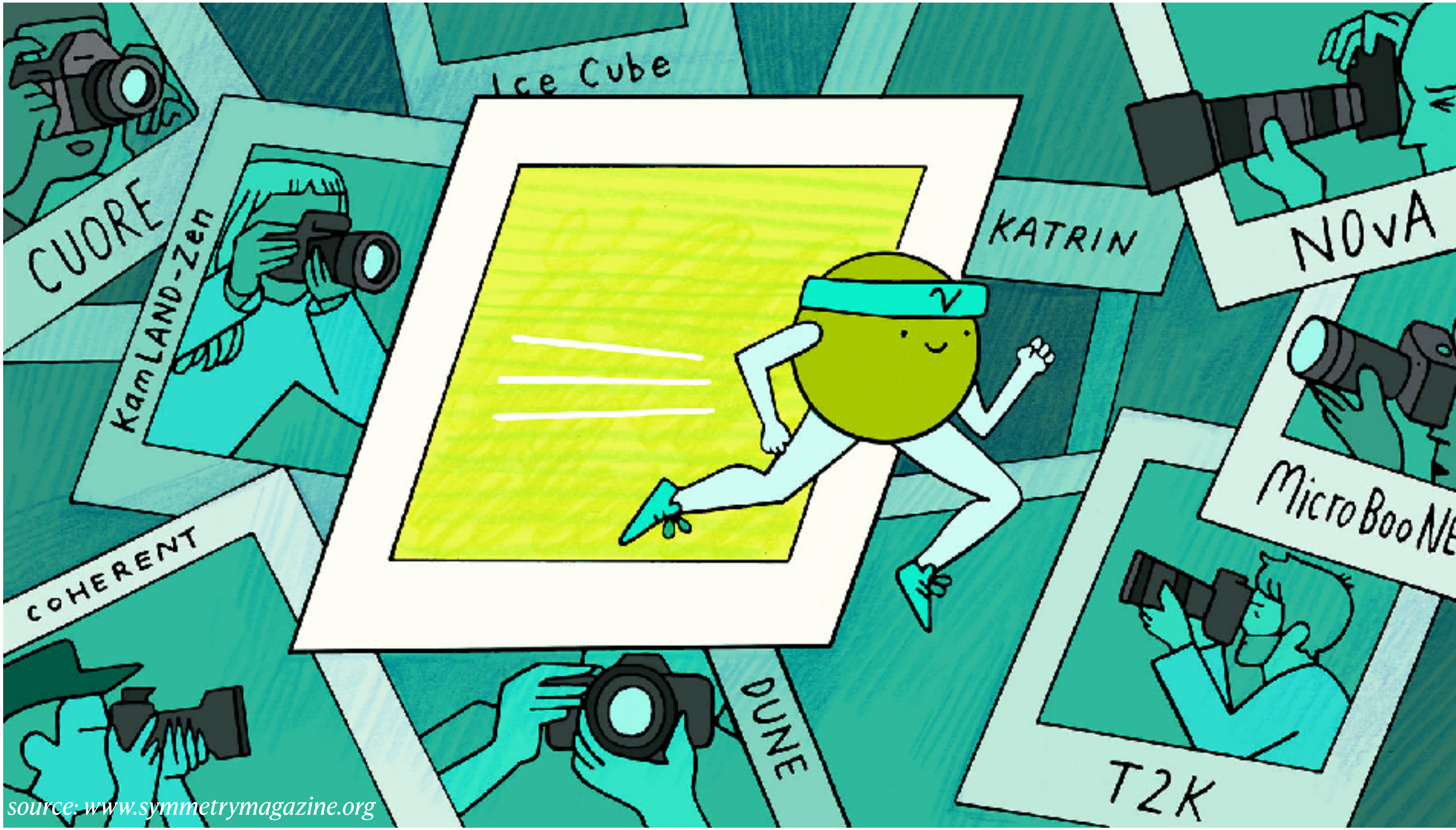
Cluster of Excellence PRISMA+ Precision Physics, Fundamental Interactions and Structure of Matter

JG|U

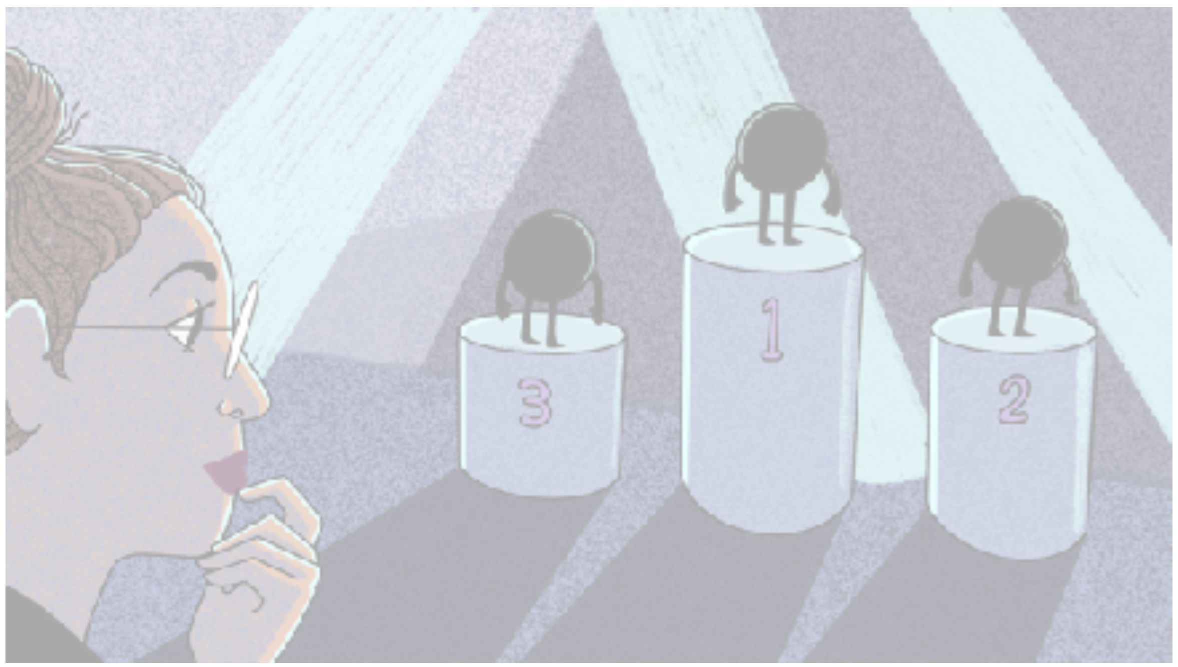
Alexander von Humboldt Stiftung/Foundation

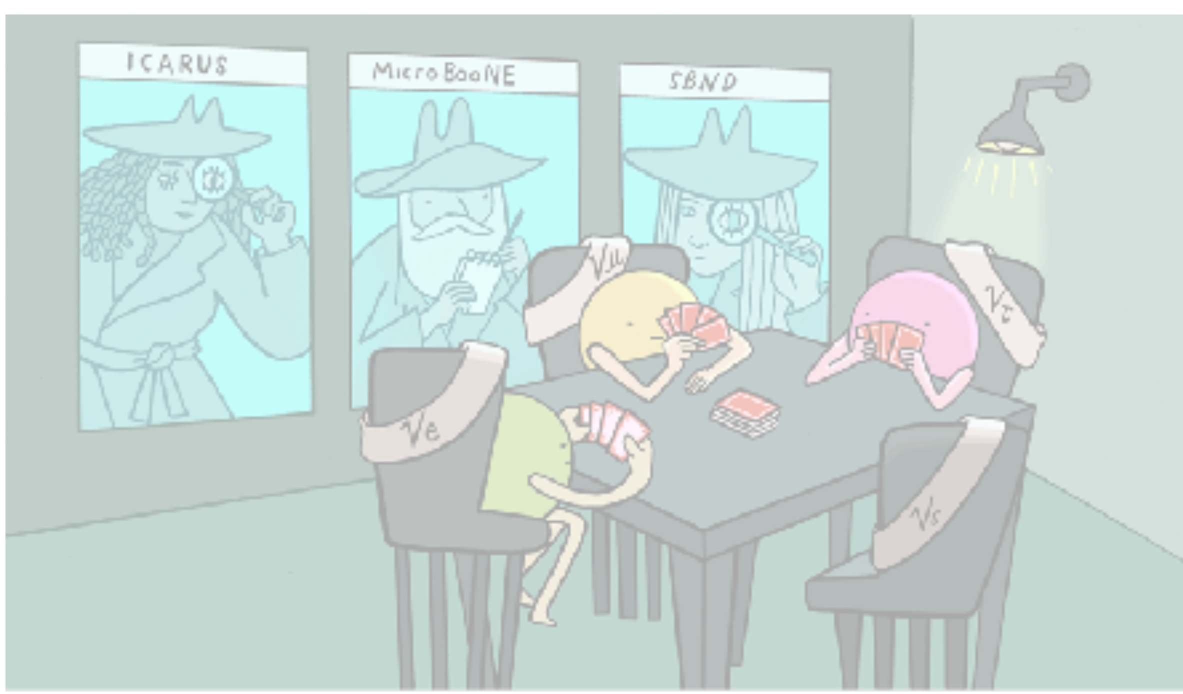
MARIE CURIE ACTIONS

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No. 101026014


Ice Cube
CUORE
KamLAND-Zen
KATRIN
NOvA
MicroBooNE
COHERENT
DUNE
T2K
source: www.symmetrymagazine.org

Neutrino Physics





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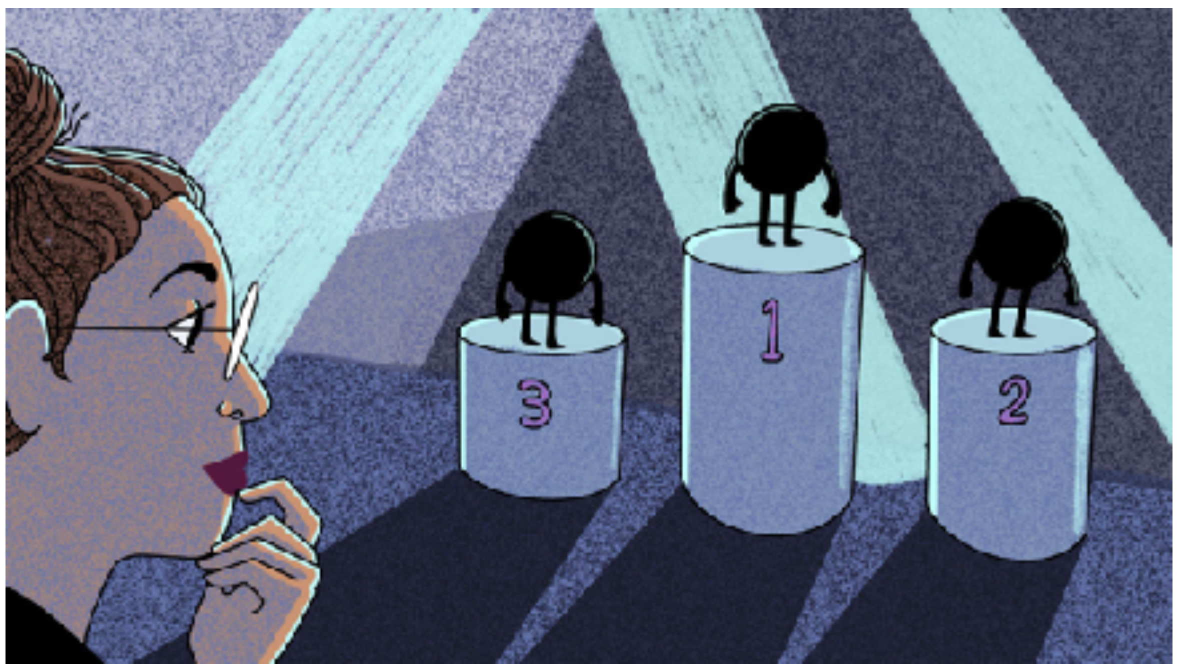

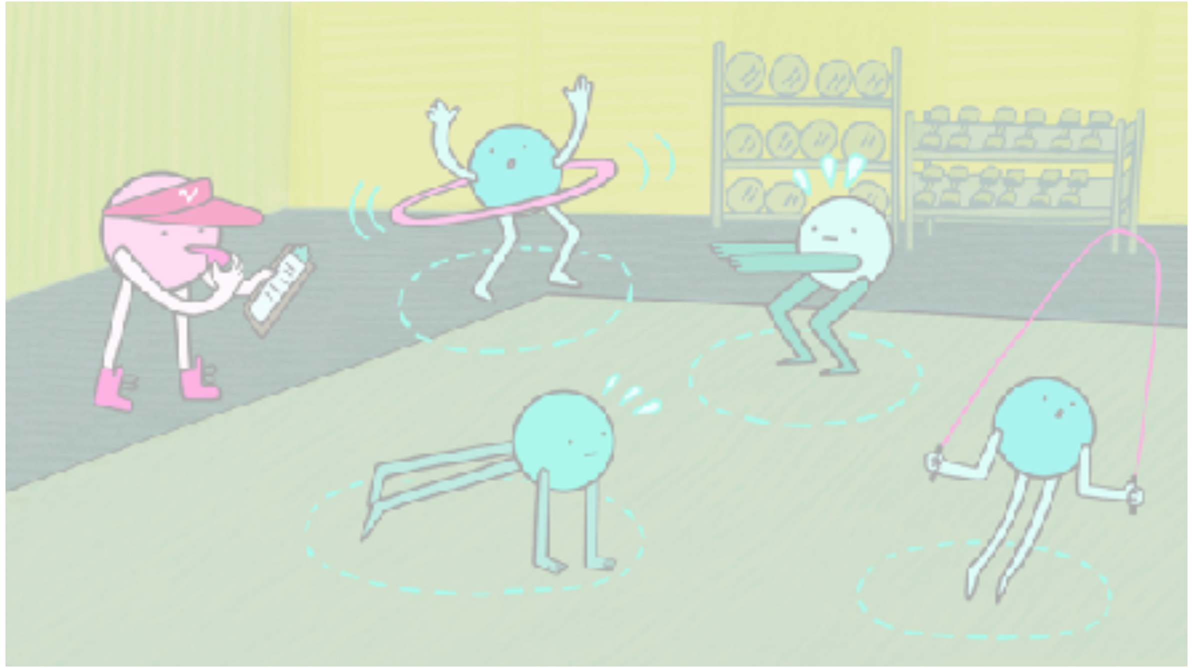

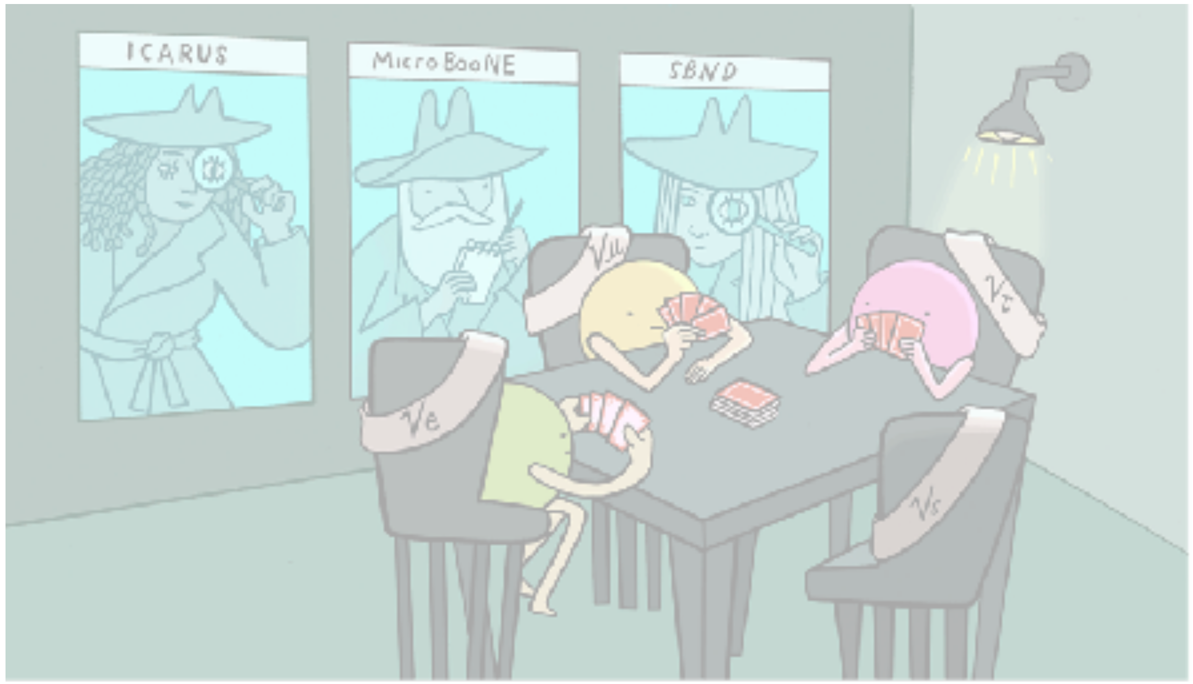

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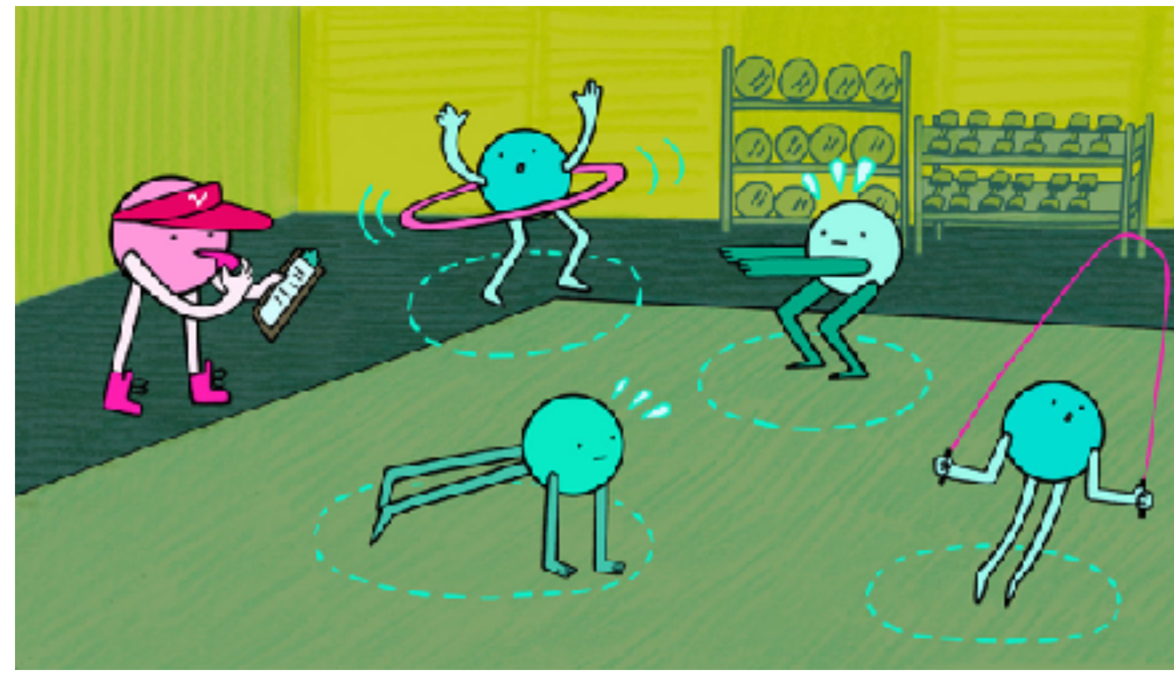
Neutrino Physics



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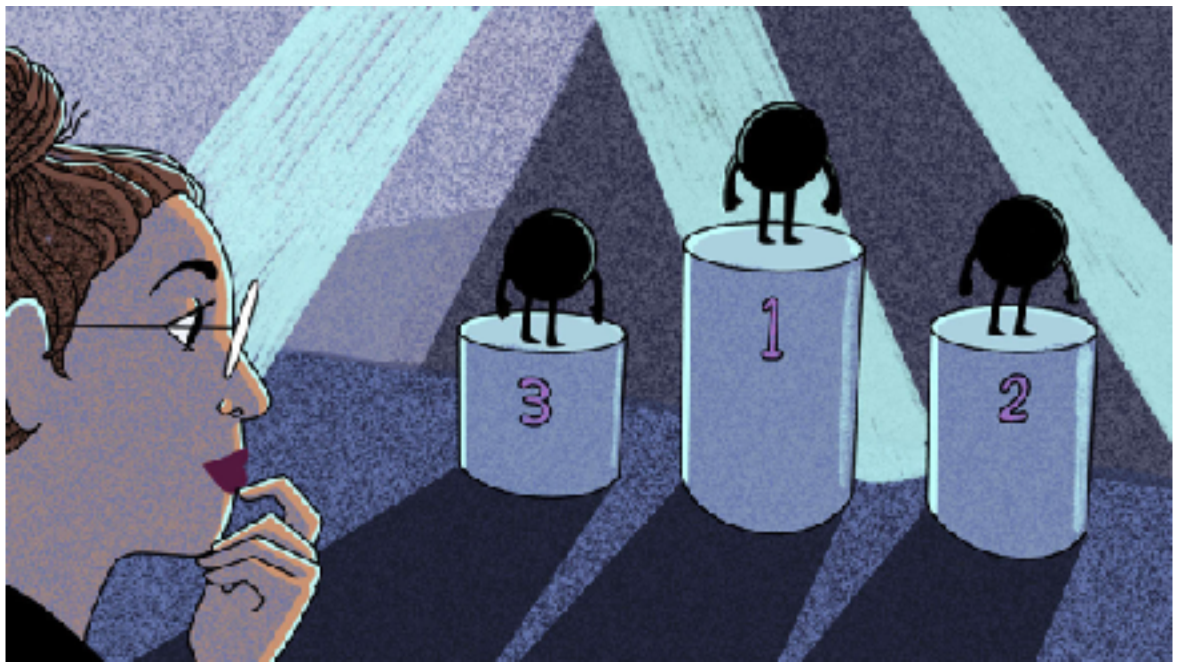

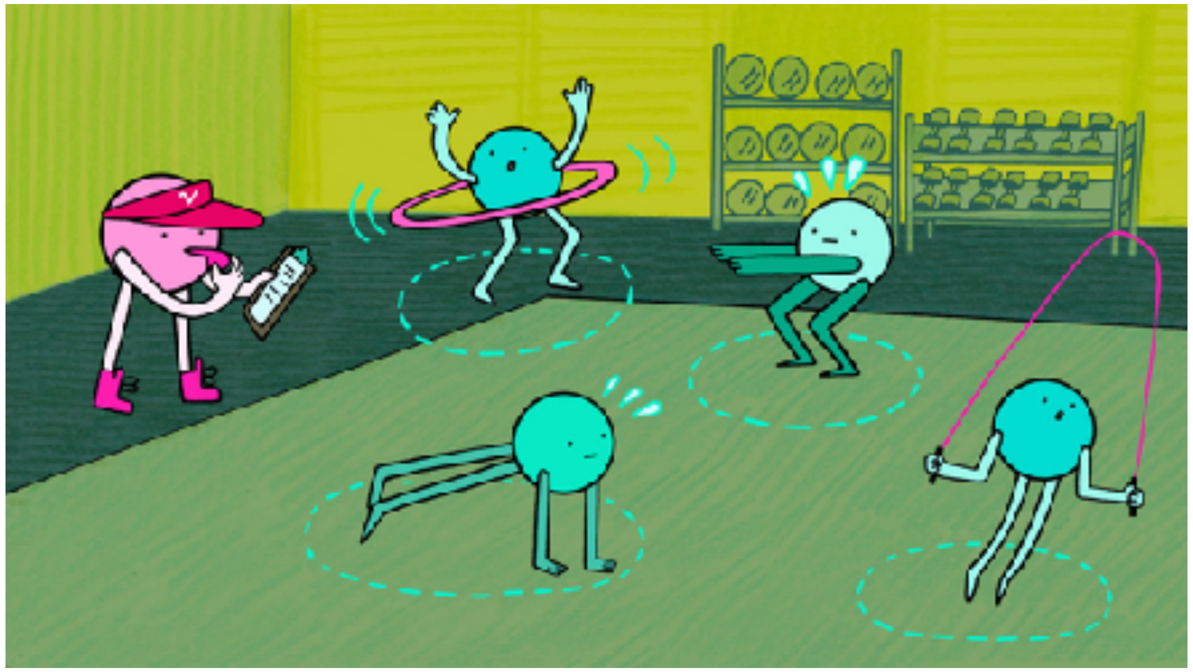

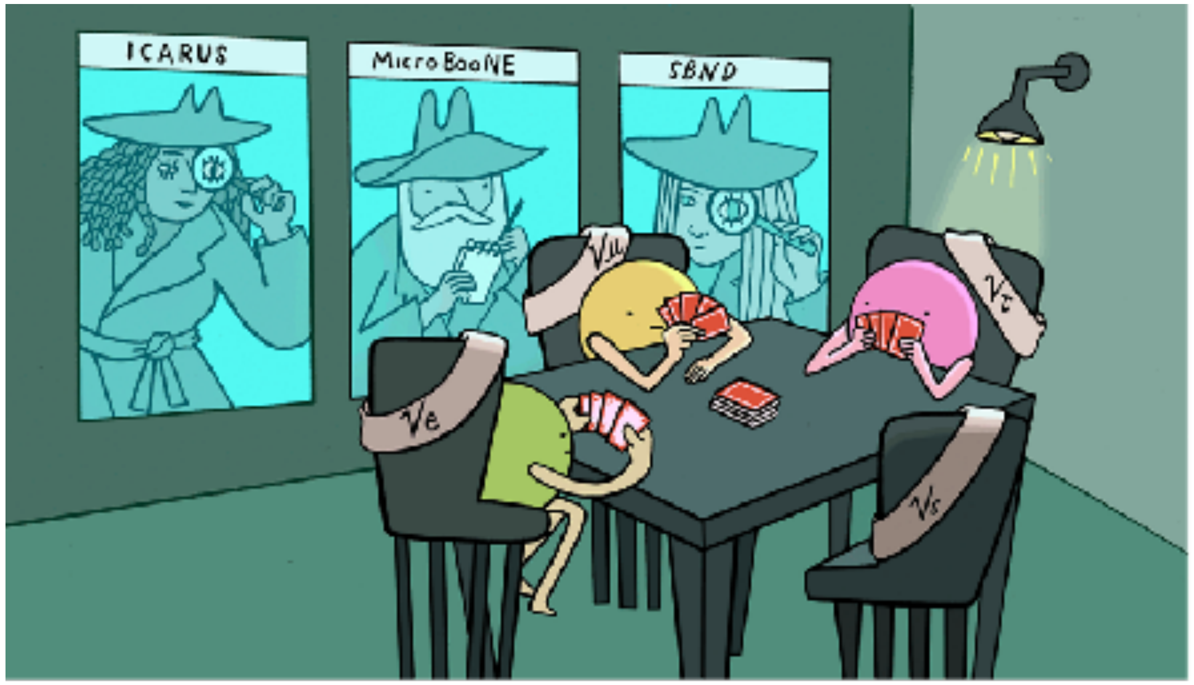

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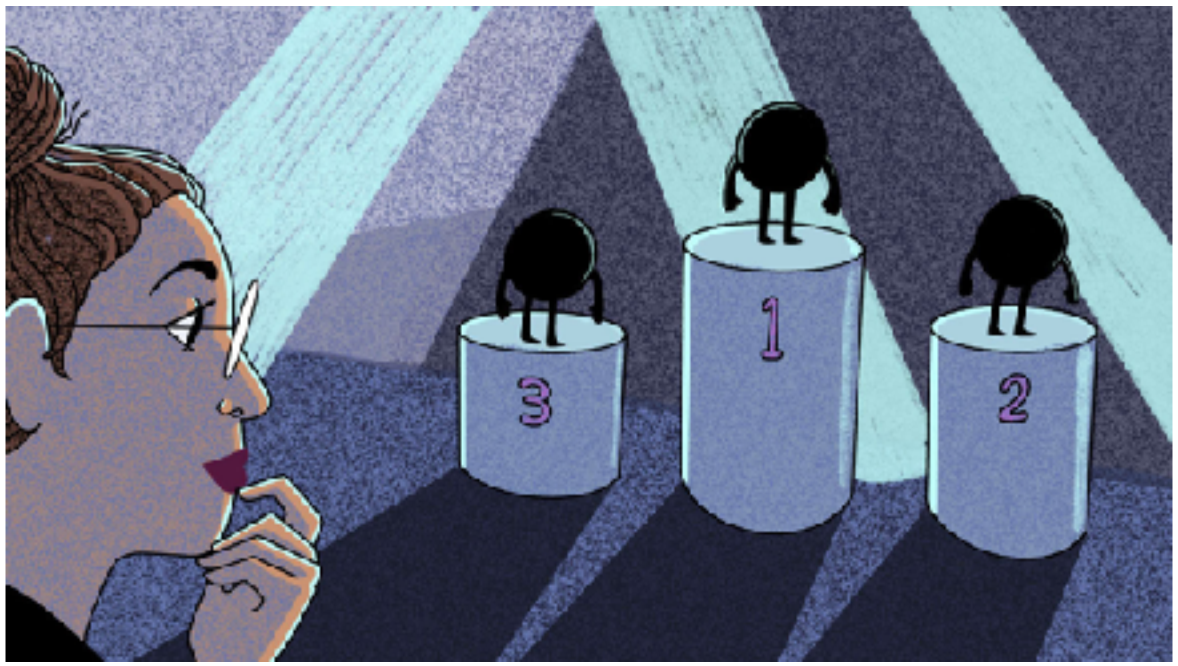
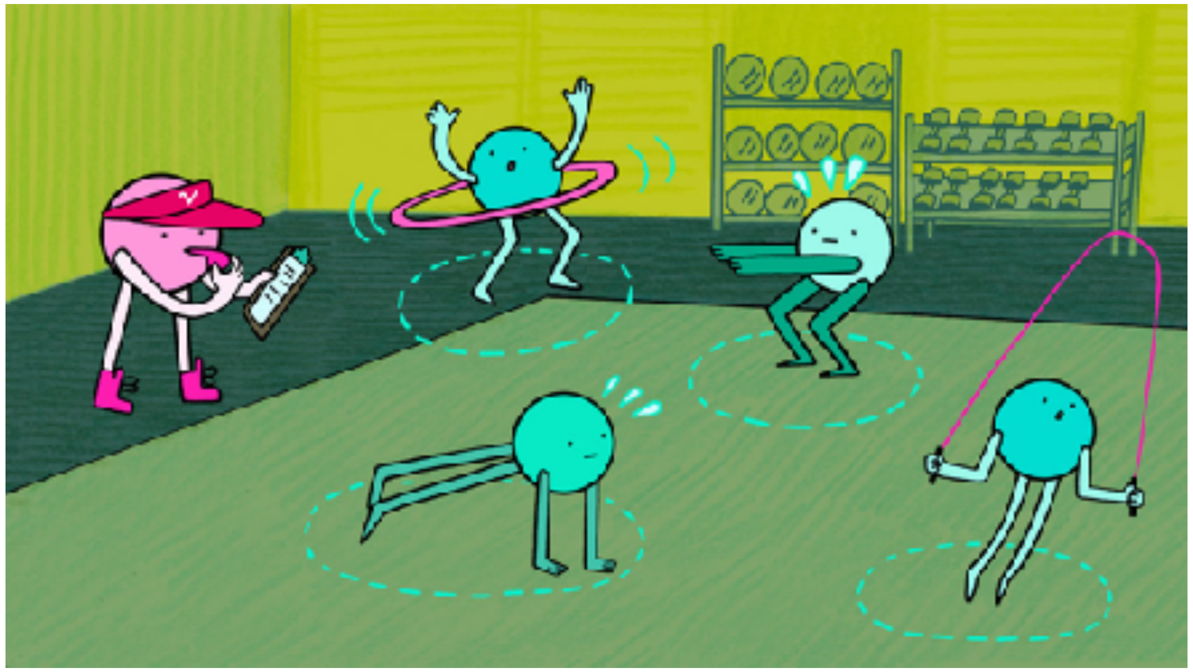
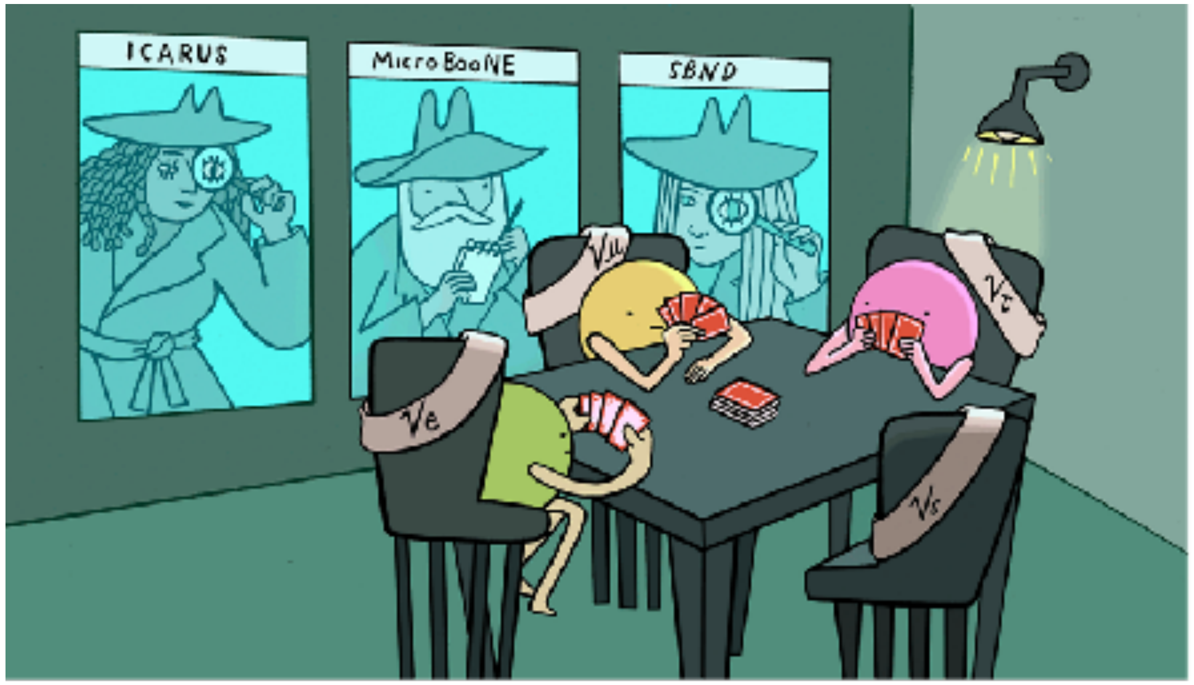


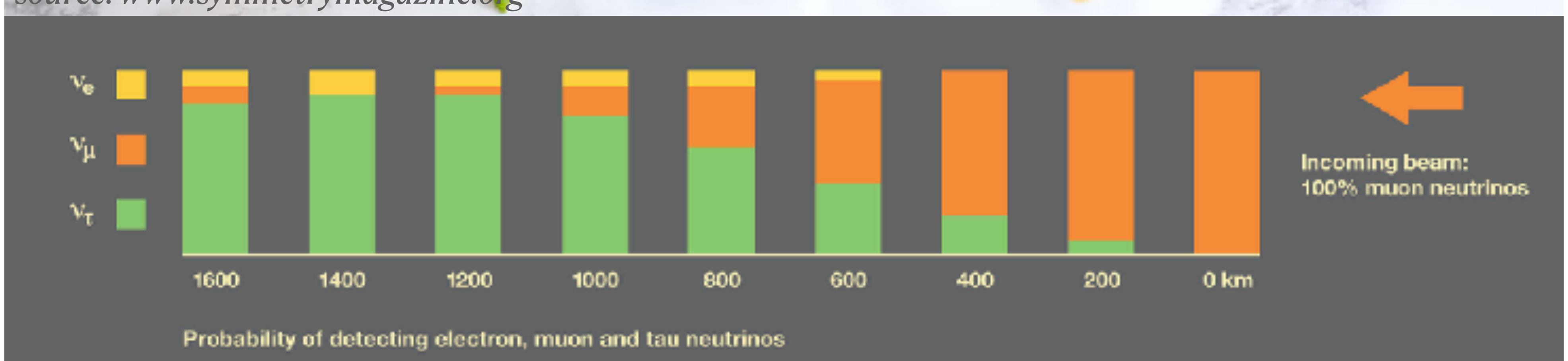




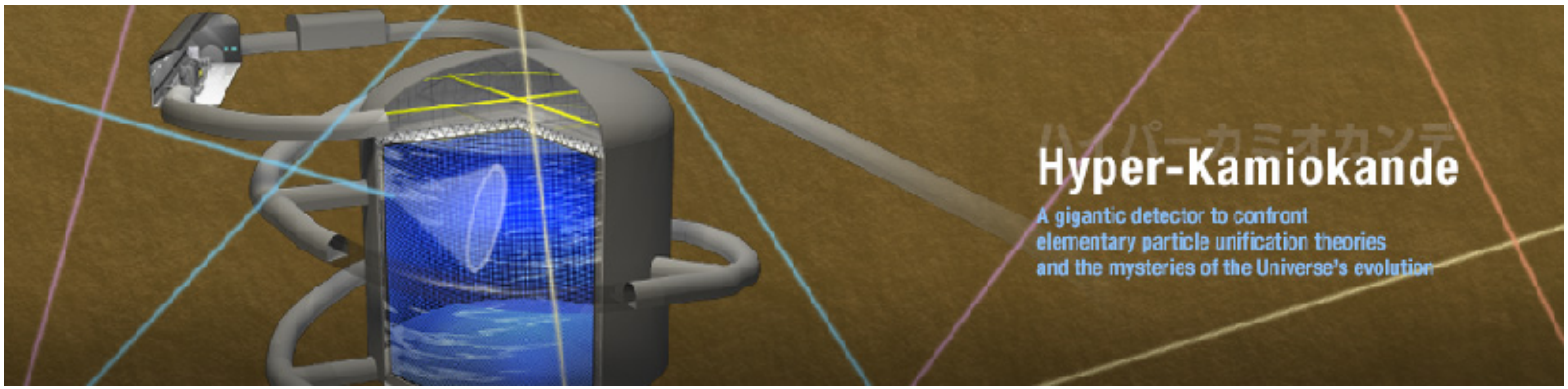
source: www.symmetrymagazine.org

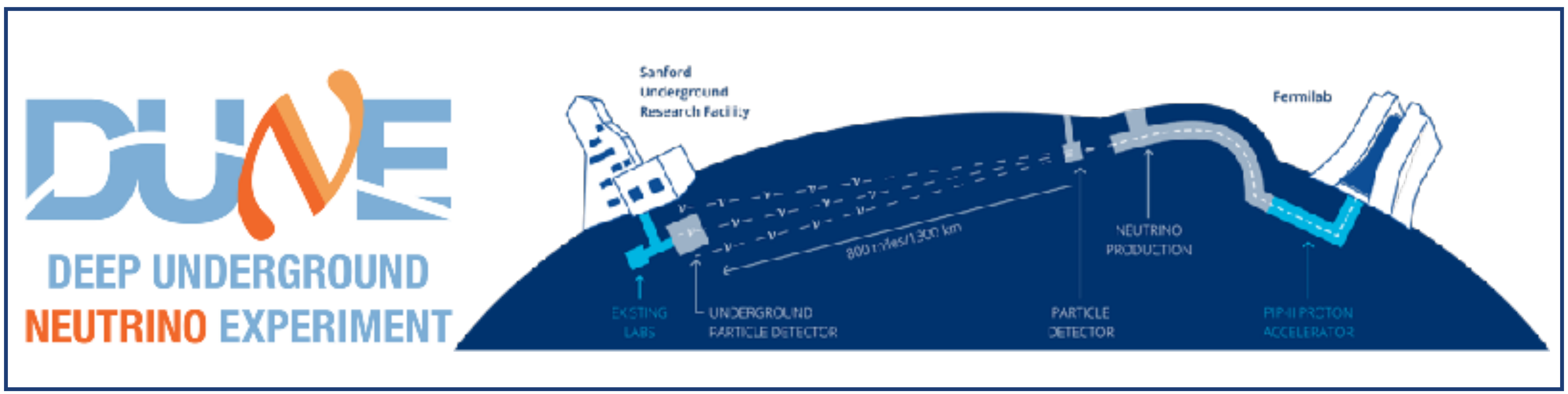
Neutrino oscillations


source: www.symmetrymagazine.org



Next generation experiments

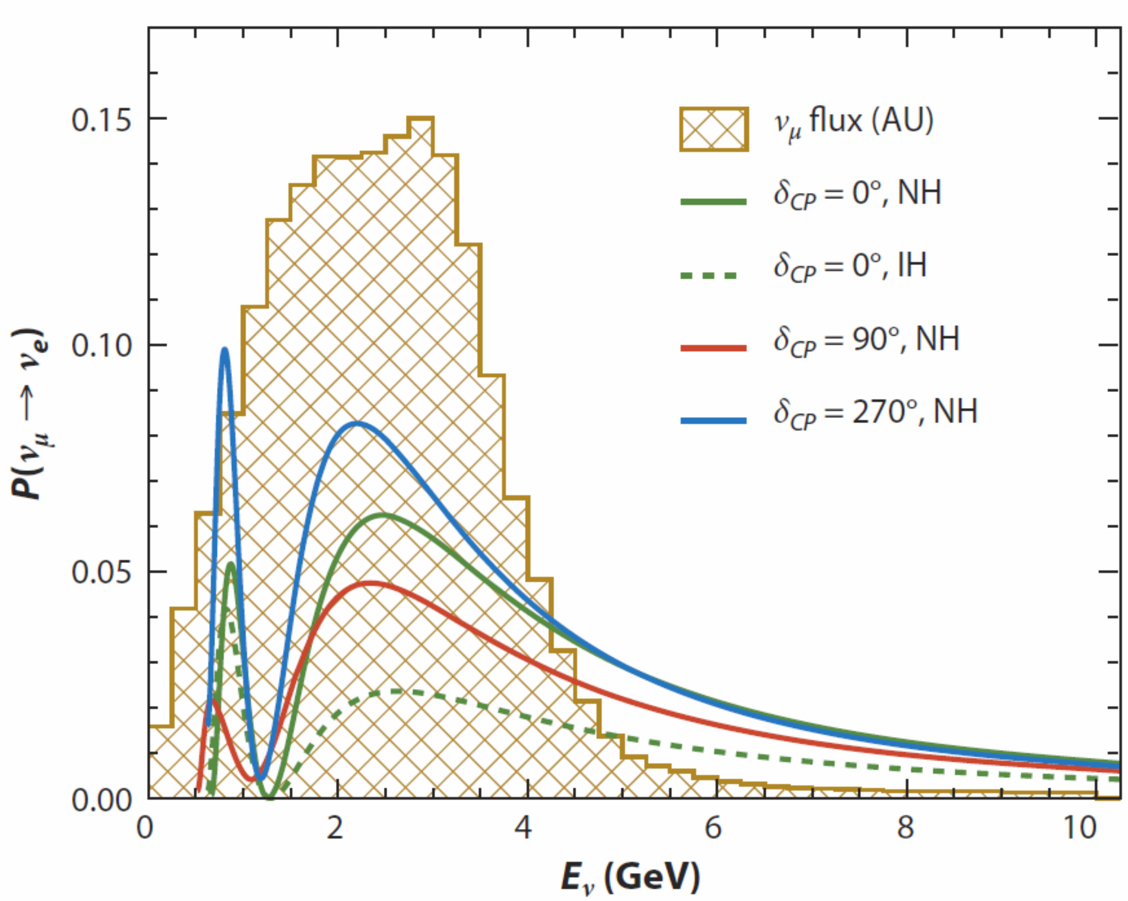




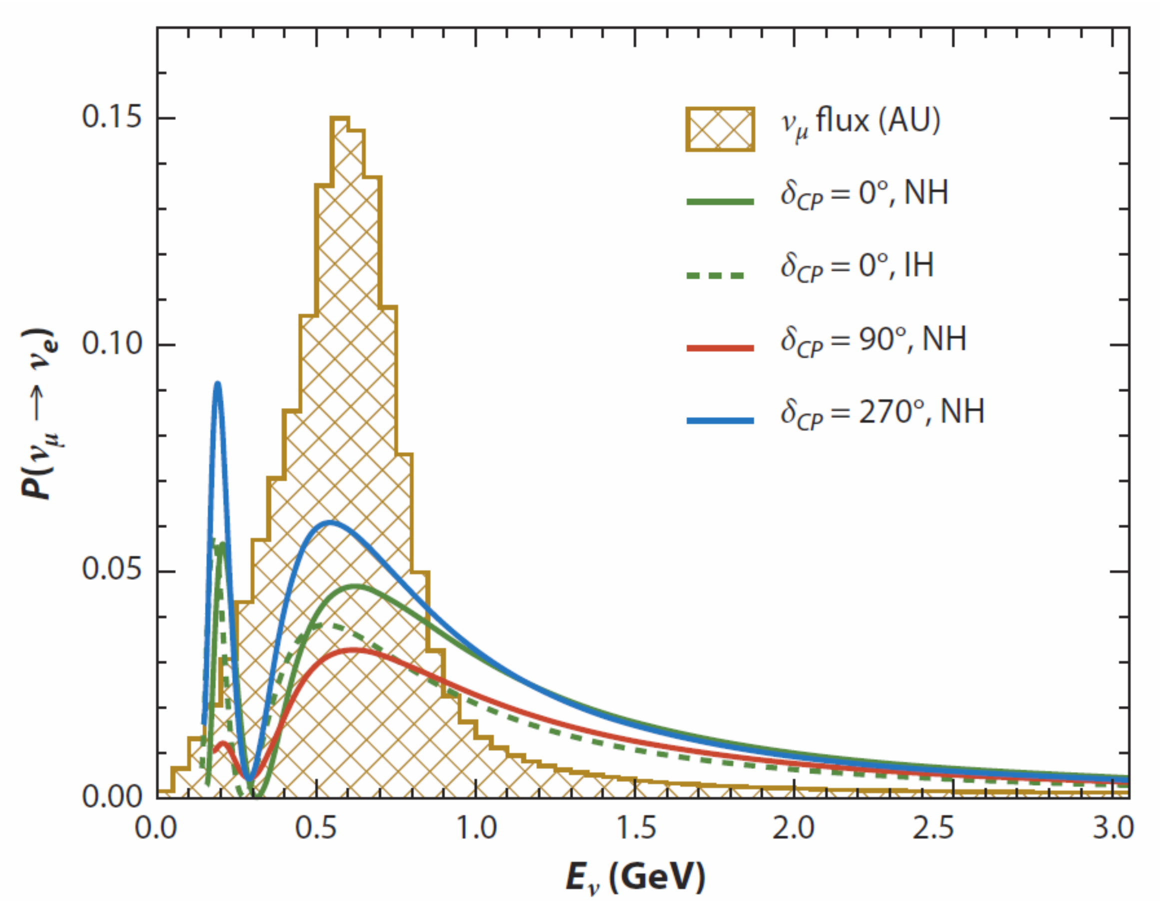
- ✓ **CP-violation measurement**
- ✓ **Determining ν mass ordering**
- ✓ Proton decay searches
- ✓ Cosmic neutrino observation

Aims & challenges

DUNE

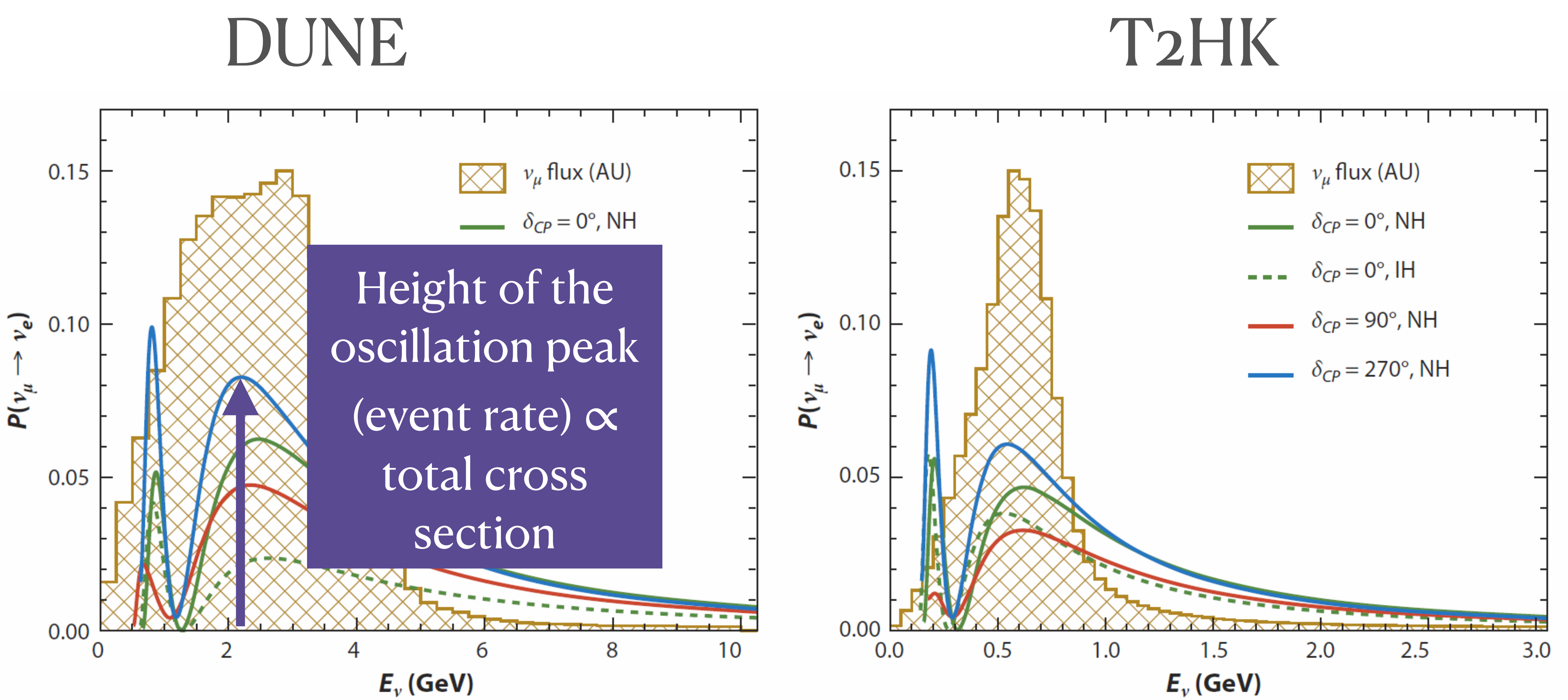


T2HK



From: Diwan et al, Ann. Rev.Nucl. Part. Sci 66 (2016)

Aims & challenges



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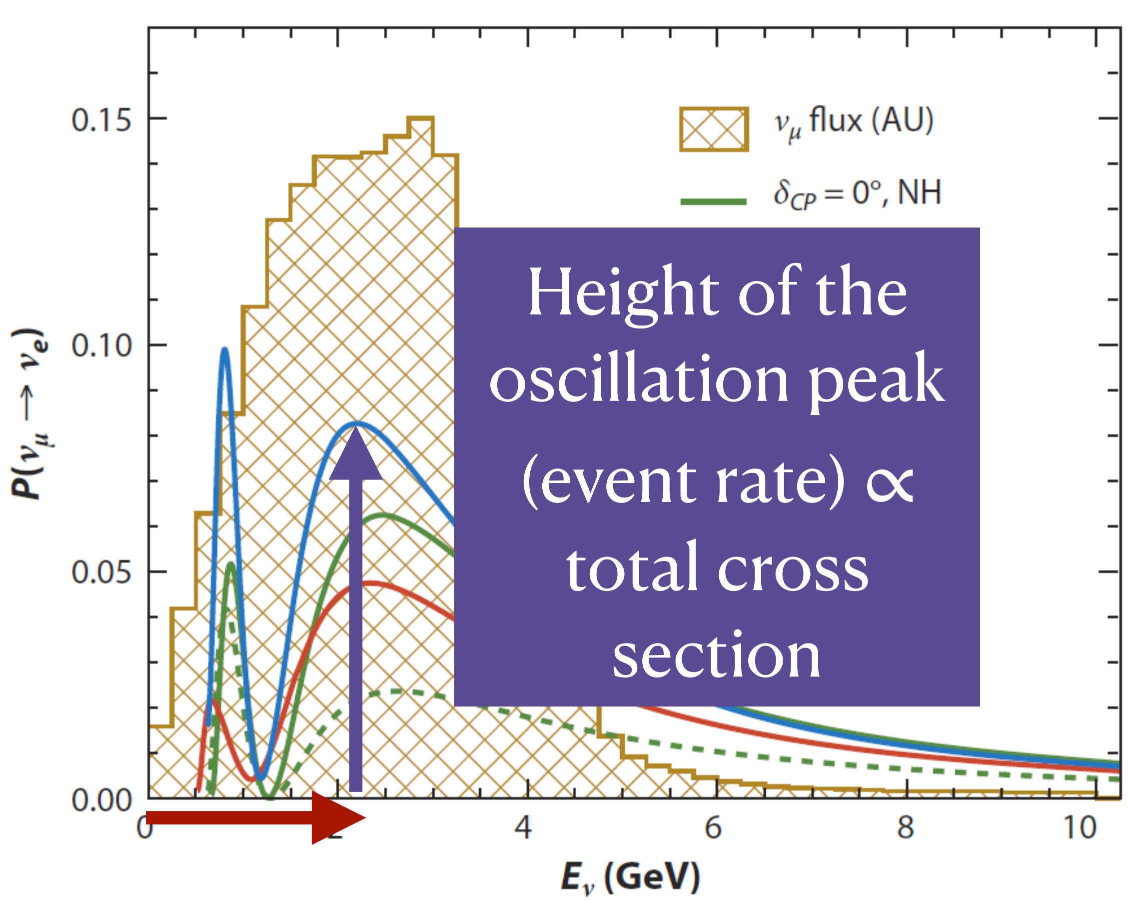
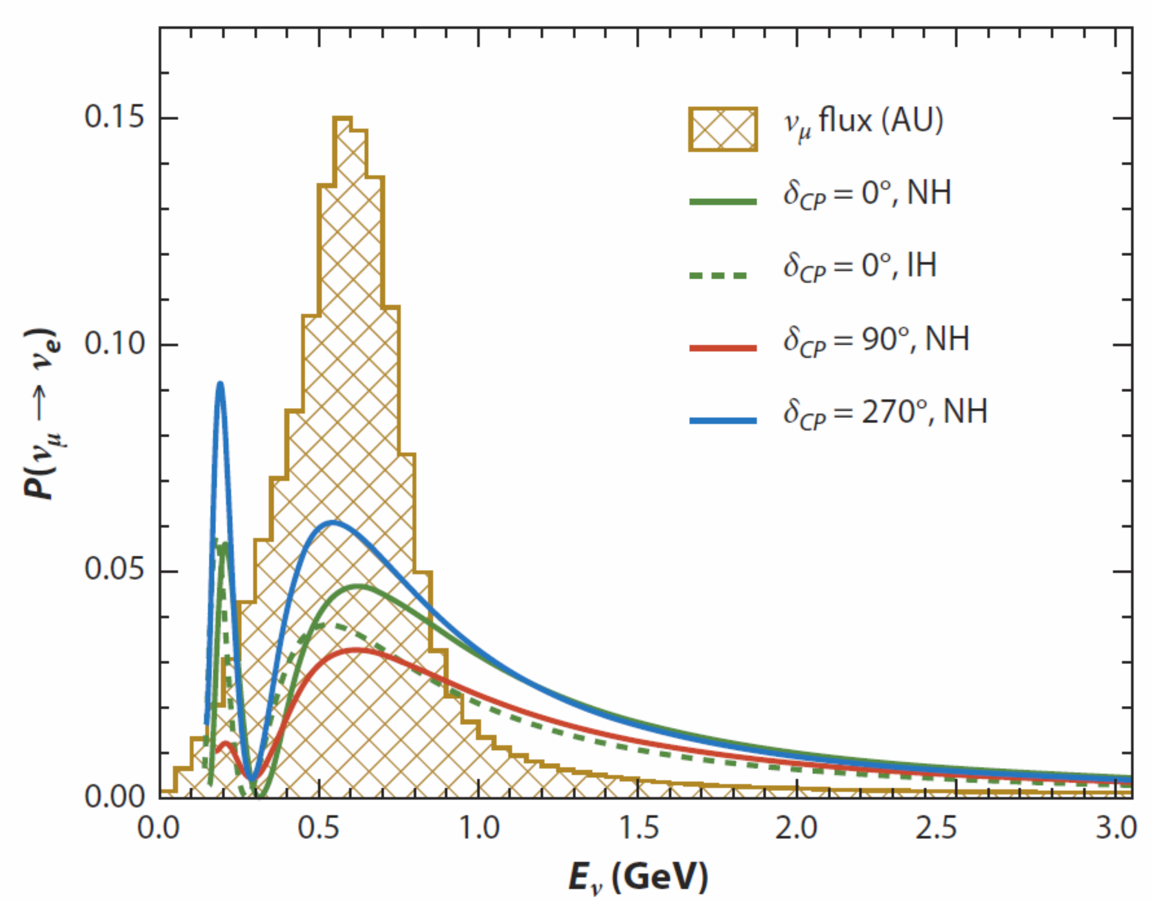


Height of the oscillation peak (event rate) ∝ total cross section

T2HK



Position of the oscillation peak depends on energy reconstruction

DUNE aims at uncertainties < 1% meaning O(25 MeV) precision of energy reconstruction

Aims & challenges

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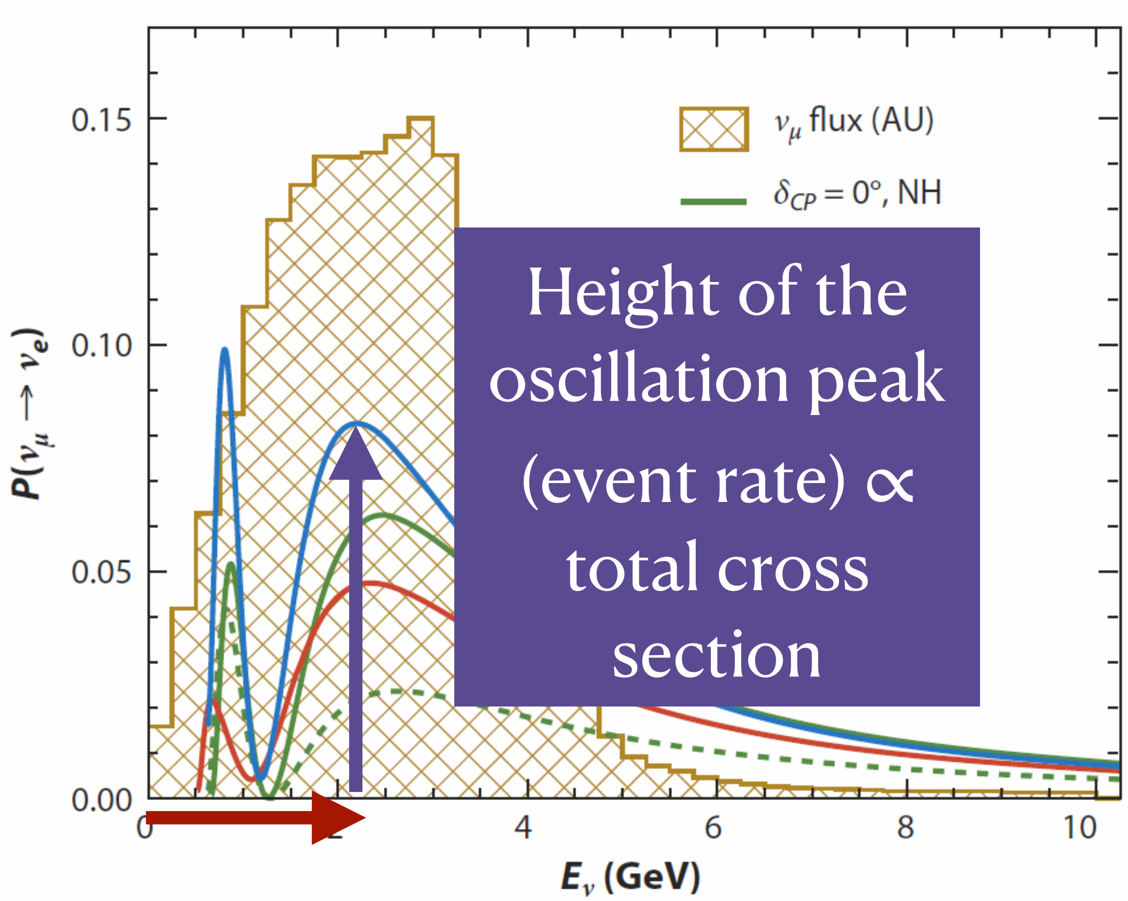
DUNE



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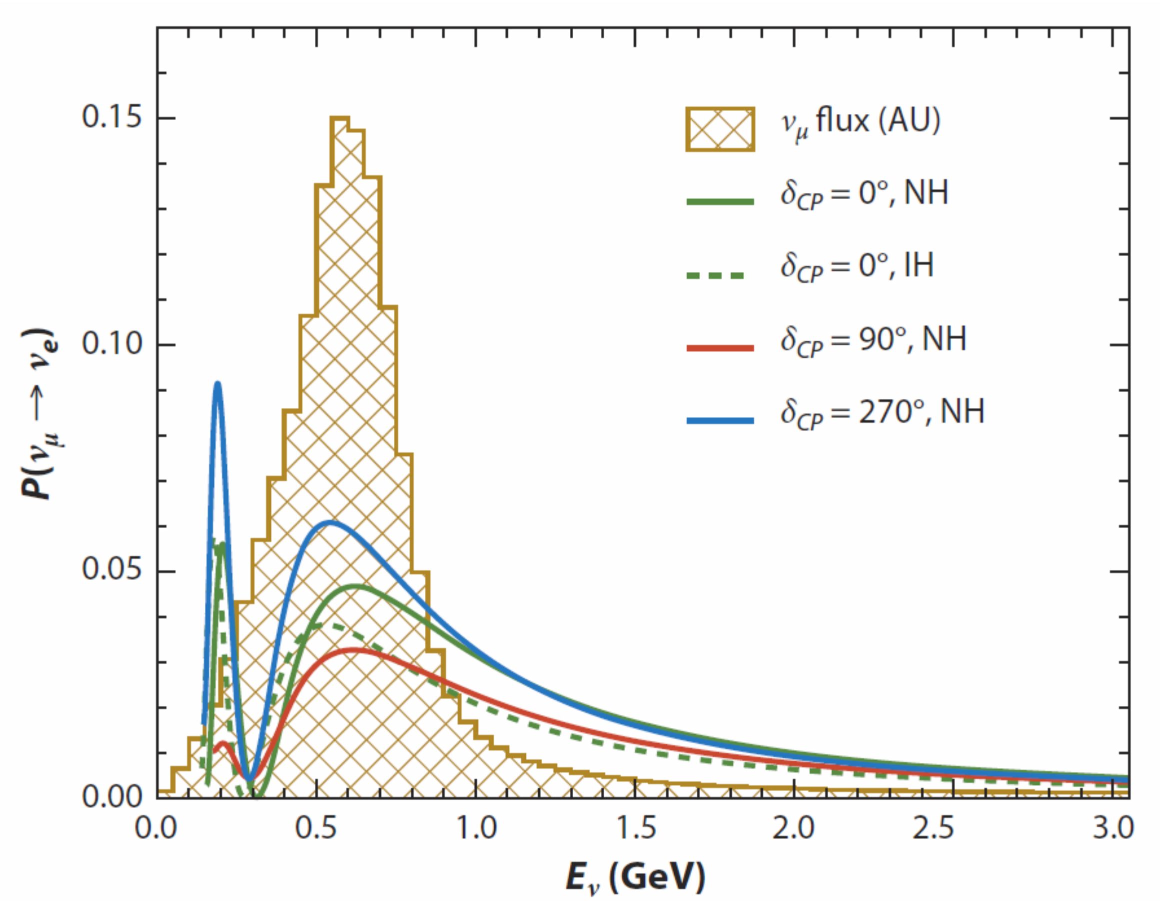


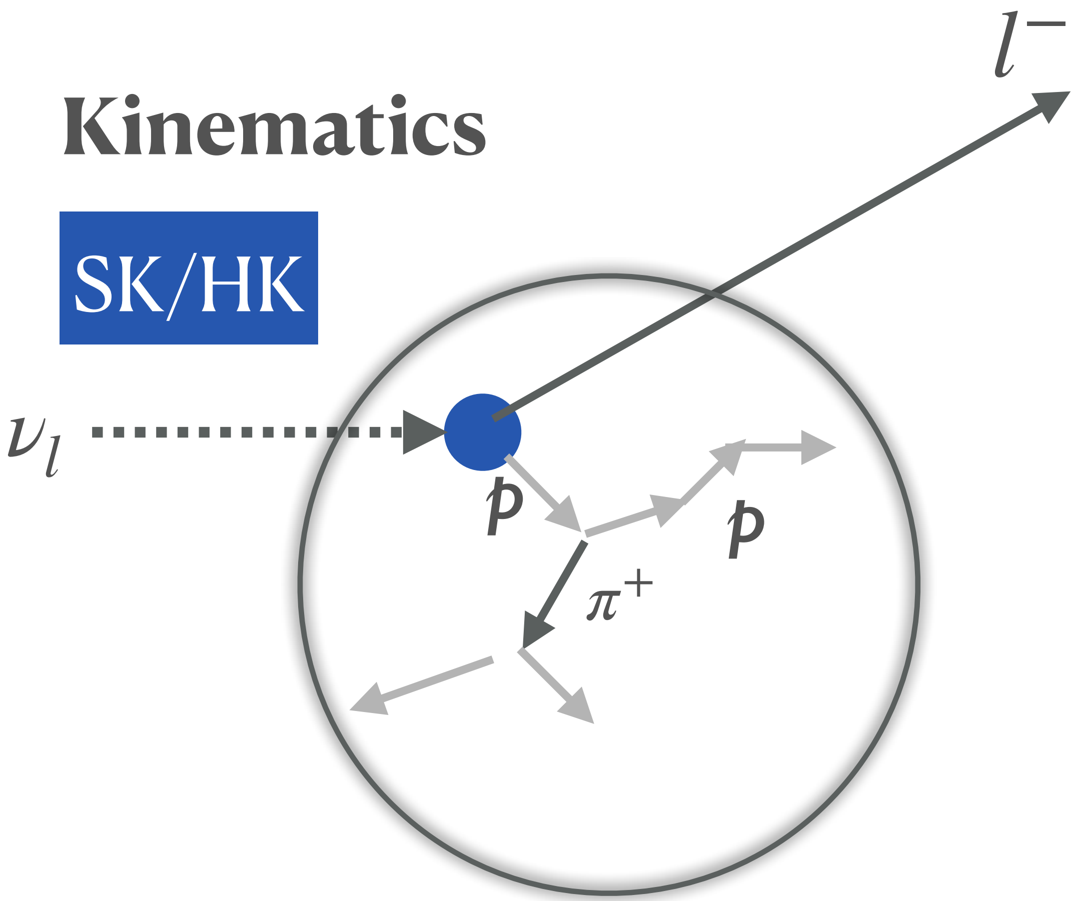
Position of the oscillation peak depends on energy reconstruction

DUNE aims at uncertainties < 1% meaning O(25 MeV) precision of energy reconstruction

Systematic errors should be small since statistics will be high.

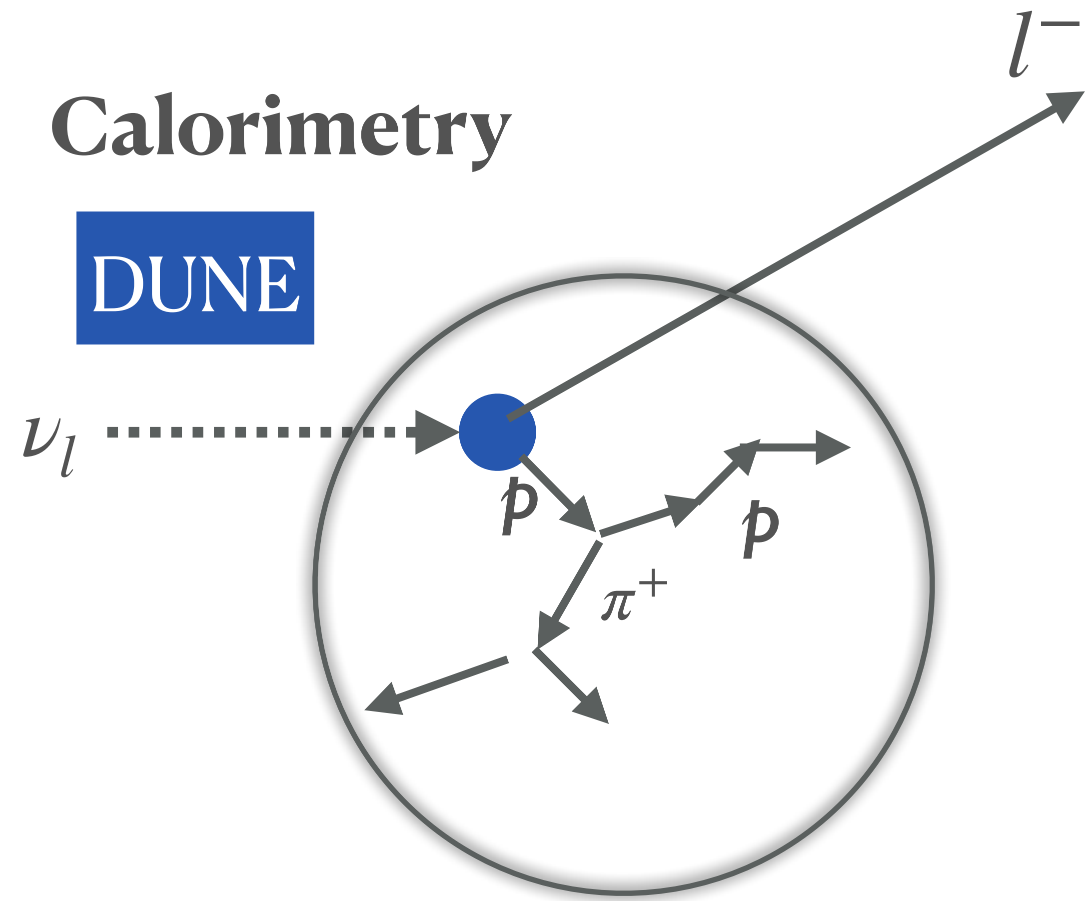
Energy reconstruction

Kinematics



- ✓ depends on lepton reconstruction
- ✓ relies on identification of interaction channel (for quasi-elastic works well)

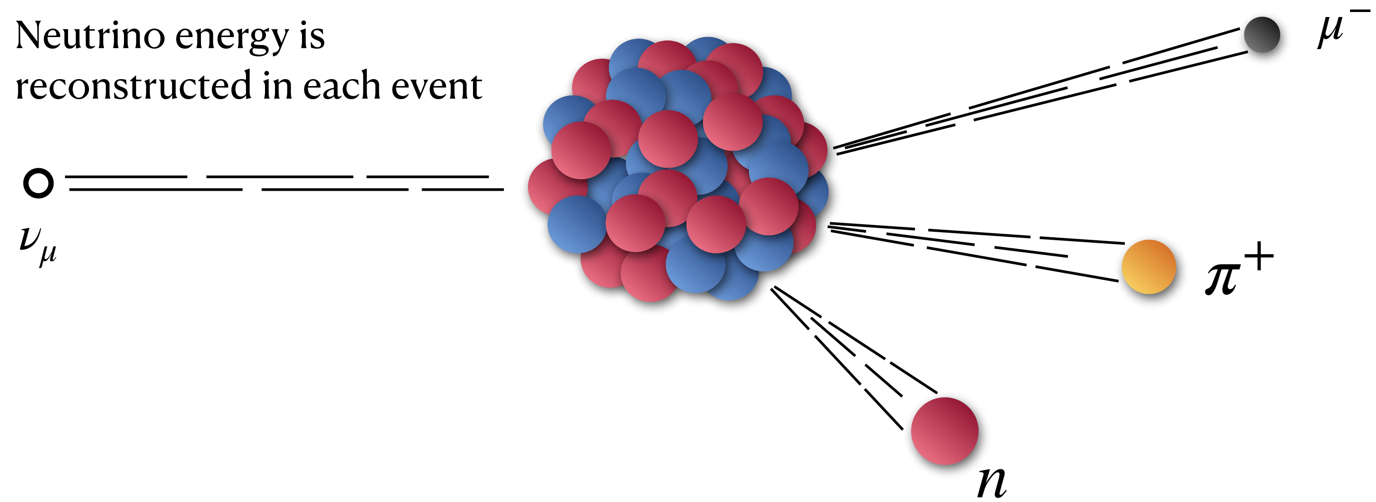
Calorimetry



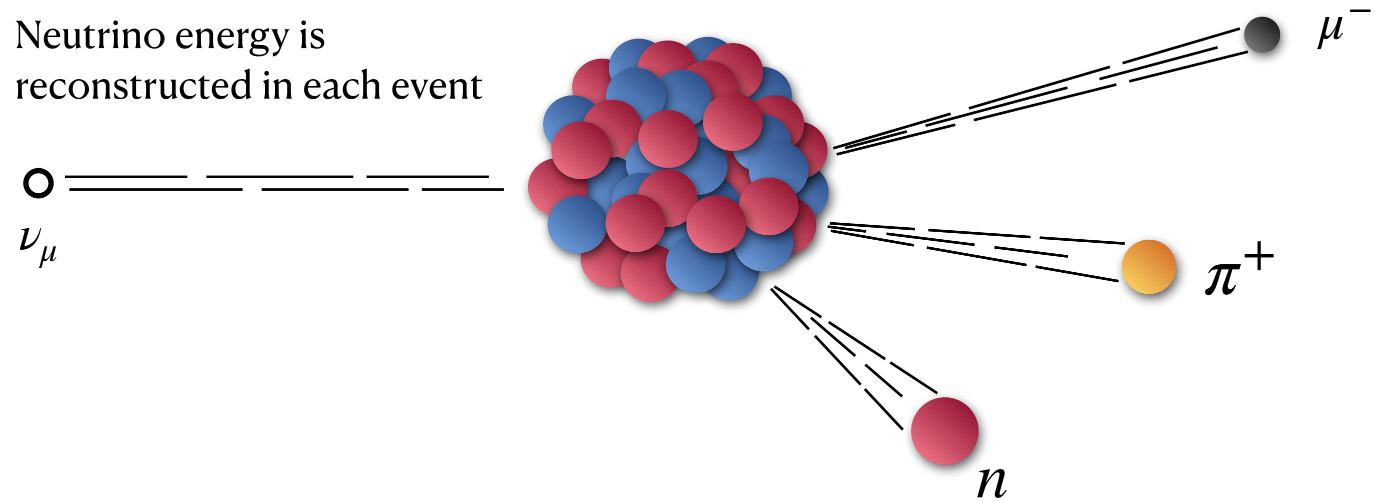
- ✓ energy conservation
- ✓ relies on visible energy
- ✓ hadron masses influence the energy balance

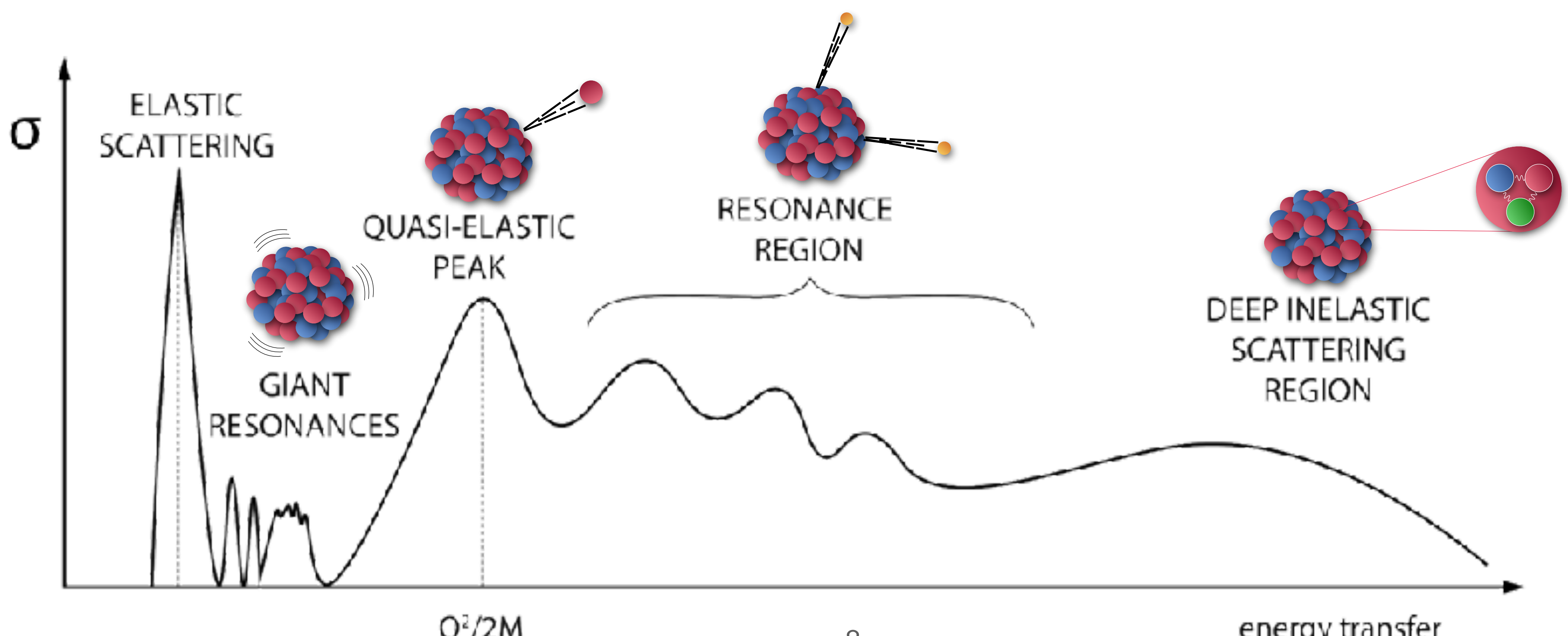
Nuclear models implemented in **Monte Carlo** event generators play crucial role.

Motivation

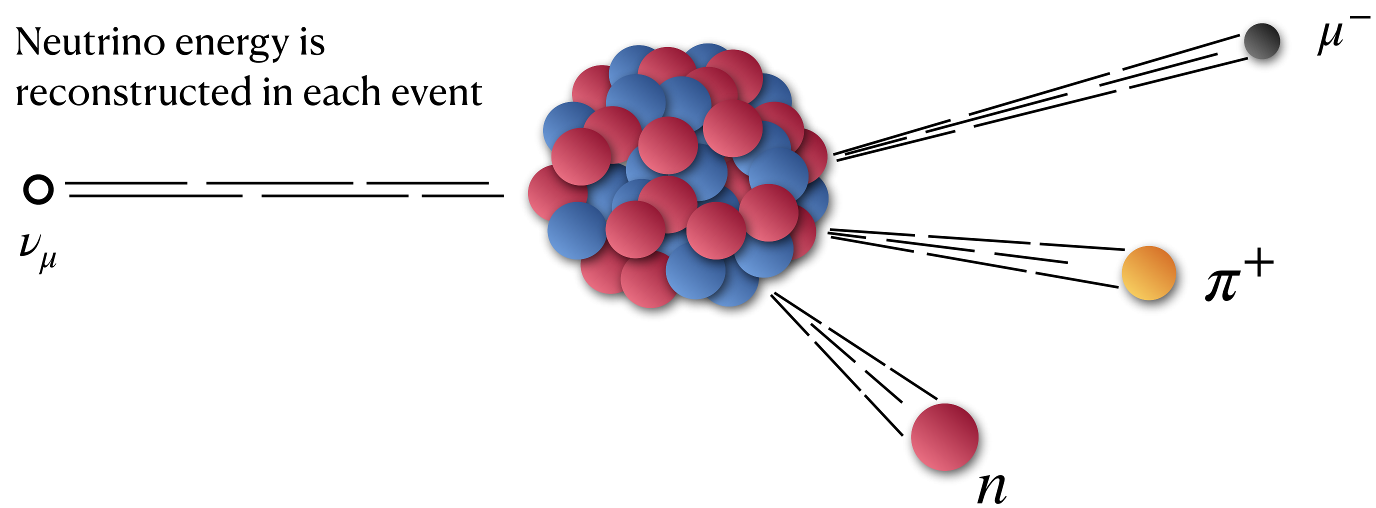


Motivation


Neutrino energy is
reconstructed in each event
ν_μ
μ^-
π^+
n


σ
ELASTIC
SCATTERING
GIANT
RESONANCES
QUASI-ELASTIC
PEAK
RESONANCE
REGION
DEEP INELASTIC
SCATTERING
REGION
$Q^2/2M$
energy transfer

Motivation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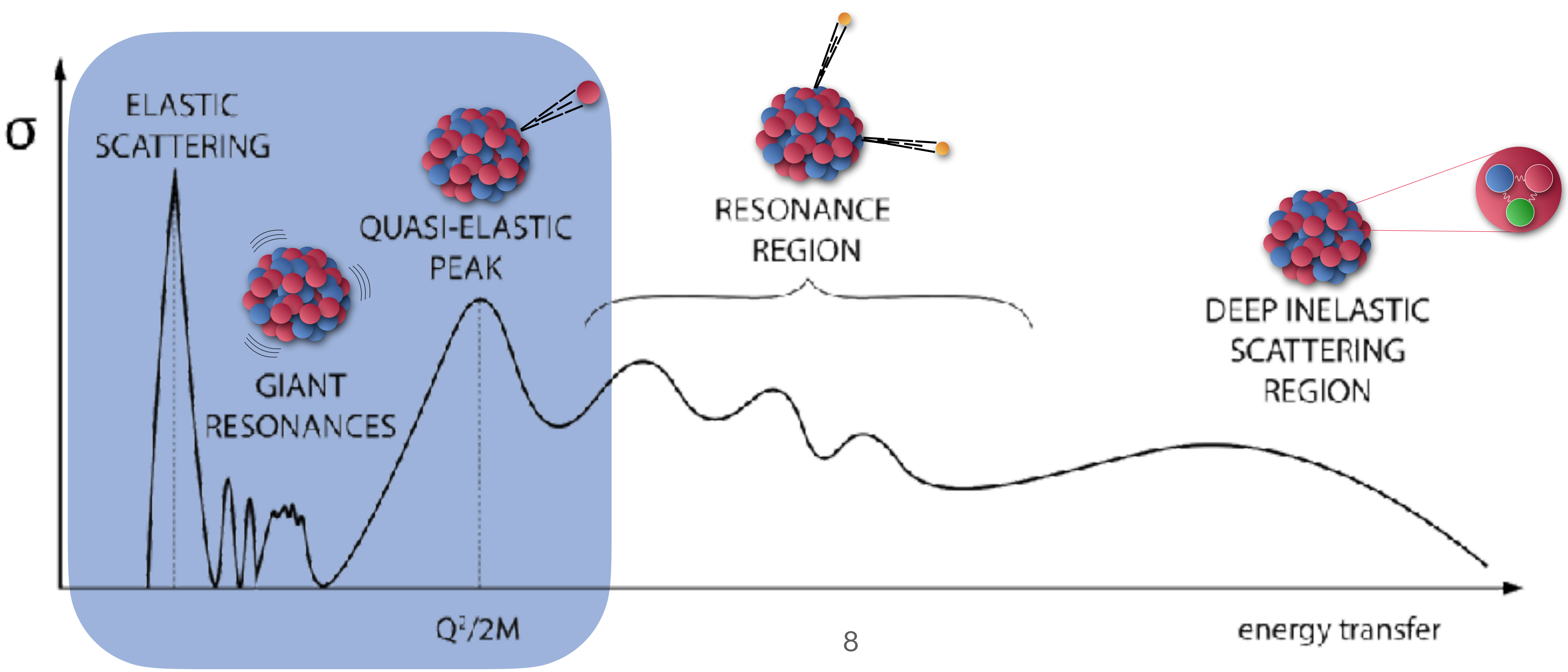
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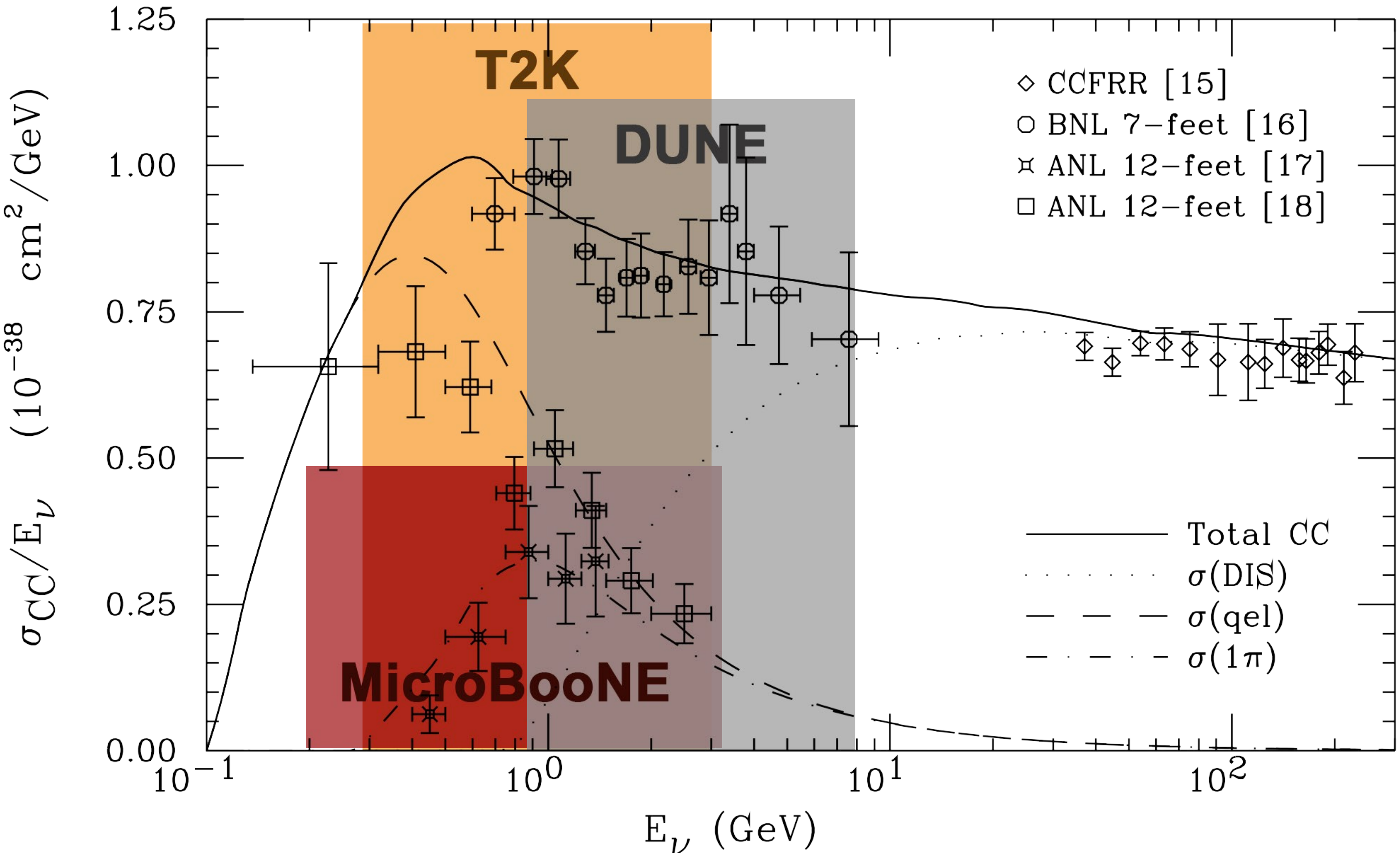
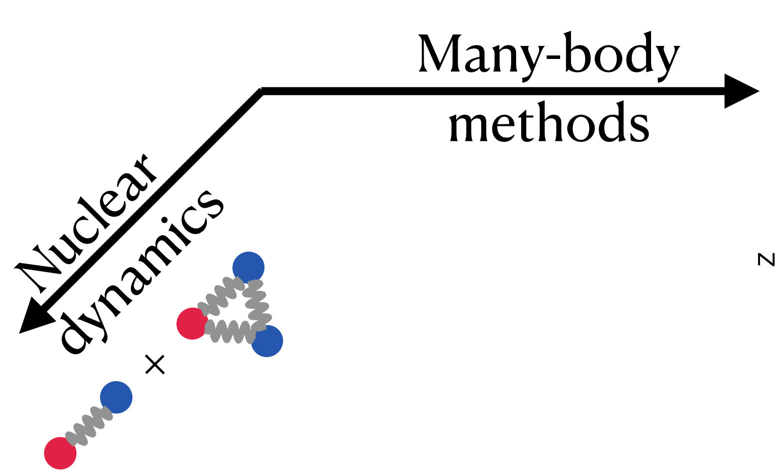
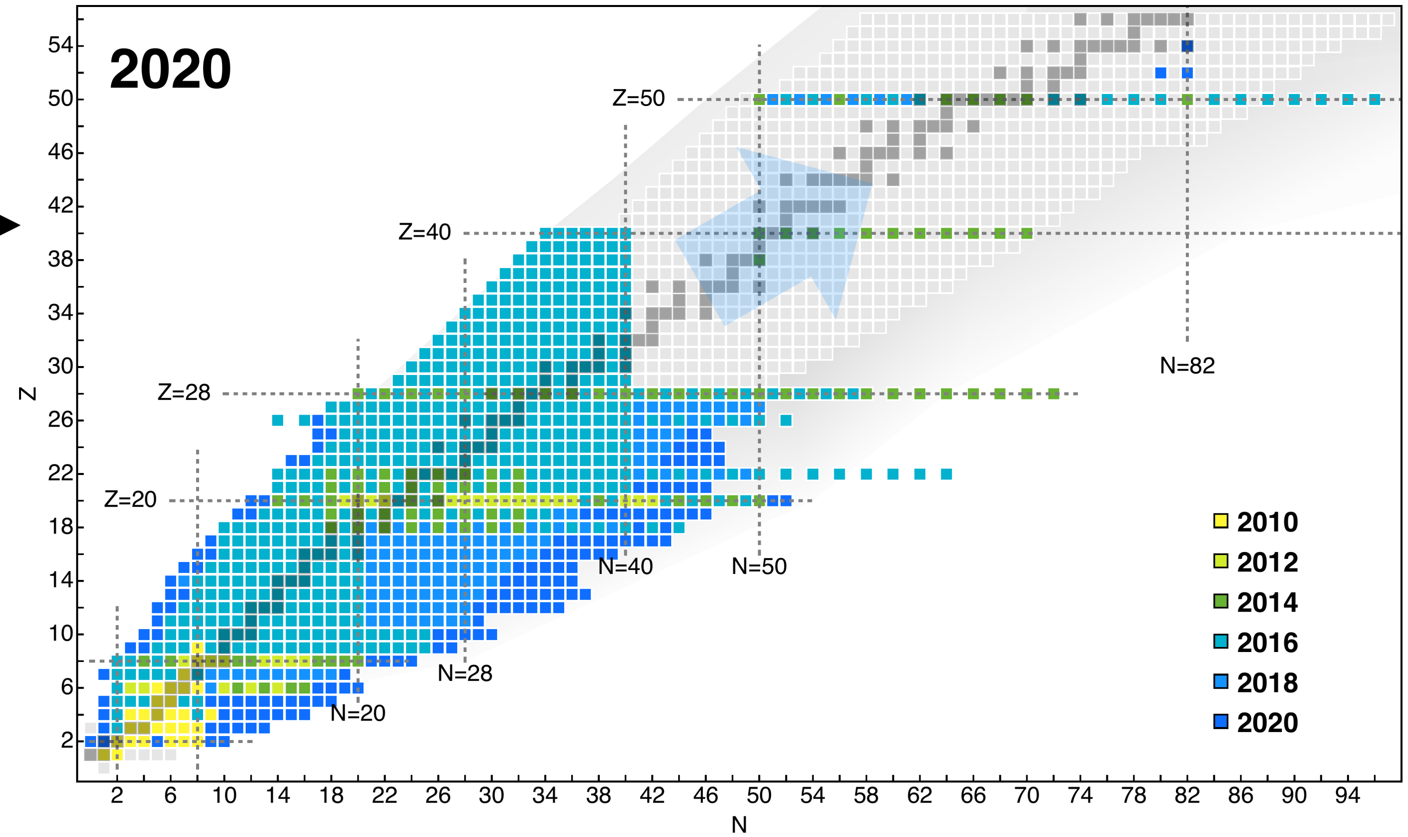
Why is QE important?



From: P. Lipari et. atl., PRL 74 (1995)

Motivation

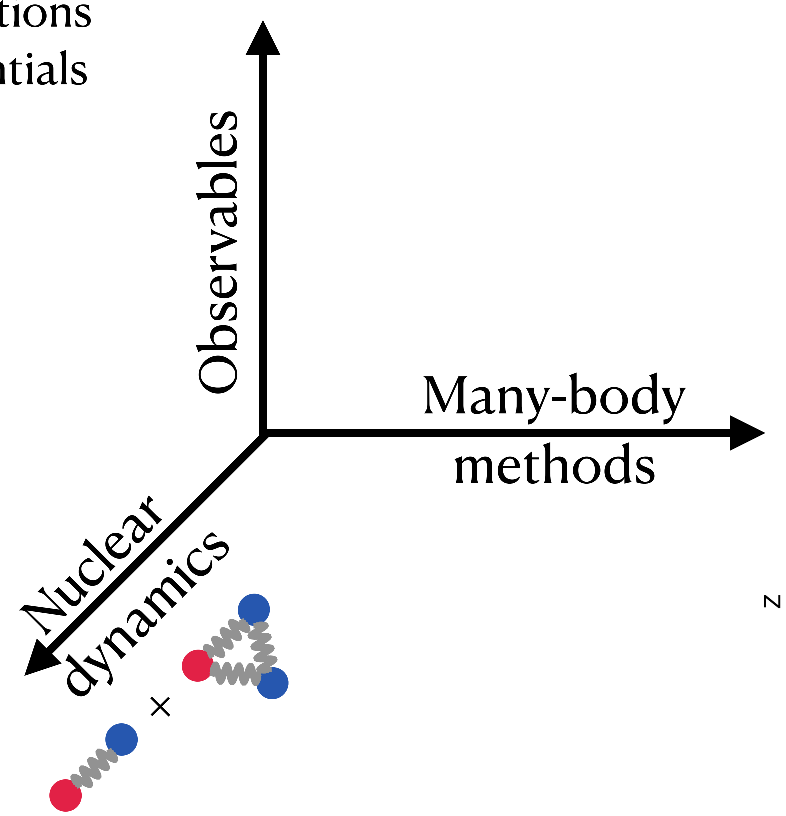


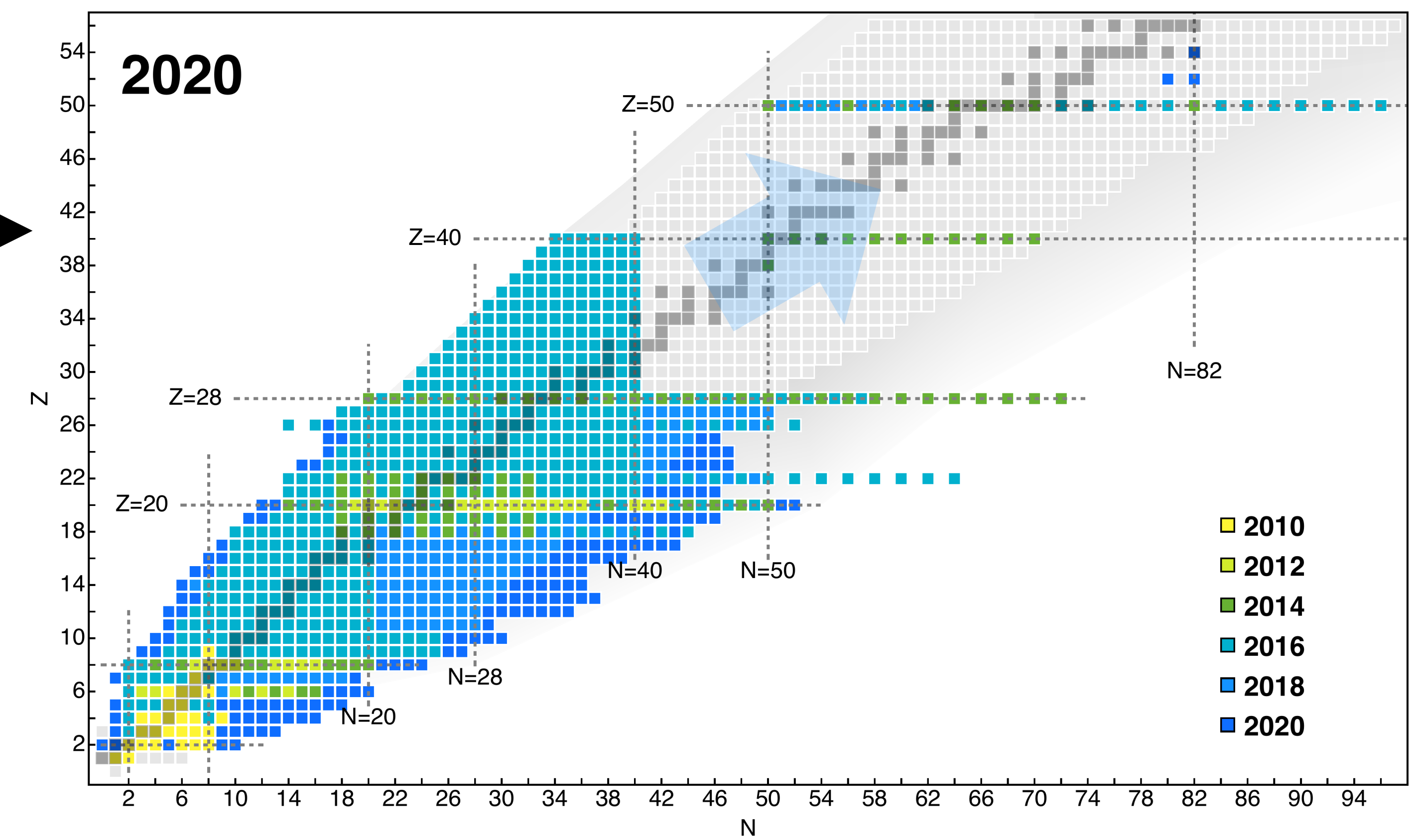


H. Hergert, *Front.in Phys.* 8 (2020) 379

Motivation

➡ Nuclear responses
➡ Spectral functions
➡ Optical potentials
...





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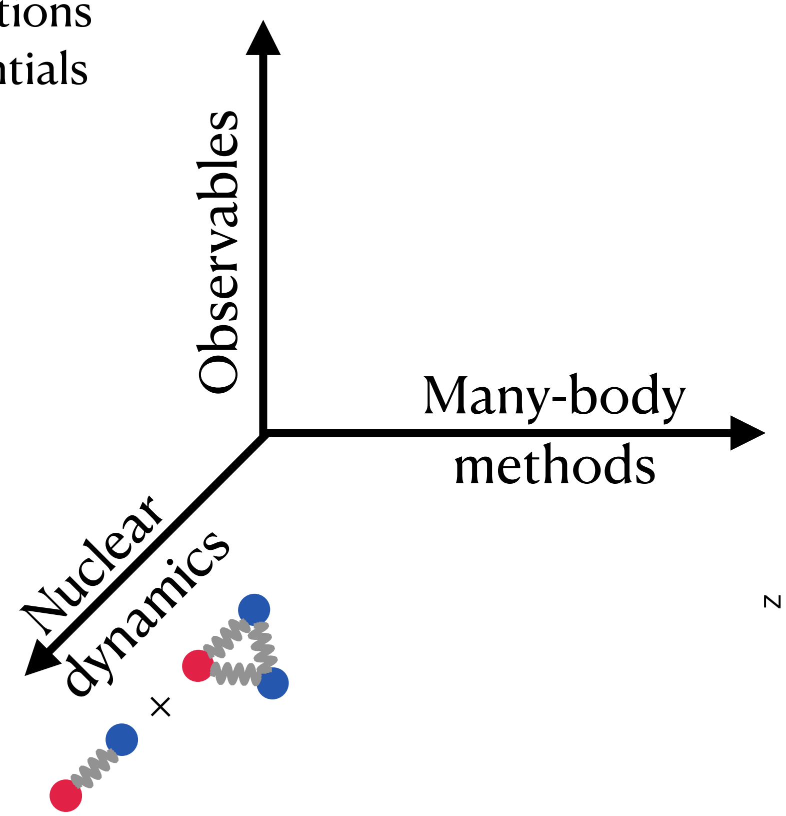
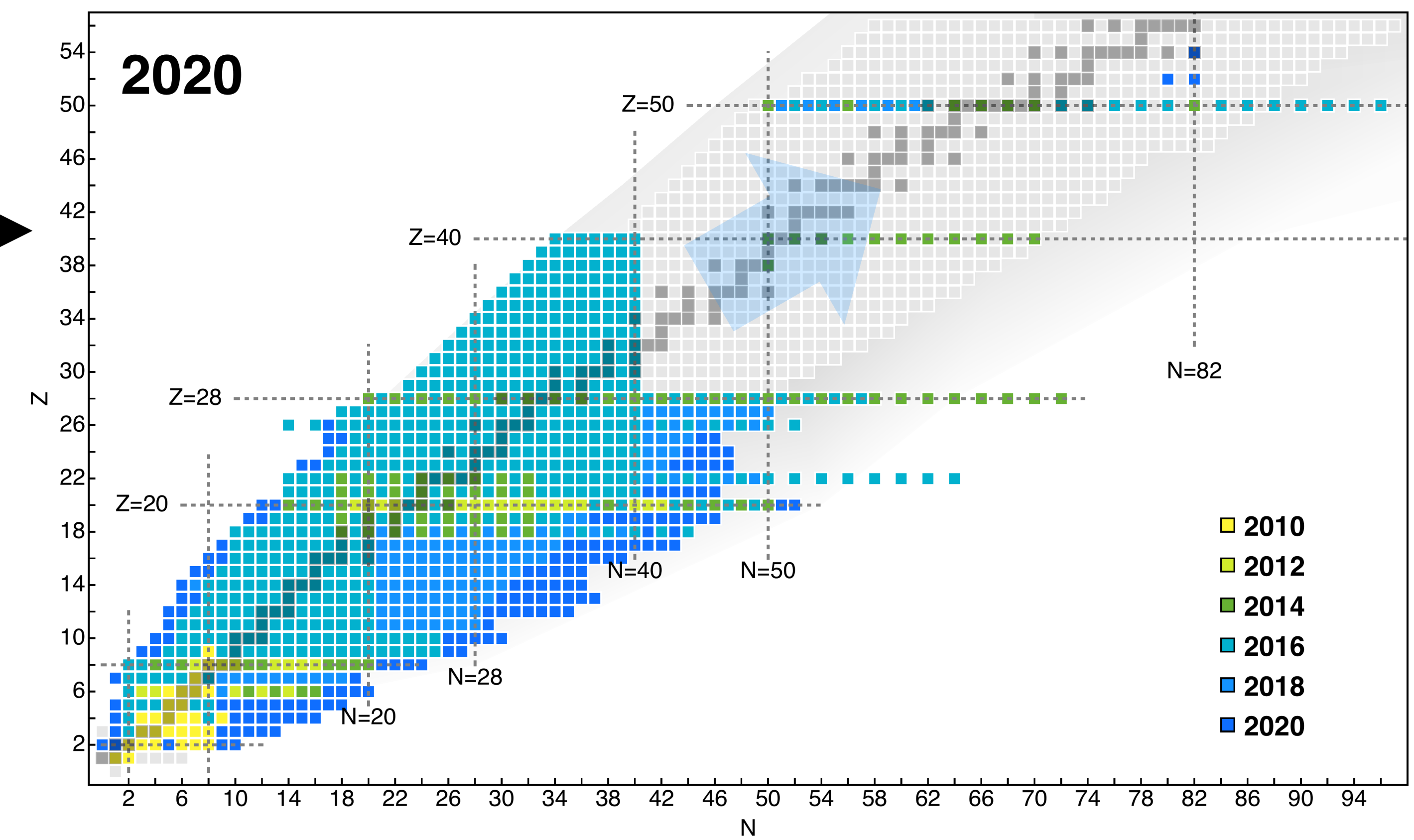


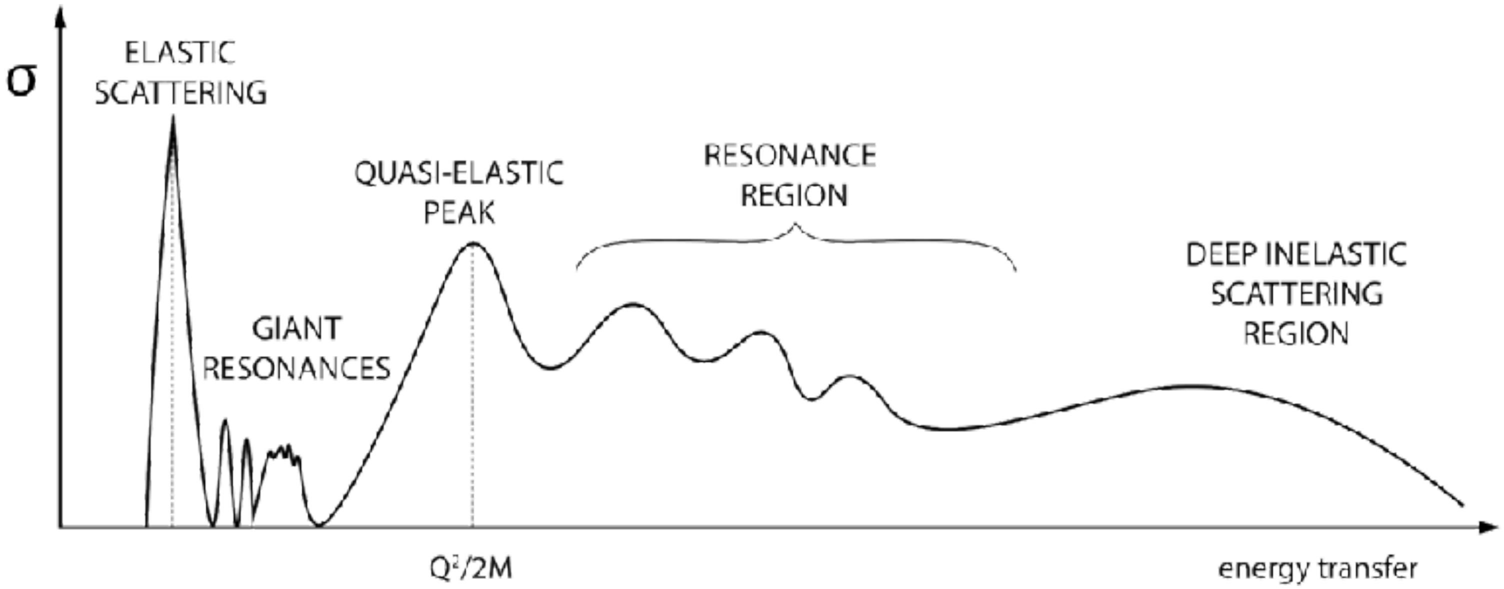


H. Hergert, *Front.in Phys.* 8 (2020) 379

➡ **Neutrinos challenge ab initio nuclear theory**

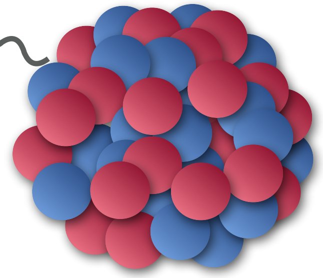
➡ **Controllable approximations within ab initial nuclear theory**

Nuclear response



$$J_\mu = (\rho, \vec{j}) \, | \, \Psi \rangle$$

$\gamma, W^\pm, Z^0$



$$\sigma \propto L^{\mu\nu} R_{\mu\nu}$$

lepton tensor — nuclear responses

$$R_{\mu\nu}(\omega, q) = \sum_f \langle \Psi \, | \, J_\mu^\dagger(q) \, | \, \Psi_f \rangle \langle \Psi_f \, | \, J_\nu(q) \, | \, \Psi \rangle \delta(E_0 + \omega - E_f)$$

Electrons for neutrinos

$$\left.\frac{d\sigma}{d\omega dq}\right|_{\nu/\bar{\nu}} = \sigma_0\left(\upsilon_{CC}R_{CC} + \upsilon_{CL}R_{CL} + \upsilon_{LL}R_{LL} + \upsilon_T R_T \pm \upsilon_{T'}R_{T'}\right)$$

$$\left.\frac{d\sigma}{d\omega dq}\right|_{e} = \sigma_M\left(\upsilon_L R_L + \upsilon_T R_T\right)$$

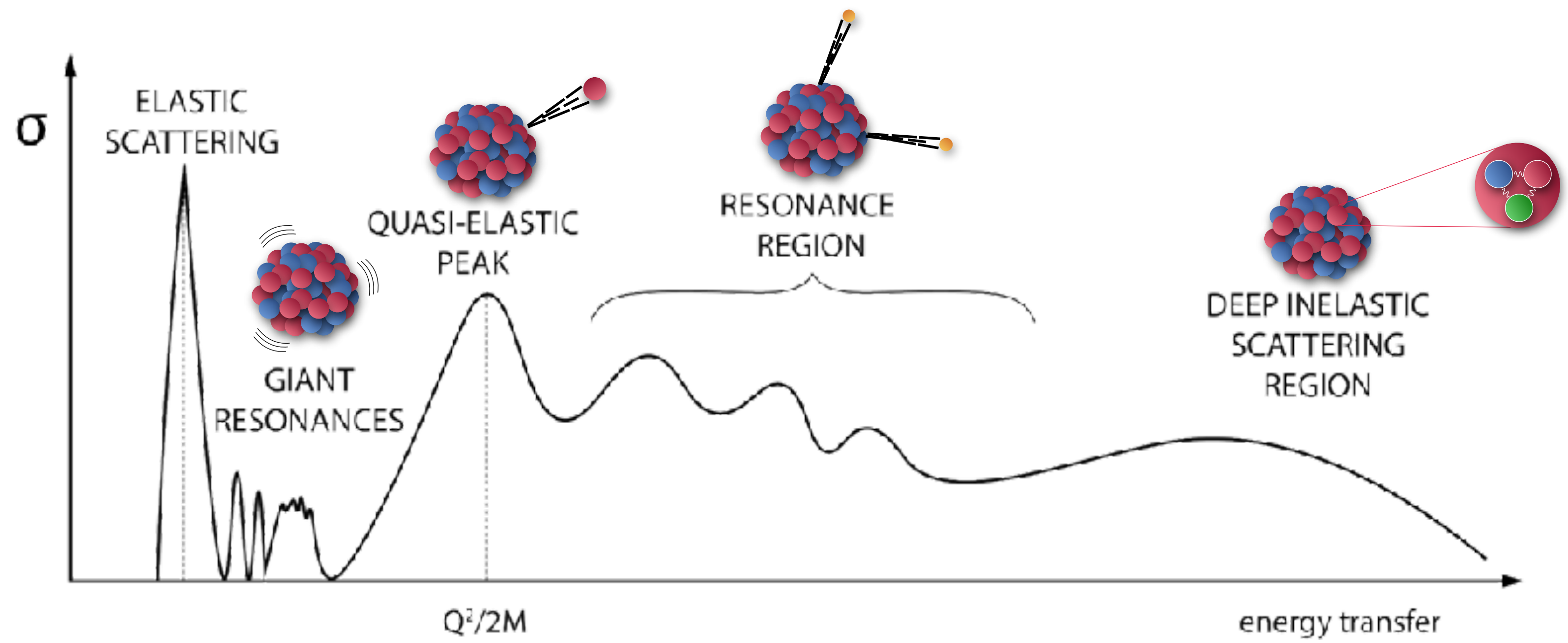
✓ much more precise data

✓ we can get access to R_L and R_T separately (Rosenbluth separation)

✓ experimental programs of electron scattering in JLab, MAMI, MESA

Quasielastic response

- Momentum transfer ~hundreds MeV
- Upper limit for ab initio methods
- Important mechanism for T2HK, DUNE
- Role of final state interactions
- Role of 1-body and 2-body currents



First step: analyse the longitudinal response

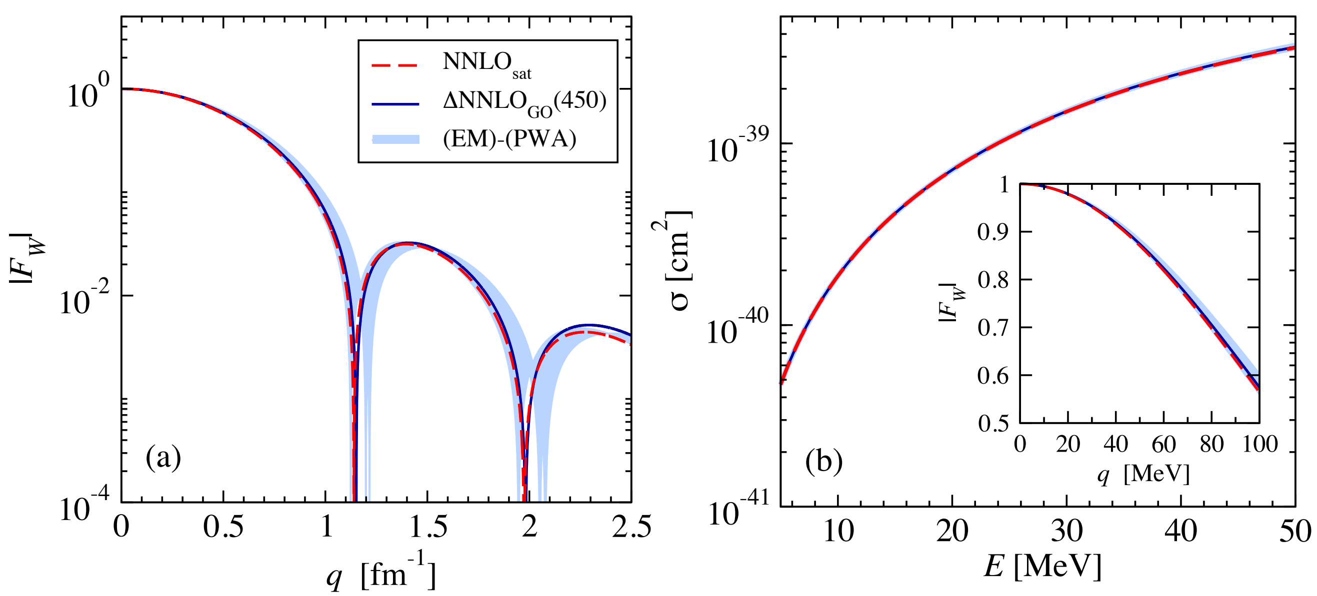
$$\left.\frac{d\sigma}{d\omega dq}\right|_e = \sigma_M\left(\upsilon_L R_L + \upsilon_T R_T\right)$$

charge operator $\hat{\rho}(q) = \sum_{j=1}^{Z} e^{iqz_j'}$

Formalism

✓ Coupled cluster (CCSD)

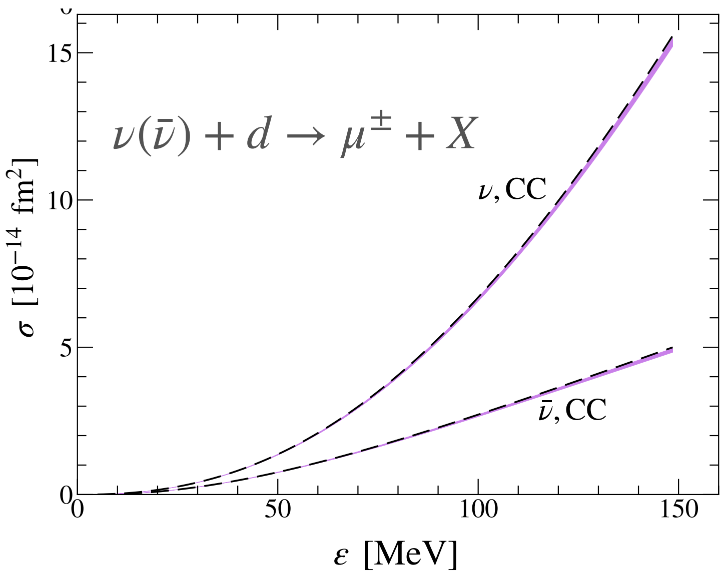
coherent elastic neutrino scattering on ^{40}Ar



C. Payne at al.
Phys.Rev.C 100 (2019) 6, 061304

✓ Electroweak currents

Multipole decomposition for 1- and 2-body EW currents



B. Acharya, S. Bacca
Phys.Rev.C 101 (2020) 1, 015505

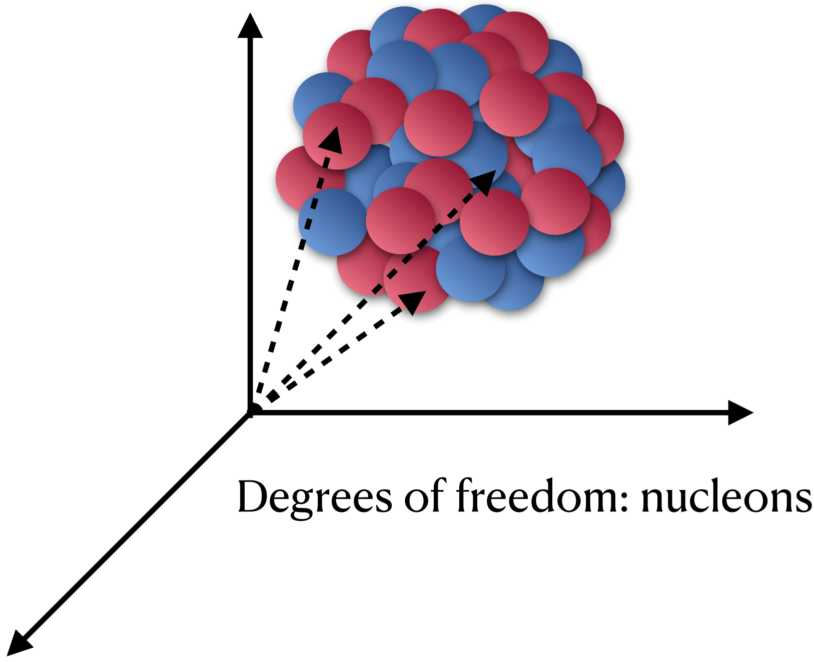
✓ Chiral potentials: NNLO$_{sat}$ and ΔNNLO$_{GO}$

A. Ekström et al. *Phys.Rev.C* 91 (2015) 5, 051301
W. Jiang at al. *Phys.Rev.C* 102 (2020) 5, 054301

Coulomb sum rule

$$m_0(q) = \int d\omega R_L(\omega, q) = \sum_{f \neq 0} |\langle \Psi_f | \hat{\rho} | \Psi \rangle|^2 = \langle \Psi | \hat{\rho}^\dagger \hat{\rho} | \Psi \rangle - |F_{el}(q)|^2$$

easier to calculate since we do not need $|\Psi_f\rangle$



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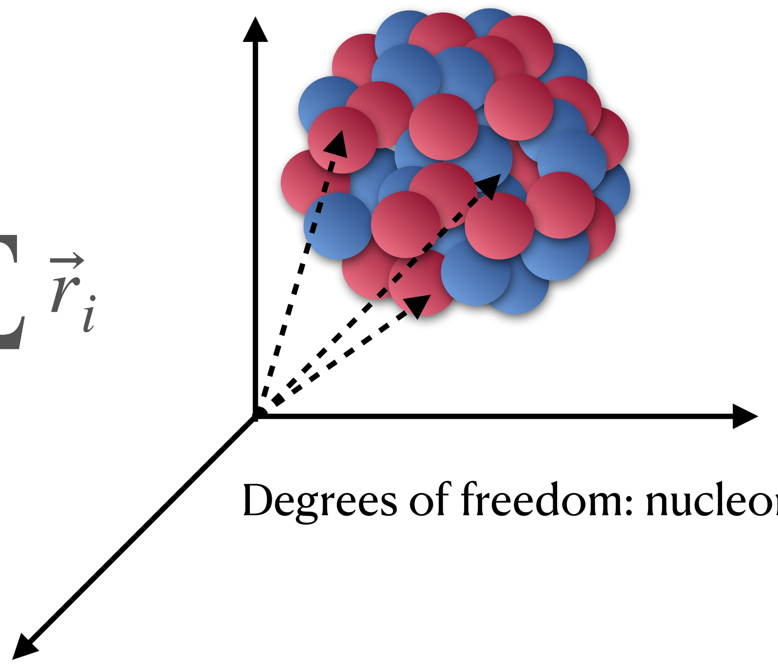
center of mass problem

$$|\Psi\rangle \text{ has 3A coordinates} \rightarrow 3(\text{A-1}) \overset{\text{intrinsic}}{\text{coordinates}} + \vec{R} = \frac{1}{A}\sum_{i}^{A} \vec{r}_i$$



With translationally non-invariant operators we may excite spurious states

Coulomb sum rule

Project out spurious states: $\hat{\rho}\,|\Psi\rangle = |\Psi_{phys}\rangle + |\Psi_{spur}\rangle$

It has been shown that to good approximation the ground state factorizes:

$$|\Psi\rangle = |\Psi_I\rangle|\Psi_{CoM}\rangle$$

center of mass wave function is a Gaussian

G. Hagen, T. Papenbrock, D. Dean *Phys.Rev.Lett.* 103 (2009) 062503

We follow a similar ansatz for the excited states:

$$\hat{\rho}\,|\Psi\rangle = |\Psi_I^{exc}\rangle|\Psi_{CoM}\rangle + |\Psi_I\rangle|\Psi_{CoM}^{exc}\rangle$$

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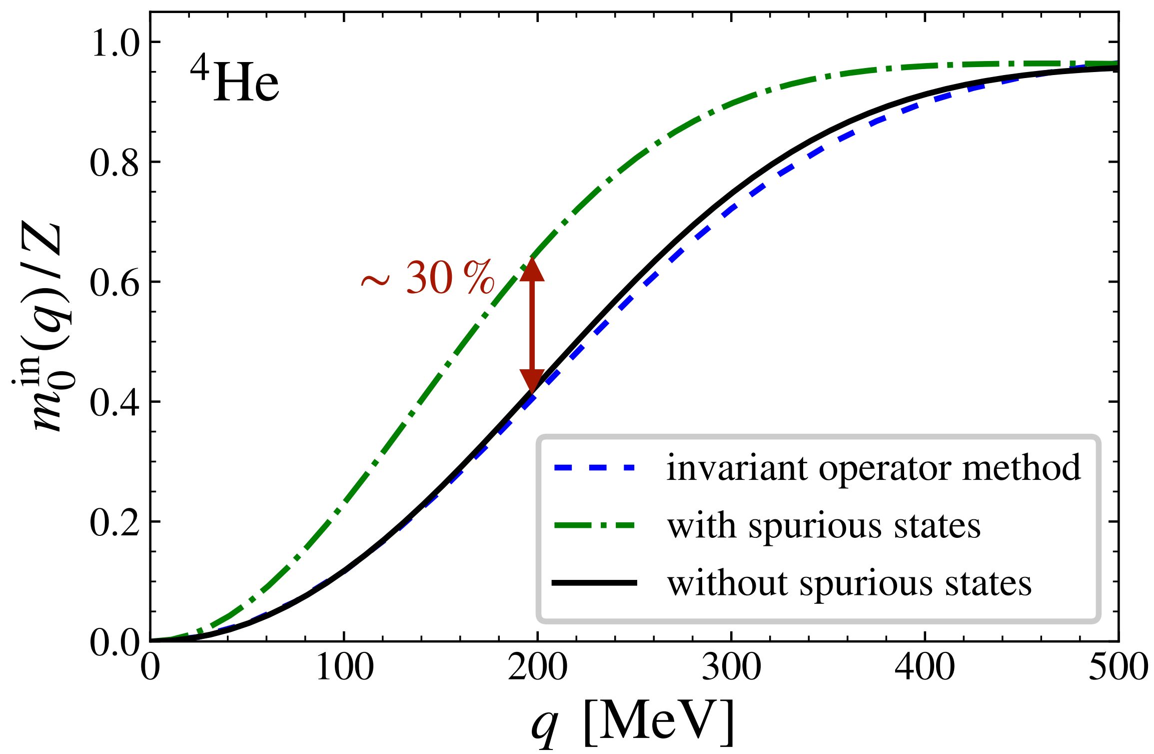
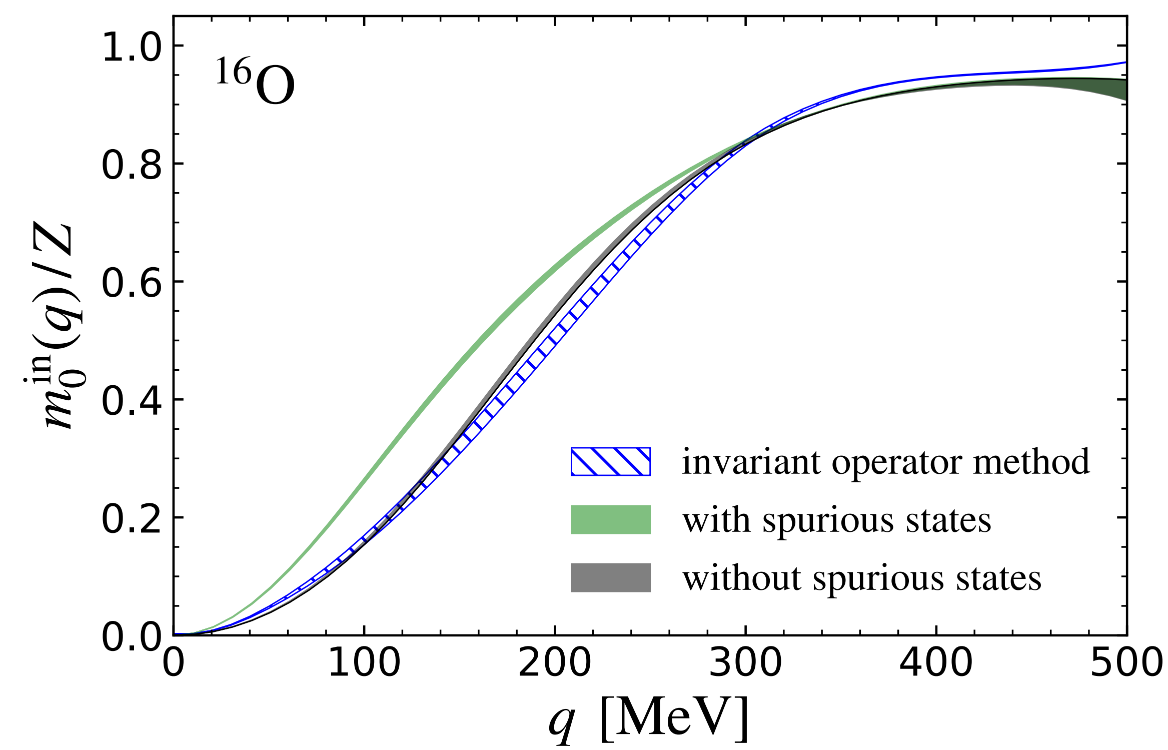


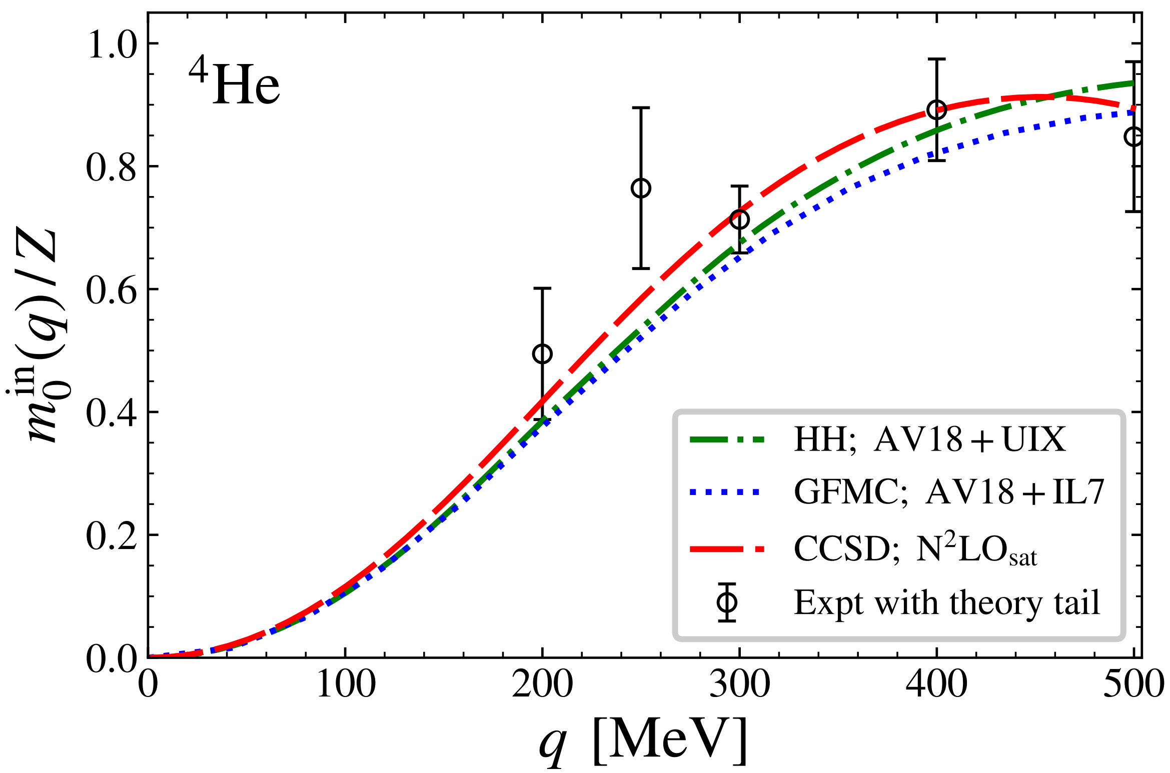


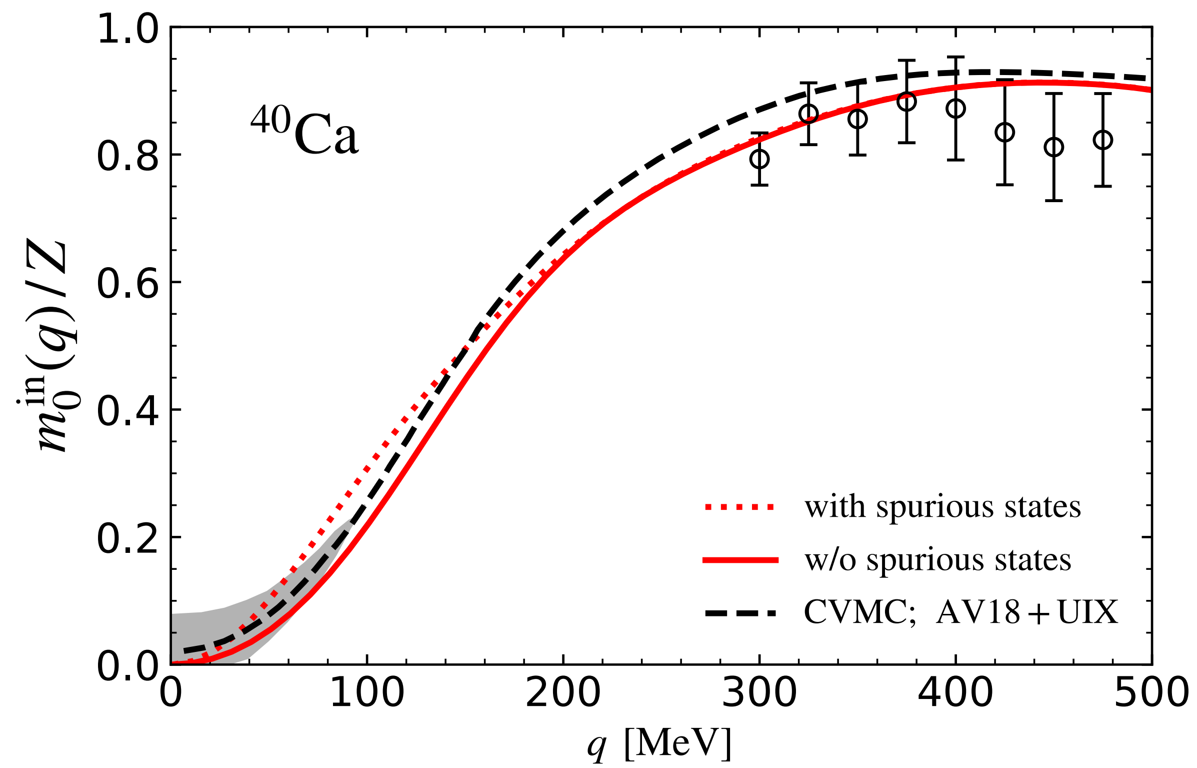
J.E.S. B. Acharya, S.Bacca, G. Hagen
Phys.Rev.C 102 (2020) 064312

CoM spurious states dominate for light nuclei

Coulomb sum rule

$$m_0(q) = \int d\omega R_L(\omega, q) = \sum_{f \neq 0} |\langle \Psi_f | \hat{\rho} | \Psi \rangle|^2 = \langle \Psi | \hat{\rho}^\dagger \hat{\rho} | \Psi \rangle - |F_{el}(q)|^2$$





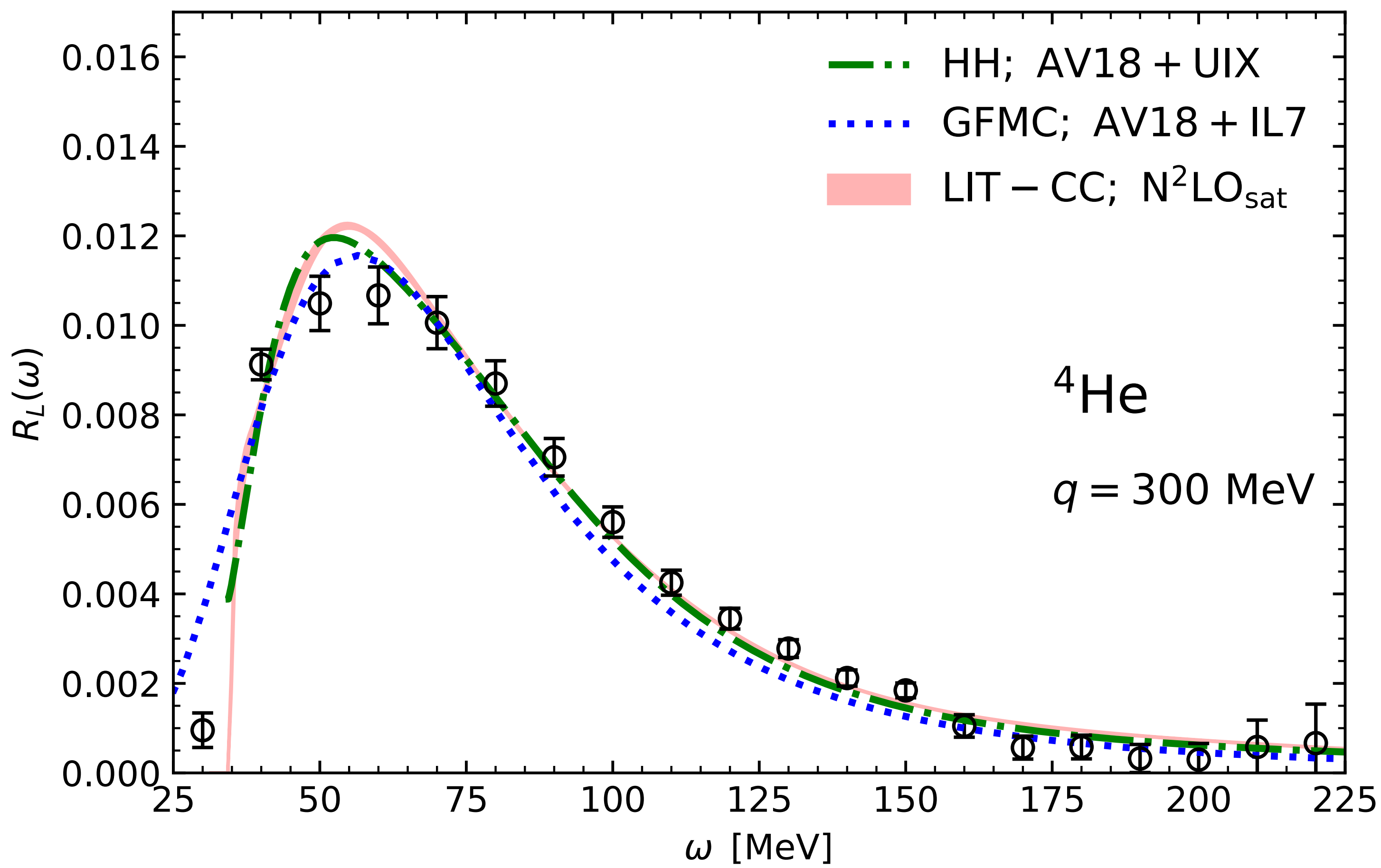
JES, B. Acharya, S.Bacca, G. Hagen Phys.Rev.C 102 (2020) 064312

PRL 127 (2021) 7, 072501 JES, B. Acharya, S. Bacca, G. Hagen

Nuclear responses

Longitudinal response

Lorentz Integral Transform + Coupled Cluster



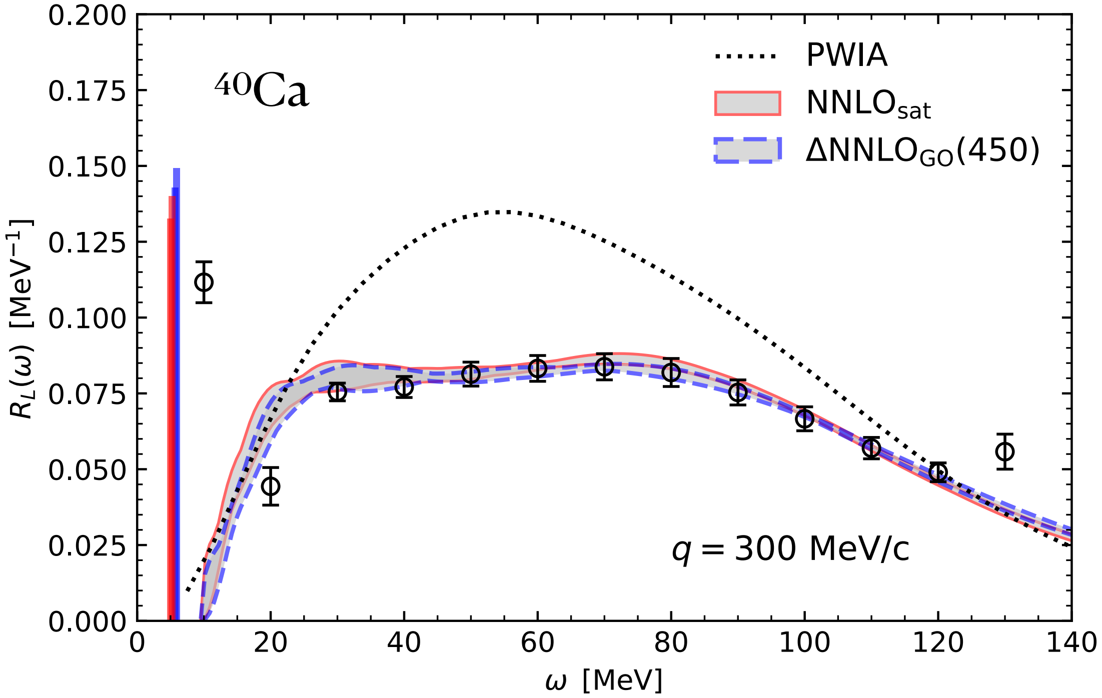
JES, B. Acharya, S. Bacca, G. Hagen; *PRL* 127 (2021) 7, 072501

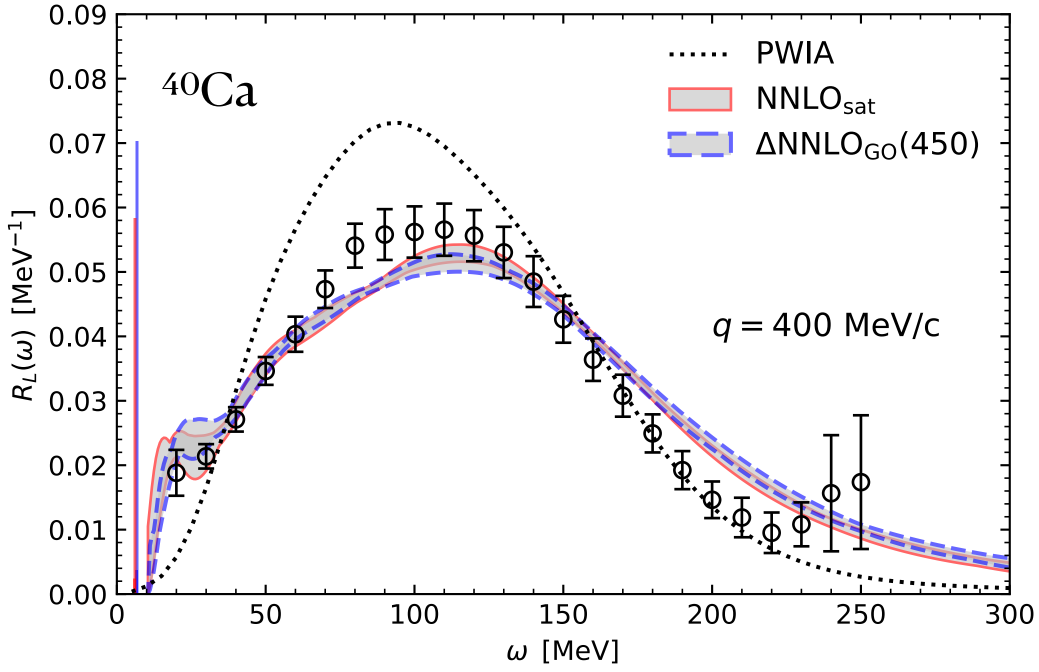
Uncertainty band: inversion procedure

$$R_{\mu\nu}(\omega, q) = \sum\!\!\!\!\!\!\int_f \langle \Psi \,|\, J_\mu^\dagger \,|\, \Psi_f \rangle \langle \Psi_f | \, J_\nu \,|\, \Psi \rangle \delta(E_0 + \omega - E_f)$$

Longitudinal response ^{40}Ca

Lorentz Integral Transform + Coupled Cluster





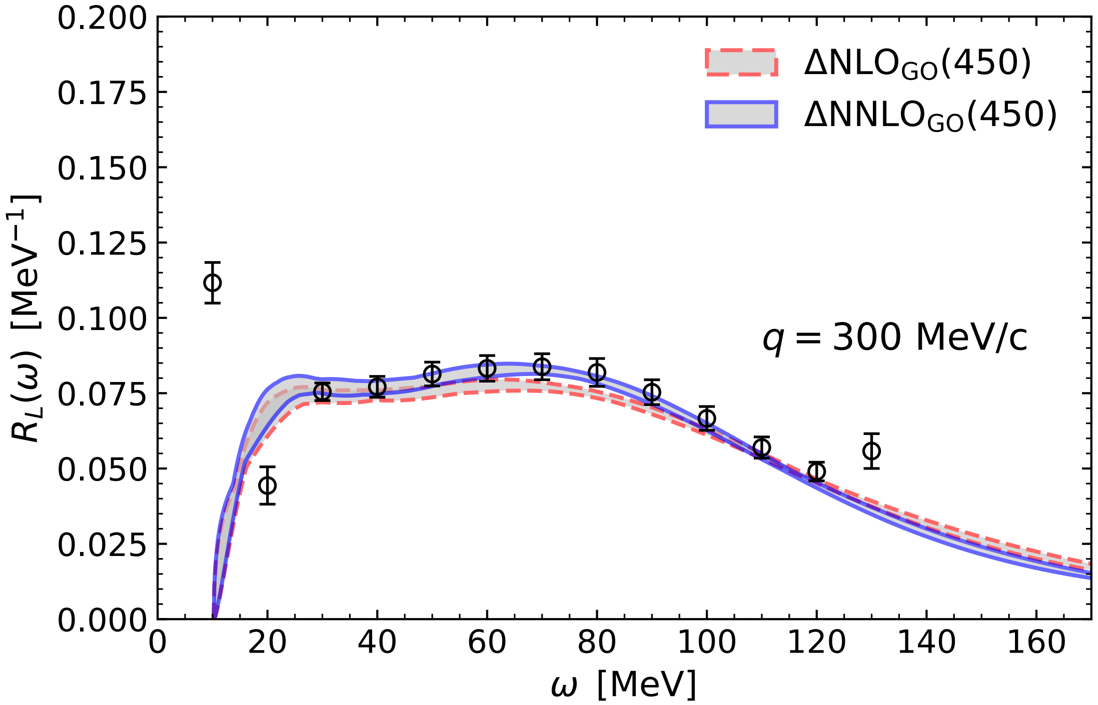
JES, B. Acharya, S. Bacca, G. Hagen; *PRL* 127 (2021) 7, 072501

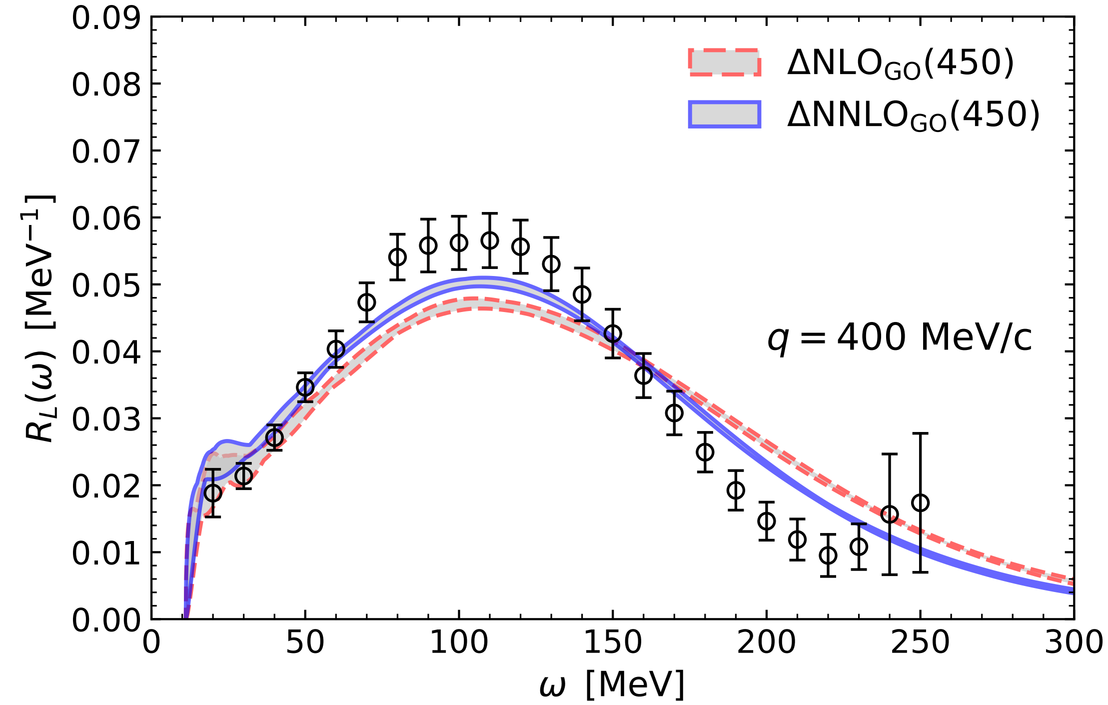
- ✓ CC singles & doubles
- ✓ varying underlying harmonic oscillator frequency
- ✓ two different chiral Hamiltonians
- ✓ *inversion procedure*

First ab-initio results for many-body system of 40 nucleons

Chiral expansion for ^{40}Ca

(Longitudinal response)



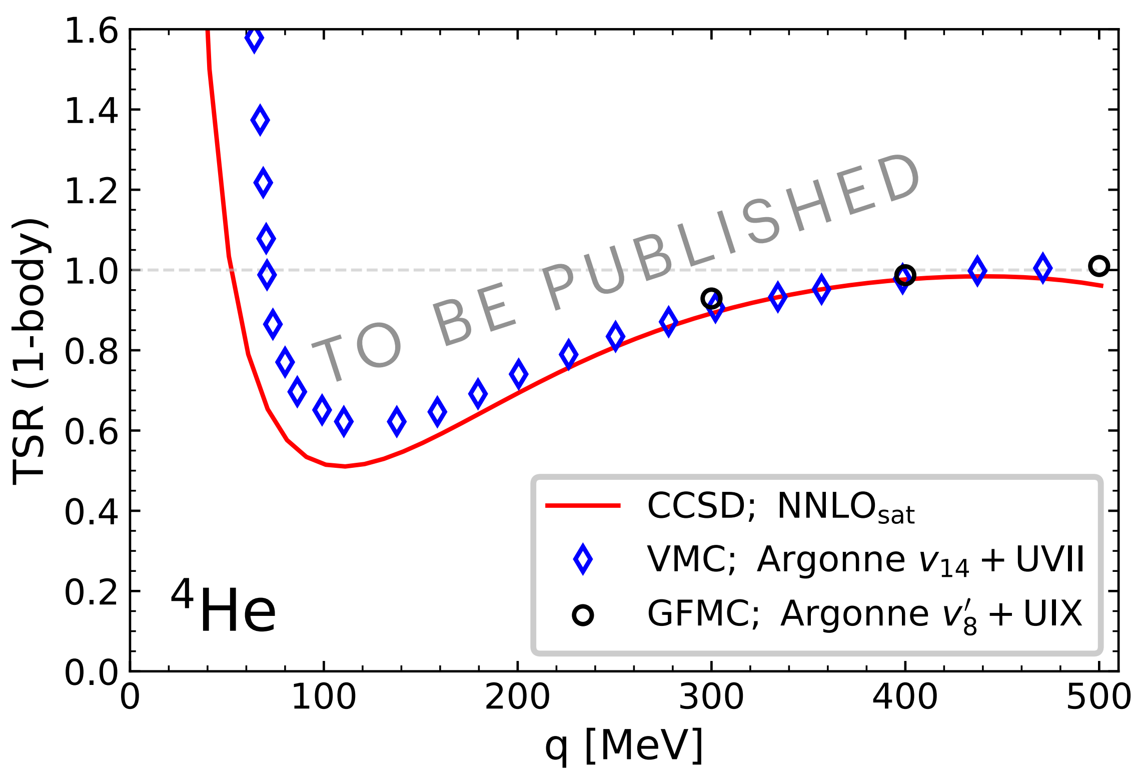


B. Acharya, S. Bacca, JES et al. Front. Phys. 1066035(2022)

- ✓ Two orders of chiral expansion
- ✓ Convergence better for lower q (as expected)
- ✓ Higher order brings results closer to the data

Transverse response

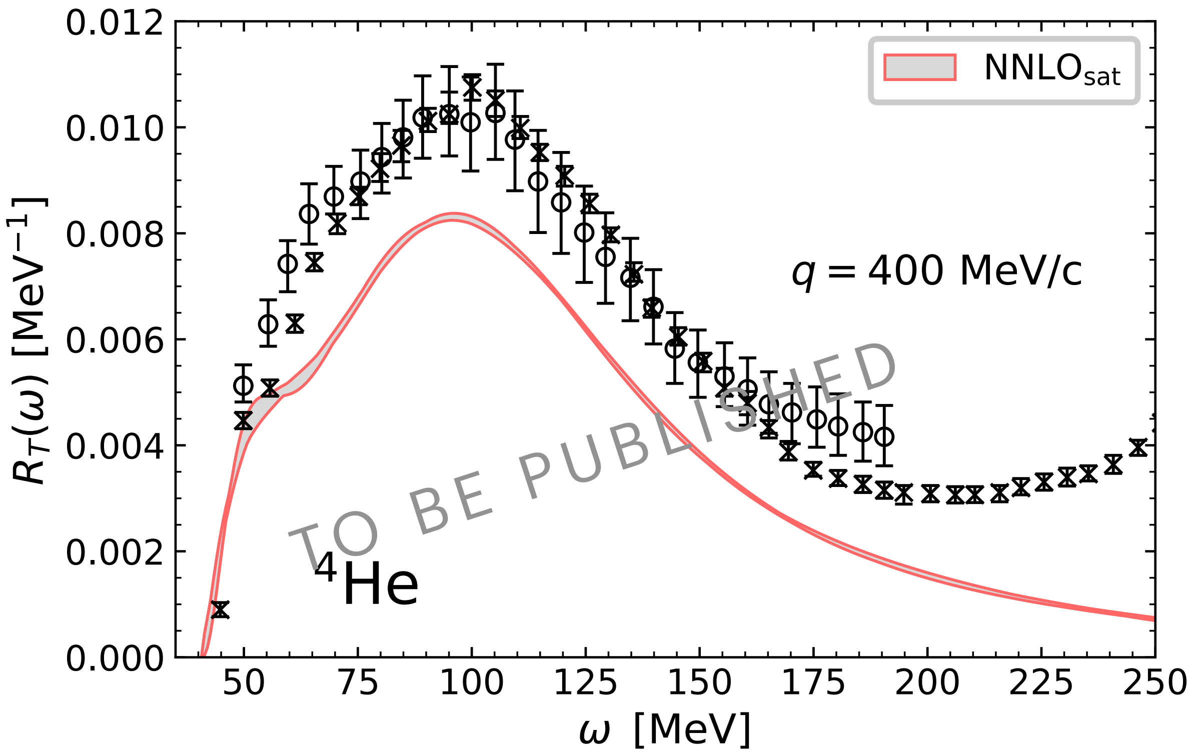
$$\mathrm{TSR}(q) = \frac{2m^2}{Z\mu_p^2 + N\mu_n^2}\frac{1}{q^2}\left(\langle\Psi|\hat{j}^\dagger\hat{j}\Psi\rangle - |\langle\Psi|\hat{j}|\Psi\rangle|^2\right)$$

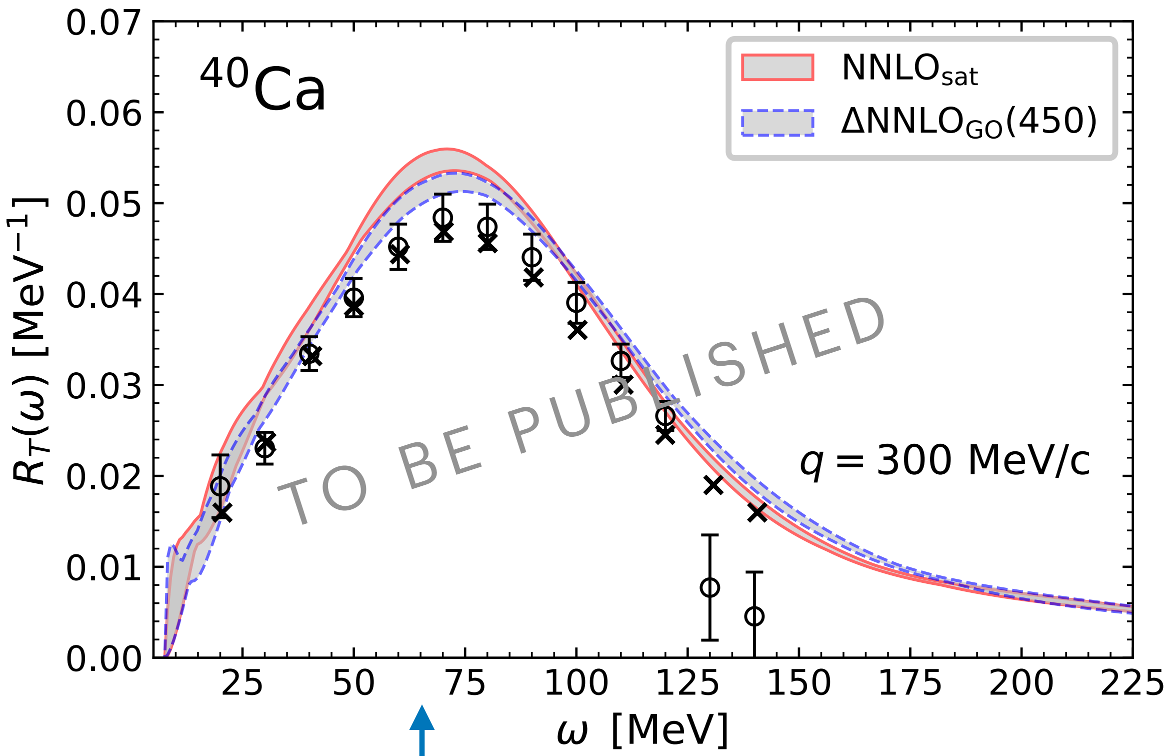


$\mathrm{TSR}(q \to 0) \propto$ kinetic energy ⟷ $\mathrm{TSR}(q \to \infty) = 1$

$$\mathbf{j}(\mathbf{q}) = \sum_i \frac{1}{2m}\epsilon_i\{\mathbf{p_i}, e^{i\mathbf{q}\mathbf{r_i}}\} - \frac{i}{2m}\mu_i\mathbf{q}\times\sigma_i e^{i\mathbf{q}\mathbf{r_i}}$$

Transverse response





➡ This allows to predict electron-nucleus cross-section

➡ Currently only 1-body current

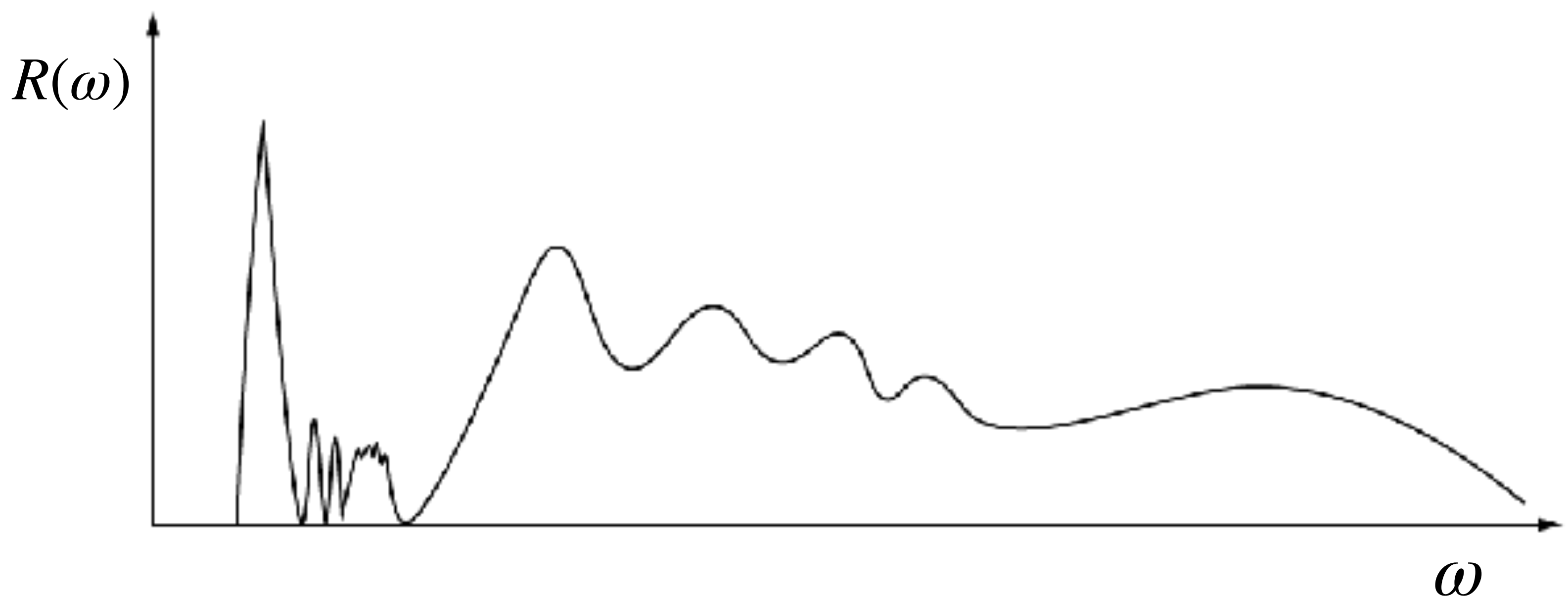
2-body currents important for 4He
→ more correlations needed?
→ 2-b currents strength depends on nucleus?

ChEK method

Chebyshev Expansion of integral Kernel

$$\Phi = \int f(\omega) R(\omega) d\omega$$

- Sum-rules
- Flux folding
- Histogram
- ...



$$\Phi \approx \tilde{\Phi} = \int f(\omega') \int K(\omega', \omega) R(\omega) d\omega d\omega'$$

expansion in Chebyshev polynomials

$$K(\omega, \sigma) = \sum_k c_k(\sigma) T_k(\omega)$$

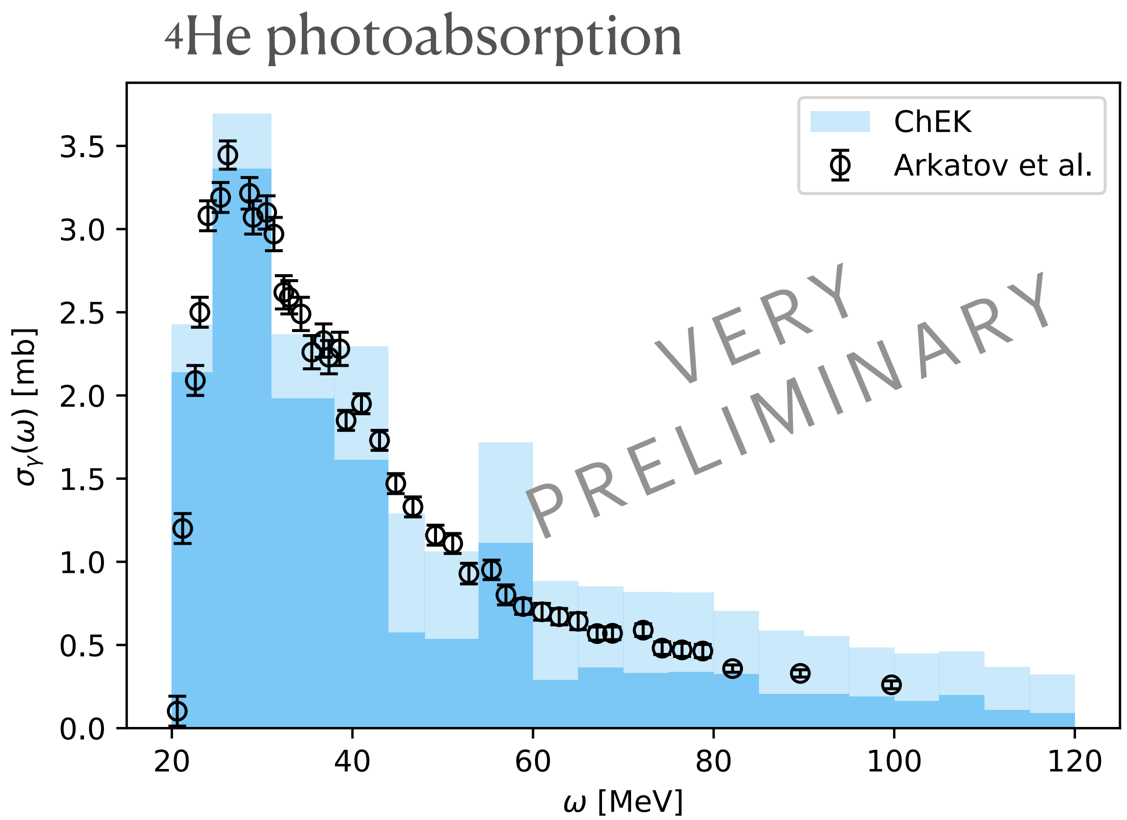
estimated error

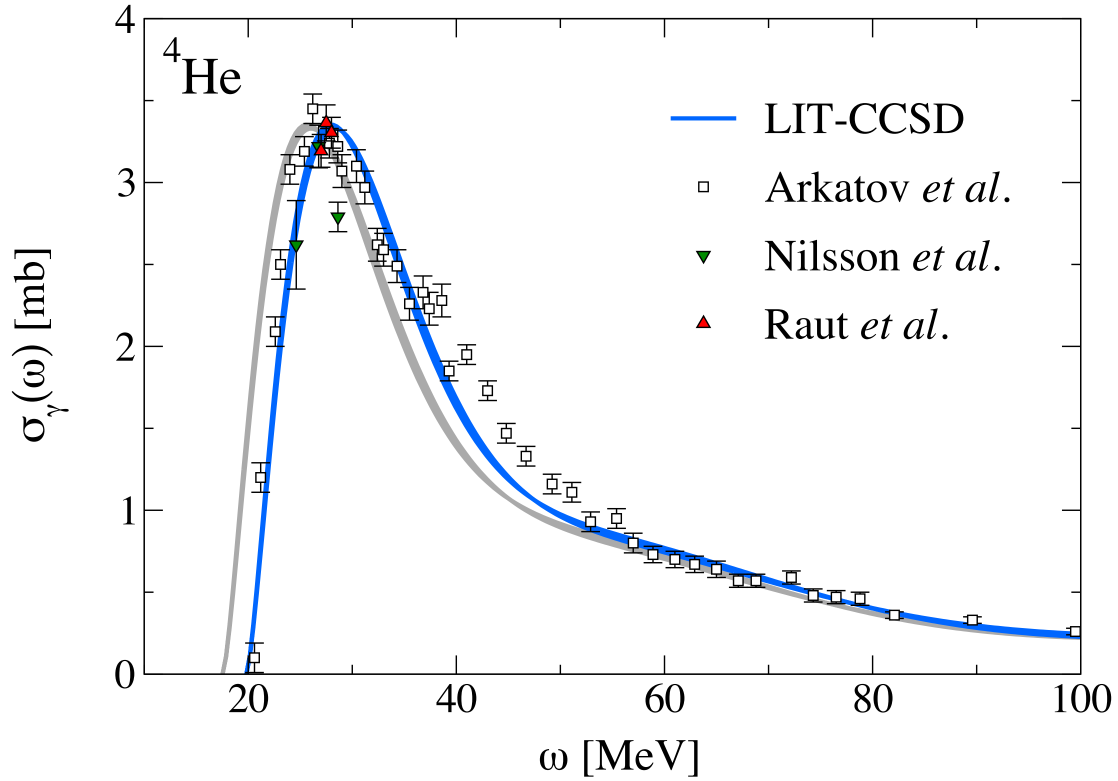
$$|\Phi - \tilde{\Phi}| < \epsilon$$

A. Roggero Phys.Rev.A 102 (2020) 2, 022409
JES, A. Roggero Phys.Rev.E 105 (2022) 055310

ChEK method

Chebyshev Expansion of integral Kernel





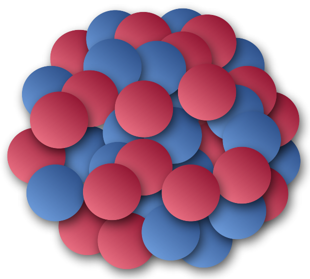
S. Bacca, N. Barnea, G. Hagen, G. Orlandini; *Phys.Rev.C* 90 (2014) 6

➡ No assumption about the shape of the response

➡ Rigorous error estimation

➡ Convenient when the response has a complicated structure

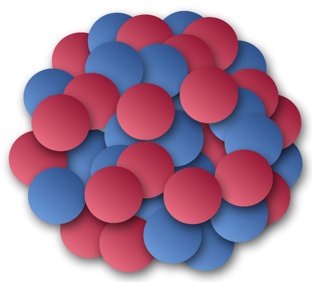
Low/high energies



$$\hat{H}|\psi_A\rangle = E|\psi_A\rangle$$

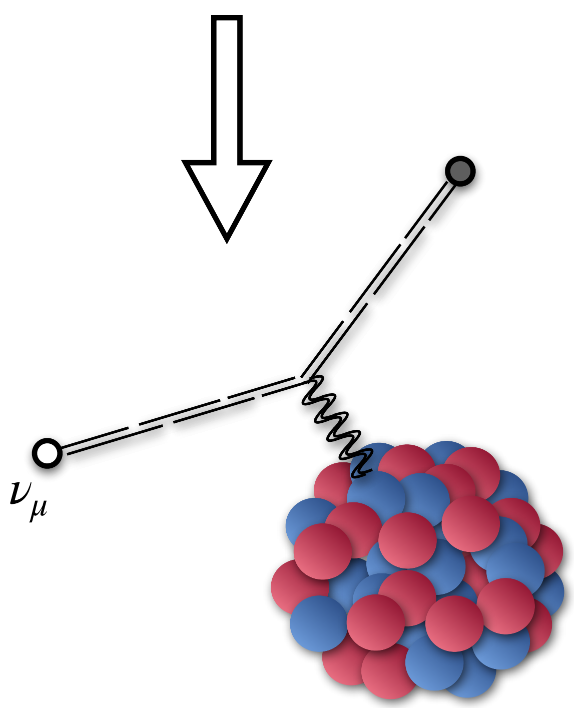
Many-body problem

Low/high energies



$$\hat{H}\,|\,\psi_A\rangle = E\,|\,\psi_A\rangle$$

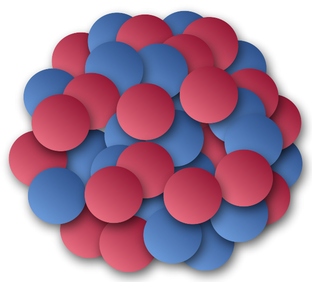
Many-body problem



$$\langle\psi_f\,|\,\hat{j}\,|\,\psi_A\rangle$$

Electroweak responses

Low/high energies



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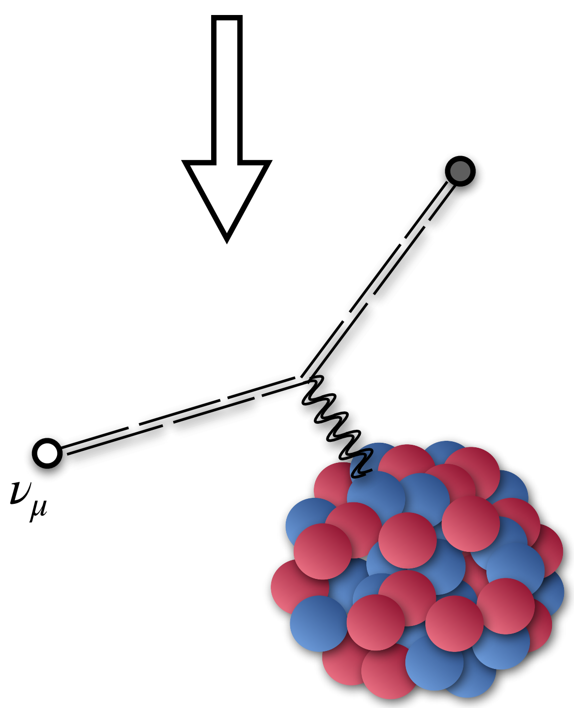
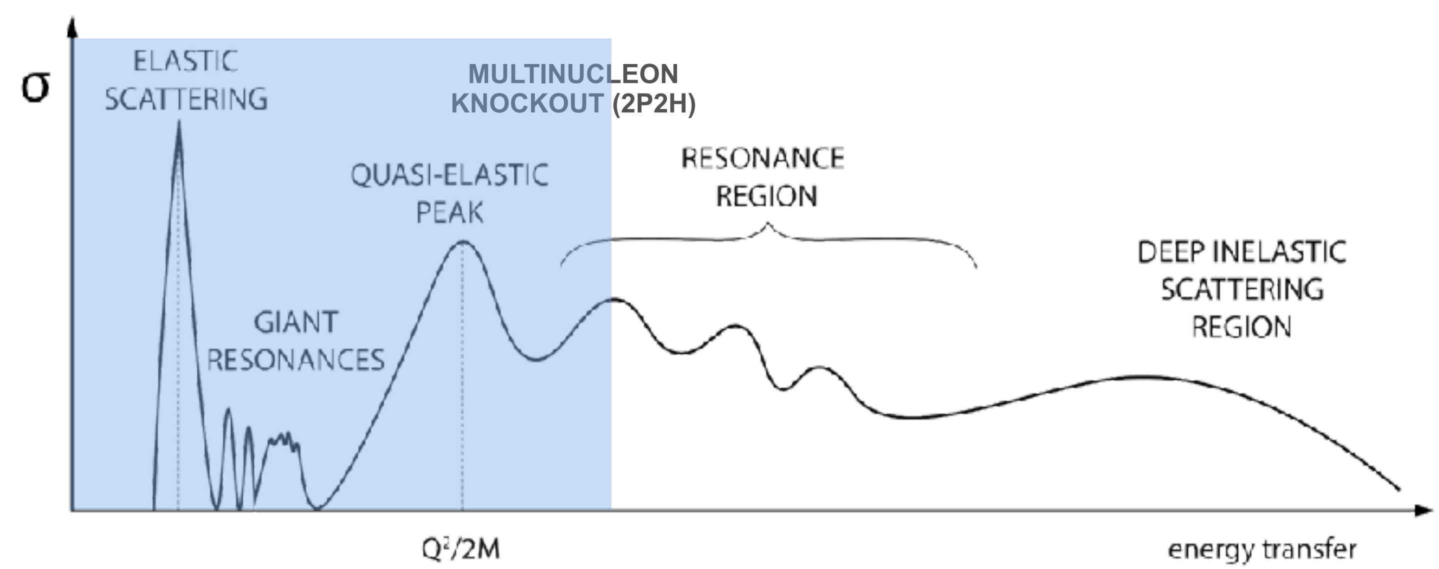
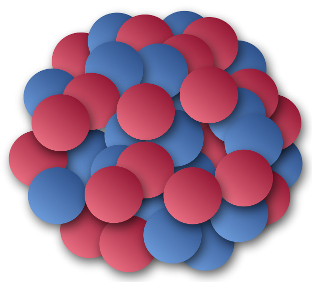


$$\langle \psi_f |\, \hat{j}\, | \psi_A \rangle$$

Electroweak responses

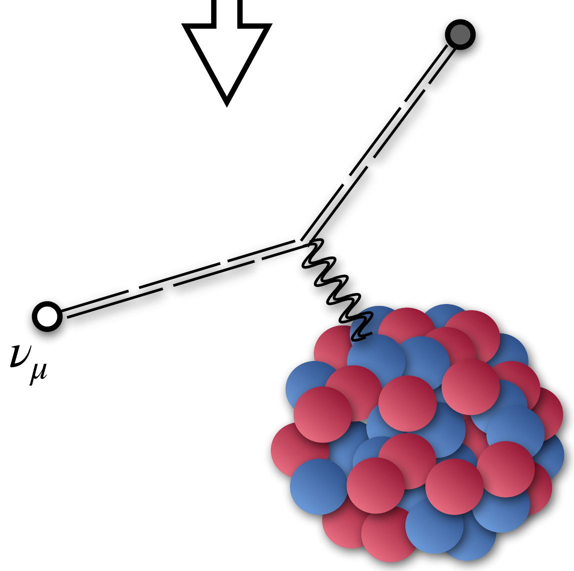


Low/high energies



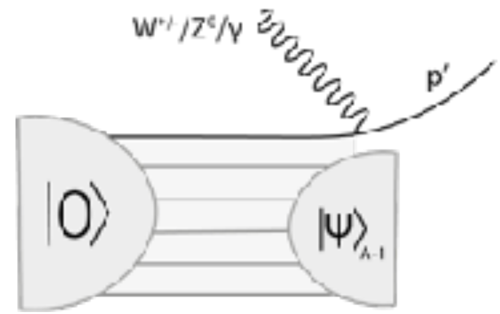
$$\hat{H}\,|\,\psi_A\rangle = E\,|\,\psi_A\rangle$$

Many-body problem

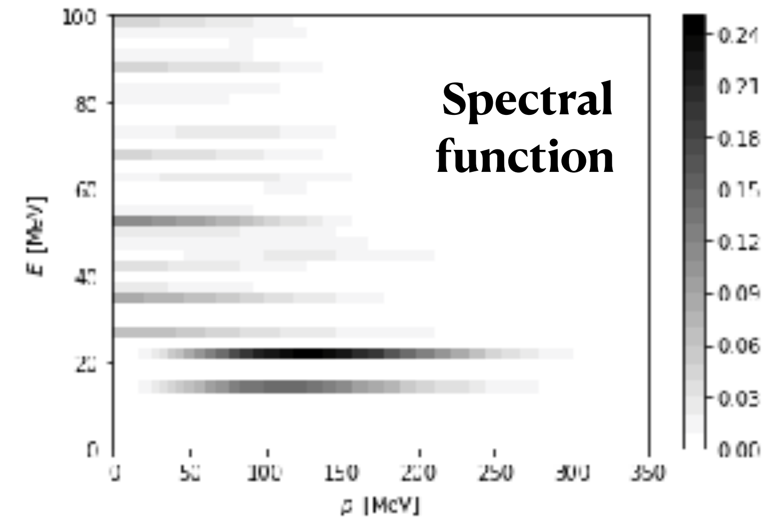


$$\langle\psi_f\,|\,\hat{j}\,|\,\psi_A\rangle$$

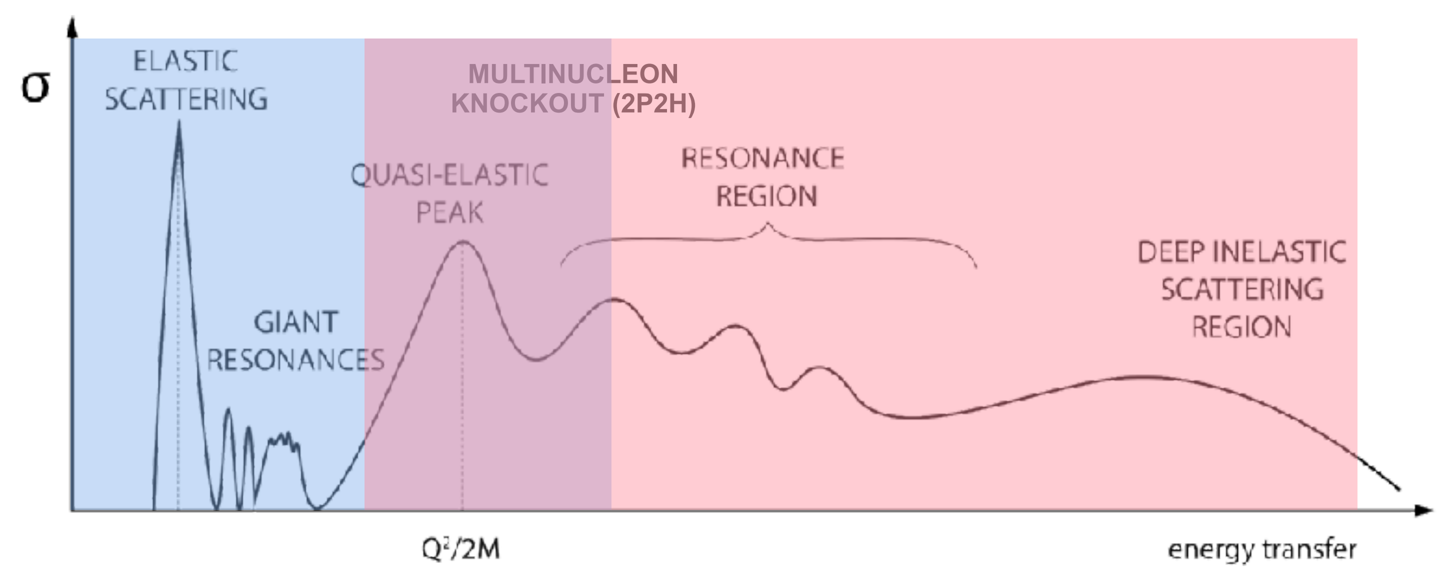
Electroweak responses



Impulse Approximation

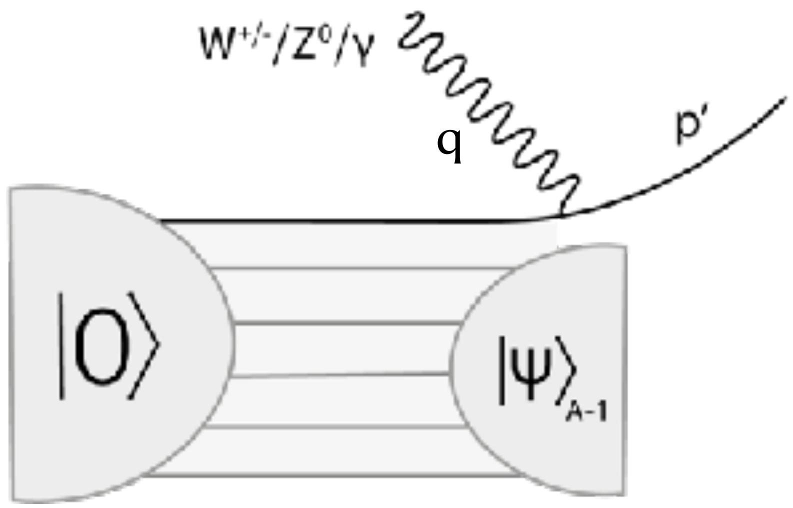


Probability density of finding nucleon $(E, \mathbf{p})$ in ground state nucleus



Spectral functions

Coupled Cluster + ChEK method

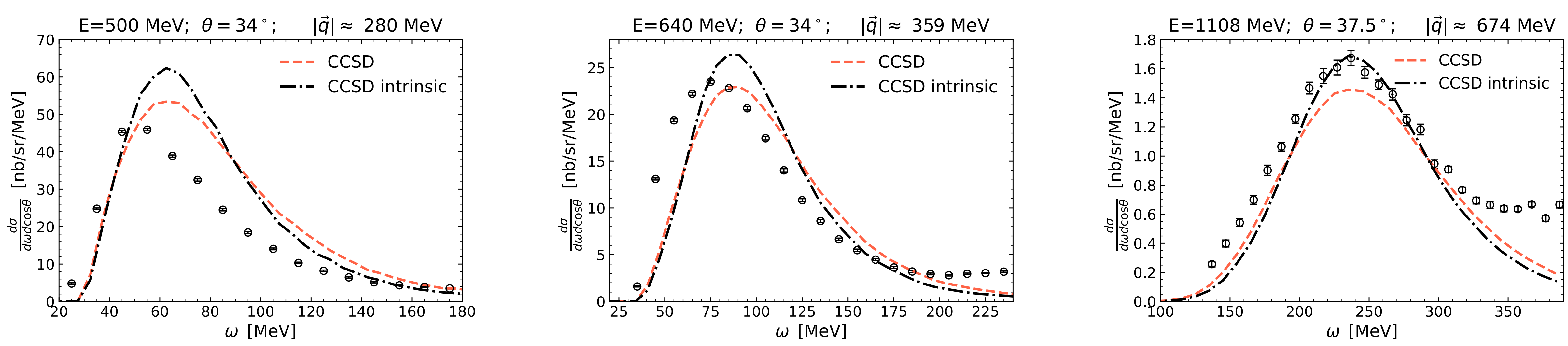


$$\sigma \propto |\mathscr{M}|^2 S(E,p)$$

Factorized interaction vertex (relativistic, pion production...)

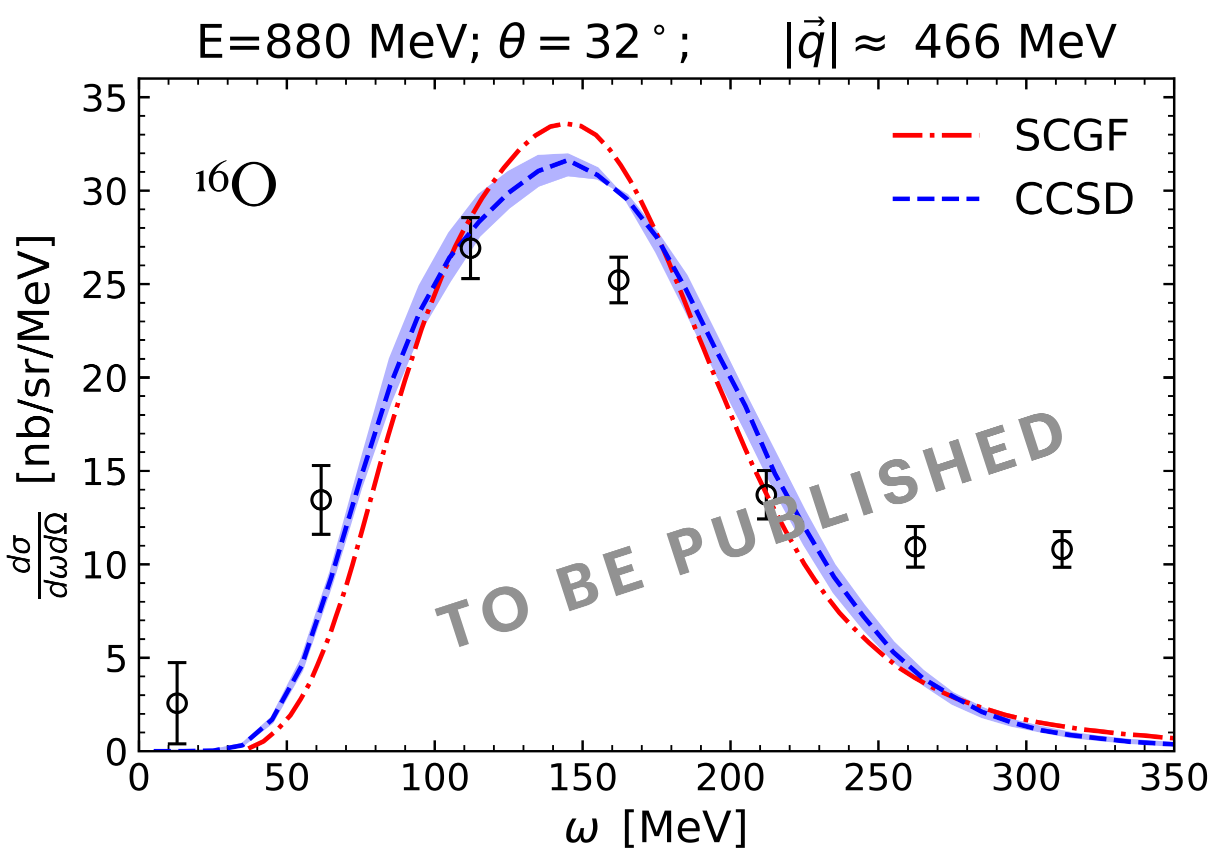
Spectral function - nuclear information

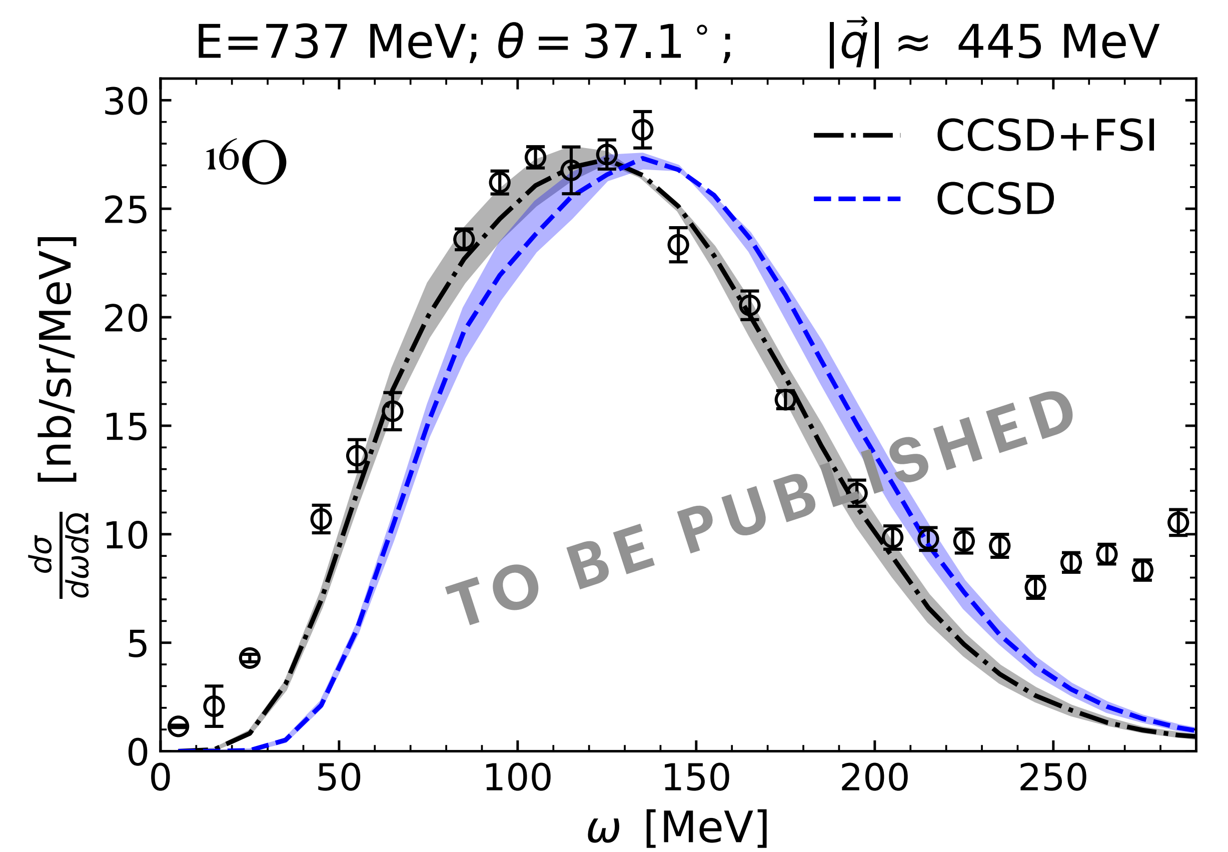
growing **q** momentum transfer → final state interactions play minor role



JES, S. Bacca, G. Hagen, T. Papenbrock *Phys.Rev.C* 106 (2022) 3, 034310

Final state interactions





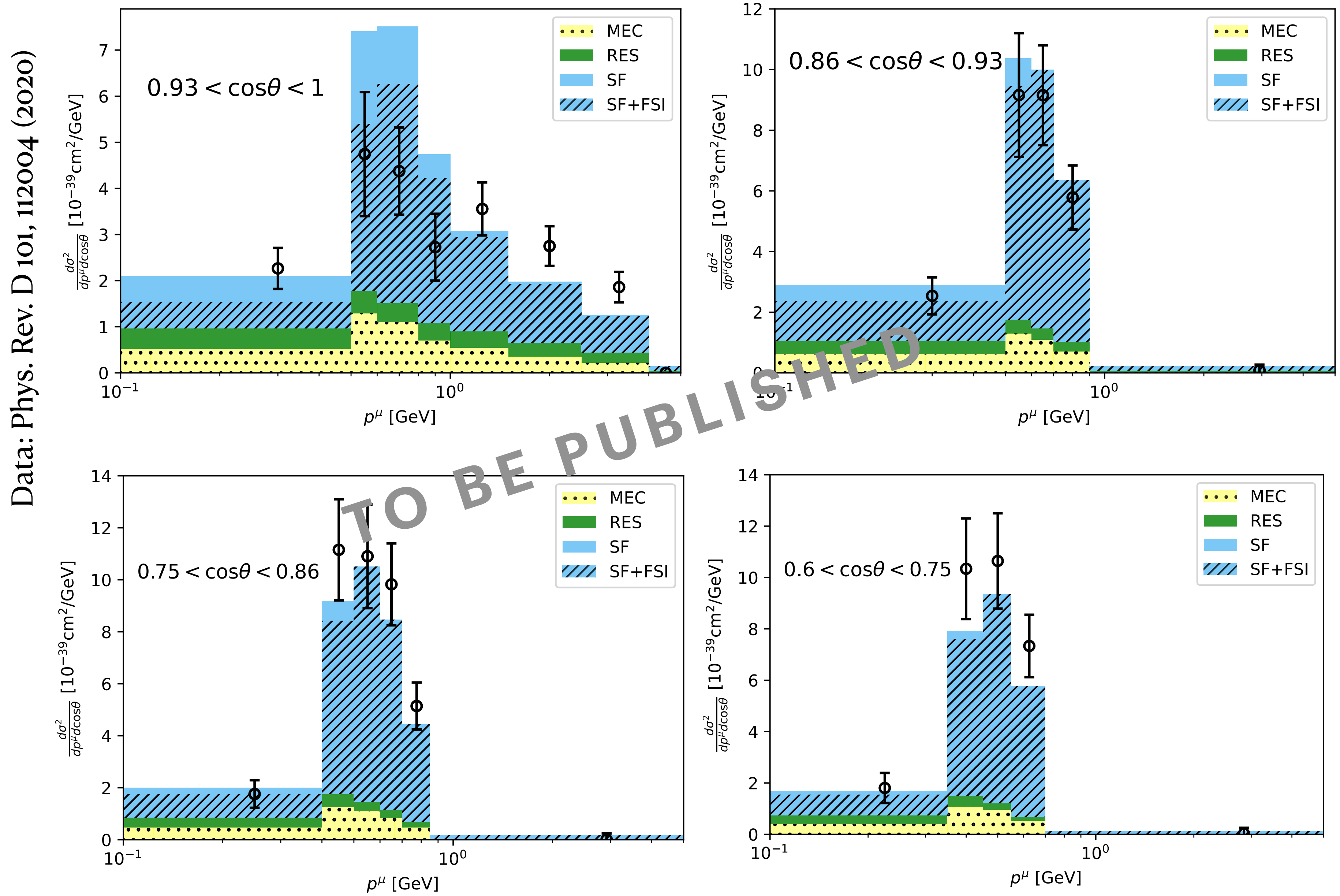
JES et al, in preparation (2022)

How to account for the FSI? Optical potential for the outgoing nucleon

Spectral function for neutrinos

$$\nu_\mu + {}^{16}\mathrm{O} \rightarrow \mu^- + X$$

- Comparison with T2K long baseline ν oscillation experiment
- CC0π events
- Spectral function implemented into NuWro Monte Carlo generator



JES et al, in preparation (2022)

Outlook

- LIT-CC benchmark for electron scattering → ready for neutrino
- Role of 2-body currents for medium-mass nuclei
- Explore possible applications of the ChEK method
- Spectral functions (within Impulse Approximation):
  - Relativistic regime
  - Semi-inclusive processes
  - Further steps: 2-body spectral functions, accounting for FSI

Thank you for attention

BACKUP

Details on inversion procedure

- Basis functions

$$R_L(\omega) = \sum_{i=1}^{N} c_i \omega^{n_0} e^{-\frac{\omega}{\beta_i}}$$

- Stability of the inversion procedure:
    - Vary the parameters n_0, β_i and number of basis functions N (6-9)
    - Use LITs of various width Γ (5, 10, 20 MeV)

Lorentz integral transform

$$L(\sigma) = \int \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} d\omega = \int \frac{R(\omega)}{(\omega + \tilde{\sigma}^*)(\omega + \tilde{\sigma})} d\omega$$

$$L(\sigma) = \int d\omega \sum_f \langle \Psi_0 | \rho^\dagger \frac{1}{\omega + \tilde{\sigma}^*} | \Psi_f \rangle \langle \Psi_f | \frac{1}{\omega + \tilde{\sigma}} \rho | \Psi_0 \rangle \delta(\omega + E_0 - E_f)$$

$$L(\sigma) = \sum_f \langle \Psi_0 | \rho^\dagger \frac{1}{E_f - E_0 + \tilde{\sigma}^*} | \Psi_f \rangle \langle \Psi_f | \frac{1}{E_f - E_0 + \tilde{\sigma}} \rho | \Psi_0 \rangle$$

$$L(\sigma) = \sum_f \langle \Psi_0 | \rho^\dagger \frac{1}{H - E_0 + \tilde{\sigma}^*} | \Psi_f \rangle \langle \Psi_f | \frac{1}{H - E_0 + \tilde{\sigma}} \rho | \Psi_0 \rangle$$

$$\langle \tilde{\Psi} | \qquad\qquad | \tilde{\Psi} \rangle$$

We need to solve

$$(H - E_0 + \tilde{\sigma}) | \tilde{\Psi} \rangle = \rho | \Psi \rangle$$

Schrodinger-like equation

Lorentz Integral Transform (LIT)

$$R_{\mu\nu}(\omega, q) = \sum\!\!\!\!\!\!\int_f \langle \Psi | J_\mu^\dagger | \Psi_f \rangle \langle \Psi_f | J_\nu | \Psi \rangle \delta(E_0 + \omega - E_f)$$

continuum spectrum

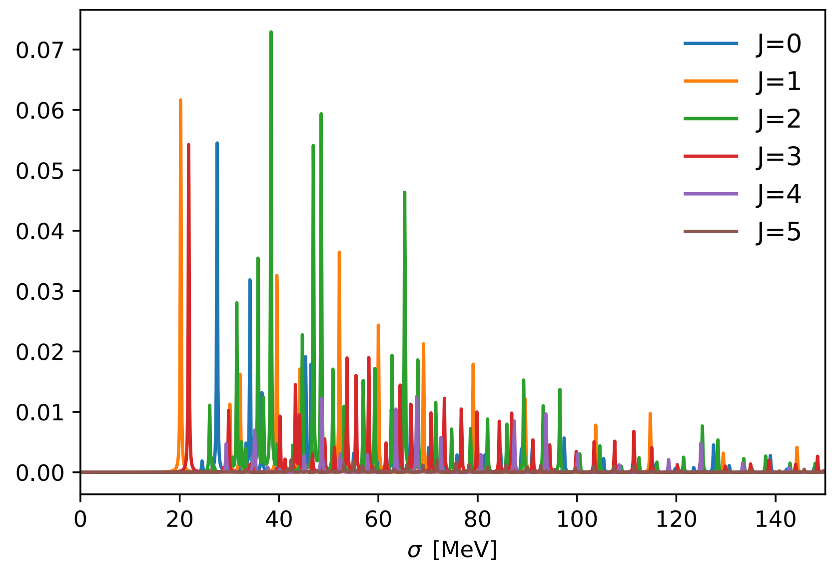
Integral transform

$$S_{\mu\nu}(\sigma, q) = \int d\omega K(\omega, \sigma) R_{\mu\nu}(\omega, q) = \langle \Psi | J_\mu^\dagger \, K(\mathscr{H} - E_0, \sigma) \, J_\nu | \Psi \rangle$$

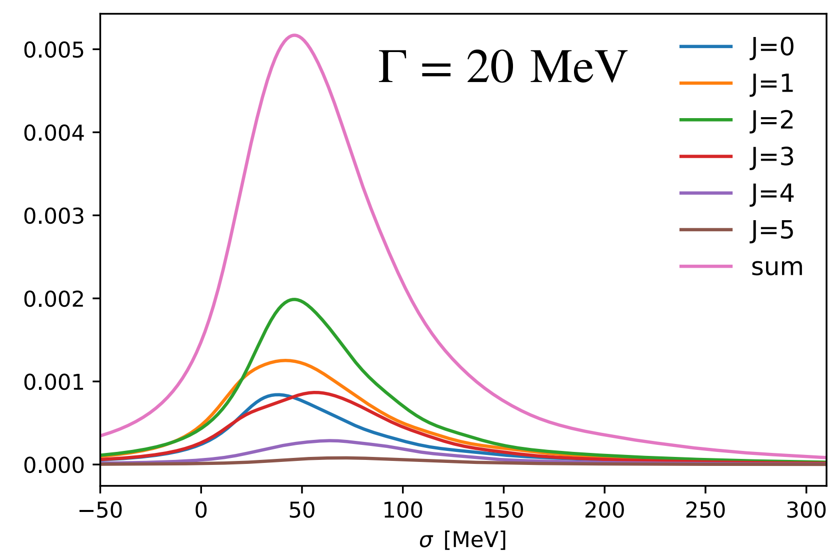
Lorentzian kernel:
$$K_\Gamma(\omega, \sigma) = \frac{1}{\pi} \frac{\Gamma}{\Gamma^2 + (\omega - \sigma)^2}$$

$S_{\mu\nu}$ has to be inverted to get access to $R_{\mu\nu}$

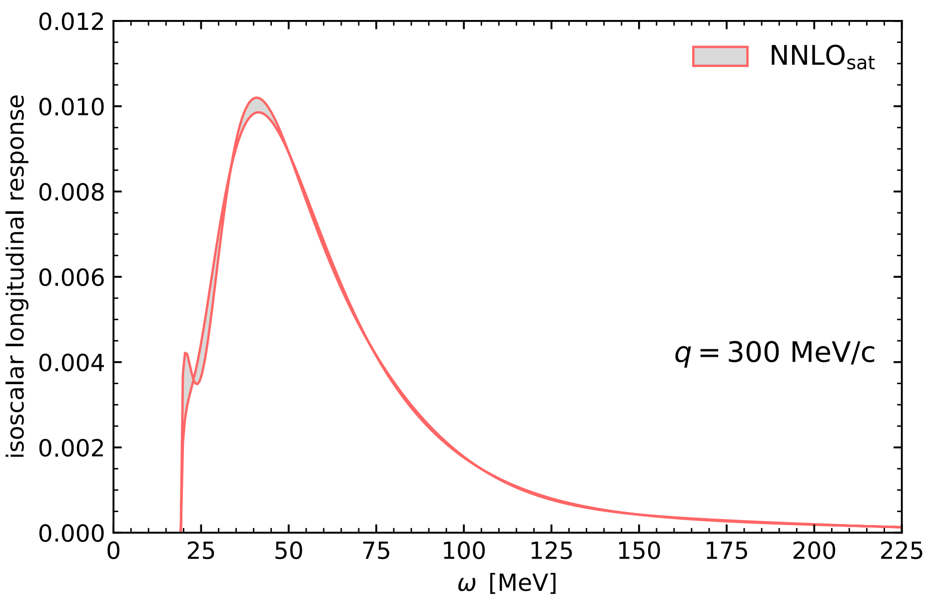
Lorentz Integral Transform



Integral transform

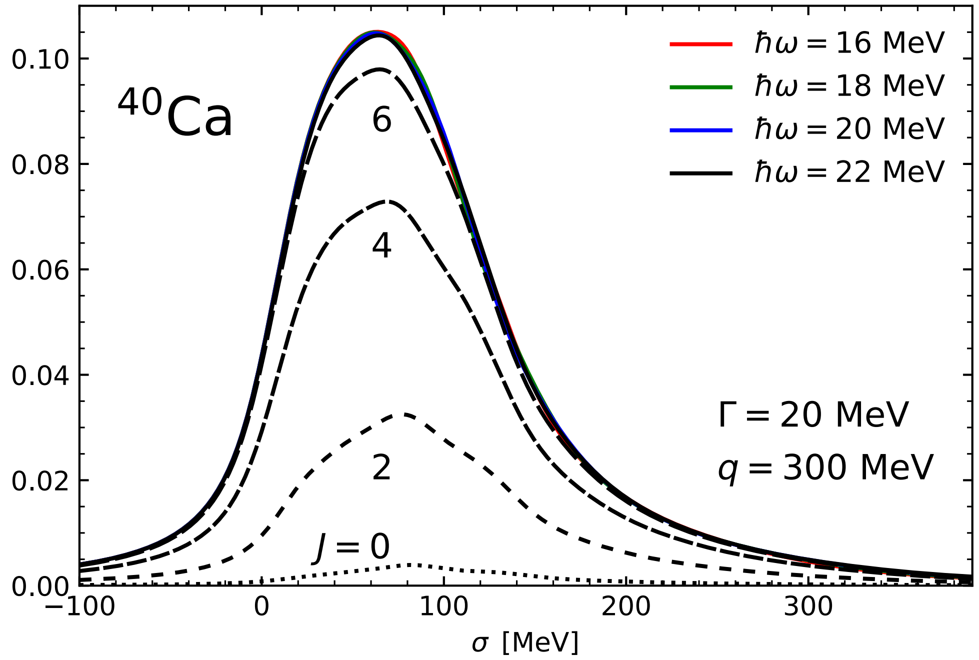


Inversion

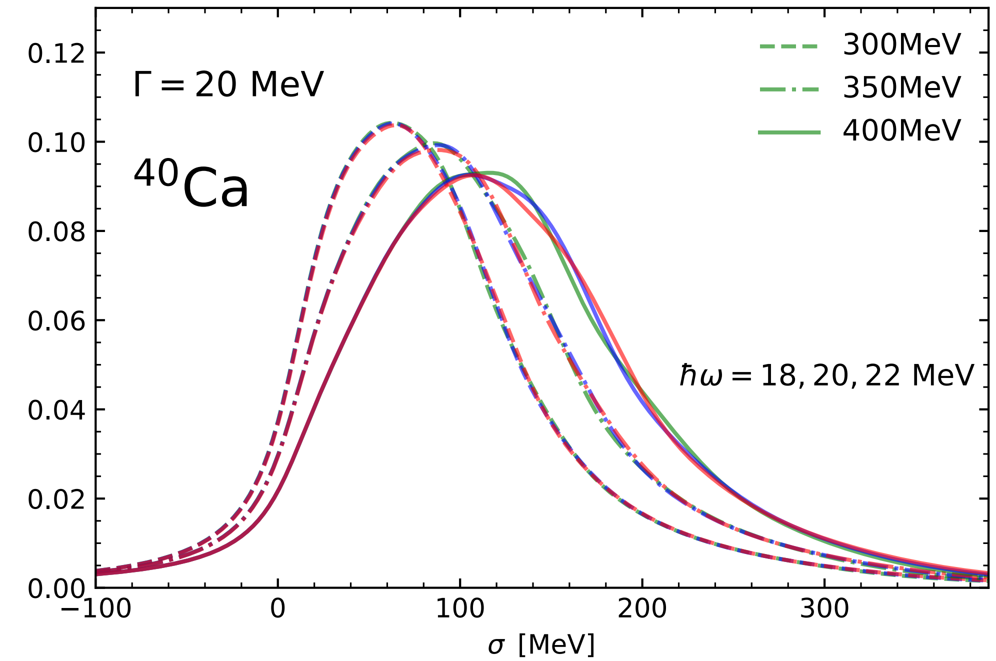


Longitudinal isoscalar response on ^{4}He at q=300 MeV

Longitudinal response ^{40}Ca

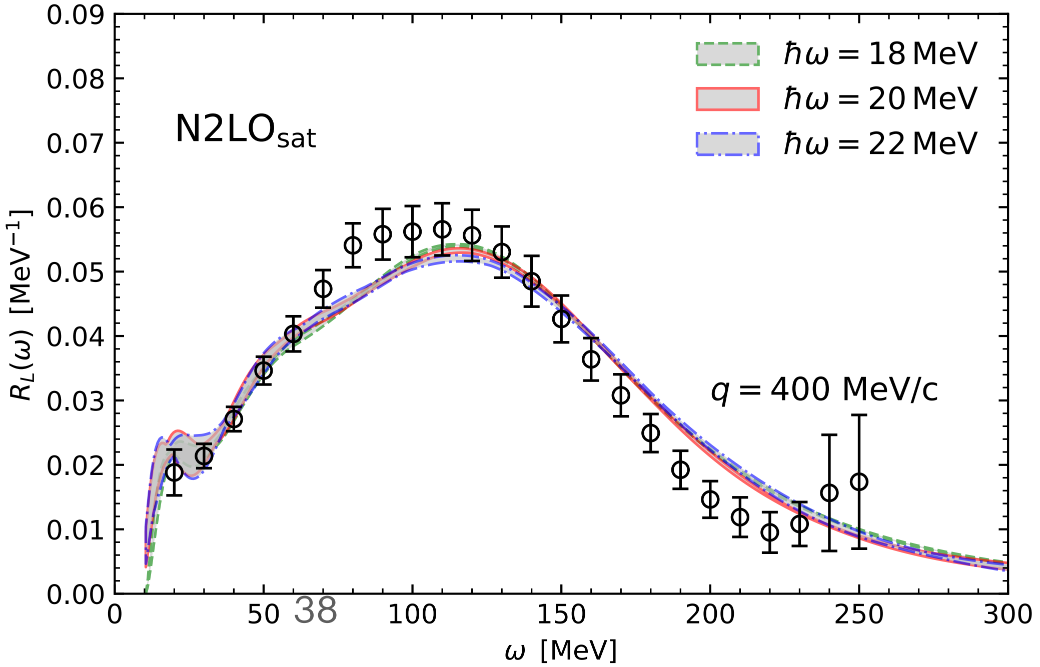


Sum over multipoles



Underlying oscillator frequency

Inversion



ChEK method

$$S_{\mu\nu}(\sigma, q) = \int d\omega K(\omega, \sigma) R_{\mu\nu}(\omega, q) = \langle \Psi | J_\mu^\dagger \; K(\mathscr{H}, \sigma) \; J_\nu | \Psi \rangle$$

- Expansion in Chebyshev polynomials

$$K(\mathscr{H}, \sigma) = \sum_{k=0}^{N} c_k(\sigma) T_k(\mathscr{H})$$

- Recursive relations of Chebyshev polynomials

$$T_0(x) = 1; \quad T_{-1}(x) = T_1(x) = x$$

$$T_{n+1}(x) = 2x T_n(x) - T_{n-1}(x)$$

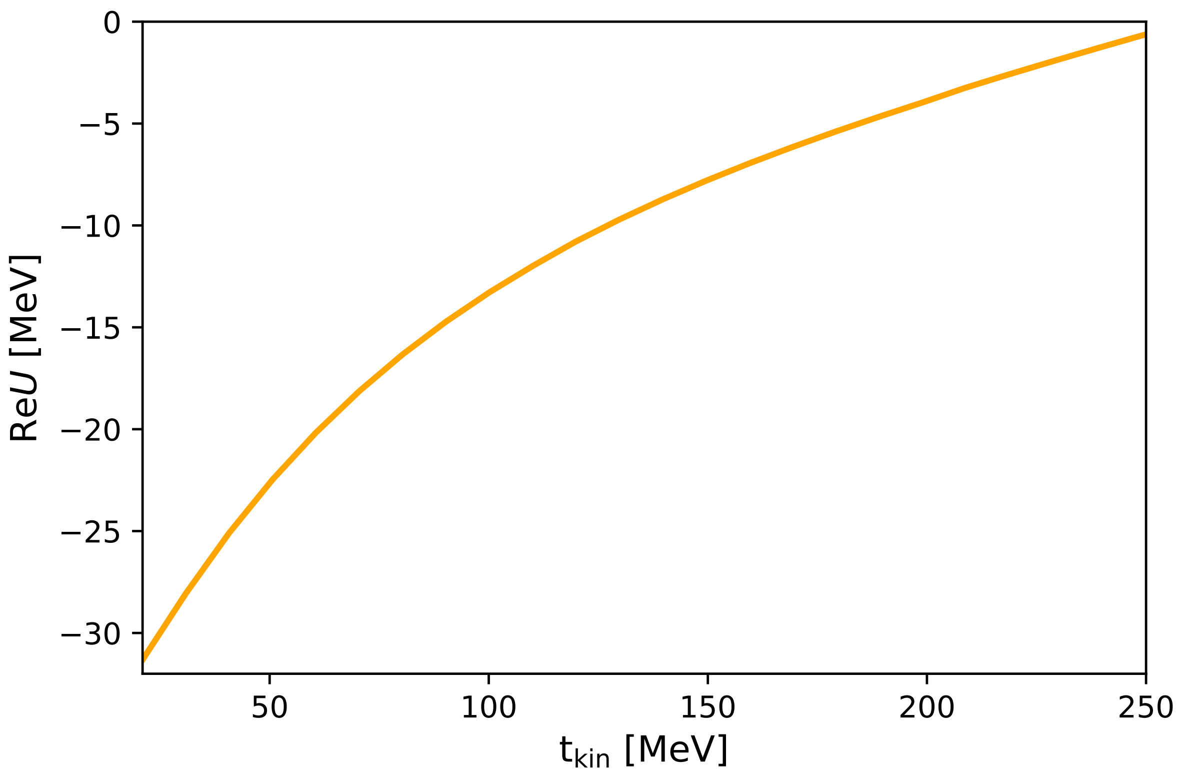
- Gives error estimate of energy integrals of local density of states $R(\omega)$

$$Q(R, f) = \int d\omega R(\omega) f(\omega)$$

Optical potential

$$W^{\mu\nu}_{\rm FSI}(q) = \int \frac{d^3\mathbf{p}}{(2\pi)^3} dE \frac{m}{E_p} \frac{m}{E_{p+q}} \left[S^n(\mathbf{p},E) w^{\mu\nu}_n(p,q) + S^p(\mathbf{p},E) w^{\mu\nu}_p(p,q)\right] \times \theta(\mathbf{p}' - p_F) \delta(\omega + E - E_{p+q} - E^{kin}_f - {\rm ReU})$$

$$w^{\mu\nu}(p,q) = \langle p+q | j^\mu | p\rangle^\dagger \langle p+q | j^\nu | p \rangle$$



Spectral function

Green's function:

$$G_h(\alpha, \beta, E) = \langle 0 | a_\beta^\dagger \frac{1}{E - (E_0 - \hat{H}) - i\epsilon} a_\alpha | 0 \rangle$$

$$\mathrm{Im} G_h(\alpha, \beta, E) = -\pi \sum\!\!\!\!\!\!\!\int_{\Psi_{A-1}} \langle 0 | a_\beta^\dagger | \Psi_{A-1} \rangle \langle \Psi_{A-1} | a_\alpha | 0 \rangle \delta\big(E - (E_0 - E_\Psi)\big)$$

Spectral function:

$$S(\mathbf{p}, E) = -\frac{1}{\pi} \sum_{\alpha,\beta} \langle \mathbf{p} | \alpha \rangle \langle \mathbf{p} | \beta \rangle^\dagger \mathrm{Im} G_h(\alpha, \beta, E)$$

Analysis of spurious states

$$\langle \Psi | \hat{\rho}^\dagger \; \hat{\rho} | \Psi \rangle$$

include a complete sum

Analysis of spurious states

$$\langle \Psi | \hat{\rho}^\dagger \sum_{f_I} |f_I\rangle |\Psi^0_{CoM}\rangle\langle\Psi^0_{CoM}| \langle f_I| + \sum_{f_{CoM}} |\Psi^0_I\rangle |f_{CoM}\rangle\langle f_{CoM}| \langle\Psi^0_I| \hat{\rho} | \Psi\rangle$$

excitation of intrinsic wave function (physical spectrum)

excitation of CoM wave function (spurious)

Analysis of spurious states

$$\langle \Psi | \hat{\rho}^\dagger \sum_{f_I} |f_I\rangle |\Psi^0_{CoM}\rangle\langle \Psi^0_{CoM}| \langle f_I| + \sum_{f_{CoM}} |\Psi^0_I\rangle |f_{CoM}\rangle\langle f_{CoM}| \langle \Psi^0_I| \hat{\rho} |\Psi\rangle$$

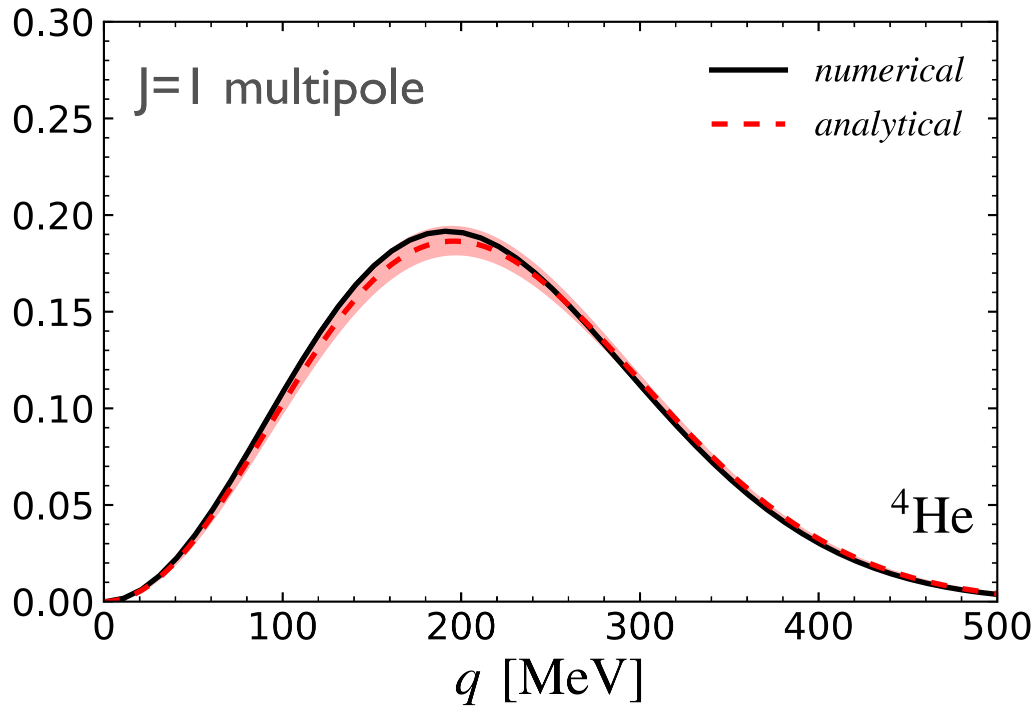
excitation of intrinsic wave function (physical spectrum)

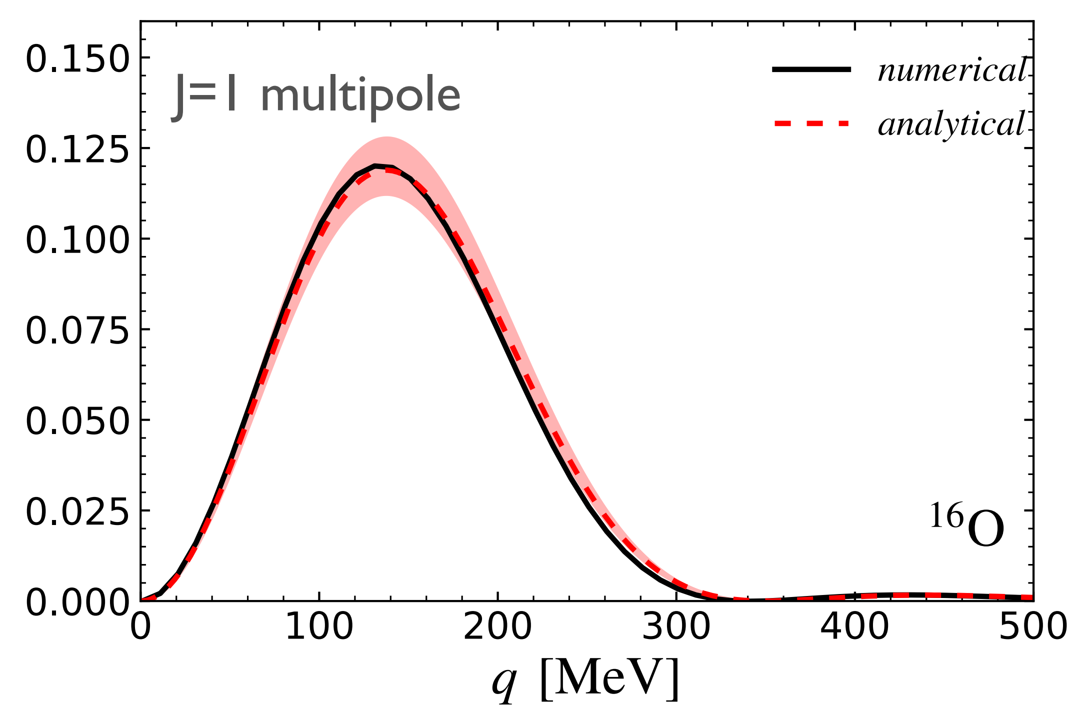
excitation of CoM wave function (spurious)

With our ansatz about $|\Psi_{CoM}\rangle$ (Gaussian) we get analytical function for spurious states

We get numerically spurious states (nonphysical excitations with energy close to 0)

Analysis of spurious states

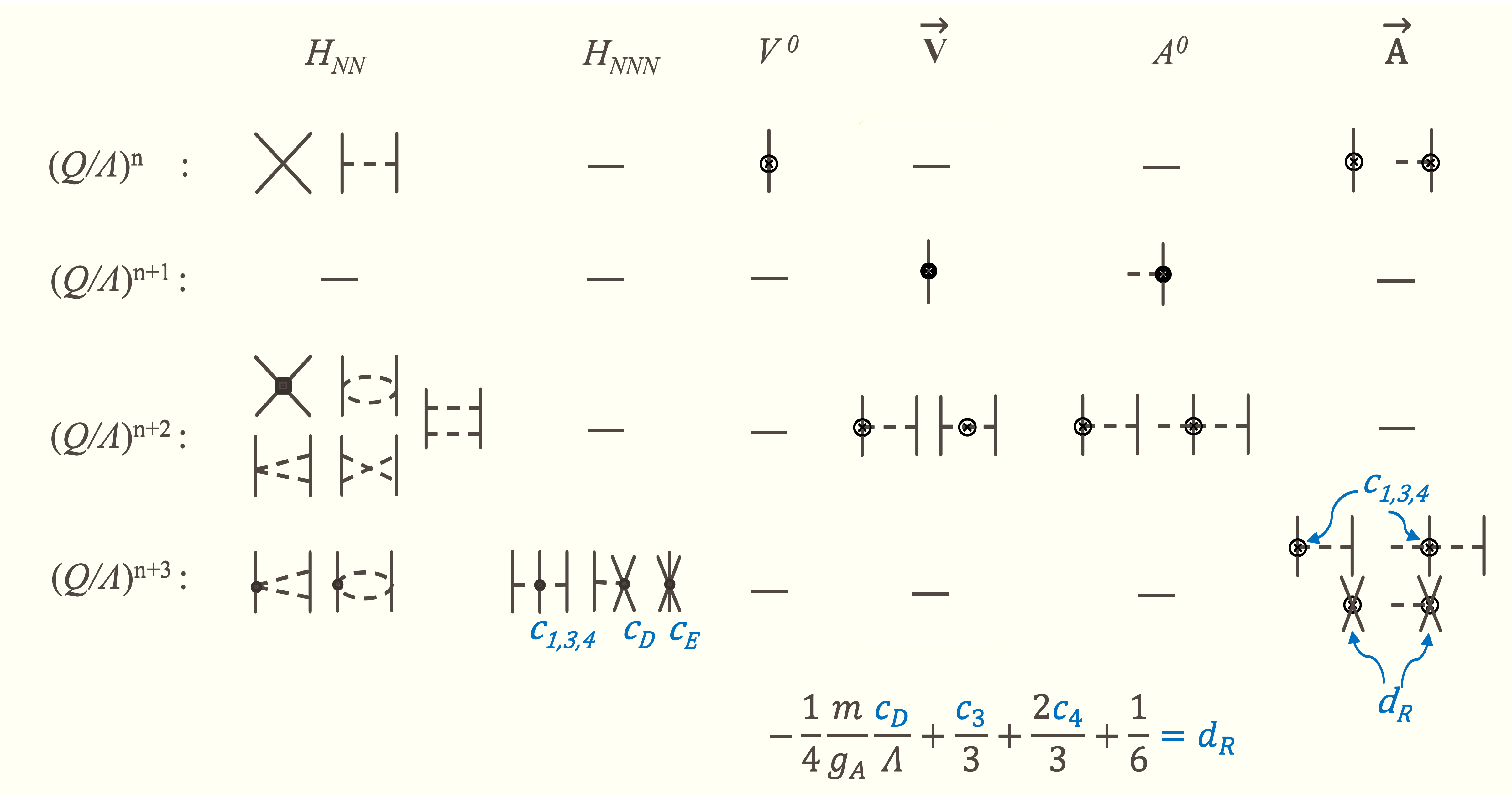




With our ansatz about $|\Psi_{CoM}\rangle$ (Gaussian) we get analytical function for spurious states

We get numerically spurious states (nonphysical excitations with energy close to 0)

Nuclear Hamiltonian and currents



*Nucleon-structure diagrams and relativistic corrections not shown

Author: Bijaya Acharya

Coupled cluster method

Reference state (Hartree-Fock): $|\Psi\rangle$

Include correlations through e^T operator

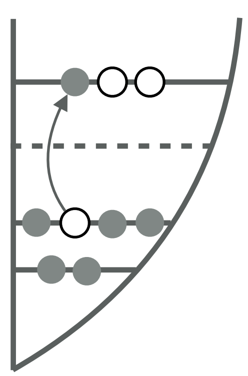
similarity transformed Hamiltonian (non-Hermitian)

$$e^{-T}\mathcal{H}e^{T}|\Psi\rangle \equiv \bar{\mathcal{H}}|\Psi\rangle = E|\Psi\rangle$$

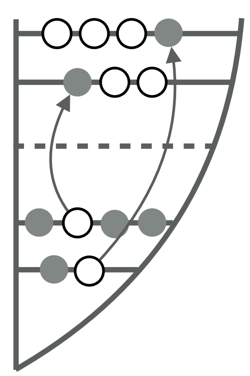
Expansion: $T = \sum t_a^i a_a^\dagger a_i + \sum t_{ab}^{ij} a_a^\dagger a_b^\dagger a_i a_j + \ldots$

←coefficients obtained through coupled cluster equations

singles



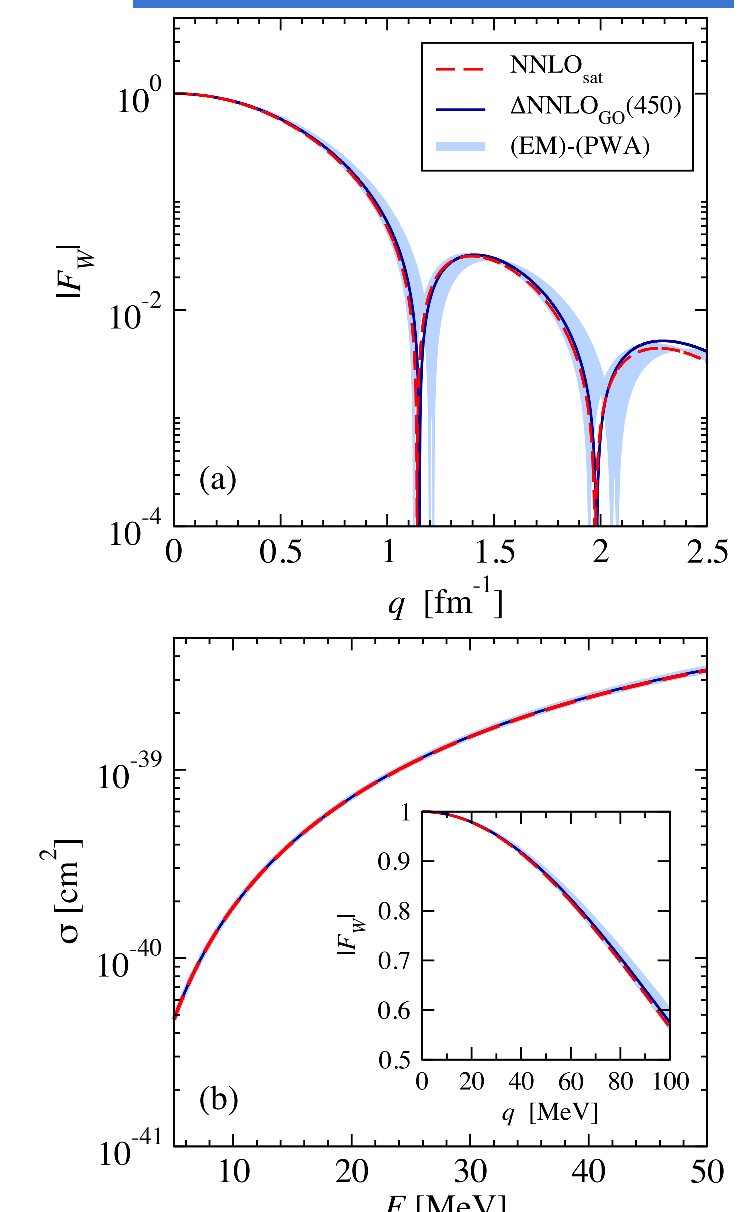
doubles



Coupled cluster method

- ✓ Controlled approximation through truncation in T
- ✓ Polynomial scaling with A (predictions for ^{100}Sn, ^{208}Pb)
- ✓ Size extensive
- ✓ Works most efficiently for doubly magic nuclei

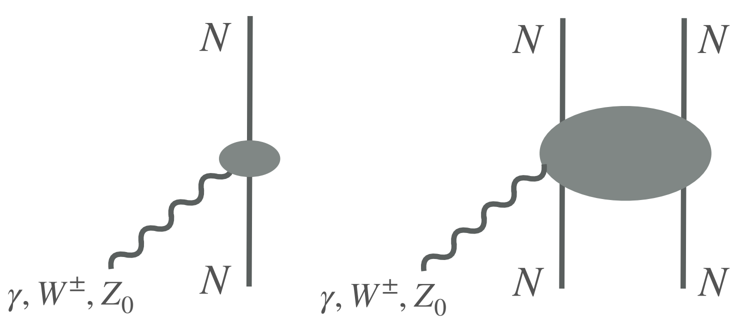
coherent elastic neutrino scattering on ^{40}Ar



C. Payne at al.
Phys.Rev.C 100 (2019) 6, 061304

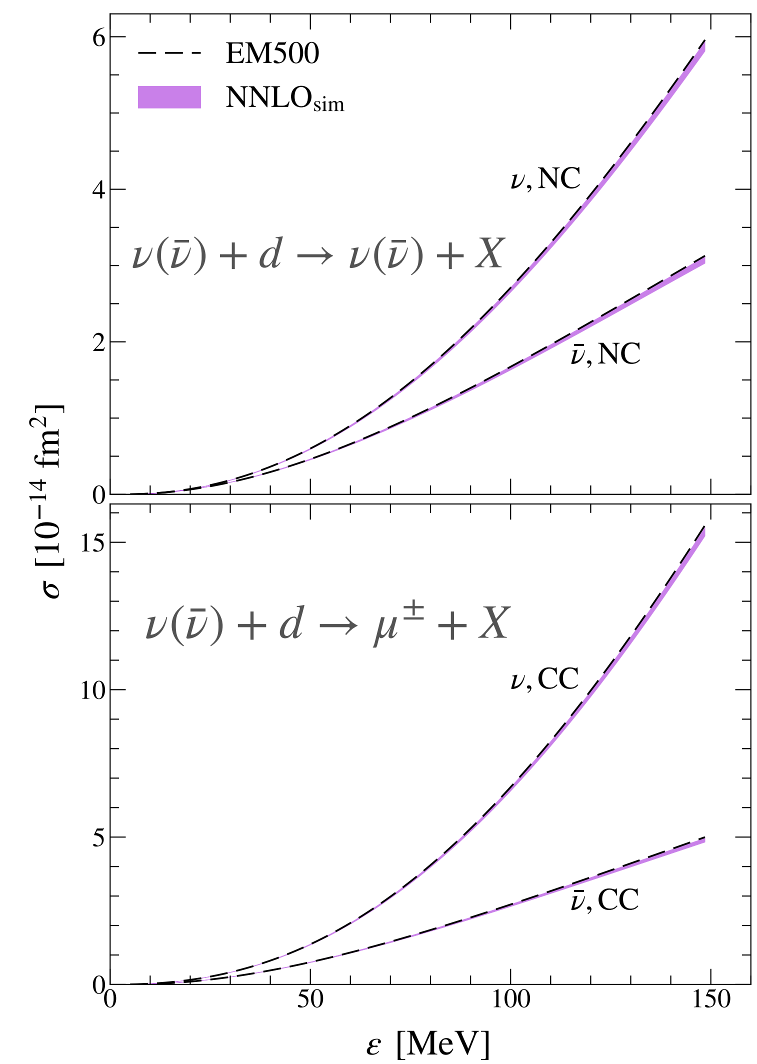
Electroweak currents

$$J = \sum_i j_i + \sum_{i<j} j_{ij} + \dots$$



known to give significant contribution for neutrino-nucleus scattering

Current decomposition into multipoles needed for various *ab initio* methods: CC, No Core Shell Model, In-Medium Similarity Renormalization Group



Multipole decomposition for 1- and 2-body EW currents

B. Acharya, S. Bacca
Phys.Rev.C 101 (2020) 1, 015505