Spectral functions from quantum Monte Carlo

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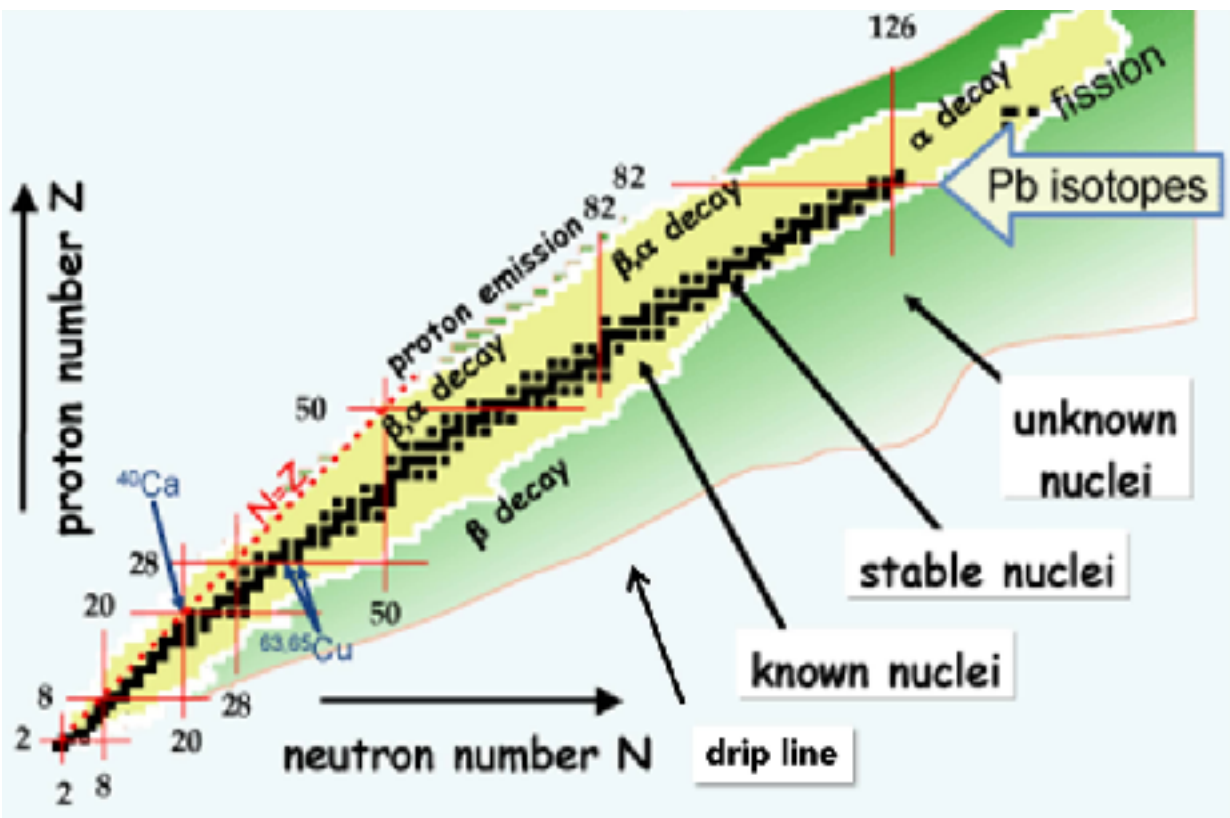
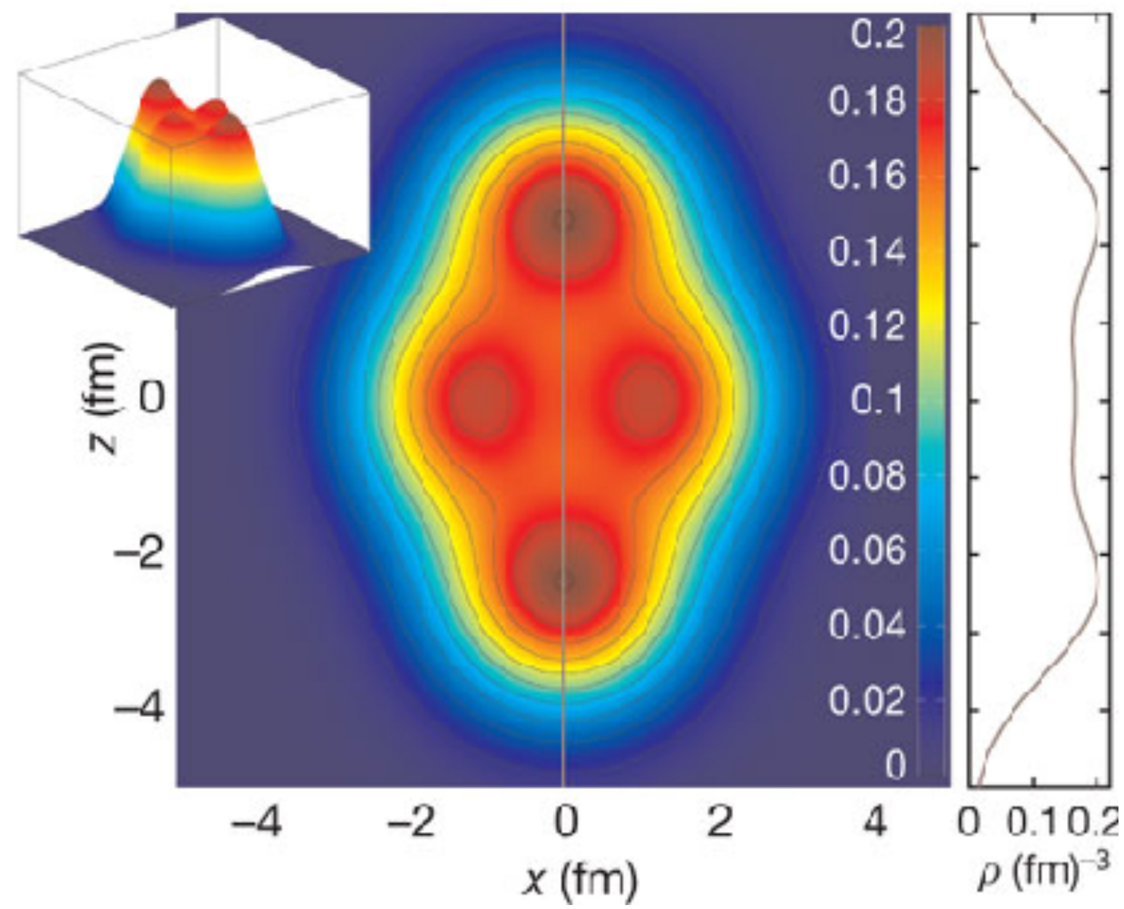
The *basic model* of nuclear physics

- Atomic nuclei are strongly interacting many-body systems exhibiting fascinating properties including: shell structure, pairing and superfluidity, deformation, and self-emerging clustering.





•The basic model of nuclear physics aims at understanding the properties of atomic nuclei and nucleonic matter in terms of the individual interactions among the neutrons and the protons

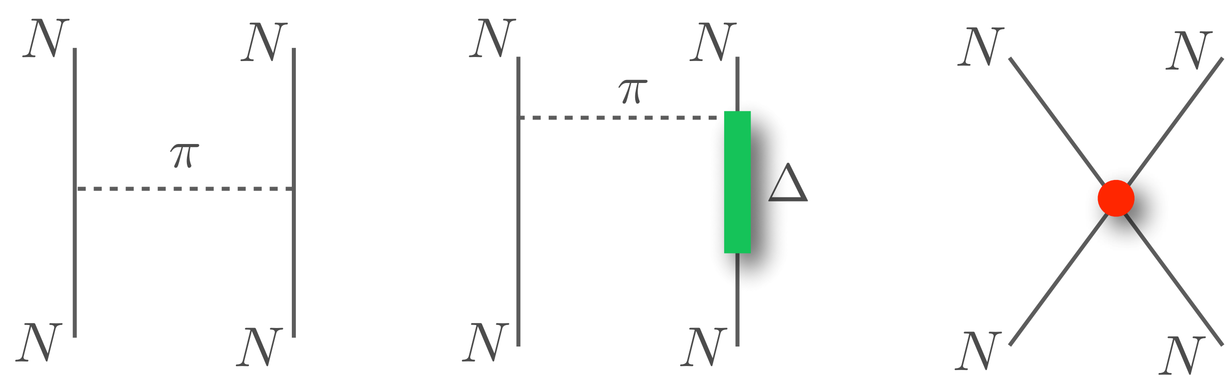
Nuclear Hamiltonian

- Nuclear ab-initio approaches are based on the non relativistic hamiltonian

$$H=\sum_i \frac{\mathbf{p}_i^2}{2m}+\sum_{i<j} v_{ij}+\sum_{i<j<k} V_{ijk}+\ldots$$

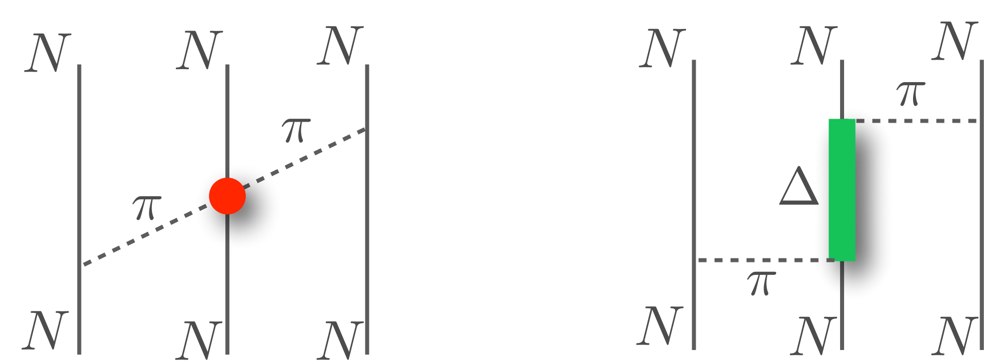
- Argonne v_{18} is a finite, local, configuration-space potential controlled by ~4300 np and pp scattering data below 350 MeV of the Nijmegen database

$$v_{ij}=\sum_{p=1}^{18} v^p(r_{ij})O_{ij}^p$$



- Three-nucleon interactions effectively include the lowest nucleon excitation, the Δ(1232) resonance, end other nuclear effects

$$V_{ijk}^{3\mathrm{N}}=A_{2\pi}^{PW}O_{ijk}^{2\pi,PW}+A_{2\pi}^{SW}O_{ijk}^{2\pi,SW}+A_{3\pi}^{\Delta R}O_{ijk}^{3\pi,\Delta R}+A^R O_{ijk}^R$$



Variational Monte Carlo (VMC)

A fundamental step towards a first-principle description of atomic nuclei is the solution of the many-body Schrödinger equation

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

- In VMC, one assumes a form for the trial wave function and optimizes its variational parameters

$$E_T = \langle\Psi_T|H|\Psi_T\rangle \geq E_0$$

- The short-range behavior of the trial wave function is modeled by Jastrow-like correlations

$$\Psi_T = \left(1 + \sum_{i<j<k} F_{ijk}\right)\left(\mathcal{S}\prod_{i<j} F_{ij}\right)\Phi_A(J, M, T, T_z)$$

- They reflect the spin-isospin dependence of the two- three-nucleon interactions

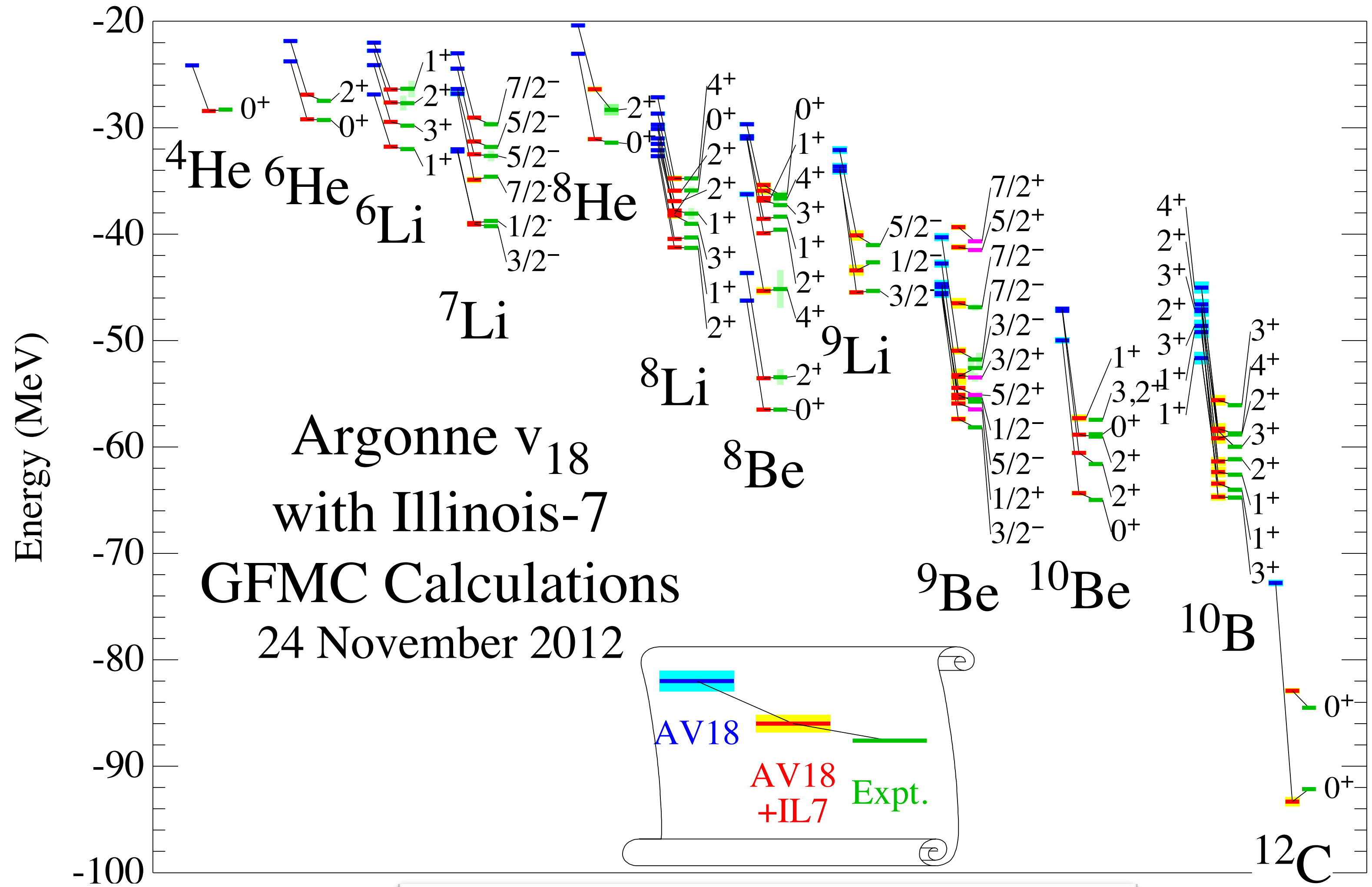
$$F_{ij} \simeq \sum_p f^p(r_{ij})O^p_{ij} \qquad F_{ijk} = \sum_x \epsilon_x V^x_{ijk}(\tilde{r}_{ij}, \tilde{r}_{ik}, \tilde{r}_{jk})$$

Green's function Monte Carlo

- Green's function Monte Carlo methods use an imaginary-time projection technique to enhance the ground-state component of a starting trial wave function.

$$\lim_{\tau\to\infty} e^{-(H-E_0)\tau}|\Psi_T\rangle = \lim_{\tau\to\infty}\sum_n c_n\, e^{-(E_n-E_0)\tau}|\Psi_n\rangle = c_0|\Psi_0\rangle$$

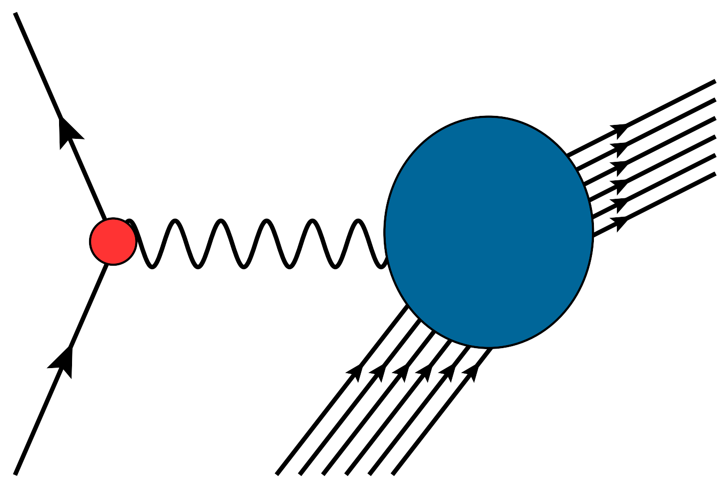
- Suitable to solve of A ≤ 12 nuclei with ~1% accuracy



J. Carlson et al. RMP **87**, 1067 (2015)

Electron-nucleus scattering

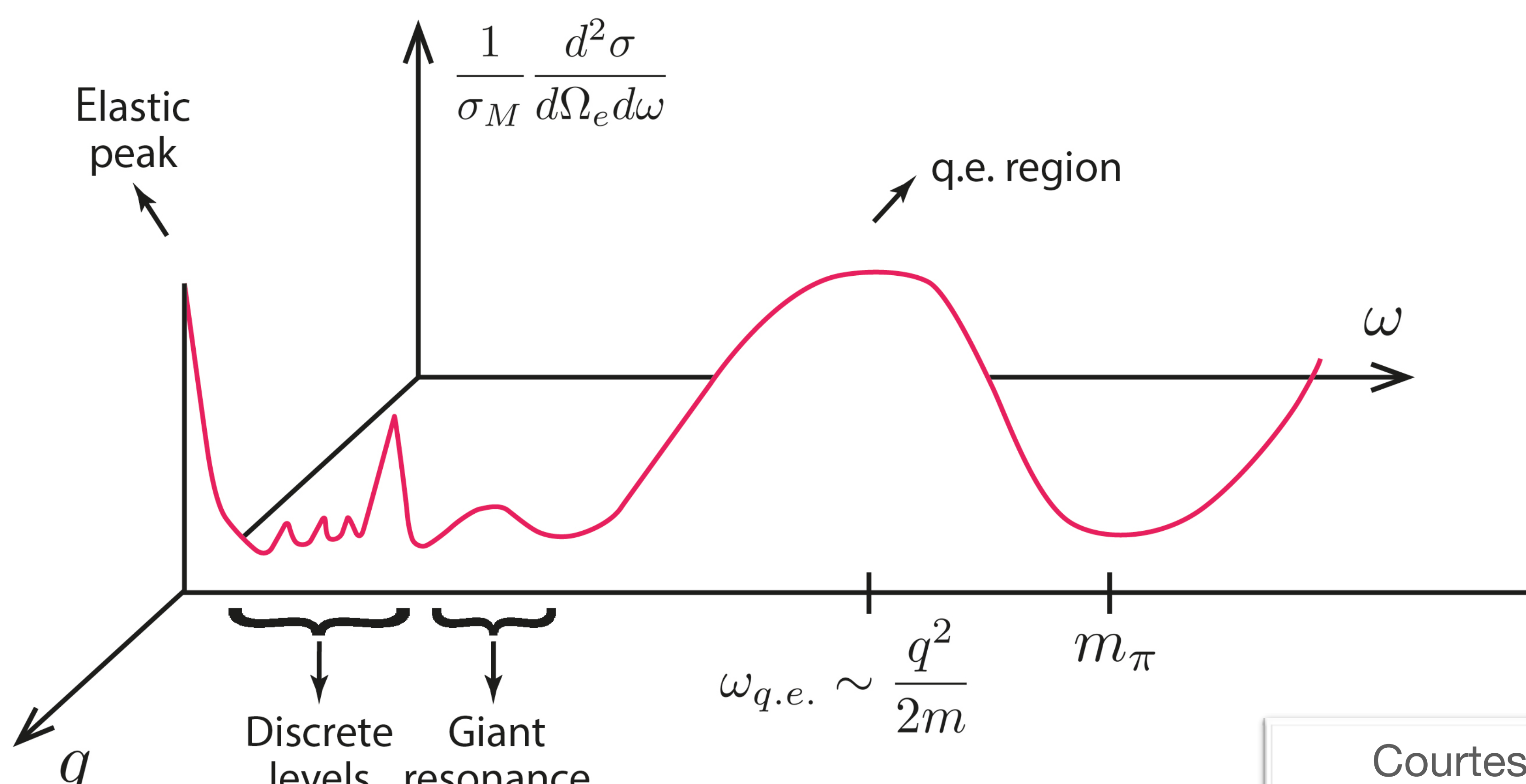
In the Born approximation, the differential cross section of the inclusive electron-nucleus scattering is



$$\left(\frac{d\sigma}{dE'd\Omega}\right)_e = \left(\frac{d\sigma}{d\Omega}\right)_{\rm M} \left[A_L\, R_L + A_T\, R_T\right] ,$$

$$R_\alpha(\mathbf{q},\omega) = \sum_f \langle\Psi_0|J^{\mu\,\dagger}|\Psi_f\rangle\langle\Psi_f|J^\nu|\Psi_0\rangle\delta(\omega - E_f + E_0) ,$$

Schematic representation of the inclusive cross section as a function of the energy loss.

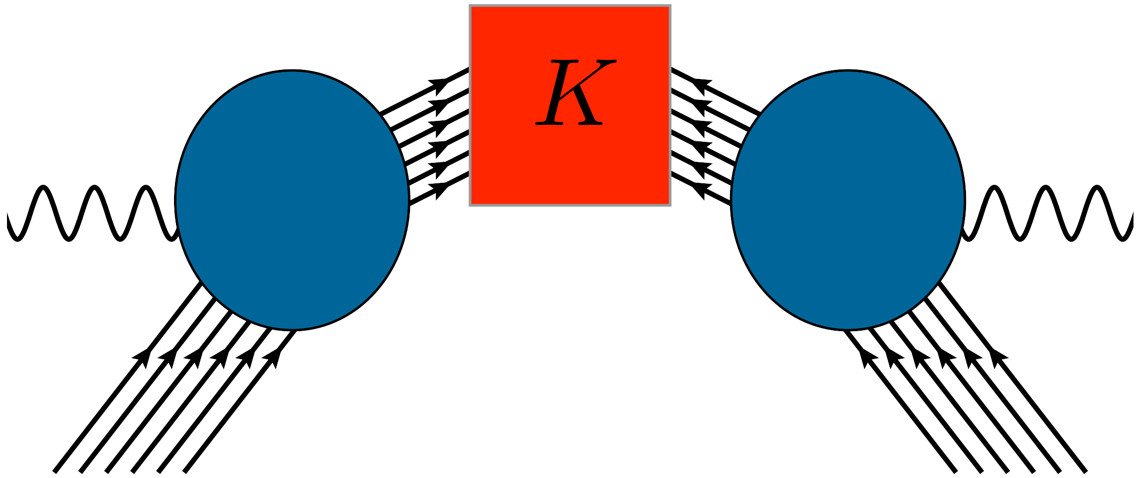


Courtesy of Saori Pastore

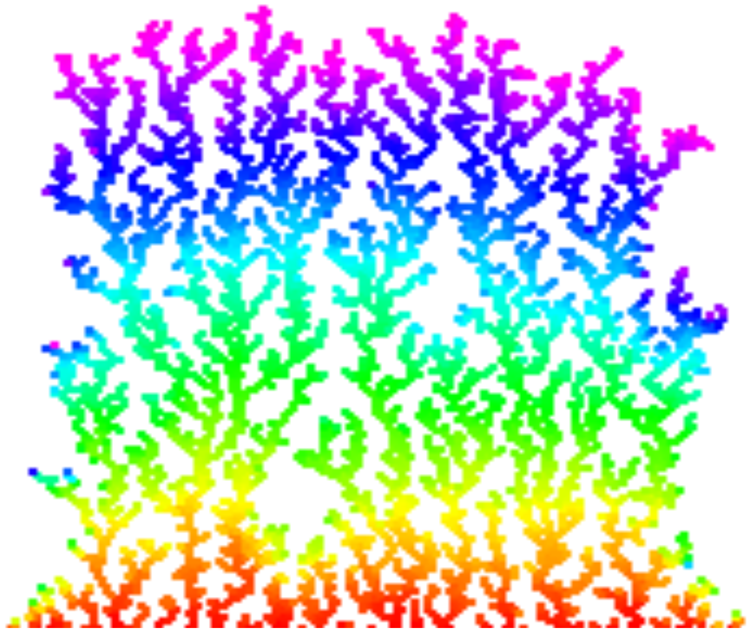
Inclusive cross-section from GFMC

- The energy dependence of the response functions can be inferred from their Laplace transforms

$$E_{\alpha\beta}(\tau, \mathbf{q}) \equiv \int d\omega e^{-\omega\tau} R_{\alpha\beta}(\omega, \mathbf{q})$$



- Using the completeness of the final states, the Euclidean responses are expressed in terms of ground-state expectation values that are computed within **Green's function Monte Carlo**

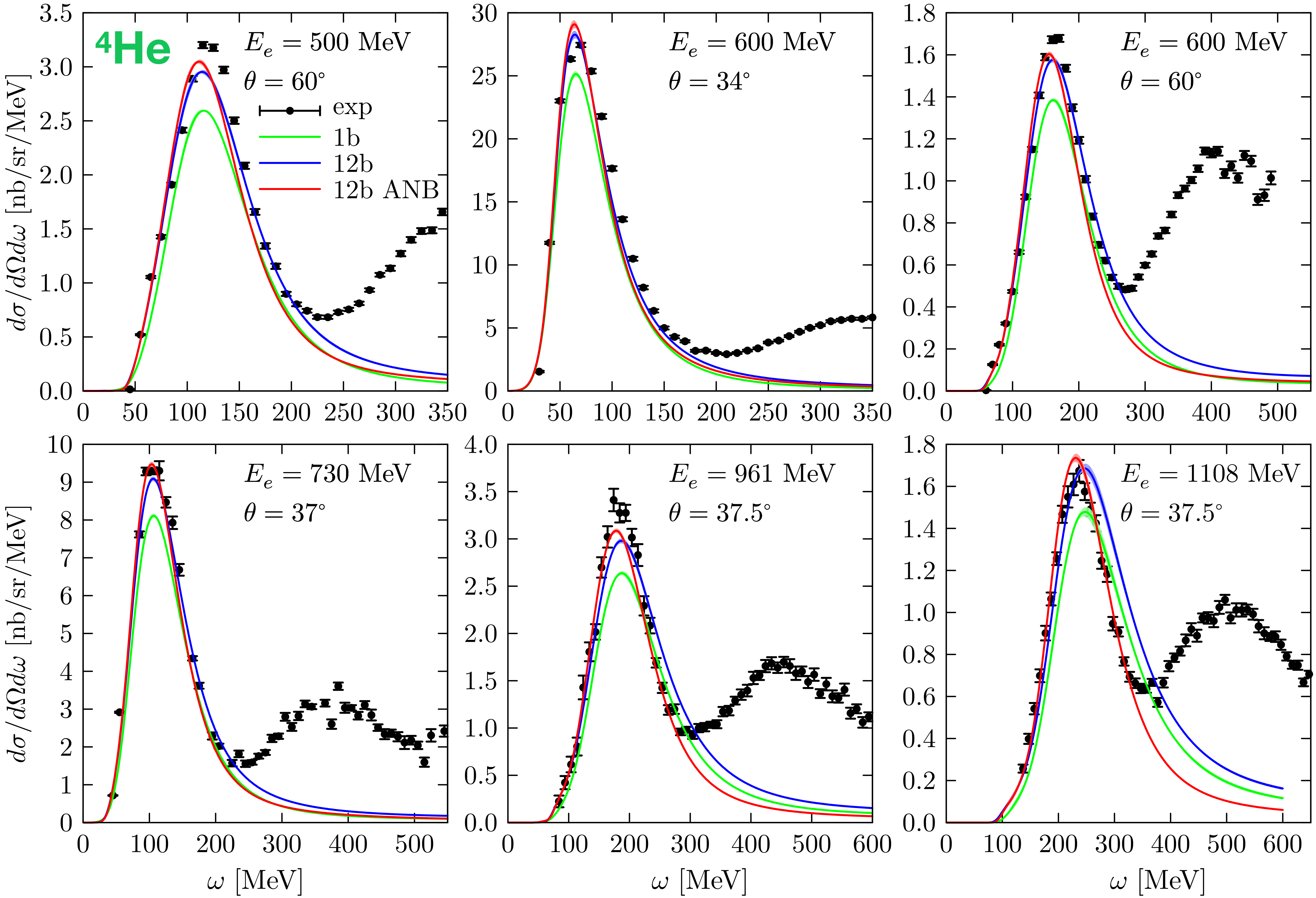


$$E_{\alpha\beta}(\tau, \mathbf{q}) = \langle \Psi_0 | J_\alpha^\dagger(\mathbf{q}) e^{-(H-E_0)\tau} J_\beta(\mathbf{q}) | \Psi_0 \rangle$$

Analogous techniques are used in Lattice QCD and condensed matter Physics

N. Rocco et al. PRC **97** 055501(2018)

Inclusive cross-section from GFMC

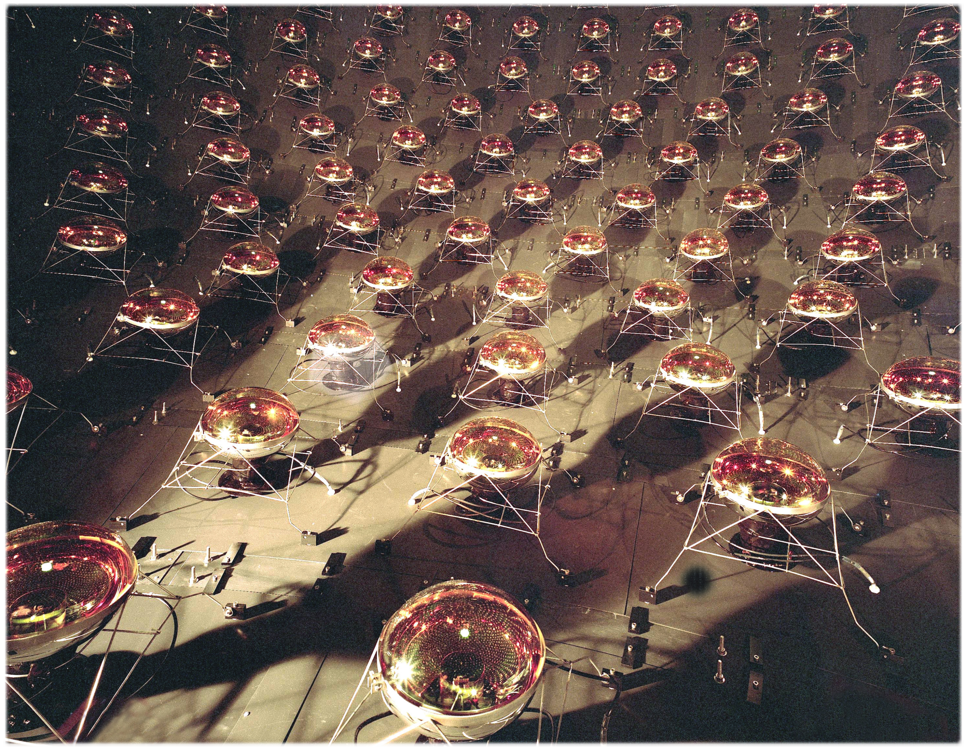


Neutrino experiments

Neutrino-oscillation and 0νββ experiments are (also) sensitive to the high-momentum components of the nuclear wave function

- Charge-parity (CP) violating phase and the mass hierarchy will be measured
- Determine whether the neutrino is a Majorana or a Dirac particle
- Need for including nuclear dynamics; mean-field models inadequate to describe neutrino-nucleus interaction

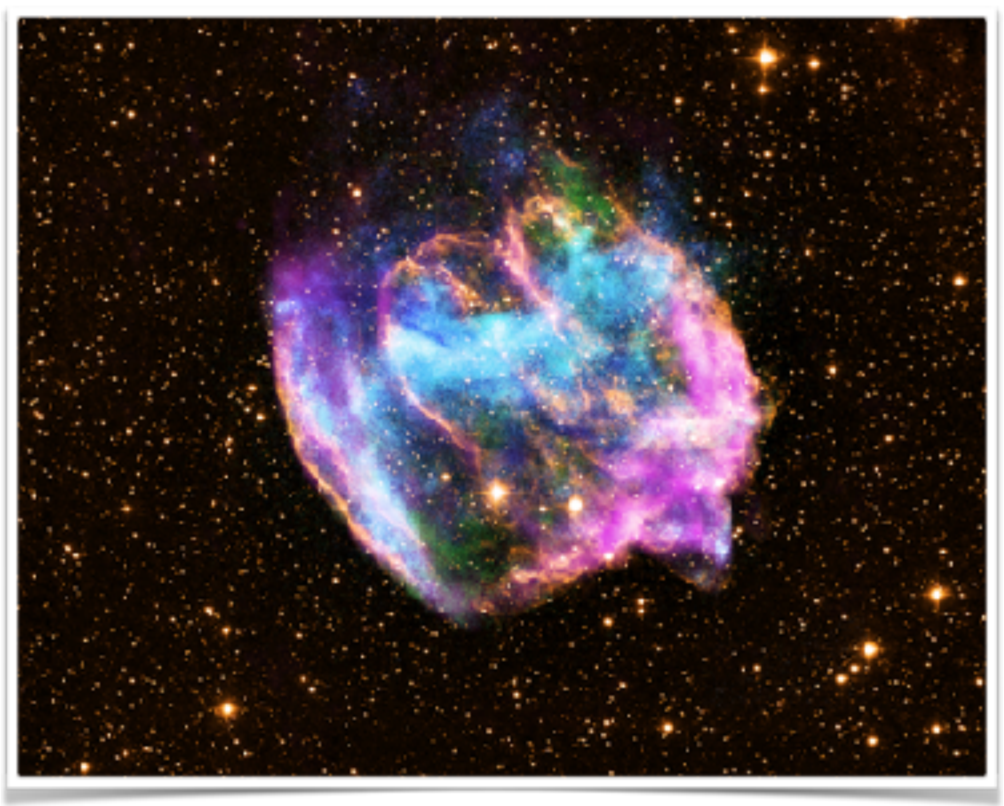
- A large body of experimental data for the electromagnetic cross sections of ^{4}He and ^{12}C (and many other nuclei) is available.
- A model unable to describe electron-nucleus scattering is (very) unlikely to describe neutrino-nucleus scattering.



Multi-messenger astronomy

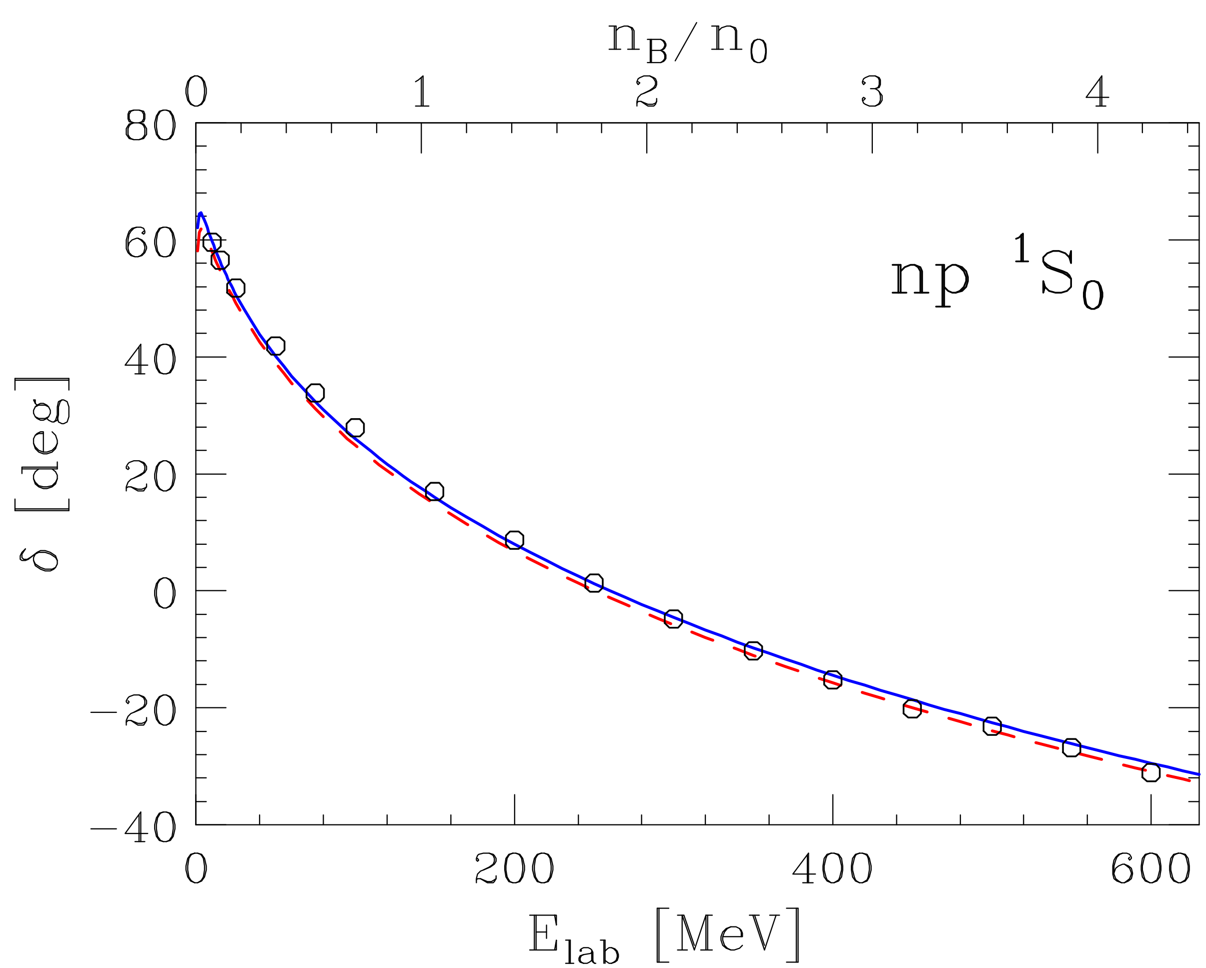
The capacity to explain scattering data at large energy is critical to assess the ability of a potential model to describe the properties of nuclear matter in the high-density region

- Gravitational waves have been detected!
- Supernovae neutrinos will be detected by the current and next generation neutrino experiments
- Nuclear dynamics determines the structure and the cooling of neutron stars



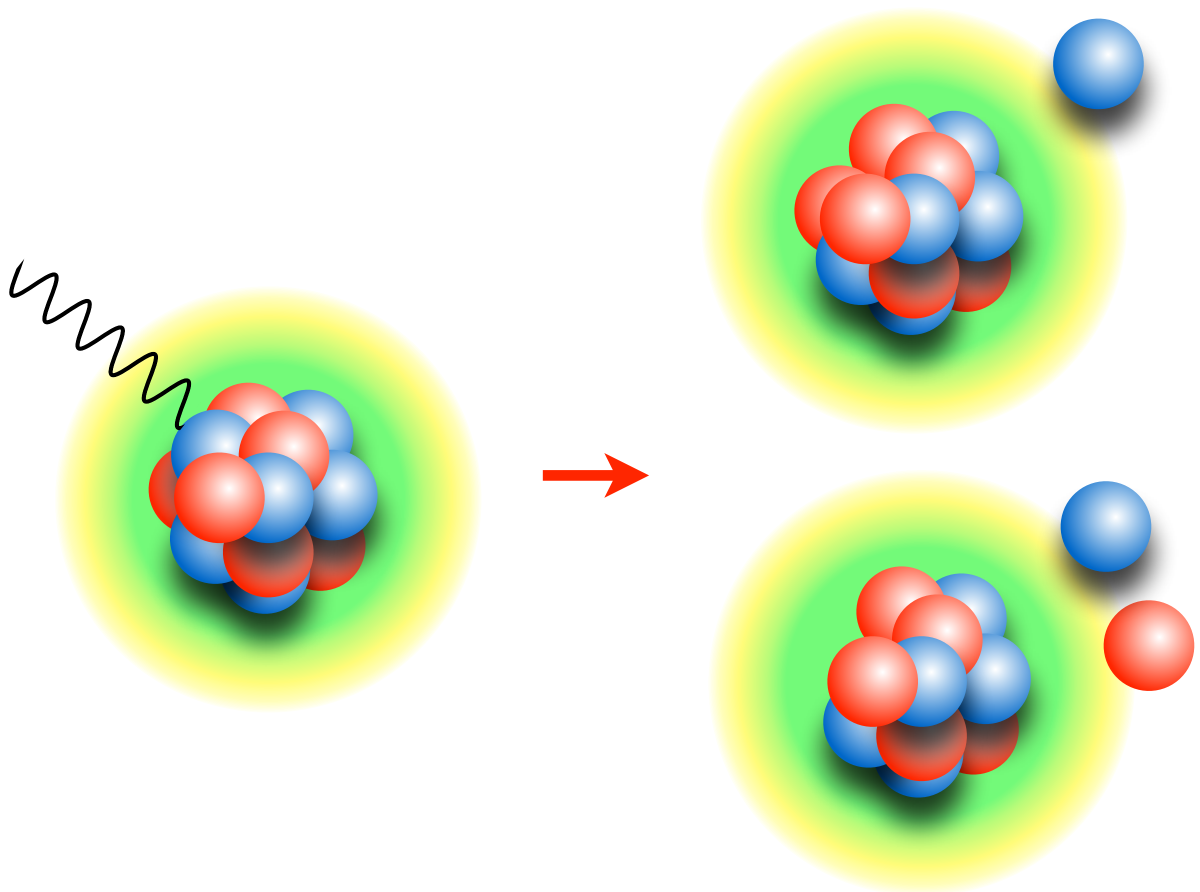
For head-on collisions, the kinetic energy in the laboratory frame is related to the density as

$$E_{\rm lab} = 4\,\frac{k_F^2}{2m} = \frac{2}{m}\left(\frac{6\pi^2 n_B}{\nu}\right)^{2/3}$$



High momentum-transfer regime

- At (very) large momentum transfer, scattering off a nuclear target reduces to the sum of scattering processes involving bound nucleons → short-range correlations.



$$|\Psi_f\rangle \simeq |p_1\rangle \otimes |\Psi_f\rangle_{A-1}$$

$$|\Psi_f\rangle \simeq |p_1, p_2\rangle \otimes |\Psi_f\rangle_{A-2}$$

- Relativistic effects play a major role and need to be accounted for along with nuclear correlations (Non-trivial interplay between them)

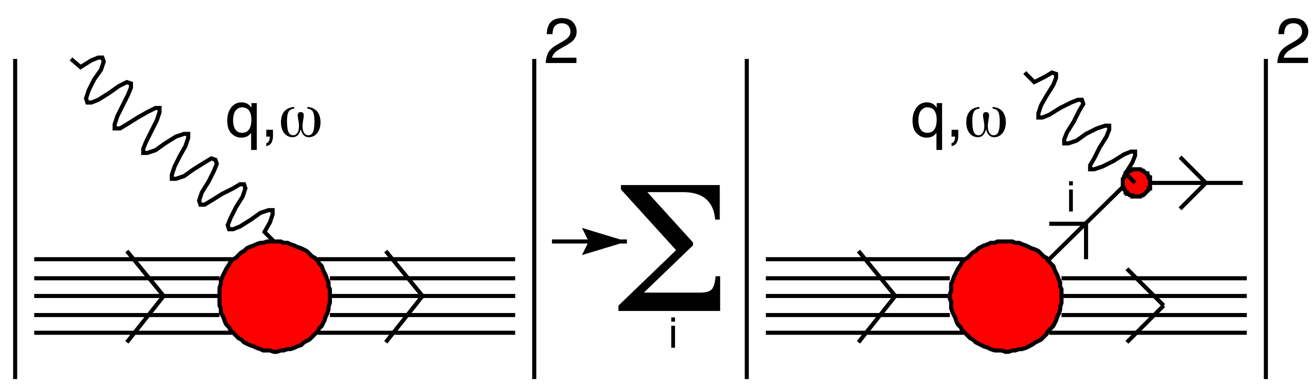
- Resonance-production and deep inelastic scattering processes need to be included

High momentum-transfer regime

Reminder $$R_{\alpha\beta}(\omega,\mathbf{q})=\sum_f\langle\Psi_0|J^\dagger_\alpha(\mathbf{q})|\Psi_f\rangle\langle\Psi_f|J_\beta(\mathbf{q})|\Psi_0\rangle\delta(\omega-E_f+E_0)$$

At large momentum transfer, scattering off a nuclear target reduces to the incoherent sum of scattering processes involving individual bound nucleons

$$J^\mu\to\sum_i j_i^\mu$$
$$|\psi_f^A\rangle\to|p\rangle\otimes|\psi_f^{A-1}\rangle$$
$$E_f=E_f^{A-1}+e(\mathbf{p})$$



Inserting a single-particle state completeness, we isolate the current matrix element

$$\langle\psi_f^A|J_\alpha|\psi_0^A\rangle\to\sum_k[\langle\psi_f^{A-1}|\otimes\langle k|]\,|\psi_0^A\rangle\langle p|\sum_i j^I_\alpha|k\rangle\ .$$

Keeping only the incoherent contribution (dominant in this regime), the one-body response reads

$$R_{\alpha\beta}=\sum_{p,k,f}\sum_i\langle k|{j^i_\alpha}^\dagger|p\rangle\langle p|j^i_\beta|k\rangle|\langle\psi_0^A|[|\psi_f^{A-1}\rangle\otimes|k\rangle]|^2\delta(\omega-e(\mathbf{p})-E_f^{A-1}+E_0^A)$$

High momentum-transfer regime

Reminder $R_{\alpha\beta} = \sum_{p,k,f} \sum_i \langle k | {j_\alpha^i}^\dagger | p \rangle \langle p | j_\beta^i | k \rangle | \langle \psi_0^A | [| \psi_f^{A-1} \rangle \otimes | k \rangle] |^2 \delta(\omega - e(\mathbf{p}) - E_f^{A-1} + E_0^A)$

Momentum-conservation in the single-nucleon vertex and the identity

$$\delta(\omega - e(\mathbf{p}) - E_f^{A-1} + E_0^A) = \int dE \, \delta(\omega + E - e(\mathbf{p})) \, \delta(E + E_f^{A-1} - E_0^A)$$

Allow one to rewrite the response function as

Covariant normalization
of the four-spinors

$$R_{\alpha\beta} = \int \frac{d^3k}{(2\pi)^3} dE P_h(\mathbf{k}, E) \frac{m_N^2}{e(\mathbf{k}) e(\mathbf{k}+\mathbf{q})} \sum_i \langle k | {j_\alpha^i}^\dagger | k+q \rangle \langle k+q | j_\beta^i | k \rangle \delta(\omega + E - e(\mathbf{k}+\mathbf{q}))$$

The hole spectral function yields the probability of removing a nucleon with momentum **k** from the target ground state leaving the residual system with excitation energy *E*.

$$P_h^{1h}(\mathbf{k}, E) \rightarrow \sum_f | \langle \Psi_0^A | [| k \rangle \otimes | \Psi_f^{A-1} \rangle] |^2 \delta(E - E_f^{A-1} + E_0^A)$$

High momentum-transfer regime

Reminder $$P_h(\mathbf{k}, E) = \sum_f |\langle\psi_0^A|[|k\rangle \otimes |\psi_f^{A-1}\rangle]|^2 \delta(E + E_f^{A-1} - E_0^A)$$

Using the Sokhotski-Plemelj theorem and the completeness of the A-1 states, the hole spectral function can be expressed in terms of the hole Green's function

$$P_h(\mathbf{k}, E) = \frac{1}{\pi} \mathrm{Im} \langle 0| a^\dagger_{\mathbf{k}} \frac{1}{E + (H - E_0^A) - i\epsilon} a_{\mathbf{k}} |0\rangle \,.$$

The integral of the spectral function over the removal energy is the momentum distribution

$$n(\mathbf{k}) = \langle\psi_0^A| a^\dagger_k a_k |\psi_0^A\rangle = \int dE P(\mathbf{k}, E) \,.$$

Taking $E_f^{A-1} - E_0 = \epsilon$ constant, the hole spectral function is sometimes approximated by

$$P_h(\mathbf{k}, E) \simeq n(\mathbf{k})\delta(E - \epsilon)$$

Hole SF from correlated-basis function

The hole SF of finite nuclei is expressed as a sum of two contributions, displaying distinctly different energy and momentum dependences

$$P_h(\mathbf{k},E) = P_h^{1h}(\mathbf{k},E) + P_h^{\rm corr}(\mathbf{k},E)$$

The 1h terms corresponds to discrete excitations of the A-1 final states

$$P_h^{1h}(\mathbf{k},E) \to \sum_{\bar f} |\langle \Psi_0^A|[|k\rangle \otimes |\Psi_{\bar f}^{A-1}\rangle]|^2 \delta(E - E_{\bar f}^{A-1} + E_0^A)$$

Computing this term in principle requires evaluating single-nucleon overlaps. Within the CBF theory, it is obtained from a modified mean-field scheme

$$P_h^{1h}(\mathbf{k},E) = \sum_{\alpha\in\{\rm F\}} Z_\alpha |\phi_\alpha(\mathbf{k})|^2 F_\alpha(E - e_\alpha) \ ,$$

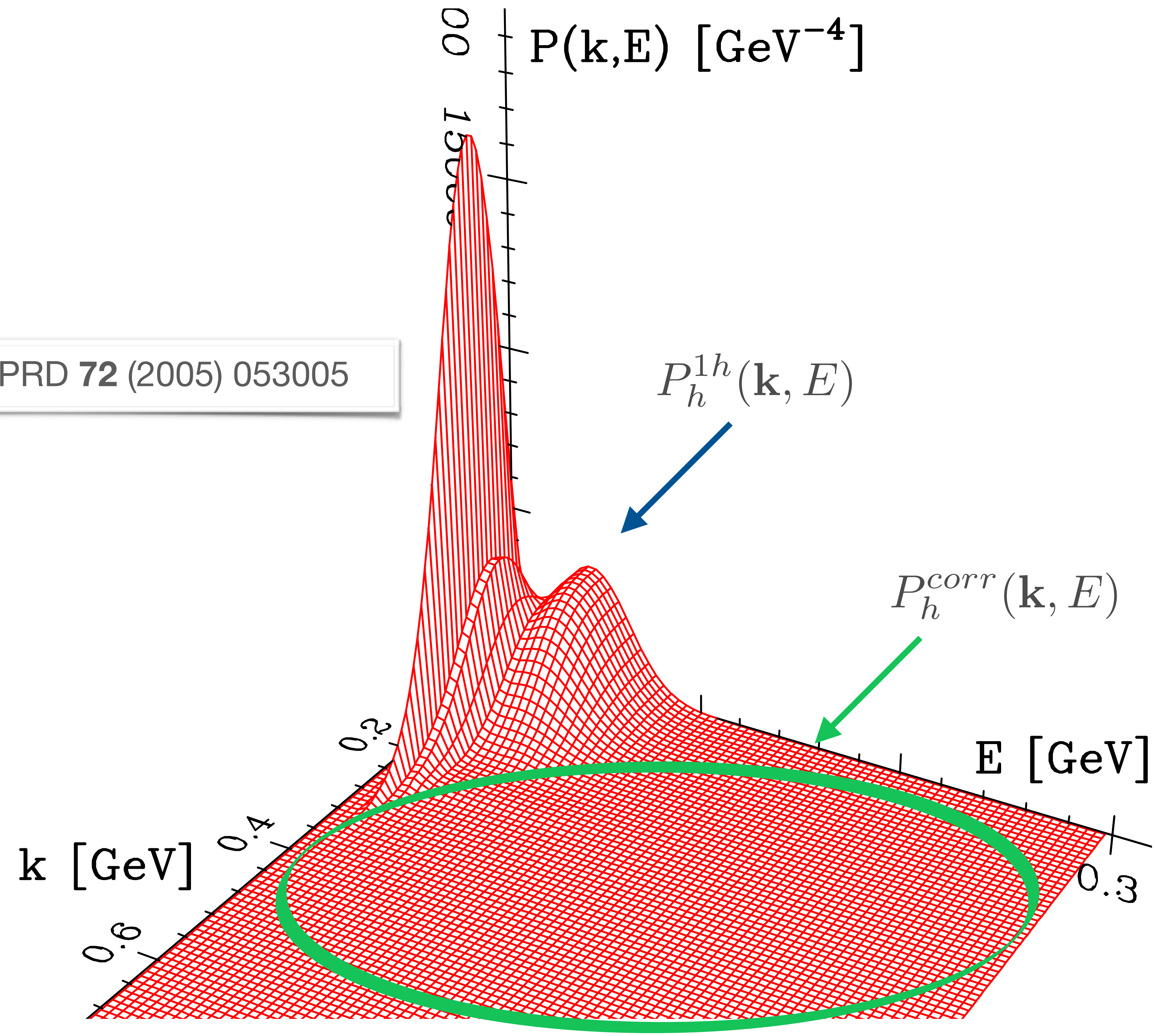
The high-momentum component, corresponding to the A-1 final state in the continuum, is obtained from CBF by calculations in infinite nuclear matter

$$P_h^{\rm corr}(\mathbf{k},E) = \int d^3R \ \rho_A(\mathbf{R}) P_{h,\,NM}^{\rm corr}(\mathbf{k},E;\rho_A(\mathbf{R}))\ ,$$

Hole SF from correlated-basis function

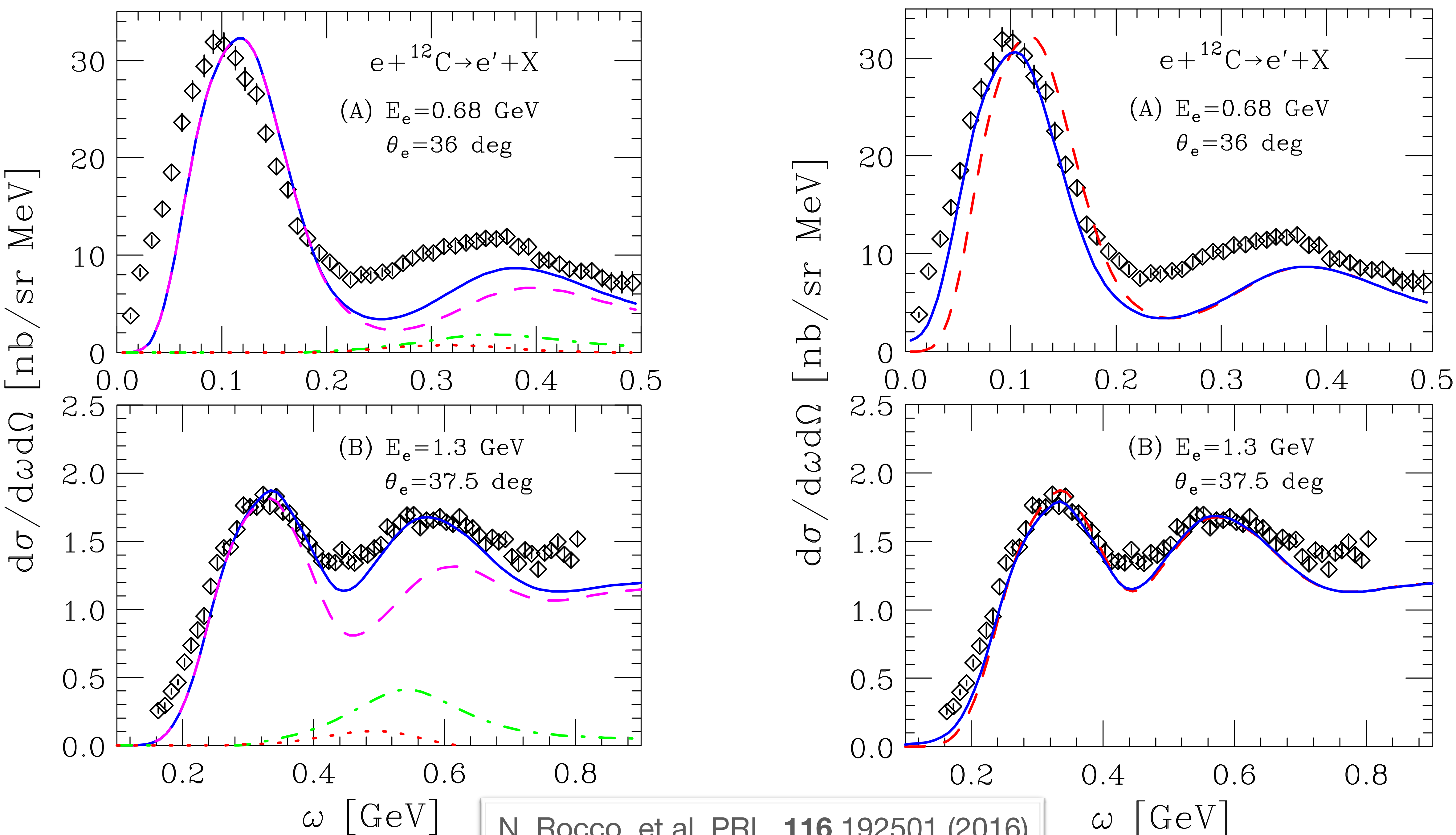
The hole SF of finite nuclei is expressed as a sum of two contributions, displaying distinctly different energy and momentum dependences

O. Benhar et al. PRD **72** (2005) 053005



Including two-body currents

Using relativistic MEC requires the extension of the factorization scheme to two-nucleon emissions $\longleftrightarrow$ $|\Psi_f^A\rangle \rightarrow |p_1 p_2\rangle \otimes |\Psi_f^{A-2}\rangle$

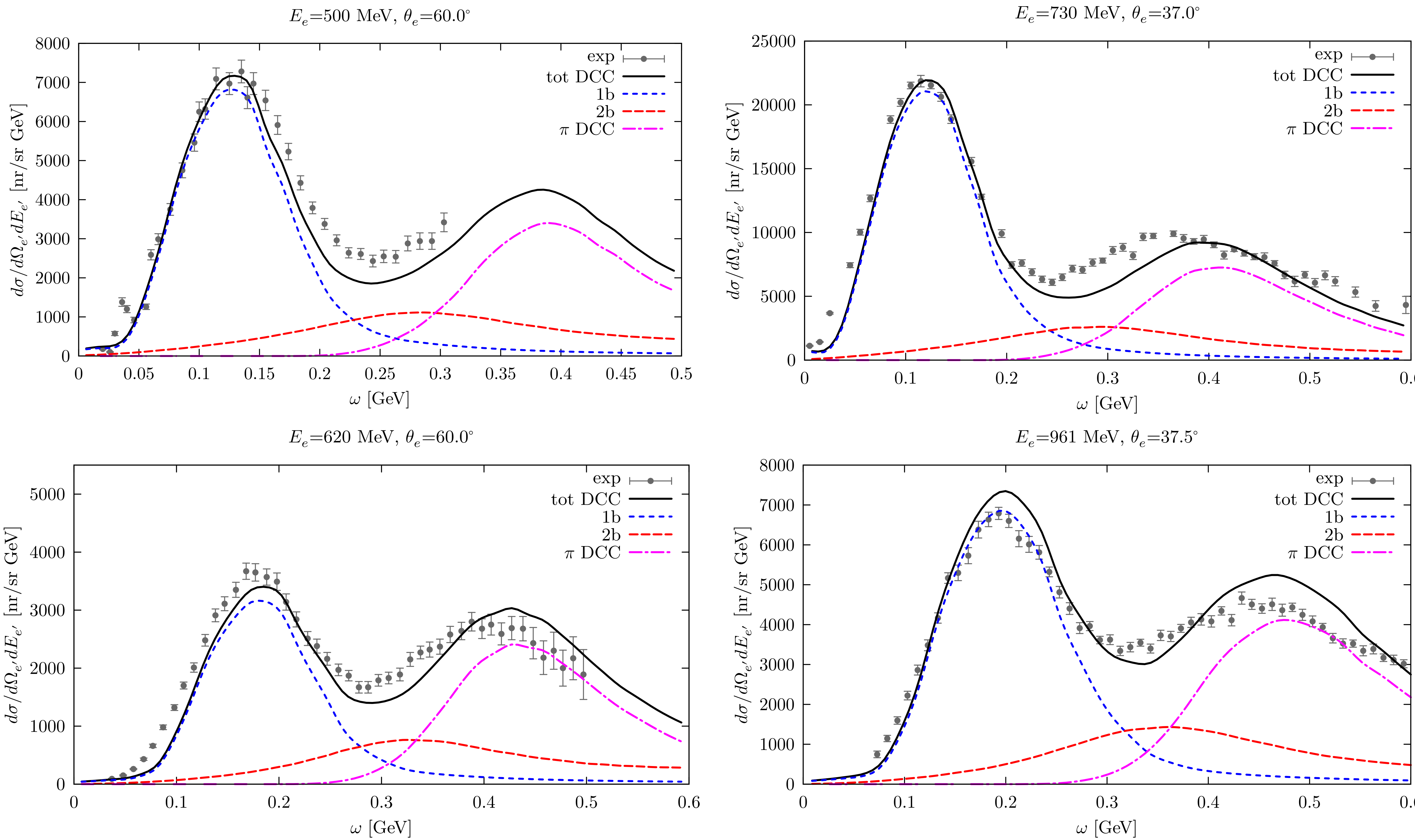


N. Rocco, et al. PRL. **116** 192501 (2016)

Inclusion of pion-production mechanisms

The factorization scheme can be further extended to include “real” pions in the final state

$$|\Psi_f^A\rangle \rightarrow |p_1 p_2\rangle \otimes |\Psi_f^{A-2}\rangle$$



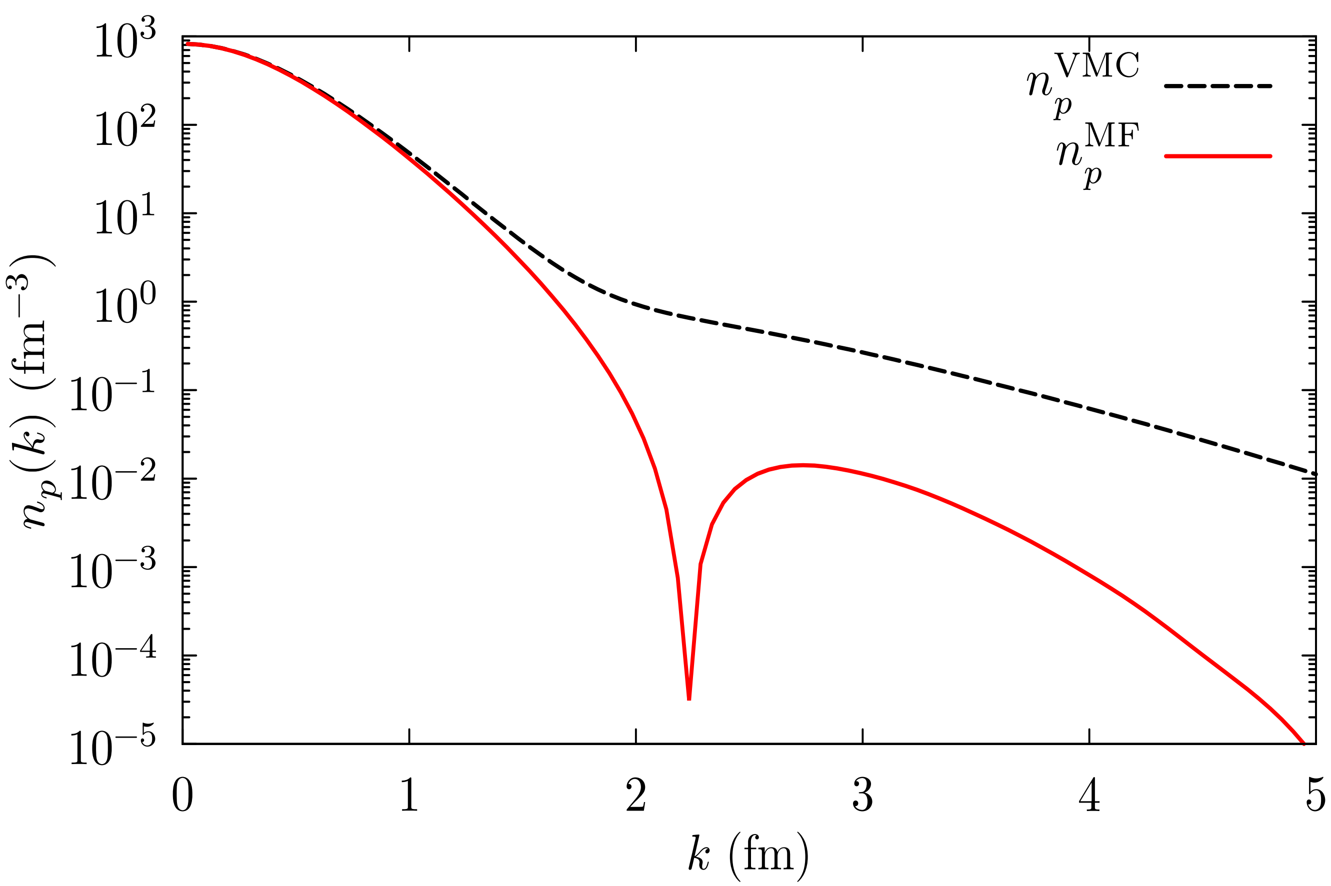
The VMC Spectral Function of ^{4}He

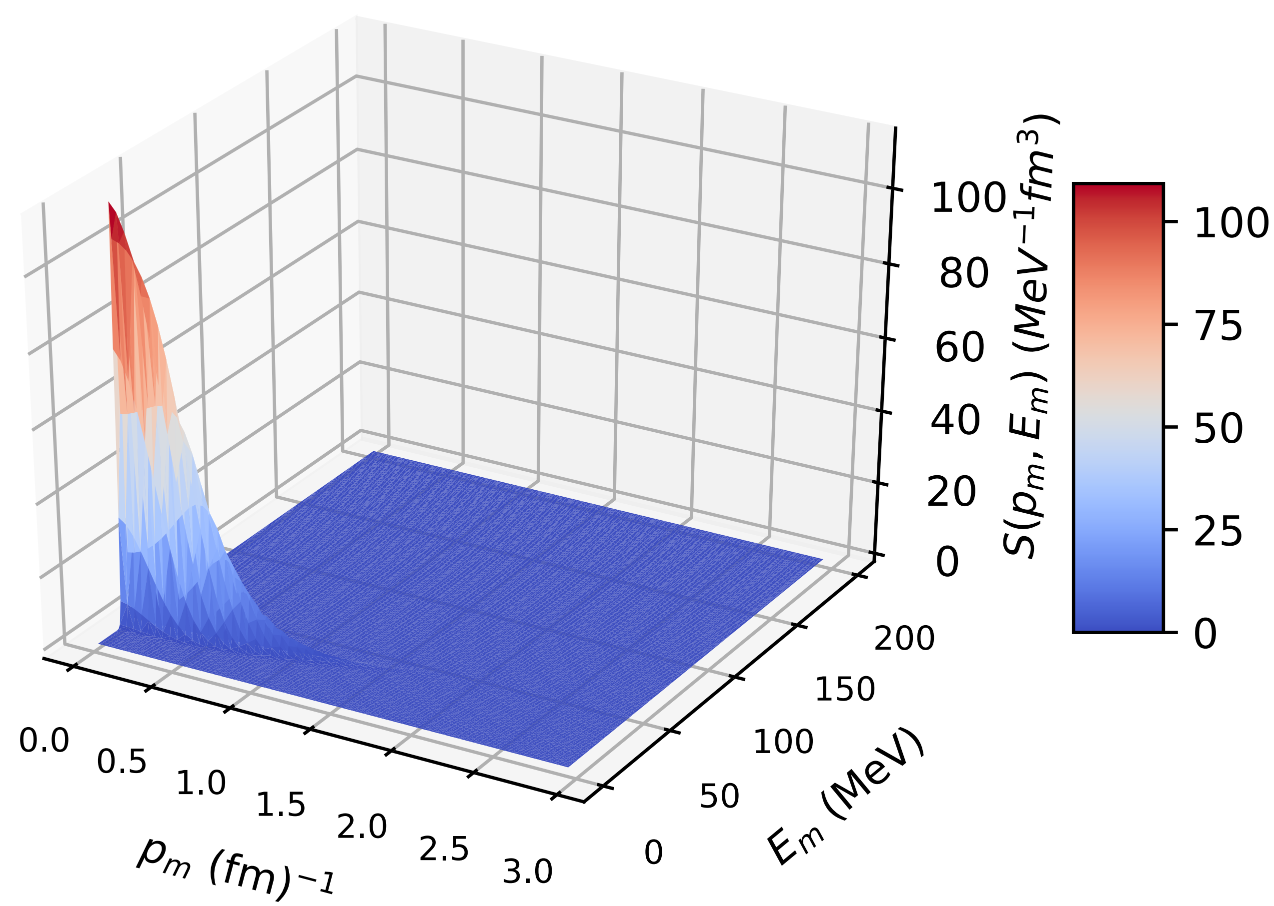
Since there are no excited states in ^{3}H, the 1h contribution is simply given by

$$P_h^{1h}(\mathbf{k},E) = \sum_{\bar f} |\langle\Psi_0^A|[|k\rangle \otimes |\Psi_{\bar f}^{A-1}\rangle]|^2 \delta(E - E_{\bar f}^{A-1} + E_0^A)$$

$$= \langle\Psi_0^{^4\mathrm{He}}|[|k\rangle \otimes |\Psi_0^{^3\mathrm{H}}\rangle]|^2 \delta\left(E - E_0^{^3\mathrm{H}} - \frac{k^2}{2M^{^3\mathrm{H}}} + E_0^{^4\mathrm{He}}\right)$$

The single-nucleon overlap can be (and have been) computed by Bob Wiringa within VMC (center of mass motion fully accounted for)



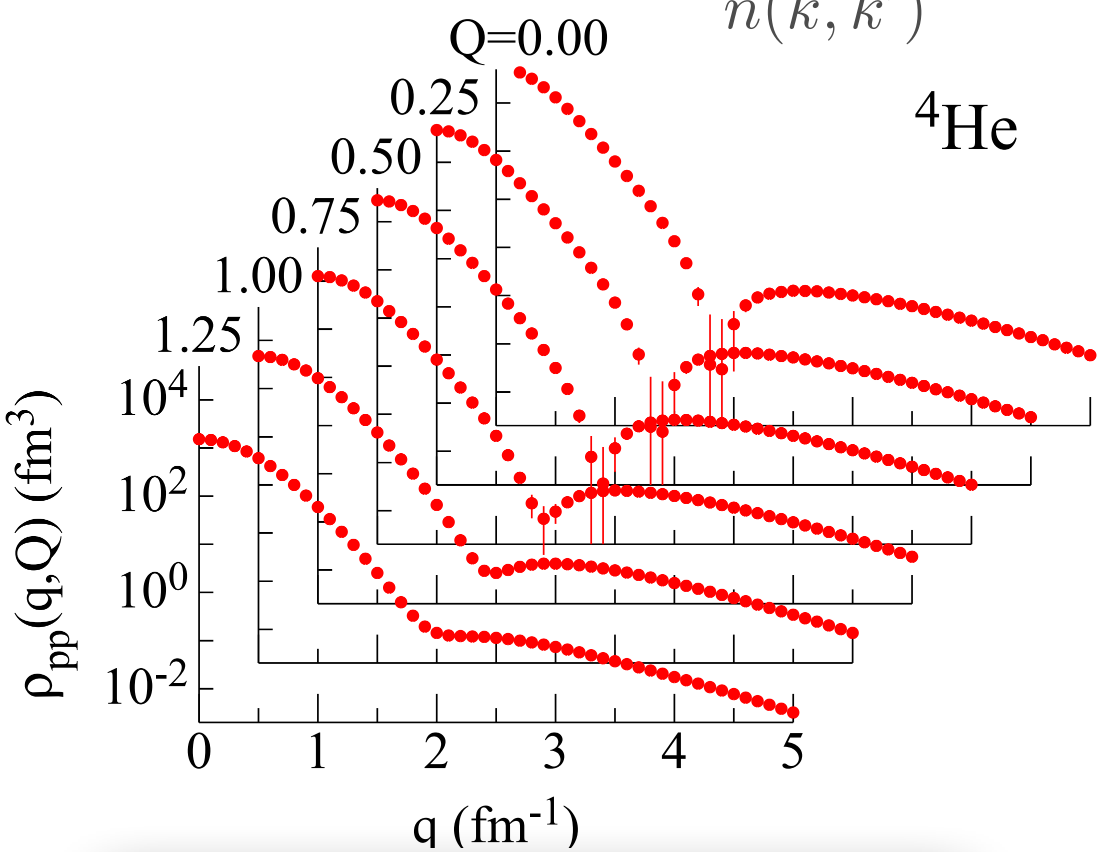


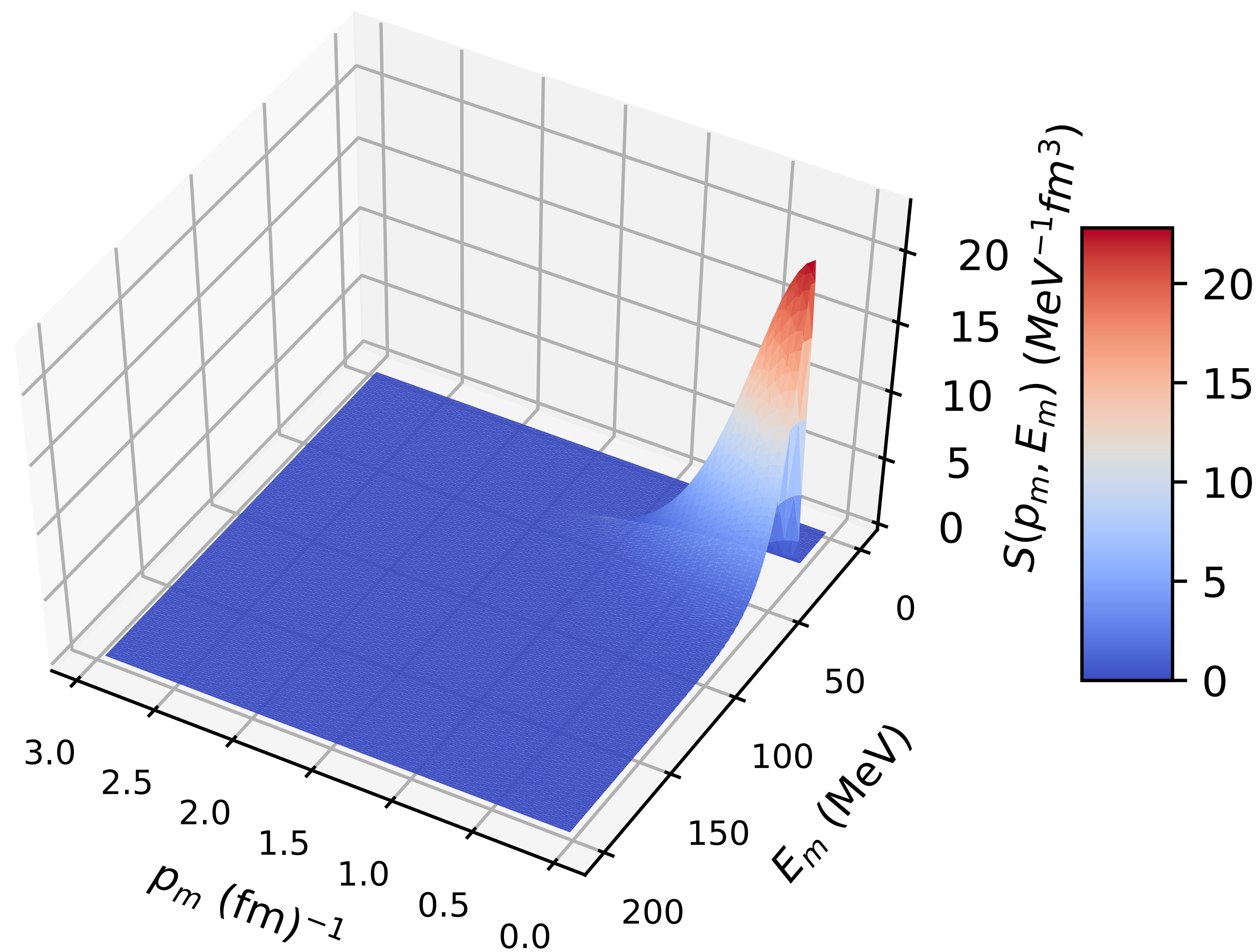
The VMC Spectral Function of ^{4}He

To determine the correlation component we utilize the two-nucleon momentum distributions computed within VMC

$$P_h^{corr}(\mathbf{k},E) \simeq \sum_f |\langle\Psi_0^A|[|kk'\rangle \otimes |\Psi_f^{A-2}\rangle]|^2 \delta\left(E - E_f^{A-2} + E_0^A - e(\mathbf{k}') - \frac{(\mathbf{k}+\mathbf{k}')^2}{2M_{^2\mathrm{H}}}\right)$$

$$\simeq \underbrace{\langle\Psi_0^A|\,|kk'\rangle\langle kk'|\,|\Psi_0^A\rangle}_{n(k,k')}\delta\left(E - \epsilon^{A-2} + E_0^A - e(\mathbf{k}') - \frac{(\mathbf{k}+\mathbf{k}')^2}{2M_{^2\mathrm{H}}}\right)$$





R.B. Wiringa, et al, PRC **89**, 024305 (2014)

The VMC Spectral Function of ^{4}He

Following the strategy outlined in

PHYSICAL REVIEW C VOLUME 47, NUMBER 5 MAY 1993

Scattering of GeV electrons by light nuclei

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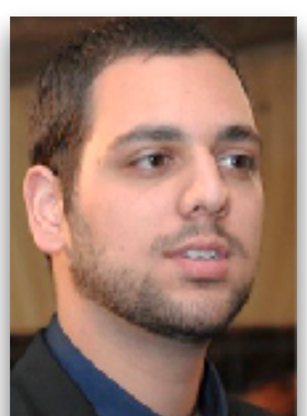
Department of Physics, University of Illinois, 1110 West Green Street, Urbana, Illinois 61801
(Received 12 November 1992)

we initially weighed the relative contributions to recover the full momentum distribution

$$P_p(\mathbf{k},E) = P_p^{\mathrm{MF}}(\mathbf{k},E) + f(\mathbf{k})P_p^{\mathrm{corr}}(\mathbf{k},E) \quad \Longleftrightarrow \quad f(\mathbf{k}) = 1 - \frac{n_p^{\mathrm{MF}}(\mathbf{k})}{n_p(\mathbf{k})}$$



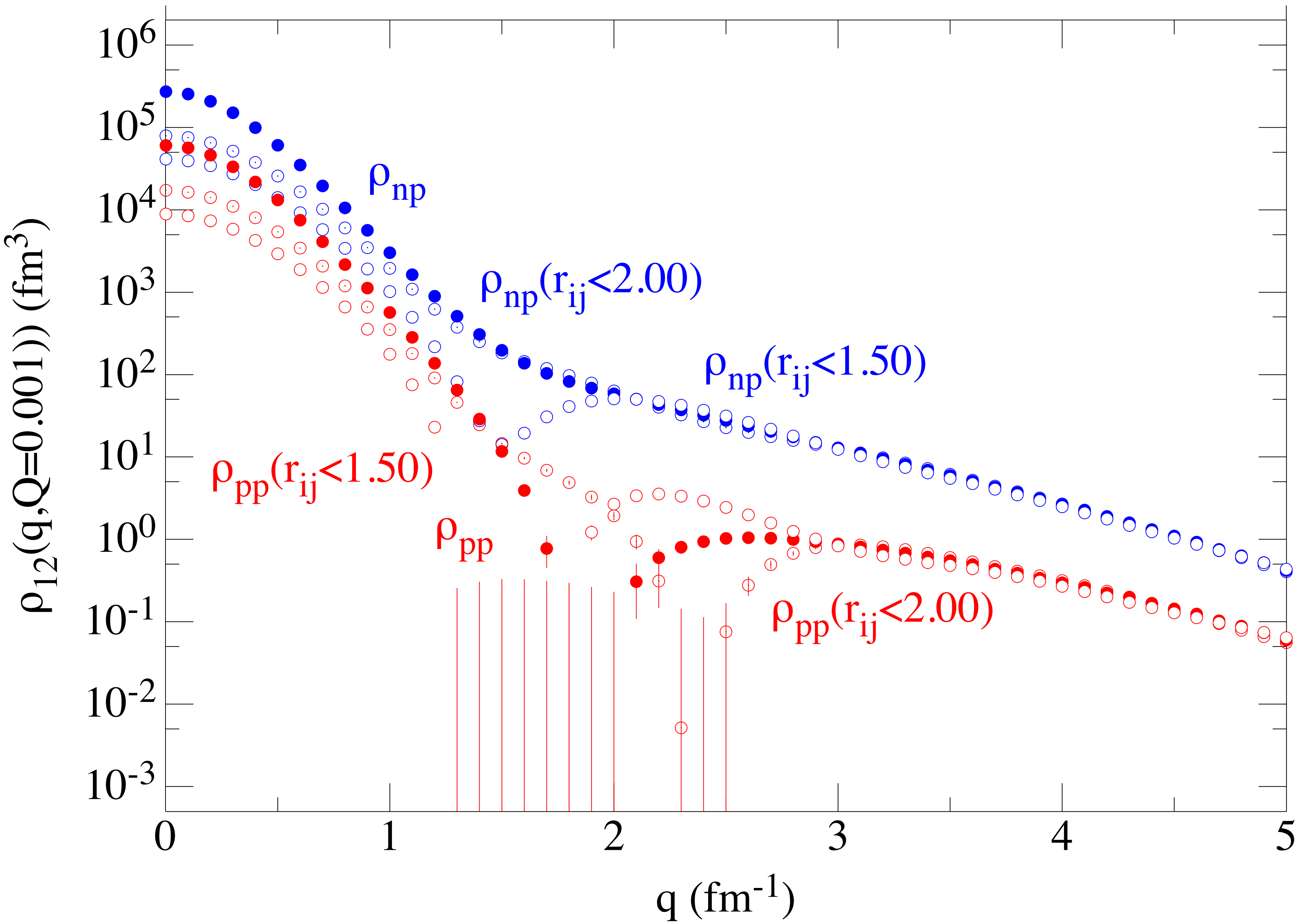
YOU ARE ALSO INCLUDING PAIRS THAT ARE **NOT** SHORT-RANGE CORRELATED!

The VMC Spectral Function of ^{4}He

Ideally, one should orthogonalize with the single-nucleon overlap

$$|k'\rangle \otimes |\Psi_f^{A-2}\rangle \rightarrow |k'\rangle \otimes |\Psi_f^{A-2}\rangle - |\Psi_{\bar{f}}^{A-1}\rangle\langle\Psi_{\bar{f}}^{A-1}|[|k'\rangle \otimes |\Psi_f^{A-2}\rangle]$$

Inspired by the contact formalism, we put a cut on the relative distance of the pair



The VMC Spectral Function of ^{4}He

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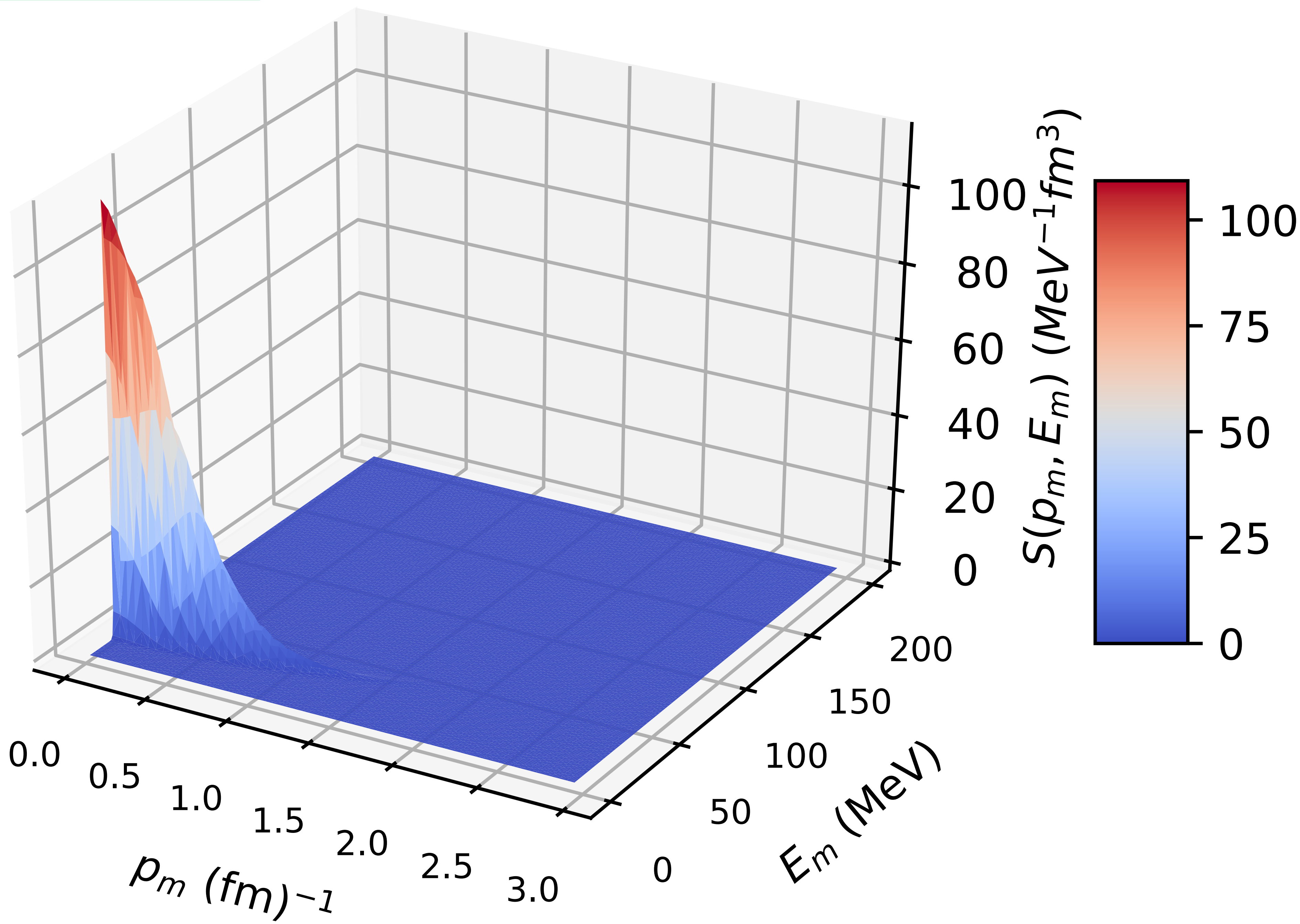

Conclusions & Plans in this direction

Conclusions

- Quantum Monte Carlo is suitable to compute cross-sections, not only responses, including relativistic effects in the kinematics
- VMC calculations of the spectral function are feasible for nuclei up to ^{12}C

Ongoing Plans

- Use the VMC hole SF of ^{4}He to compute inclusive cross sections (to begin with)
- Use Bob's overlap and two-body momentum distributions to compute the VMC hole SF of ^{12}C
- GFMC calculations of the spectral function of light nuclei using imaginary-time techniques

$$\int dE e^{-E\tau} P_h(\mathbf{k}, E) \sim \frac{\langle \Psi_0 | a^\dagger_{\mathbf{k}} e^{-(H-E_0)\tau} a_{\mathbf{k}} | \Psi_0 \rangle}{\langle \Psi_0 | e^{-(H-E_0)\tau} | \Psi_0 \rangle}$$

- Study nuclei up to ^{16}O with the AFDMC method