Making Sense of Structure/Reaction 'Non-observables'

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August, 2011

What is a 'non-observable'?

- I don't mean in-principle non-observables
 - T.D. Lee: "The root of all symmetry principles lies in the assumption that it is impossible to observe certain basic quantities; these will be called 'non-observables'."
 - E.g., you can't measure absolute position or time
- True observables are directly measurable quantities
 - E.g., cross sections and energies
 - Association with a Hermitian operator is not enough!
- I mean scale- and scheme-dependent quantities
 - E.g., spectroscopic factors depend on scheme (do ANC's?)
 - Questions to address:
 - Is there a consistent extraction from experiment such that they can be applied in other processes?
 - Can one convert between different prescriptions?
 - What is the ambiguity or convention dependence?
 - Note: Many quantities can be *in-practice* observables depending on the physics context (e.g., negligible ambiguity)

Partial list of 'non-observables' references

- Equivalent Hamiltonians in scattering theory, H. Ekstein, (1960)
- Measurability of the deuteron D state probability, J.L. Friar, (1979)
- Problems in determining nuclear bound state wave functions, R.D. Amado, (1979)
- Nucleon nucleon bremsstrahlung: An example of the impossibility of measuring off-shell amplitudes, H.W. Fearing, (1998)
- Are occupation numbers observable?, rjf and H.-W. Hammer, (2002)
- Unitary correlation in nuclear reaction theory: Separation of nuclear reactions and spectroscopic factors, A.M. Mukhamedzhanov and A.S. Kadyrov, (2010)
- Non-observability of spectroscopic factors, B.K. Jennings, (2011)
- How should one formulate, extract, and interpret 'non-observables' for nuclei?, rjf and A. Schwenk, (2010) [in J. Phys. G focus issue on Open Problems in Nuclear Structure Theory, edited by J. Dobaczewski]

From rjf and A. Schwenk essay [J. Phys. G 37 (2010)]

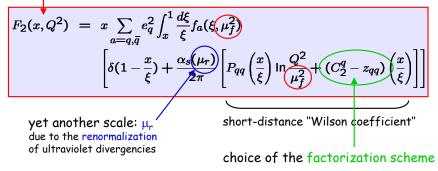
- The general structure is that a measured quantity such as a cross section is decomposed as a convolution of subsidiary pieces, usually based on a factorization principle.
- This decomposition is not unique, and so we refer here to the extracted quantities as 'non-observables'.
- The quotes are intended to soften the implication that it is improper to talk about them; nevertheless, unless the conventions (e.g., scale and scheme dependence) are controlled and specified, there will be ambiguities that will be entangled with the structure and reaction approximations.
- The challenge is to formulate and carry out experimental extractions and theoretical calculations of non-observables systematically and consistently.

Parton distributions as paradigm [Marco Stratman]

Deep-inelastic scattering (DIS) according to pQCD

the physical structure fct. is independent of μ_f (this will lead to the concept of renormalization group eqs.)

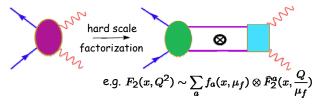
both, pdf's and the short-dist. coefficient depend on μ_f (choice of μ_f : shifting terms between long- and short-distance parts)



Parton distributions as paradigm [Marco Stratman]

Factorization schemes

pictorial representation of factorization:



the separation between long- and short-distance physics is not unique



- 1. choice of μ_f : defines borderline between long-/short-distance
- 2. choice of scheme: re-shuffling finite pieces

July, 25-28 2005

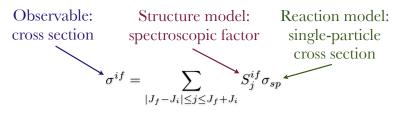
PHENIX Spin Fest @ RIKEN Wako

Parton distributions as paradigm: Lessons

- The momentum distribution for a given hadron is not unique
 - With parton distributions one would not talk about the results at a particular *Q*² as being "the" quark or gluon momentum distribution as opposed to distributions for lower or higher *Q*².
 - Dependence on *Q*², which serves as the resolution scale and can be changed by renormalization group (RG) evolution, and the PDF analysis at NLO must be performed in a specific renormalization and factorization scheme (e.g., MS or DIS)
 - Controlled factorization allows PDF's from one process to be used in other processes (and at other scales)!
 - For consistency, hard-scattering cross section calculations used for the input processes or that use the extracted PDFs have to be implemented with the same scheme
 - There is careful treatment of the uncertainties in the PDFs; not considered sufficient to just compare different extractions. Instead, Lagrange Multiplier and Hessian techniques have been developed to estimate PDF uncertainties.
- Can we formulate our stucture/reaction theory to have the same control as with PDFs using factorization?

What are the low-energy nuclear physics analogs?

• E.g., from D. Bazin ECT* talk, 5/2011



- Questions:
 - How general/robust is this factorization?
 - What does it mean to be *consistent* between structure and reaction models?
 - How does scheme dependence come in?
 - What are the trade-offs? (E.g., does simpler structure mean more complicated reaction?)

The source of convention or scheme dependence

- General form: cross section as convolution
 - but individual parts are not unique
- Short-range unitary transformation U leaves m.e.'s invariant:

$$O_{mn} \equiv \langle \Psi_m | O | \Psi_n \rangle = \left(\langle \Psi_m | U^{\dagger} \right) UOU^{\dagger} \left(U | \Psi_n \rangle \right) = \langle \widetilde{\Psi}_m | \widetilde{O} | \widetilde{\Psi}_n \rangle$$

But the matrix elements of *O* itself between the transformed states are in general modified:

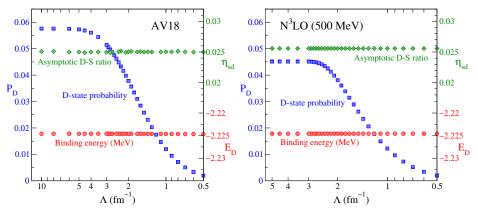
$$\widetilde{O}_{mn} \equiv \langle \widetilde{\Psi}_m | O | \widetilde{\Psi}_n \rangle \neq O_{mn} \implies \text{e.g., } \langle \Psi_n^{A-1} | a(\mathbf{r}) | \Psi_0^A \rangle \text{ changes}$$

- Field theory version: the equivalence principle says that only on-shell quantities can be measured. Field redefinitions change off-shell dependence only.
- Claim: In a low-energy effective theory, there is no preferred set of states (or preferred Hamiltonian) so transformations that modify *short-range* unresolved physics generate equally acceptable states. So $\widetilde{O}_{mn} \neq O_{mn} \Longrightarrow$ ambiguous.

Quantities that vary with convention or scheme

- deuteron D-state probability [e.g., Friar, PRC 20 (1979)]
- off-shell effects (e.g., from NN bremsstrahlung) [Fearing/Scherer, PRC 62 (2000)]
- occupation numbers [Hammer/rjf, PLB 531 (2002)]
- spectroscopic factors [Mukhamedzhanov/Kadyrov, PRC 82 (2010)]
- proton radius (cf. charge radius) [Polyzou, PRC 58 (1998)]
- short-range part of wave functions (SRC's)
- wound integrals
- short-range potentials; e.g., contribution of short-range 3-body forces
- and so on ...

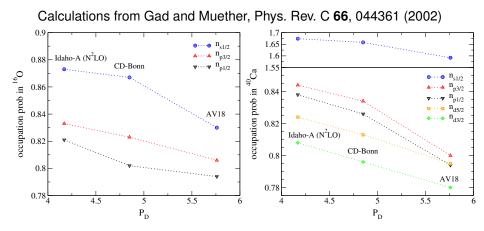
Deuteron true and scheme-dependent observables



• Unitary transformations labeled by Λ ($V_{\text{low }k}$ here)

- \implies soften interactions by lowering resolution (how far?)
- \implies reduced short-range and tensor correlations
- D-state probability changes (cf. spectroscopic factors)
- Asymptotic D-S ratio is unchanged (cf. ANC's)

Correlation of *P*_D **with spectroscopic factors**



- Increased occupation probability with increased non-locality and correlated reduction in short-range tensor strength
- Is the correlation quantitatively predictable?

Cutoff dependence in coupled cluster calculations

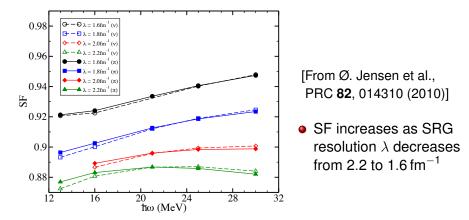
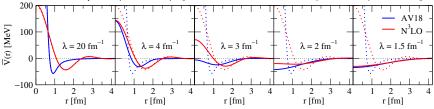


FIG. 4: (Color online) Spectroscopic factor SF(1/2⁻) for neutron and proton removal as a function of the oscillator spacing $\hbar\omega$ for nucleon-nucleon interactions with different cutoffs in a model space with N = 6.

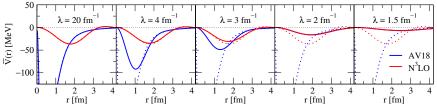
Wave functions are more single-particle-like as Λ/λ decreases, but do reaction operators become significantly less one-body?

Changing the scheme: (short-range) NN potential

- V_{low k} or SRG unitary transformations to soften interactions
- Project non-local NN potential: $\overline{V}_{\lambda}(r) = \int d^3r' V_{\lambda}(r, r')$
 - Roughly gives action of potential on long-wavelength nucleons
- Central part (S-wave) [Note: The V_{λ} 's are all phase equivalent!]

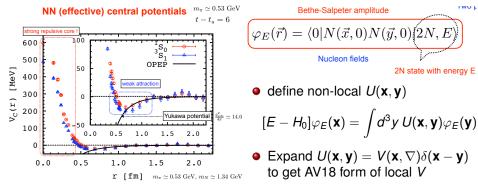


• Tensor part (S-D mixing) [graphs from K. Wendt]



Determining the nuclear potential from lattice QCD

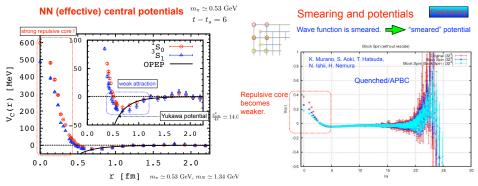
[S. Aoki, Hadron interactions in lattice QCD, arXiv:1107.1284]



- Why not just calculate energy as function of separation $\implies V(r)$?
 - Only works in heavy mass limit (e.g., works for B-mesons)
- But is this unique? No!
 - choice of nucleon interpolating field \Longrightarrow different $V(\mathbf{x})$
 - choice of "wave function" smearing (changes overlap)

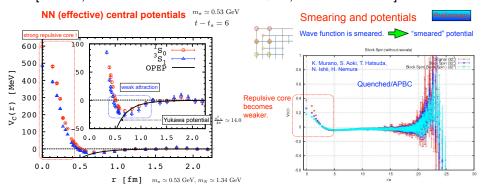
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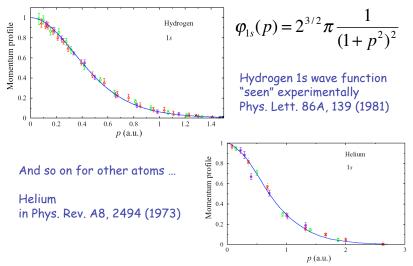
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Determining the nuclear potential from lattice QCD [S. Aoki, *Hadron interactions in lattice QCD*, arXiv:1107.1284]



- "... the potential depends on the choice of nucleon operator..." which "... is considered to be a 'scheme' to define the potential."
- "Is such a scheme-dependent quantity useful? The answer to this question is probably 'yes', since the potential is useful to understand or describe the phenomena."
- Claim: useful to choose a scheme that yields good convergence of the velocity expansion (close to local)

Are wave functions measurable? [from W. Dickhoff] Atoms studied with the (e,2e) reaction



But compare approximations for (*e*, 2*e*) on atoms to those for (*e*, *e'p*) on nuclei! (Impulse approx., FSI, vertex, ...)

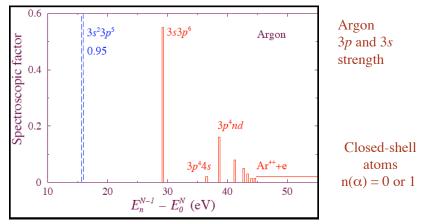
Spectroscopic factors in atoms

For a bound final N-1 state the spectroscopic factor is given by S =

$$S = \int d\vec{p} \left| \left\langle \Psi_n^{N-1} \left| a_{\vec{p}} \right| \Psi_0^N \right\rangle \right|$$

For H and He the 1s electron spectroscopic factor is 1 For Ne the valence 2p electron has S=0.92 with two additional fragments, each carrying 0.04 at higher energy

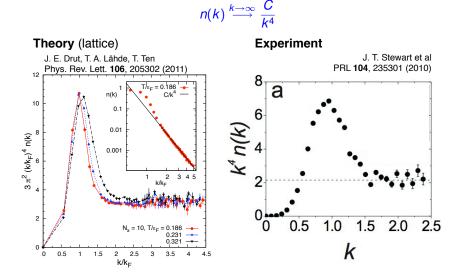
each carrying 0.04, at higher energy.



One-body scattering, small scheme dependence \implies robust SF

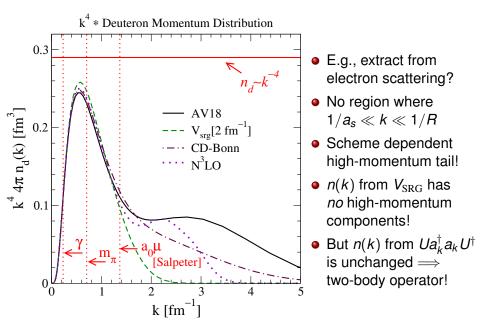
Unitary cold atoms: Is *n*(*k*) observable?

• Tail of momentum distribution + contact [Tan; Braaten/Platter]



• When $R/a_s \ll kR \ll 1 \implies$ tiny scheme dependence

Is the tail of n(k) for nuclei measurable? (cf. SRC's)



Using EFT and field redefinitions as tool

• EFT:
$$\mathcal{L}_{\text{eft}} = \psi^{\dagger} \left[i \frac{\partial}{\partial t} + \frac{\nabla^2}{2M} \right] \psi - \frac{C_0}{2} (\psi^{\dagger} \psi)^2 - \frac{D_0}{6} (\psi^{\dagger} \psi)^3 + \dots$$

- general short-range interactions, but not unique!
- Try simple field redefinition to check scheme dependence:

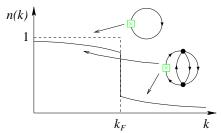
$$\psi \longrightarrow \psi + \alpha \frac{4\pi}{\Lambda^3} (\psi^{\dagger} \psi) \psi \qquad \alpha \sim \mathcal{O}(1) \Longrightarrow \text{``natural''} \Longrightarrow \text{estimate!}$$

- "new" vertices: 2–body off-shell \triangle , 3–body o $\propto \frac{8\pi\alpha}{\Lambda^3} C_0(\psi^{\dagger}\psi)^3$
- asymptotic "on-shell" quantities (S-matrix elements) must be unchanged by redefinition
- Energy density is model (α) independent *if* all terms kept
 - sum of new terms is zero, so energy is unchanged

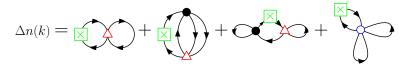
• What about momentum occupation number?

Occupation No. \Longrightarrow **Momentum Distribution**

• Insert $a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} \Longrightarrow \boxtimes$



• But nonzero contribution $\Delta n(k)$ from induced vertices:

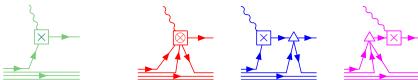


- There is no preferred definition for transformed operator
 - \implies only defined for specific convention
 - \implies momentum distributions for different schemes differ

Analysis of (e,e'p) Experiments? [cf. (e,2e) on atoms]

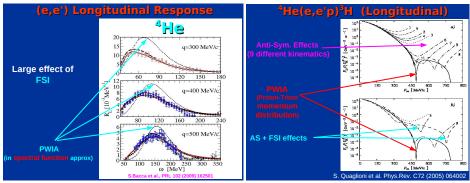
- Suppose external source *J*(*x*) coupled to fermions
 - EFT: need most general current coupled to J(x) for all α
- Consider lowest order with simplest ($\alpha = 0$) current

• if $\alpha = 0$, just impulse approximation $J\psi^{\dagger}\psi$



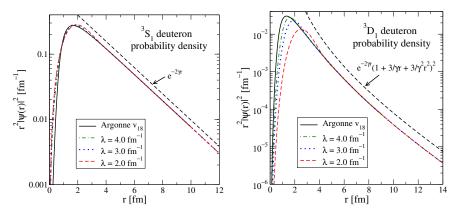
- if α ≠ 0 [recall ψ → ψ + α^{4π}/_{Λ³}(ψ[†]ψ)ψ], then same cross section *only* if vertex contribution from modified operator *and* modified final (and initial) state interactions are included
- There are *always* contributions from all three at each order
 - sub-leading pieces are mixed by field redefinitions \implies isolating $J\psi^{\dagger}\psi$ is model dependent
 - How large is ambiguity? Set by natural size $\alpha \sim \mathcal{O}(1)$

Ab initio electron scattering with LIT [from G. Orlandini]



- Ab initio calculations of longitudinal (*e*, *e'*) response functions show importance of FSI for quasi-elastic regime
 - $\bullet\,$ PWIA fails for quasi-elastic peak and at low ω
 - FSI effects decrease with q in peak but not at low ω
- Direct proton knockout and neglect of FSI tested for (*e*, *e*'*p*)
 - Both antisymmetrization effects and FSI play important roles
 - Approximate estimates of FSI effects can be poor

Why are ANC's different? Coordinate space



- ANC's, like phase shifts, are asymptotic properties \implies short-range unitary transformations do not alter them [e.g., see Mukhamedzhanov/Kadyrov, PRC 82 (2010)]
- In contrast, SF's rely on interior wave function overlap
- (Note difference in S-wave and D-wave ambiguities)

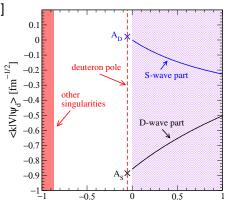
Why are ANC's different?

[based on R.D. Amado, PRC 19 (1979)]

$$\begin{array}{l} \mathbf{\hat{k}}^{2} \langle \mathbf{k} | \psi_{n} \rangle + \langle \mathbf{k} | \mathbf{V} | \psi_{n} \rangle = -\frac{\gamma_{n}^{2}}{2\mu} \langle \mathbf{k} | \psi_{n} \rangle \\ \Longrightarrow \langle \mathbf{k} | \psi_{n} \rangle = -\frac{2\mu \langle \mathbf{k} | \mathbf{V} | \psi_{n} \rangle}{k^{2} + \gamma_{n}^{2}} \\ \mathbf{\hat{k}} \langle \mathbf{r} | \psi_{n} \rangle = \int \frac{d^{3}k}{(2\pi)^{3}} e^{i\mathbf{k}\cdot\mathbf{r}} \langle \mathbf{k} | \psi_{n} \rangle \\ & \stackrel{|\mathbf{r}| \to \infty}{\longrightarrow} A_{n} e^{-\gamma_{n}r} / r \end{array}$$

integral dominated by pole from 1.

) extrapolate $\langle {f k} | {m V} | \psi_n
angle$ to $k^2 = -\gamma_n^2$



 k^{2} [fm⁻²]

- Or, residue from extrapolating on-shell T-matrix to deuteron pole
 invariant under unitary transformations
- Inverse scattering puzzle: A_n uniquely determined because assumed longest-range part of V from one-pion exchange

• Next vertex singularity at $-(\gamma + m_{\pi})^2 \Longrightarrow$ same for FSI

Momentum space

More questions and some possible answers

How should one choose a scheme/convention?

- To make calculations easier or more convergent
 - QCD running coupling and scale: improved perturbation theory; choosing a gauge: e.g., Coulomb or Lorentz
 - (Near-) local potential: quantum Monte Carlo methods work
 - Low-*k* potential: many-body perturbation theory works, or to make microscopic connection to shell model
- Better interpretation or intuition \Longrightarrow predictability
- Use range of schemes to test calculations and learn physics

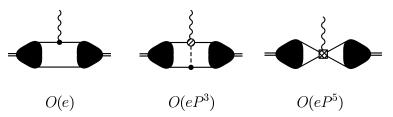
Can we (should we) use a reference Hamiltonian?

- That is, to allow us to make comparisons
- If so, which one? (cleanest extraction from experiment?)

More questions and some possible answers

How do we match Hamiltonians and operators?

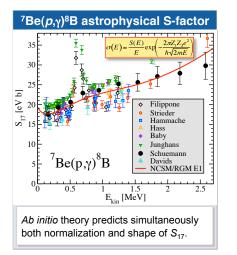
- Use EFT perspective
 - E.g., electromagnetic currents [D.R. Phillips, nucl-th/0503044]



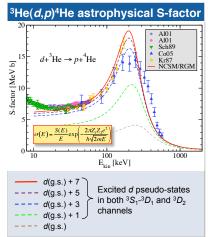
- Model independent because complete (up to some order)
- Can identify consistent operator and interaction
- Tells you when new info is required
- Use RG as tool to evolve consistent operators

Can EFT or RG help to construct optical potentials?

Is it ok to fine-tune SRG λ ? [e.g. Navratil, Quaglioni, Roth]



- arXiv:1105.5977
- SRG $\lambda = 1.86 \, \text{fm}^{-1}$
- match separation energy



- arXiv:1009.3965
- SRG $\lambda = 1.5 \, \text{fm}^{-1}$
- low $\lambda \Longrightarrow$ more convergent

What about long-range correlations?

- SF calculations with FRPA
- N³LO Hamiltonian
 - Soft ⇒ small SRC
 - SRC contribution changes dramatically with lower resolution
- Compare short-range correlations (SRC) to long-range correlations from particle-vibration coupling
- LRC \gg SRC!!
- Are long-range correlations scheme dependent?

C. Barbieri, PRL 103 (2009)

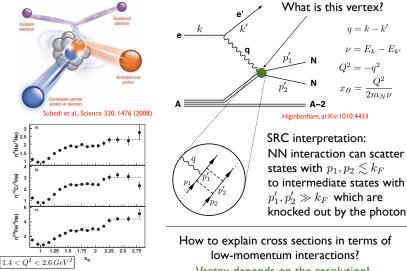
TABLE I. Spectroscopic factors (given as a fraction of the IPM) for valence orbits around ⁵⁶Ni. For the SC FRPA calculation in the large harmonic oscillators space, the values shown are obtained by including only SRC, SRC and LRC from particle-vibration couplings (full FRPA), and by SRC, particle-vibration couplings and extra correlations due to configuration mixing (FRPA + ΔZ_o). The last three columns give the results of SC FRPA and SM in the restricted 1*p0f* model space. The $\Delta Z_o s$ are the differences between the last two results and are taken as corrections for the SM correlations that are not already included in the FRPA formalism.

	10 osc. shells			Exp. [29]	1p0f space		
	FRPA (SRC)	Full FRPA	FRPA + ΔZ_{α}		FRPA	SM	ΔZ_{α}
⁵⁷ Ni:							
$\nu 1 p_{1/2}$	0.96	0.63	0.61		0.79	0.77	-0.02
$\nu 0 f_{5/2}$	0.95	0.59	0.55		0.79	0.75	-0.04
$\nu 1 p_{3/2}$	0.95	0.65	0.62	0.58(11)	0.82	0.79	-0.03
⁵⁵ Ni:							
$\nu 0 f_{7/2}$	0.95	0.72	0.69		0.89	0.86	-0.03
57Cu:							
$\pi 1 p_{1/2}$	0.96	0.66	0.62		0.80	0.76	-0.04
$\pi 0 f_{5/2}$	0.96	0.60	0.58		0.80	0.78	-0.02
$\pi 1 p_{3/2}$	0.96	0.67	0.65		0.81	0.79	-0.02
55Co:							
$\pi 0 f_{7/2}$	0.95	0.73	0.71		0.89	0.87	-0.02

Parton distributions as paradigm: Factorization

- PDF analysis: part of convolution for cross section can be calculated reliably for given experimental conditions so that the remaining part can be extracted as a universal quantity, to be related to other processes and kinematic conditions
- For hard-scattering processes with large momentum transfer scale *Q*, *factorization* allows separation of momentum and distance scales in reaction
 - The time scale for binding interactions in the rest frame is time dilated in the center-of-mass frame, so the interaction of an electron with a hadron in deep-inelastic scattering is with single non-interacting partons
 - Short-distance part calculated systematically in low-order perturbative QCD; long-distance part identified in PDF's (momentum distribution for partons in hadrons)
- PDF's relate deep inelastic scattering of leptons, Drell-Yan, jet production, and more
 - Measure in limited set of reactions and then perturbative calculations of hard scattering and PDF evolution enable first principles predictions of cross sections for other processes

Case study: Large Q² electron scattering



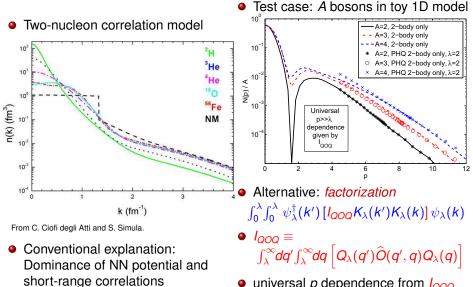
Egiyan et al. PRL 96, 1082501 (2006)

Vertex depends on the resolution!

• K. Hebeler/E. Anderson \implies evolve *operators* to low resolution

Nuclear scaling: $n_A(p) \approx C_A n_D(p)$ at large p

(Frankfurt et al.)



- universal p dependence from Iooo
- C_A factor from low-momentum m.e.

Factorization with SRG [Anderson et al., arXiv:1008.1569]

- If $k < \lambda$ and $q \gg \lambda \Longrightarrow$ factorization: $U_{\lambda}(k,q) \to K_{\lambda}(k)Q_{\lambda}(q)$
- Operator product expansion for nonrelativistic wf's (see Lepage)

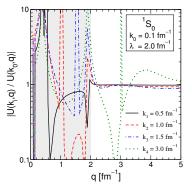
$$\Psi^{\infty}_{\alpha}(\boldsymbol{q}) \approx \gamma^{\lambda}(\boldsymbol{q}) \int_{0}^{\lambda} p^{2} d\boldsymbol{p} \ \boldsymbol{Z}(\lambda) \Psi^{\lambda}_{\alpha}(\boldsymbol{p}) + \eta^{\lambda}(\boldsymbol{q}) \int_{0}^{\lambda} p^{2} d\boldsymbol{p} \ \boldsymbol{p}^{2} \ \boldsymbol{Z}(\lambda) \Psi^{\lambda}_{\alpha}(\boldsymbol{p}) + \cdots$$

• Construct unitary transformation to get $U_{\lambda}(k, q) \approx K_{\lambda}(k)Q_{\lambda}(q)$ $U_{\lambda}(k, q) = \sum_{\alpha} \langle k | \psi_{\alpha}^{\lambda} \rangle \langle \psi_{\alpha}^{\infty} | q \rangle \rightarrow \Big[\sum_{\alpha}^{\alpha_{low}} \langle k | \psi_{\alpha}^{\lambda} \rangle \int_{0}^{\lambda} p^{2} dp \ Z(\lambda) \Psi_{\alpha}^{\lambda}(p) \Big] \gamma^{\lambda}(q) + \cdots$

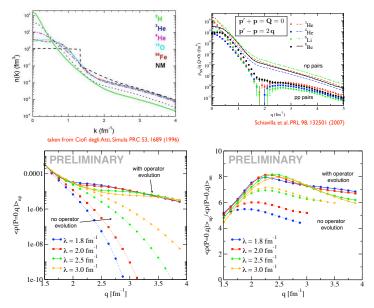
Test of factorization of U:

 $\frac{U_{\lambda}(k_{i}, q)}{U_{\lambda}(k_{0}, q)} \rightarrow \frac{K_{\lambda}(k_{i})Q_{\lambda}(q)}{K_{\lambda}(k_{0})Q_{\lambda}(q)},$ so for $q \gg \lambda \Rightarrow \frac{K_{\lambda}(k_{i})}{K_{\lambda}(k_{0})} \xrightarrow{\text{LO}} 1$

• Look for plateaus: $k_i \leq 2 \text{ fm}^{-1} \leq q$

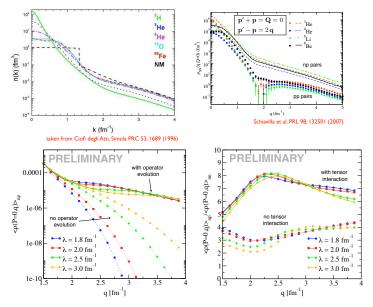


Simpler calculations of pair densities



Many-body perturbation theory may be sufficient at low resolution!

Simpler calculations of pair densities



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Recap

- Summary points
 - Scheme-dependent observables are robust for some systems, but not generally for nuclei! Must specify it! (e.g., V_{NN···N}, Ô's)
 - SF's are scheme-dependent, ANC's are (generally) not
 - surface-integral formulation sounds promising!
 - Unitary transformations show natural scheme dependence
 - Parton distribution functions as a paradigm
 - \implies Can we have controlled factorization?
- Questions for which EFT/RG may help
 - How should one choose a scheme/convention?
 - Can we (should we) use a reference Hamiltonian?
 - What is the scheme-dependence of SF's and other quantities?
 - Is the assumption of one-body operators viable? Required?
 - How do we match Hamiltonians and operators?
 - What can EFT or RG say about N-nucleus optical potentials?
 - What is the role of short-range/long-range correlations?
 - ...and many more!