How low-momentum interactions can constrain the nuclear density functional

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Nuclear structure near the limits, INT, Oct. 3, 2005

Collaborators: Scott Bogner, Dick Furnstahl, Andreas Nogga, Gerry Brown, Tom Kuo and Andres Zuker

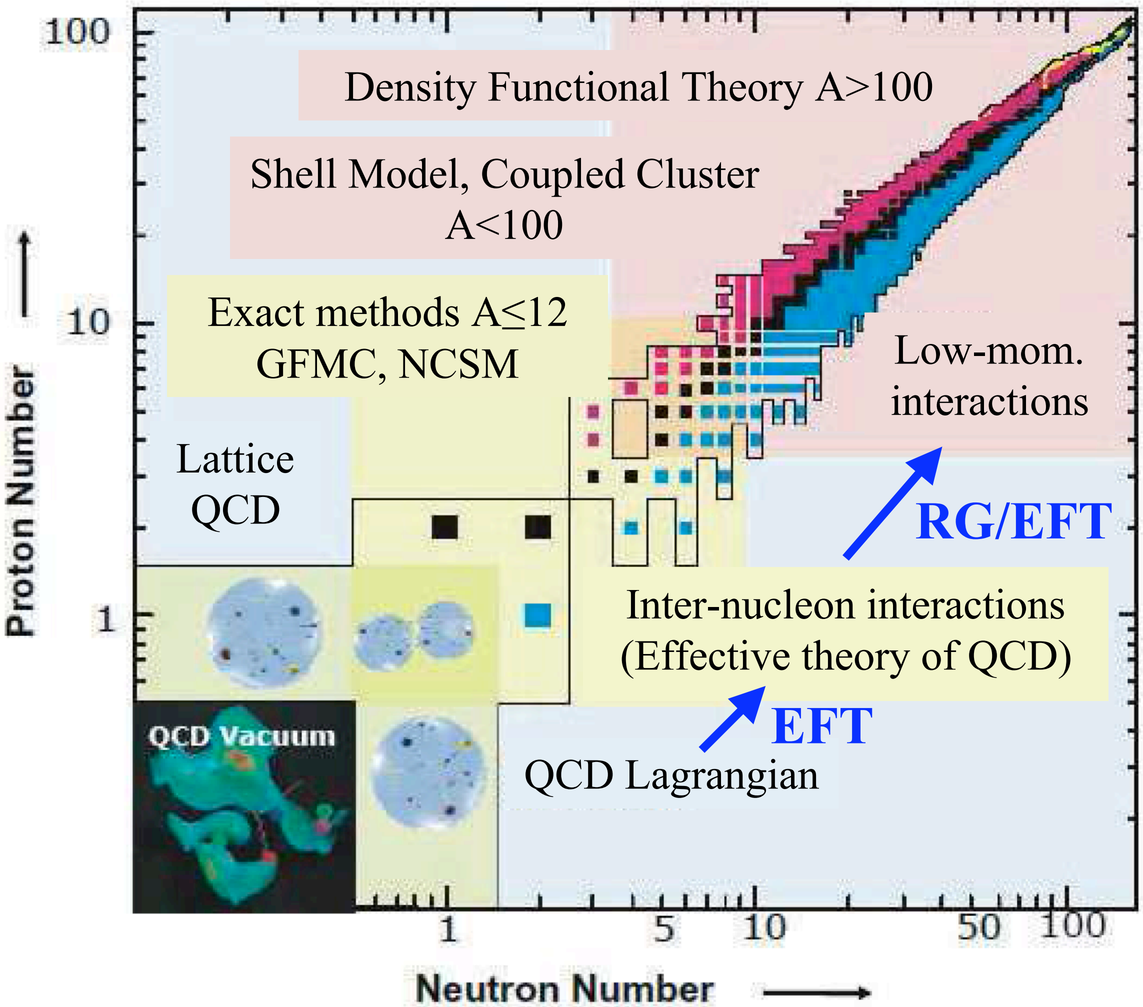
Supported by DOE

Outline

1) Motivation - Progress in nuclear interactions, exact many-body methods, constructing density functionals
2) RG applied to nuclear interactions
3) Results for nuclei and nuclear matter
4) Strategies for density-functional calculations from nuclear interactions
5) Summary

1) Motivation

Simple density functionals work: $\Delta E_{rms} \sim 1$ MeV, excitations,…
But extensions need guidance (many new parameters in general ∇^2 DF)



adapted from A. Richter @ INPC2004

Advances in nuclear interactions relevant to heavy nuclei

Constraints for DF from microscopic interactions?

Immense progress in many-body methods
nuclei accessible with CC overlap with DFT

Microscopic foundation of density functional theory

For ground state densities couple source $K_{\sigma,\sigma'}(x)$ to density $\psi^\dagger_\sigma(x)\,\psi_{\sigma'}(x)$

see e.g., talks by Negele and Furnstahl

$$e^{W[K]} = \int \mathcal{D}[\psi^\dagger]\mathcal{D}[\psi]\; e^{-S[\psi^\dagger,\psi]+\sum_{\sigma,\sigma'}\int dx\,\psi^\dagger_\sigma(x)\psi_{\sigma'}(x)\,K_{\sigma,\sigma'}(x)}$$

S contains nuclear forces (e.g., $V_{\text{low }k} + V_{3N}$)

Path integral leads to generating functional $W[K]$

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Densities given by (with K=0 in the ground state)

$$\rho_{\sigma,\sigma'}(x) \equiv \langle \psi^\dagger_\sigma(x)\,\psi_{\sigma'}(x)\rangle = \frac{\delta W[K]}{\delta K_{\sigma,\sigma'}(x)}$$ and by inversion $K[\rho]$

Construct effective action $\Gamma[\rho] = -W[K] + K\cdot\rho$ by Legendre trafo.

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Effective action is minimal at the physical (K=0) ground state density

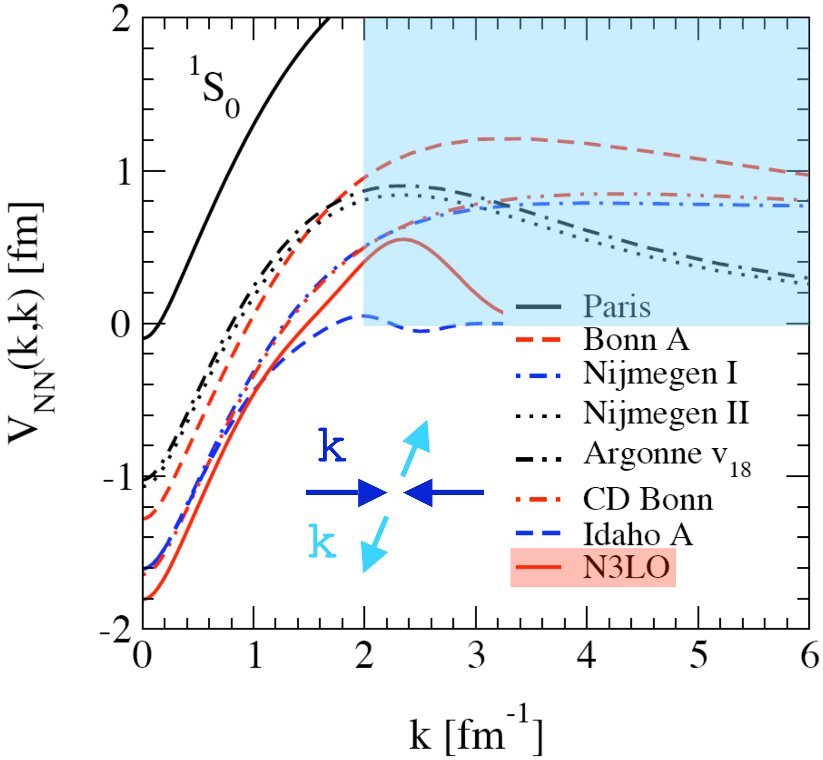
$$\left.\frac{\delta\Gamma[\rho]}{\delta\rho}\right|_{\rho=\rho_{\text{gs}}} = 0$$ with gs energy $E_{\text{gs}} = E[\rho_{\text{gs}}] = \lim_{\beta\to\infty}\frac{1}{\beta}\,\Gamma[\rho_{\text{gs}}]$

DF = effective action, degrees-of-freedom are one-body densities

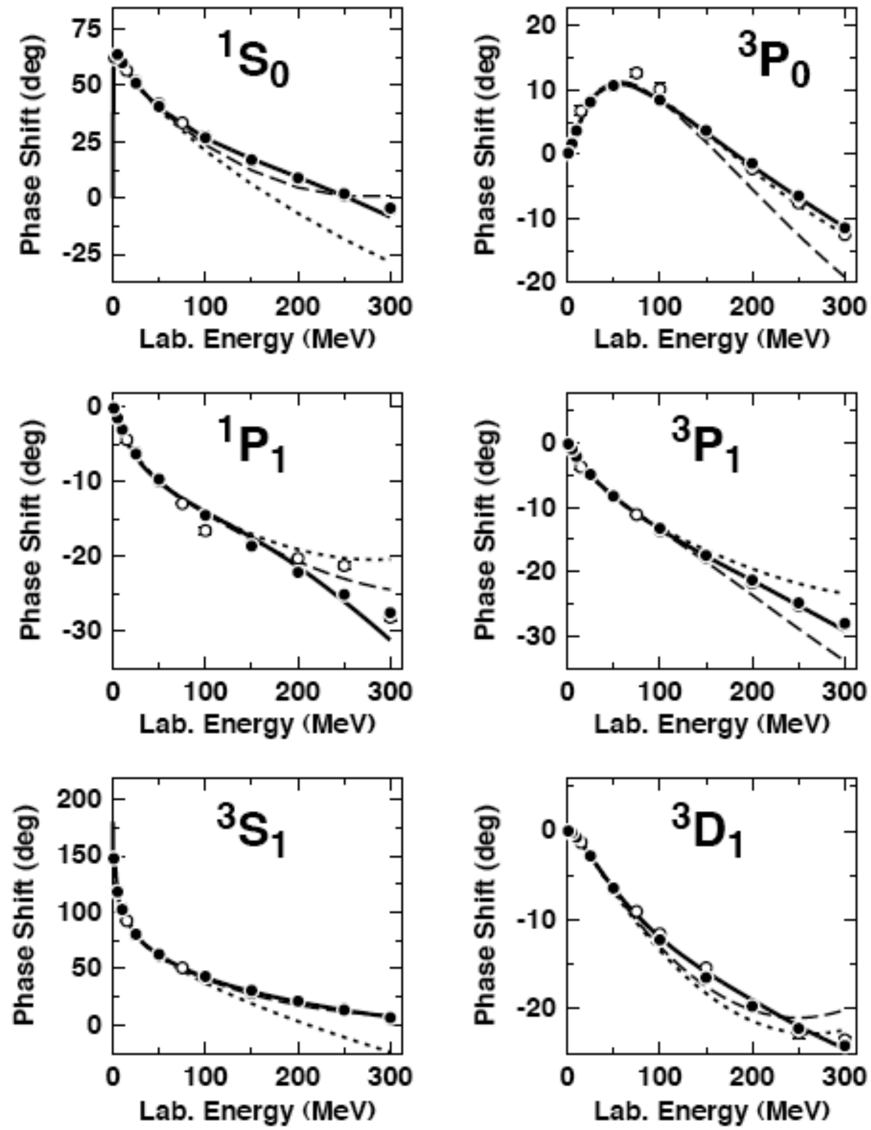
microscopic DF for dilute systems beyond LDA, Furnstahl, discussion by Engel

NN interactions well-constrained by NN scattering

Many different NN potentials fit to data below $E_{\mathrm{lab}} \lesssim 350\,\mathrm{MeV}$ (corresponding relative k < 2.1 fm^{-1})



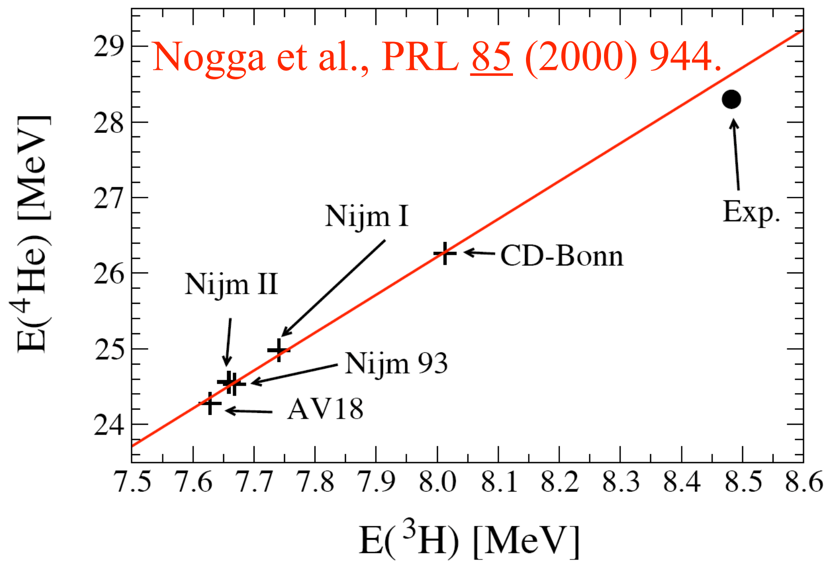
Details not constrained for momenta k > 2.1 fm^{-1}



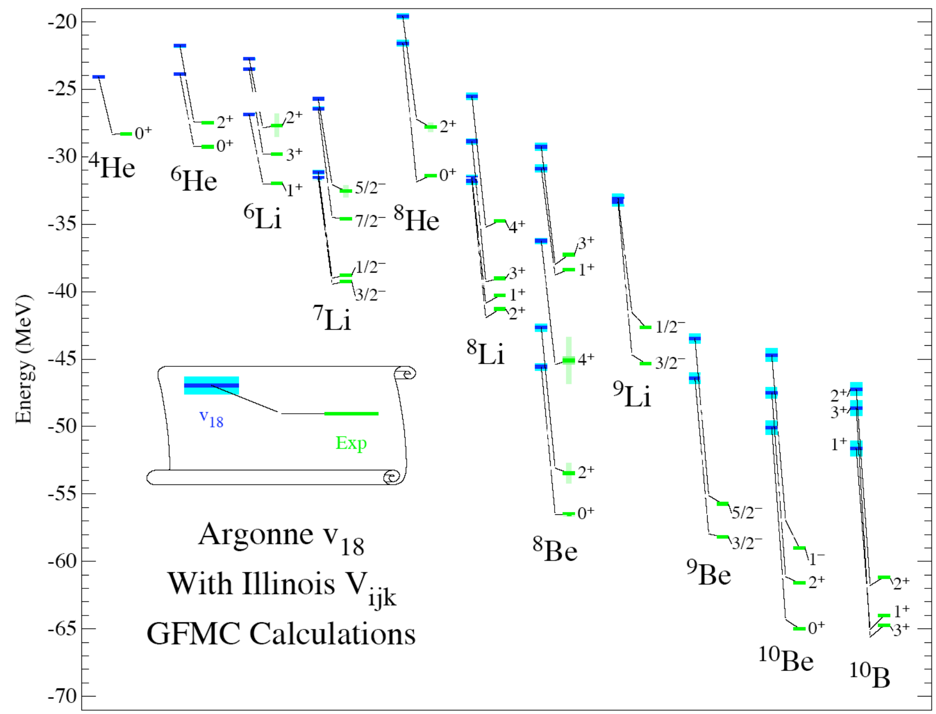
N3LO: Entem, Machleidt, PR C68 (2003) 041001

Importance of 3N interactions

All exact calculations with only NN forces miss A=3,4 nucleon binding energies



Exact GFMC results with only NN force miss A≤10 spectra

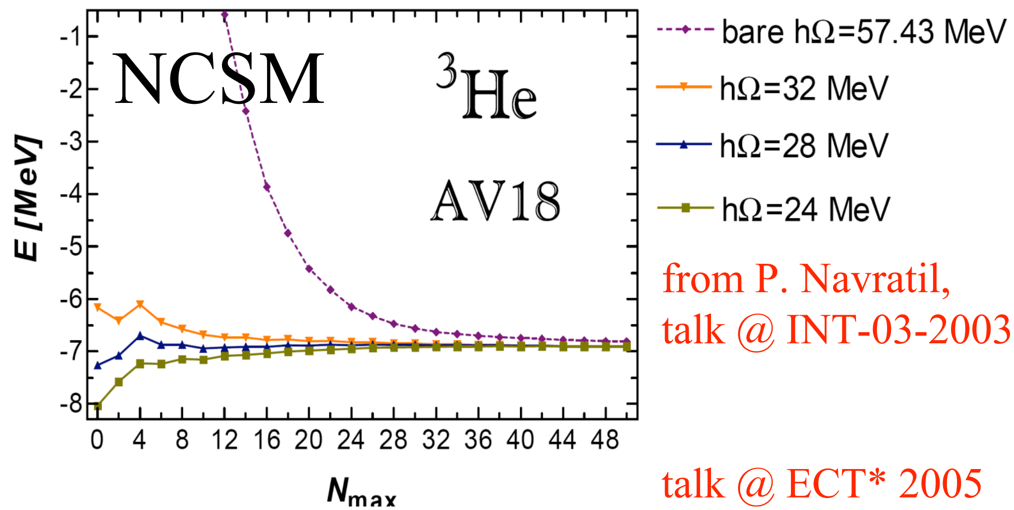


Pieper, Wiringa, Ann. Rev. Nucl. Part. Sci. 51 (2001) 53.

Size of 3N depends on V_{NN}
no "true" 3N force

Many-body applications with large-cutoff NN interactions

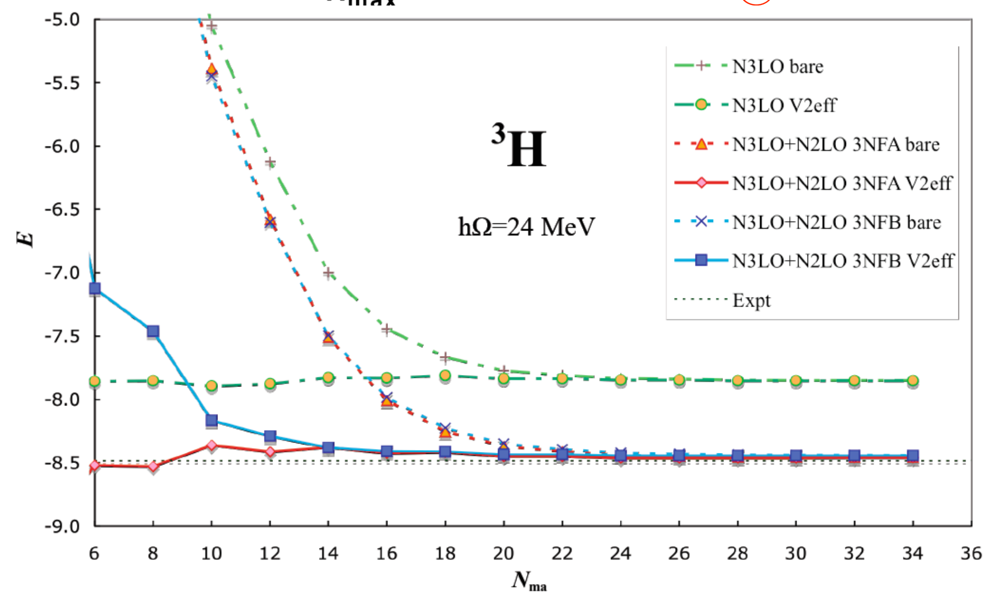
require resummations due to slow convergence with HO basis size



from P. Navratil, talk @ INT-03-2003

talk @ ECT* 2005

chiral N3LO interaction with lower cutoff (Λ≈600 MeV) leads to faster convergence

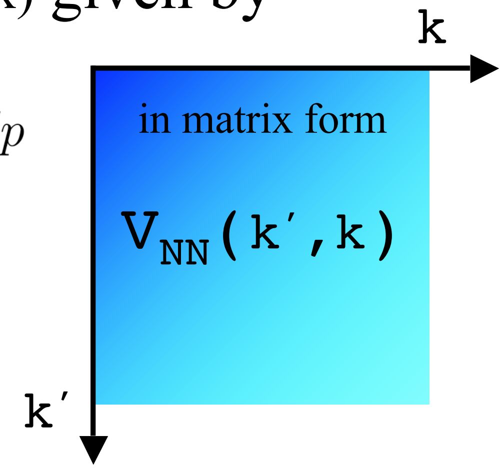


Desire **low-momentum interaction for many-body applications** where resolution is low and no need for model-dep. high-mom. parts

2) RG applied to NN interactions

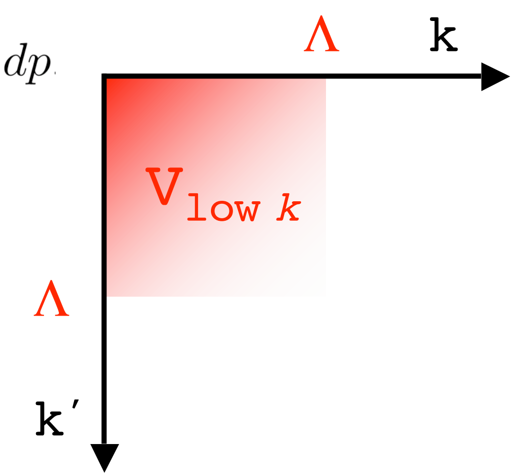
In momentum space, scattering amplitude (T matrix) given by

$$T(k', k; k^2) = V_{\rm NN}(k', k) + \frac{2}{\pi}\,\mathcal{P}\int_0^{\infty} \frac{V_{\rm NN}(k', p)\, T(p, k; k^2)}{k^2 - p^2}\, p^2 dp$$



Integrating out high-momentum modes leads to effective interaction $V_{{\rm low}\,k}$ (which reproduces the low-momentum T matrix - phase shifts, E_d)

$$T(k', k; k^2) = V_{\rm low\ k}(k', k) + \frac{2}{\pi}\,\mathcal{P}\int_0^{\Lambda} \frac{V_{\rm low\ k}(k', p)\, T(p, k; k^2)}{k^2 - p^2}\, p^2 dp$$



Changes of effective interaction with cutoff Λ are given by RG equation

$$\frac{d}{d\Lambda} V_{\rm low\ k}(k', k) = \frac{2}{\pi} \frac{V_{\rm low\ k}(k', \Lambda)\, T(\Lambda, k; \Lambda^2)}{1 - (k/\Lambda)^2}$$

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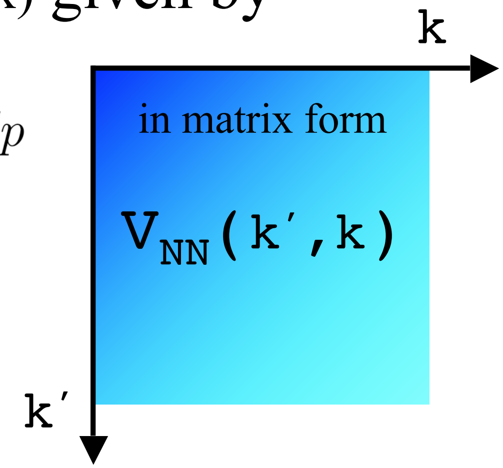

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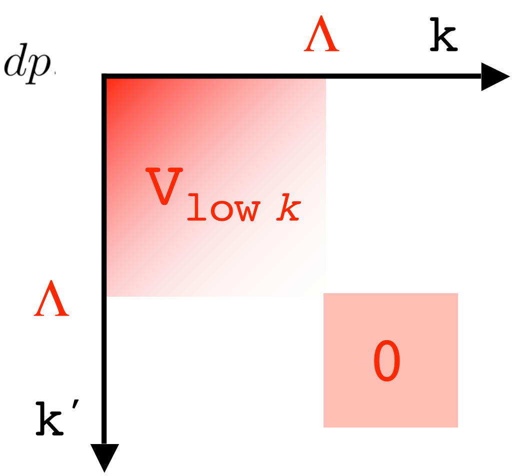

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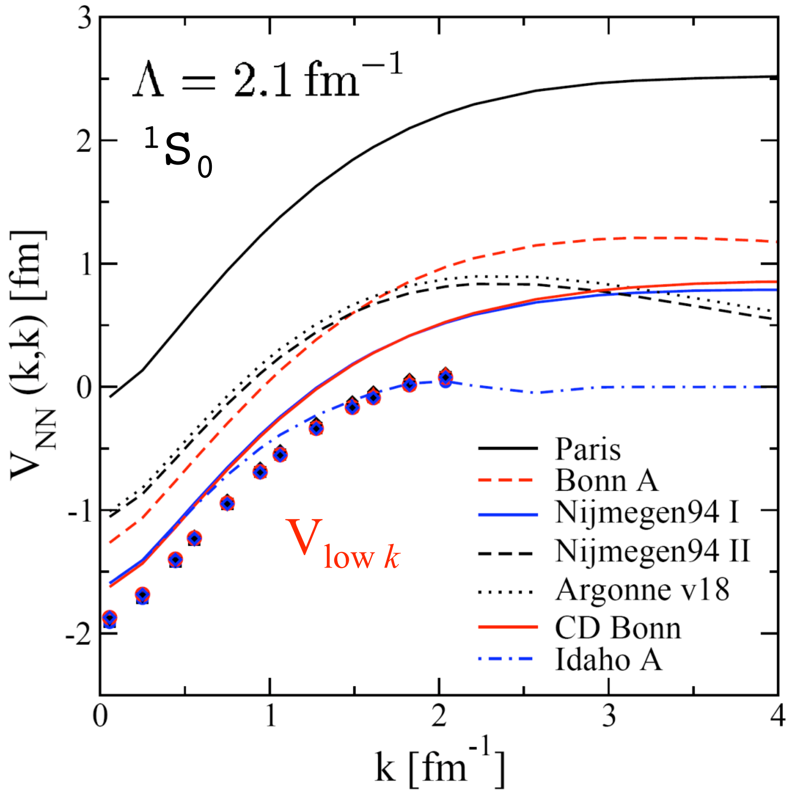
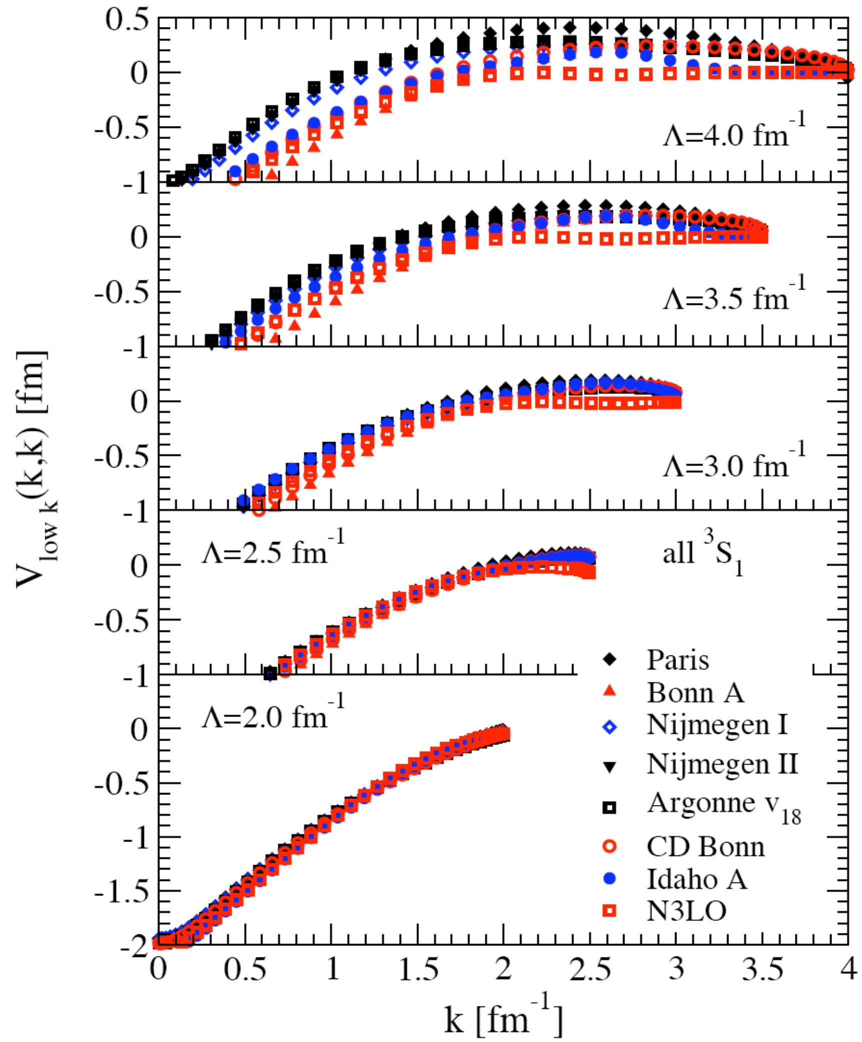
Technically equivalent to Lee-Suzuki in mom. space, with Q-block≡0

Starting from any NN interaction:
Solutions to the RG eqn. evolve
to a "universal" interaction $V_{\text{low } k}$
for cutoffs below $\Lambda \lesssim 2.1\,\text{fm}^{-1}$



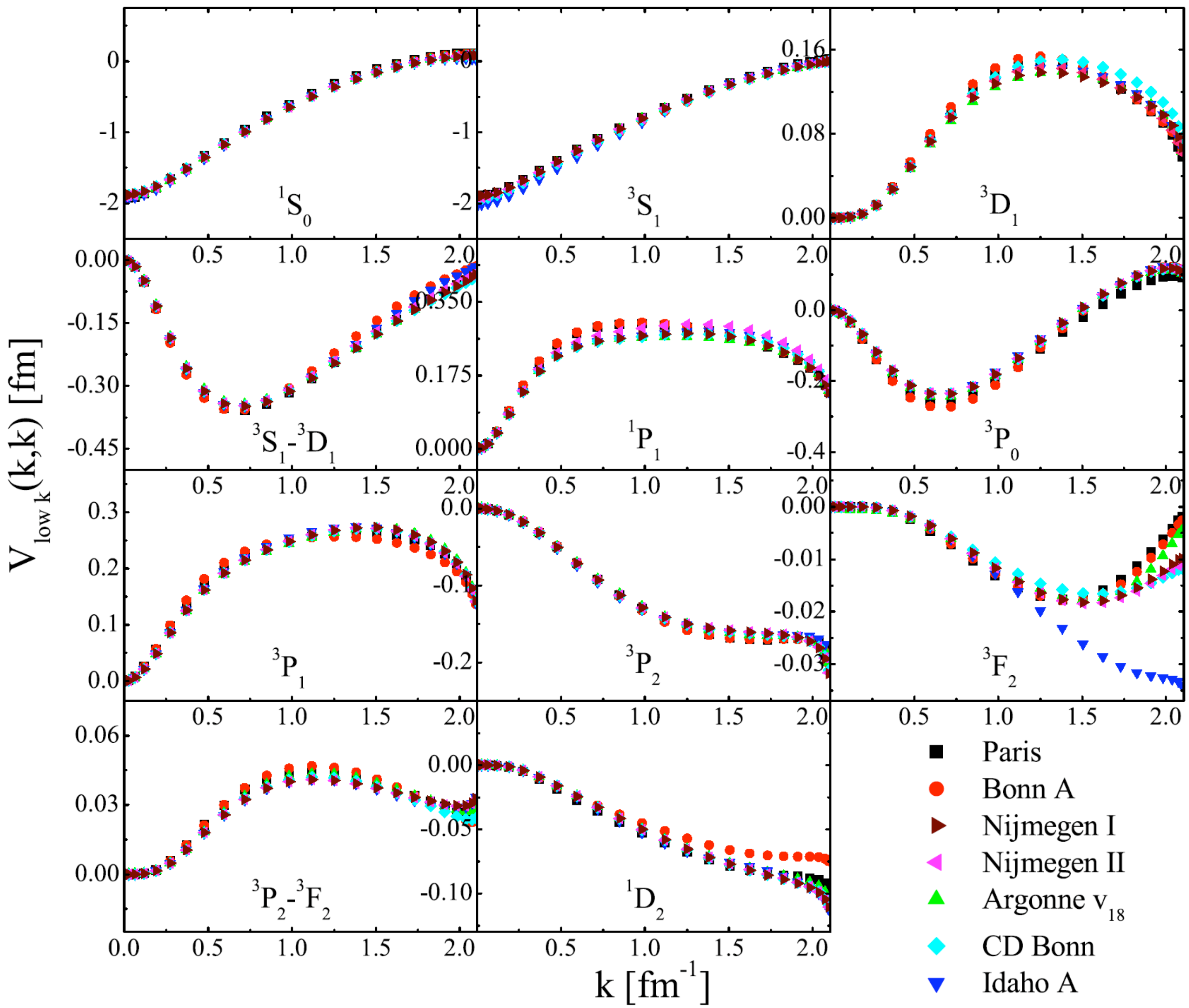
Bogner, Kuo, AS, Phys. Rep. 386 (2003) 1.



$V_{\text{low } k}(\Lambda)$ defines a class of
energy-indep. NN interactions

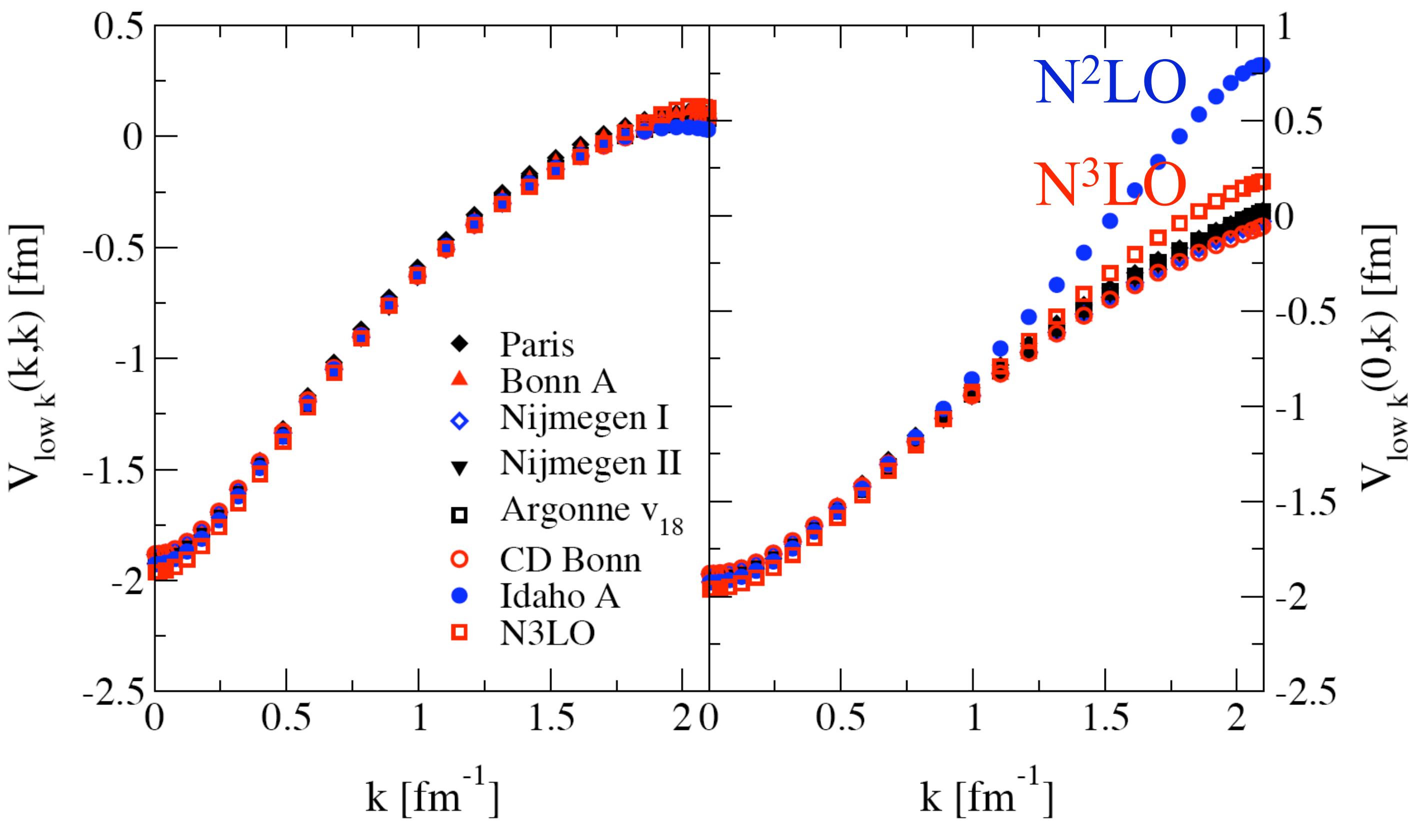
Collapse in all partial waves

due to same long-distance (π) physics and phase shift equivalence

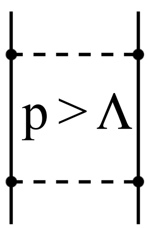


small differences related to spread in phase shift fit (Idaho misses $^3F_2$)

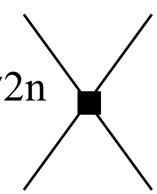
Collapse of off-shell matrix elements as well



"Universal" result indicates that $V_{\mathrm{low}\ k}$ effectively parameterizes a chiral EFT interaction with higher-order contacts

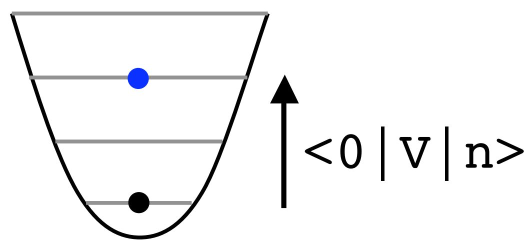


has same effect for low momenta as ∇^{2n}

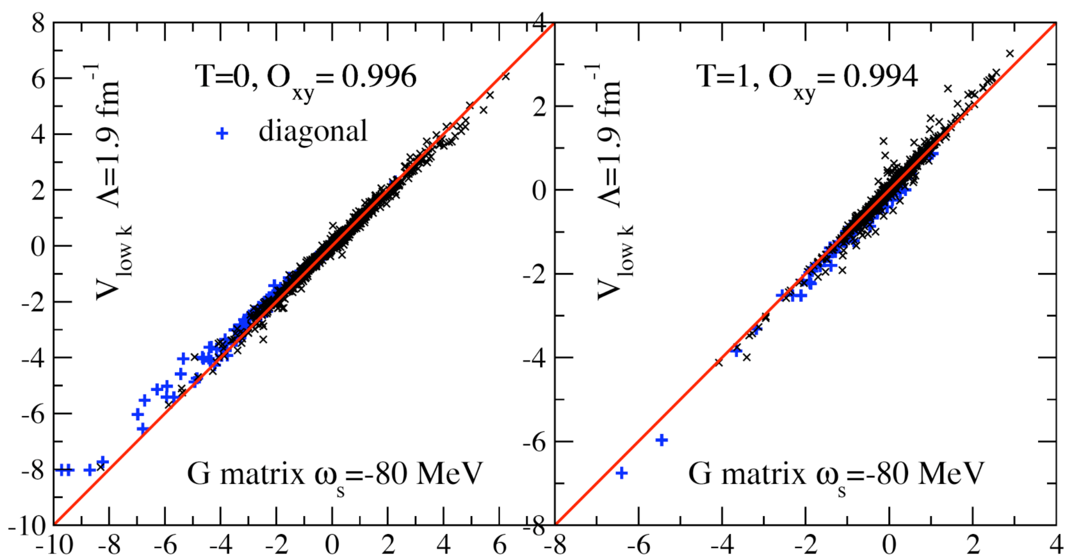


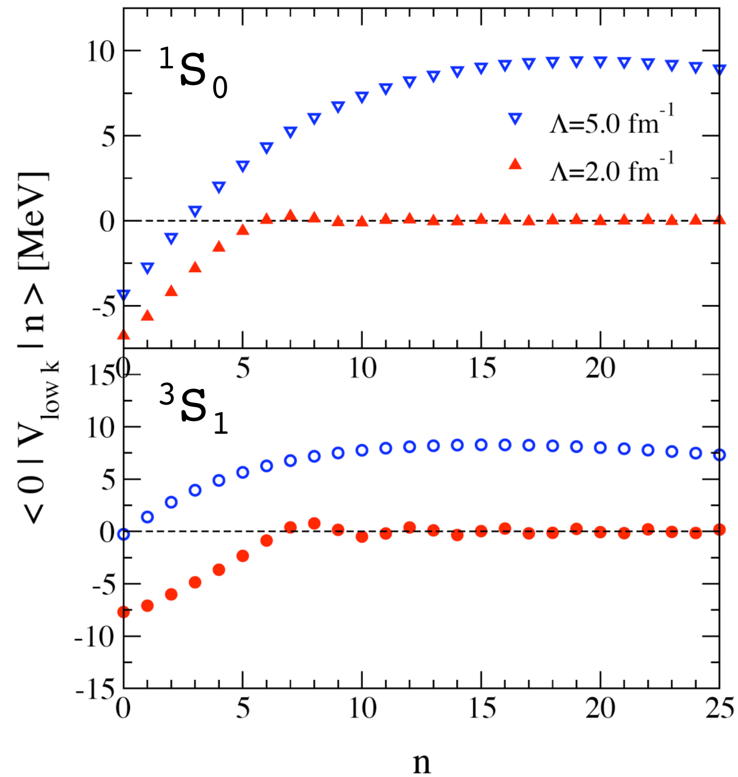
Advantages of lower cutoffs

Low-momentum interactions are tractable in a HO basis



$V_{\text{low }k}$ similar to successful G matrix pseudopotential (without drawbacks of G)





Plot of two-body $V_{\text{low }k}$ vs. G matrix elements in MeV

(4 shells) AS, Zuker, nucl-th/0501038.

What about ladders in $V_{\text{low }k}$?

3) Results for nuclei and nuclear matter

Many-body calculations with $V_{\text{low}\,k}$ make model-independent predictions, with cutoff-independent NN observables ($\chi^2 \approx 1$)

But incomplete, because 3N, 4N,… interactions are not included

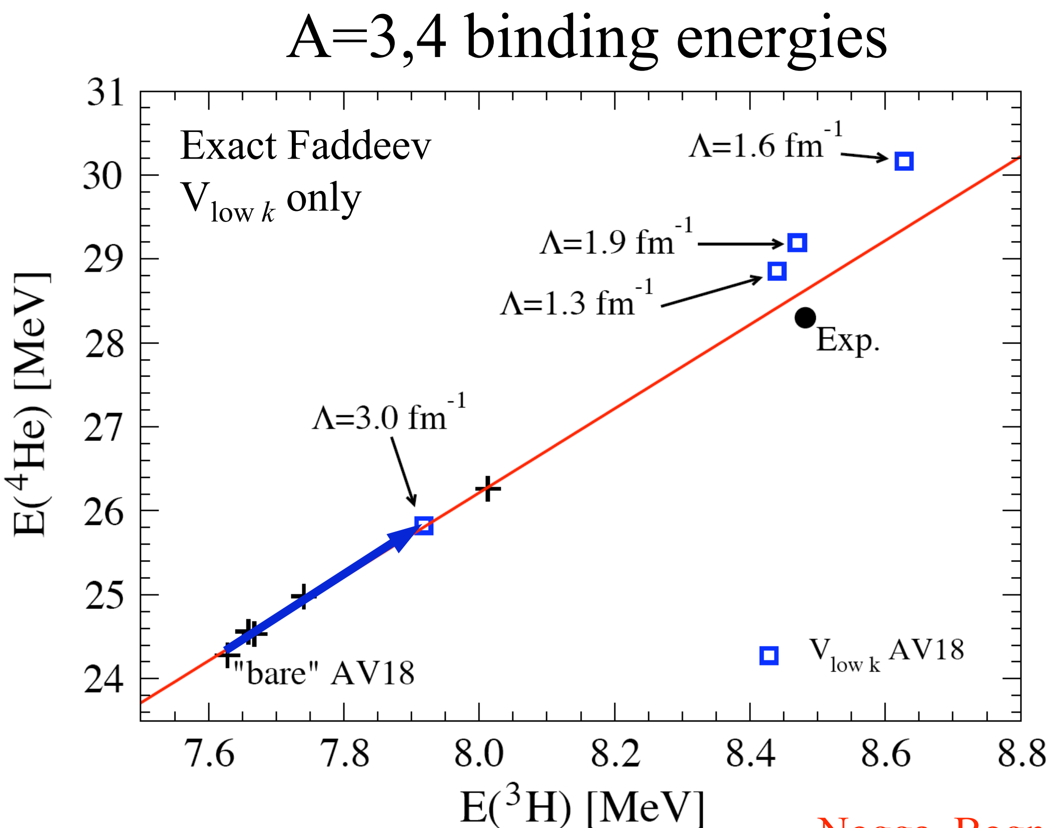
If one omits the many-body forces, calculations of low-energy 3N, 4N,… observables will be cutoff-dependent

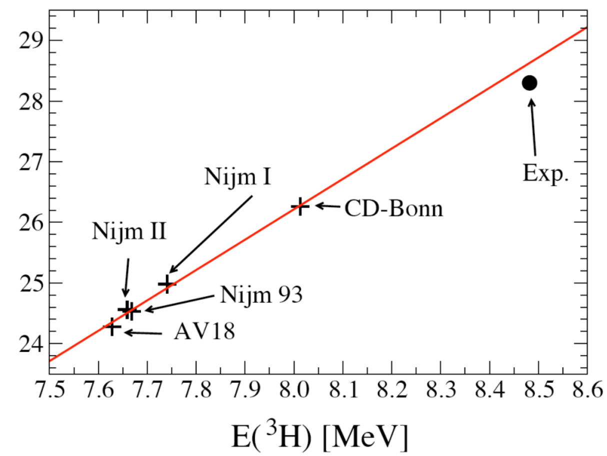
This is a feature

Varying the cutoff estimates the effects of omitted many-body interactions Nogga, Bogner, AS, PR C70 (2004) 061002(R).

Important to assess theoretical errors for predictions to extreme compositions and astrophysical densities/temperatures

Cutoff dependence due to omitted 3N forces





Nogga, Bogner, AS, PR C70 (2004) 061002(R).

Cutoff dependence shows that three-body forces are inevitable

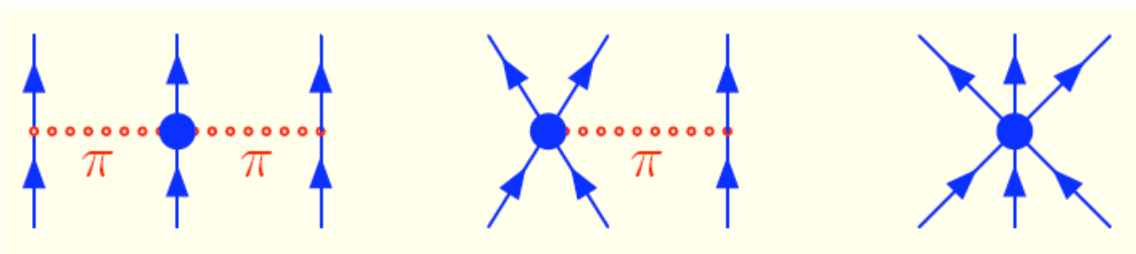
Cutoff dependence is almost linear (explains Tjon line),
with 3N contributions smaller for low-momentum interactions

Low-momentum 3N forces with only pion exchanges

organized by chiral Effective Field Theory van Kolck, PR C49 (1994) 2932; Epelbaum et al., PR C66 (2002) 064001.

operator structure of any 3N force collapses at low energies to

long (2π) intermediate (π) short-range



c-terms D-term E-term

chiral counting:
$(Q/\Lambda)^3 \sim (m_\pi/\Lambda)^3$
rel. to 2N force

c_i from NN PWA with chiral 2π exchange (c_3, c_4 important for nuclear structure)

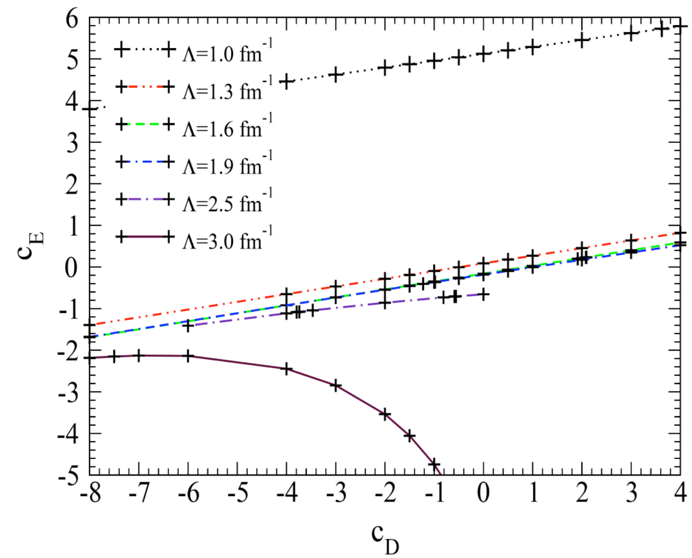
approximate 3N evolution by fitting low-energy D,E constants of leading-order chiral 3N interaction to $V_{\text{low }k}$ over a range of cutoffs

Two couplings fit to ^{3}H and ^{4}He

Linear dependences in fits, consistent with perturbative 3N contributions

$$E(^3H) = \langle T + V_{\text{low }k} + V_c \rangle + c_D \langle O_D \rangle + c_E \langle O_E \rangle$$

3N forces become perturbative for cutoffs $\Lambda \lesssim 2\,\text{fm}^{-1}$



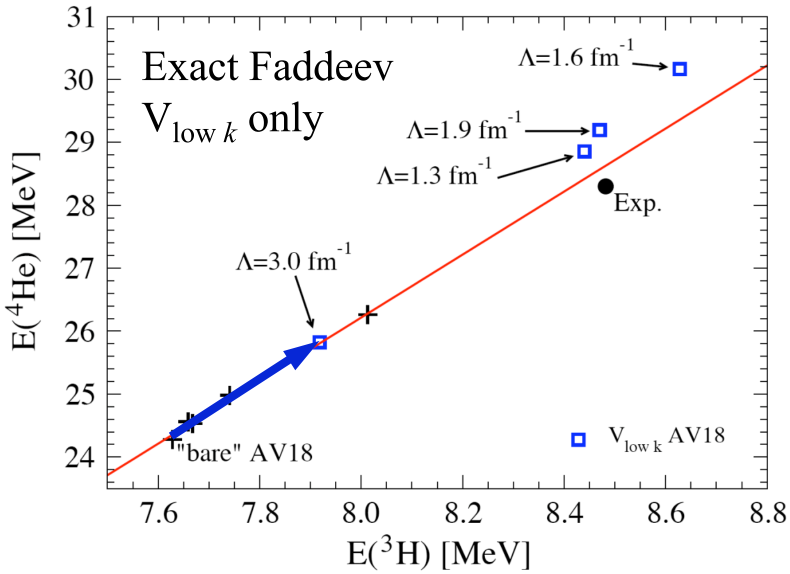
nonperturbative at larger cutoffs (also for chiral EFT with $\Lambda \approx 3\ \text{fm}^{-1}$), with expectation values beyond expected $(Q/\Lambda)^3 \sim (m_\pi/\Lambda)^3 \approx 0.1$ of NN

Λ	^{3}H T	^{3}H $V_{\text{low }k}$	^{3}H c-terms	^{3}H D-term	^{3}H E-term	^{4}He T	^{4}He $V_{\text{low }k}$	^{4}He c-terms	^{4}He D-term	^{4}He E-term	max $\lvert V_{3\text{N}}/V_{\text{low }k}\rvert$	^{4}He k_{rms}
1.0	21.06	−28.62	0.02	0.11	−1.06	38.11	−62.18	0.10	0.54	−4.87	0.08	0.55
1.3	25.71	−34.14	0.01	1.39	−1.46	50.14	−78.86	0.19	8.08	−7.83	0.10	0.63
1.6	28.45	−37.04	−0.11	0.55	−0.32	57.01	−86.82	−0.14	3.61	−1.94	0.04	0.67
1.9	30.25	−38.66	−0.48	−0.50	0.90	60.84	−89.50	−1.83	−3.48	5.68	0.06	0.70
2.5(*a*)	33.30	−40.94	−2.22	−0.11	1.49	67.56	−90.97	−11.06	−0.41	6.62	0.12	0.74
2.5(*b*)	33.51	−41.29	−2.26	−1.42	2.97	68.03	−92.86	−11.22	−8.67	16.45	0.18	0.74
3.0(∗)	36.98	−43.91	−4.49	−0.73	3.67	78.77	−99.03	−22.82	−2.63	16.95	0.23	0.80

$\approx m_\pi$

$V_{\text{low }k}$ + leading chiral 3N interaction, **no further adjustments**

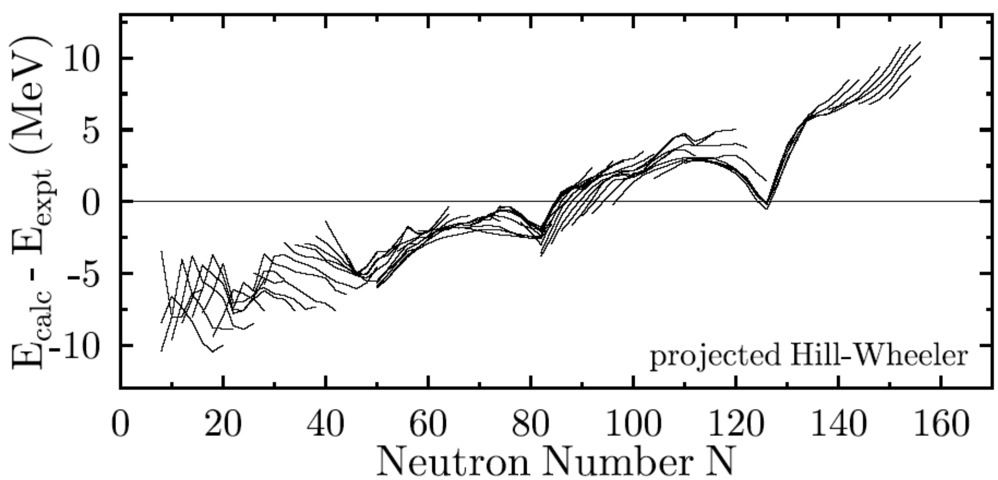
3N interaction and mass models



large-cutoff NN interactions underbind light A, overbind heavy A

low-mom. NN interactions close to A=3,4, overbind heavier A

need 3N input to correct this



similar trend in DF predictions

investigate density/isospin dependence of weak low-mom. 3N interactions

Bender et al., PRL 94 (2005) 102503.

NN scattering in free-space vs. nuclear matter

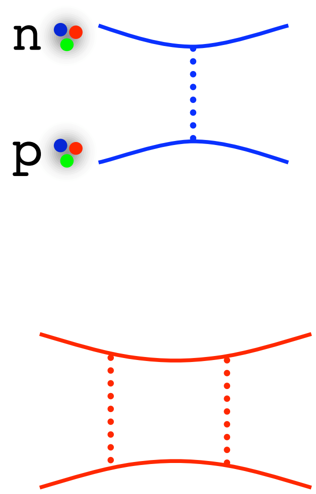
Sources of nonperturbative behavior:

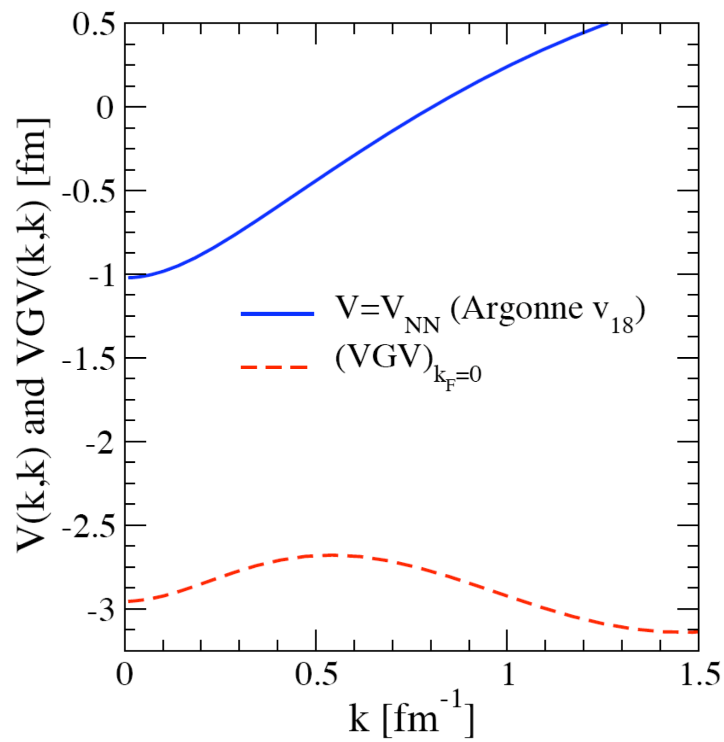
1. Iterated interactions at low momenta are nonperturbative due to near bound states $a_{^1S_0} = -23.7\,\mathrm{fm}$ $a_{^3S_1} = 5.4\,\mathrm{fm}$

2. Cores scatter strongly to high-momentum states (overwhelms 1.)

For interactions with cores:

second-order contributions larger than V_{NN}





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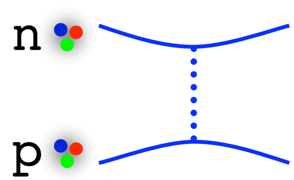
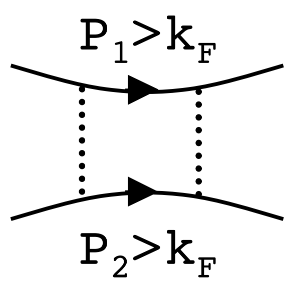
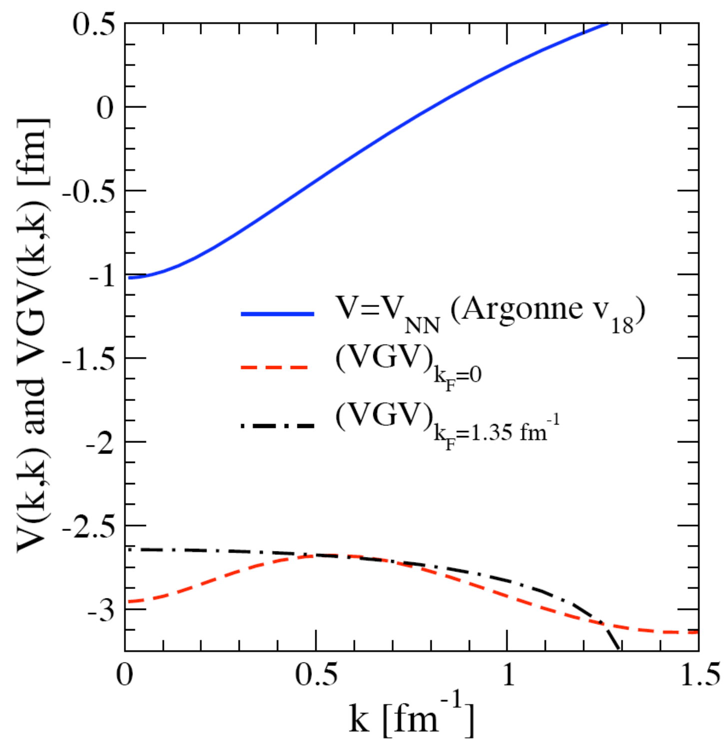


even with Pauli blocking





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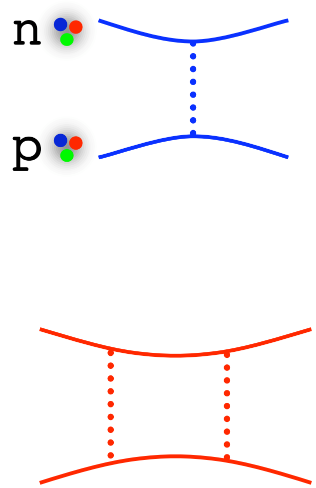
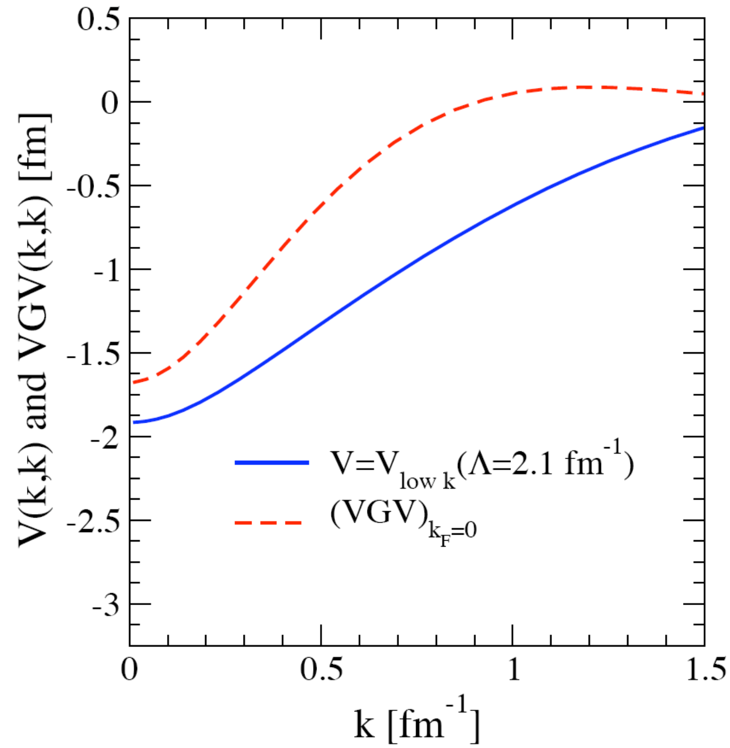
For low-momentum interactions:

free-space nonperturbative due to near-bound state





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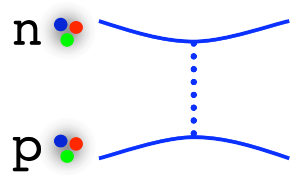
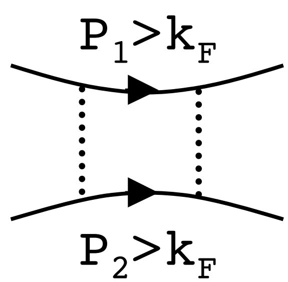
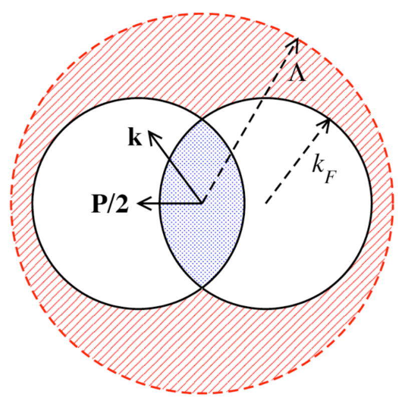
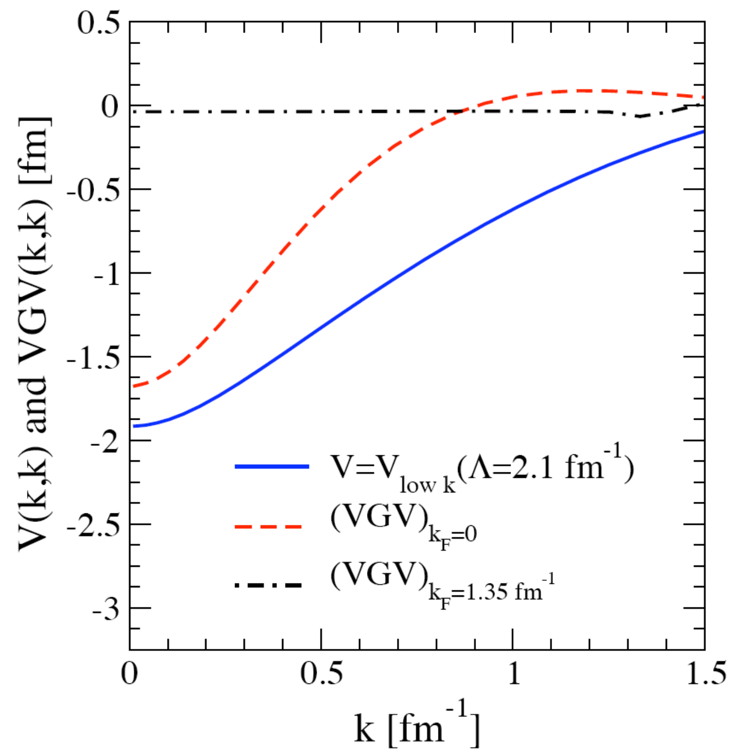


small in medium due to occupied Fermi sea

restricts phase space for two particles







mom. cutoff $k < 2.1\ \mathrm{fm}^{-1}$

$= $ density cutoff $\rho < 4\ \rho_0$

Weinberg eigenvalues

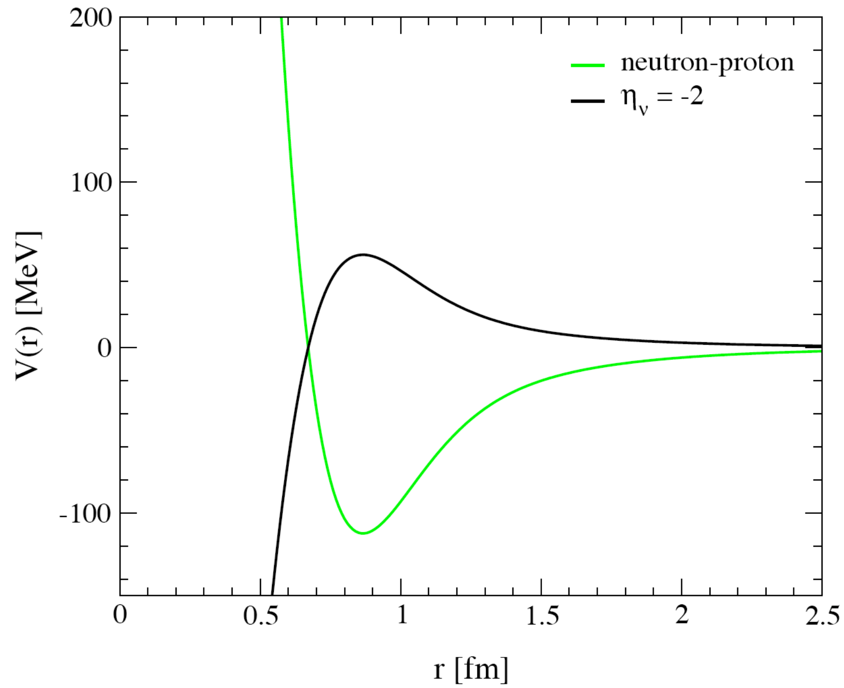
rigorously show that in-medium Born series is perturbative for $V_{\text{low } k}$ at sufficient densities Bogner, AS, Furnstahl, Nogga, nucl-th/0504043.

study spectrum of $G_0(z)V\,|\Psi_\nu(z)\rangle = \eta_\nu(z)\,|\Psi_\nu(z)\rangle$

i.e., convergence of $T(z)\,|\Psi_\nu(z)\rangle = (1+\eta_\nu(z)+\eta_\nu(z)^2+\ldots)\,V\,|\Psi_\nu(z)\rangle$

write as Schroedinger eqn. $\left(H_0 + \frac{1}{\eta_\nu(z)}V\right)|\Psi_\nu(z)\rangle = z\,|\Psi_\nu(z)\rangle$

large-cutoff interactions
have at least one large $\eta_\nu < 0$



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rigorously show that in-medium Born series is perturbative for $V_{\mathrm{low}\,k}$ at sufficient densities Bogner, AS, Furnstahl, Nogga, nucl-th/0504043.

study spectrum of $G_0(z)V\,|\Psi_\nu(z)\rangle = \eta_\nu(z)\,|\Psi_\nu(z)\rangle$

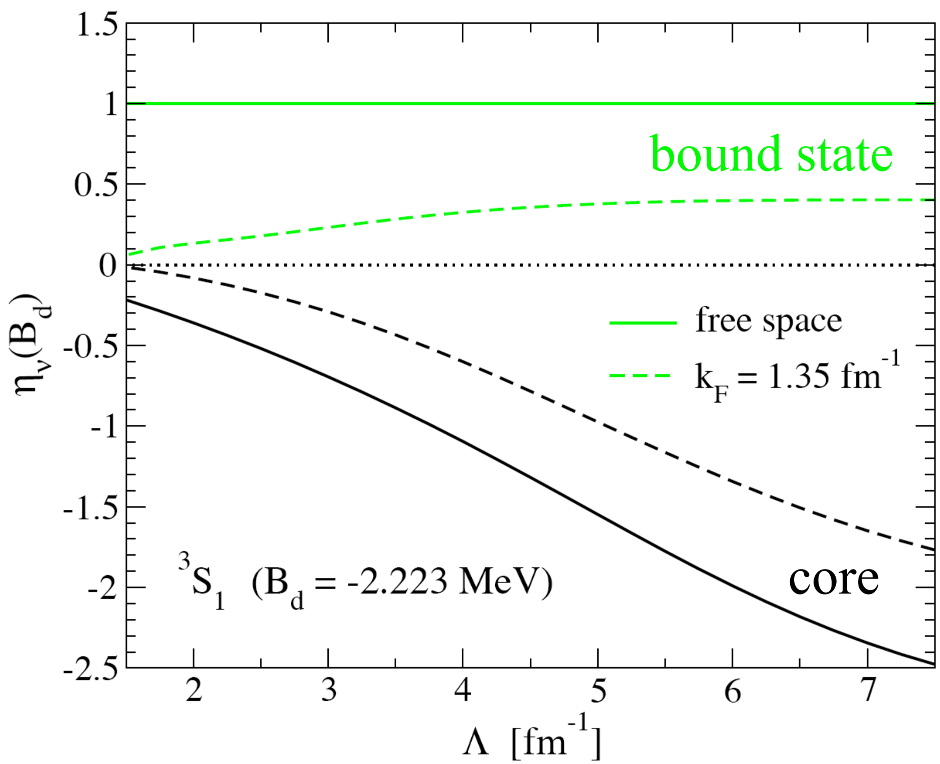
i.e., convergence of $T(z)\,|\Psi_\nu(z)\rangle = (1 + \eta_\nu(z) + \eta_\nu(z)^2 + \ldots)\,V\,|\Psi_\nu(z)\rangle$

write as Schroedinger eqn.

$$\left(H_0 + \frac{1}{\eta_\nu(z)}V\right)|\Psi_\nu(z)\rangle = z\,|\Psi_\nu(z)\rangle$$

repulsive core eigenvalue small for lower cutoffs

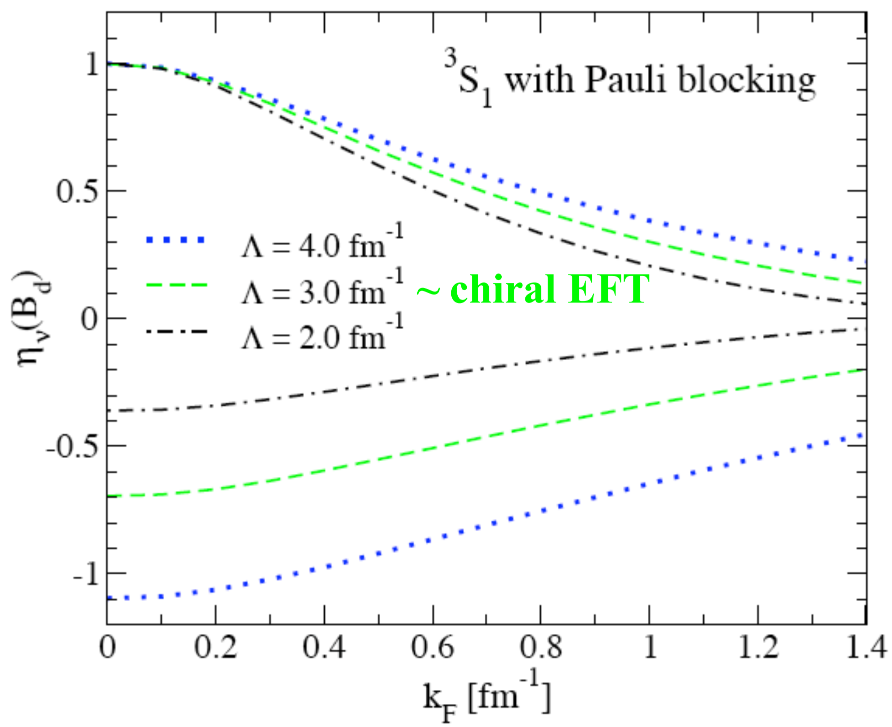
deuteron eigenvalue small in-medium (fine-tuning elim.)

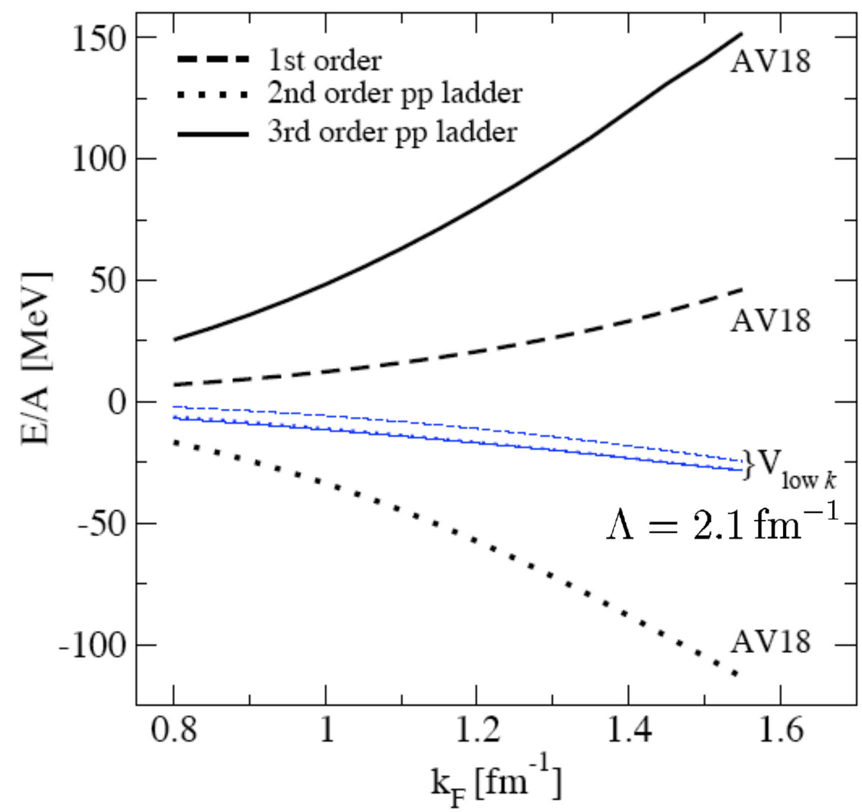


Perturbative two-body ladders

Weinberg analysis anticipates rapidly converging particle-particle contributions to nuclear matter energy for low-mom. interactions

Bogner, AS, Furnstahl, Nogga, nucl-th/0504043.

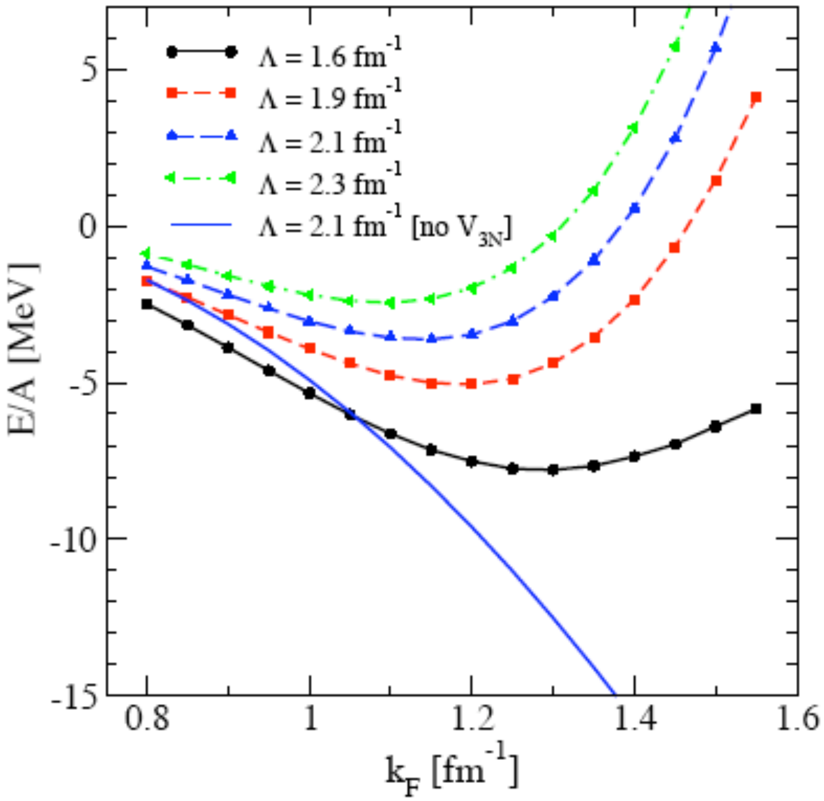




Perturbation theory in place of ladder resummations

Note second-order important (remaining tensor)

Nuclear matter with NN and 3N



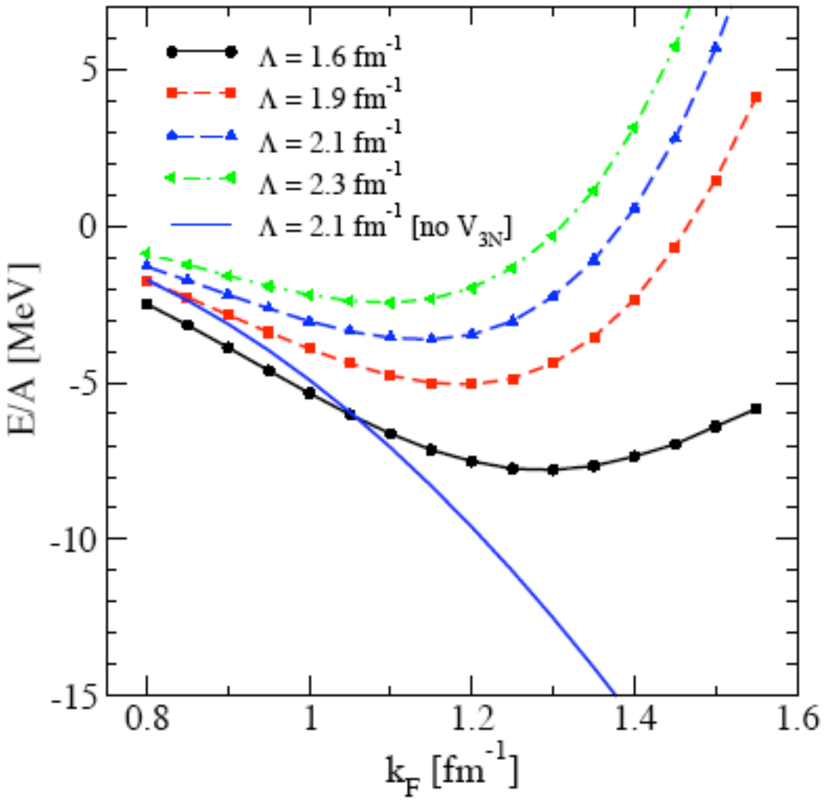
Hartree-Fock

bound, saturation from 3N force

(2π-exchange dominates, no adjustments)

Bogner, AS, Furnstahl, Nogga, nucl-th/0504043.

Nuclear matter with NN and 3N



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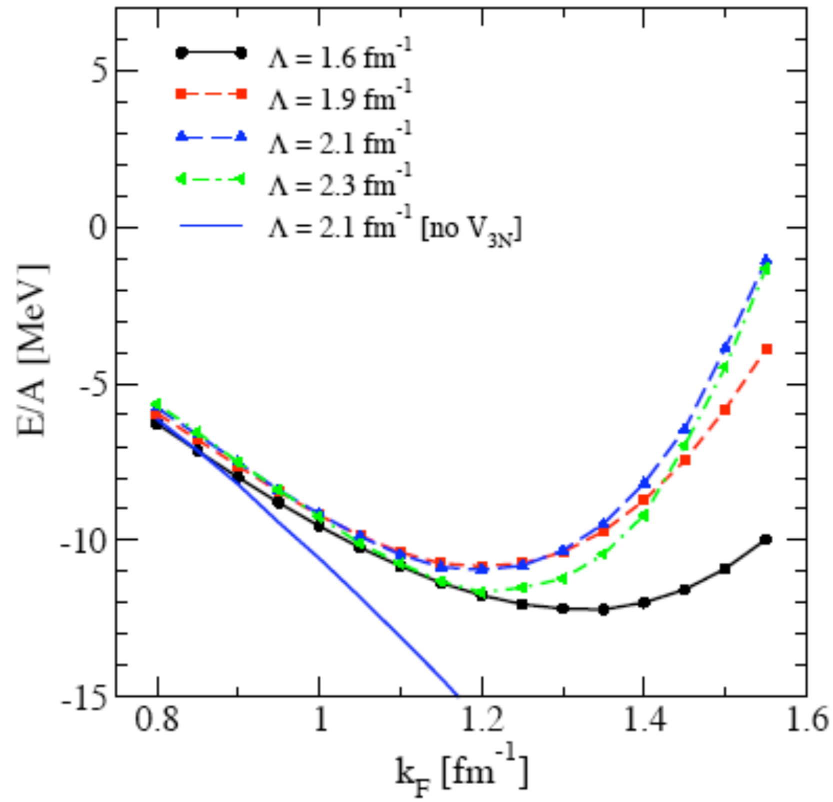


Hartree-Fock + 2nd-order

(approx. 2nd-order 3N treatment, continuous spectrum with m*)

cutoff dep. strongly reduced

Ex-corr. much weaker, use $V_{\mathrm{low}\,k} + V_{3N}$ to constrain nuclear DF

3N force remains natural in nuclear matter

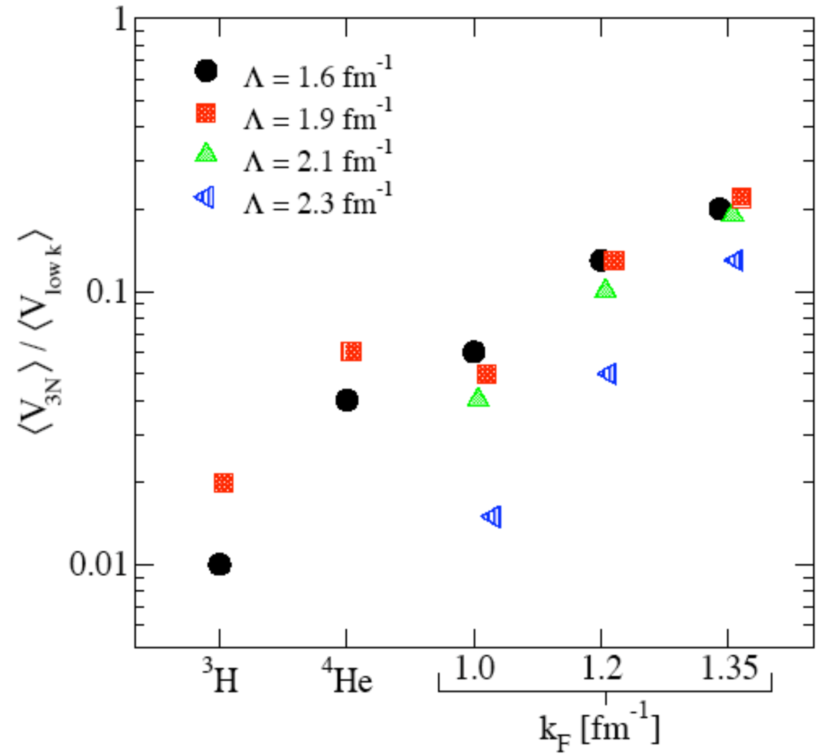
3N force drives saturation but exp. values not unnaturally large

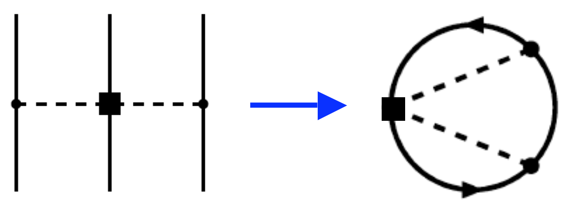
consistent with chiral EFT scaling

$$\langle V_{3\mathrm{N}} \rangle \sim (Q/\Lambda)^3 \langle V_{\mathrm{NN}} \rangle$$

$V_{\mathrm{low}\,k}$ exp. values change by ≈0.5 MeV after inclusion of 3N interaction

largest 3N contribution from 2π-part

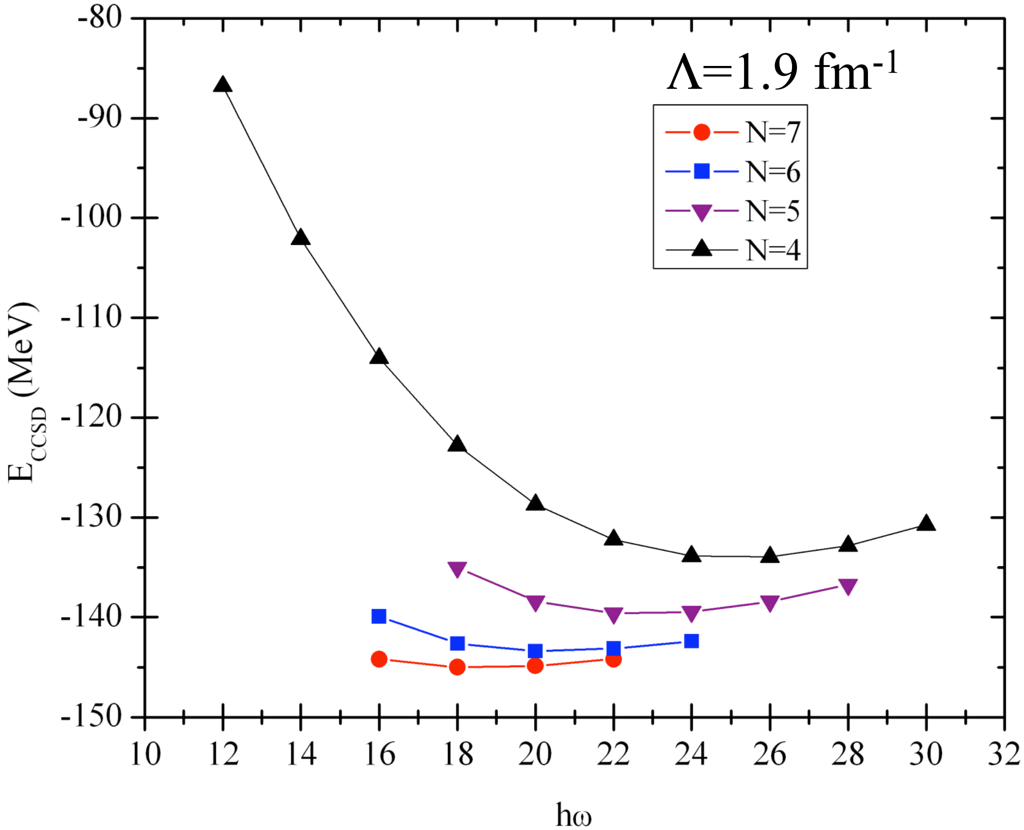




mom. dep. of 3N determines density dep.

		Hartree-Fock					Hartree-Fock + dominant second order				
k_F	Λ	T	$V_{\mathrm{low}\,k}$	V_c	V_D	V_E	T	$V_{\mathrm{low}\,k}$	V_c	V_D	V_E
1.2	1.6	17.92	−31.47	5.37	1.31	−0.64	20.86	−37.66	4.59	1.03	−0.65
	1.9	17.92	−28.95	5.61	−0.81	1.18	21.80	−37.38	3.99	−0.50	1.28
	2.1	17.92	−27.51	5.67	−1.37	1.84	22.87	−37.53	2.27	−0.37	1.82
	2.3	17.92	−26.13	5.70	−1.86	2.42	24.32	−37.95	−0.38	0.51	1.78

Coupled cluster results for $V_{\text{low }k}$



with D. Dean et al.

nearly converged

N=8, $\hbar\omega$=18 MeV: -145.85 MeV

calc. with 3N interaction in progress, is repulsive

also have ^{40}Ca results

CC method can provide exact answer for low-momentum interactions without resummations or similarity trafo.

Can test other many-body methods for same interaction

Build DF from low-momentum interactions and compare to CC results

Spin-orbit strength of low-momentum interactions

As for binding energies, interplay of NN and 3N contributions to LS splitting, individual parts depend on cutoff

CC results for different NN interactions, N=8, Gour et al., nucl-th/0507049

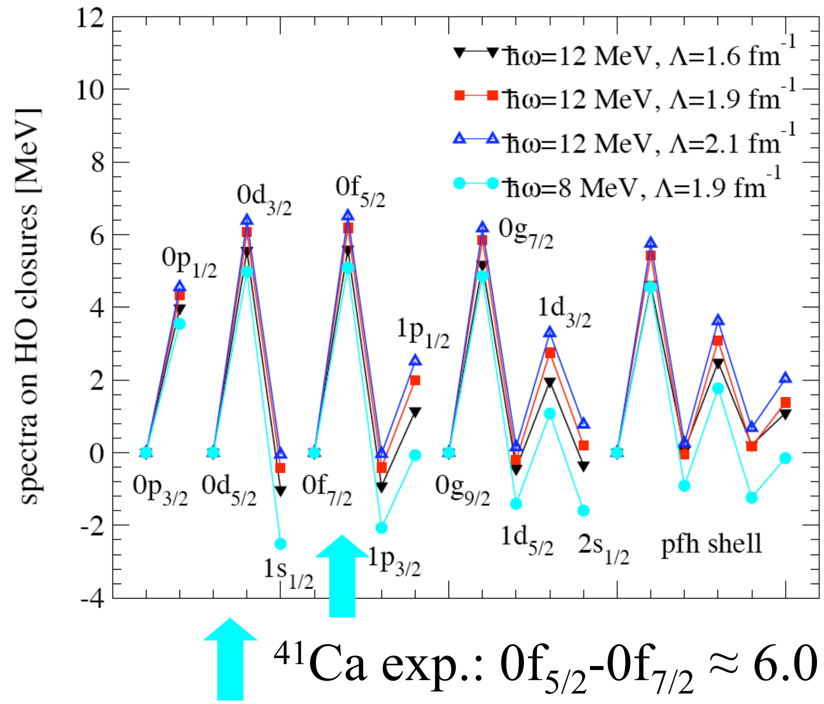
^{15}O	Expt.	N^{3}LO	CD-Bonn
3/2$^-$	6.176	6.26	7.35
1/2$^-$	0.0	0.0	0.0

^{17}O	Expt.	N^{3}LO	CD-Bonn
3/2$^+$	5.085	5.68	6.41
5/2$^+$	0.0	0.0	0.0

	Interaction			
Excited state	N^{3}LO	CD-Bonn	V_{18}	Expt
^{15}O $(3/2)_1^-$	6.264	7.351	4.452	6.176
^{15}N $(3/2)_1^-$	6.318	7.443	4.499	6.323
^{17}O $(3/2)_1^+$	5.675	6.406	3.946	5.084
^{17}O $(1/2)_1^+$	-0.025	0.311	-0.390	0.870
^{17}F $(3/2)_1^+$	5.891	6.677	4.163	5.000
^{17}F $(1/2)_1^+$	0.428	0.805	0.062	0.495

similar observation in 0ħω with $V_{\text{low }k}$

AS, Zuker, nucl-th/0501038.



^{41}Ca exp.: $0f_{5/2}$-$0f_{7/2} \approx 6.0$ MeV

^{17}O exp.: $0d_{3/2}$-$0d_{5/2} \approx 5.1$ MeV

3N contrib. to LS for N3LO or $V_{\text{low }k}$ smaller, agrees with Q/Λ expectation

4) Strategies for density-functional calculations from nuclear interactions

Revisit density-matrix expansion with low-momentum interactions

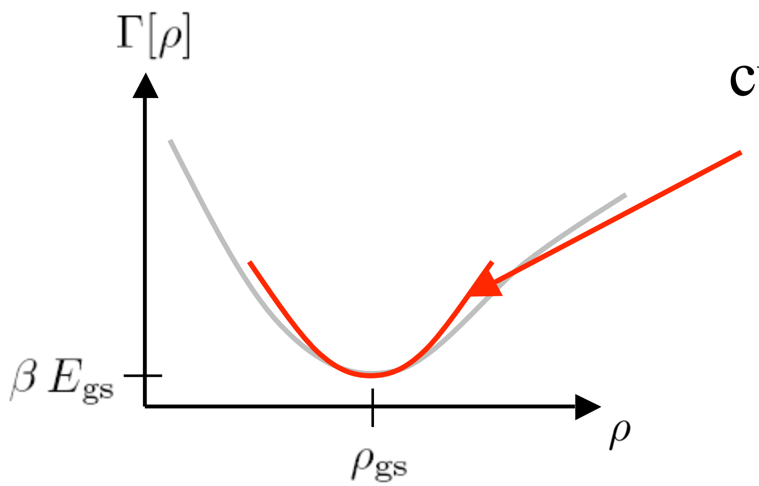
Direct constraints on general ∇^2 DF

Inversion method, provided a power counting for nuclear matter

Functional RG approach to DF Polonyi, Schwenk, formalism in nucl-th/0403011.

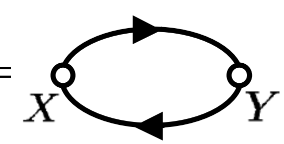
Effective action is minimal at the physical (K=0) ground state density

$$\left.\frac{\delta\Gamma[\rho]}{\delta\rho}\right|_{\rho=\rho_{\rm gs}} = 0 \quad \text{with gs energy} \quad E_{\rm gs} = E[\rho_{\rm gs}] = \lim_{\beta\to\infty} \frac{1}{\beta}\,\Gamma[\rho_{\rm gs}]$$



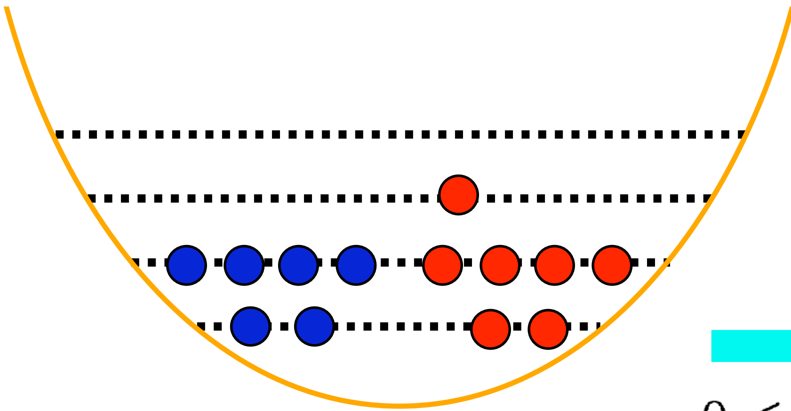
curvature will include ex-corr.

$$\left(\left.\frac{\delta^2\Gamma[\rho]}{\delta\rho\,\delta\rho}\right|_{\rho_{\rm gs}}\right)^{-1} = \left.\frac{\delta^2 W[K]}{\delta K\,\delta K}\right|_{K=0}$$

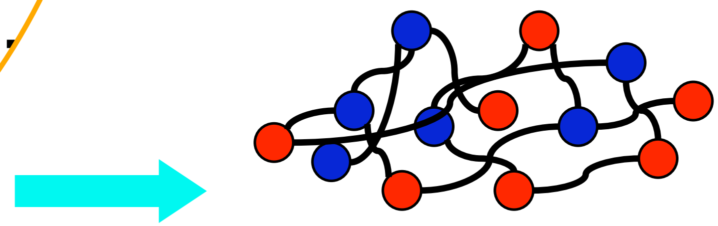
$=$ 

+ interactions

Basic idea of functional RG approach



$0 \leqslant \lambda \leqslant 1$



start from non-interacting fermions in a background potential (a simple guess for the mean field)

gradually switch off background potental while turning on the microscopic interactions

$$S_{\lambda,1}[\psi^\dagger,\psi] = \sum_\sigma \int dx\, \psi_\sigma^\dagger(x) \left(\partial_t - \frac{1}{2m}\nabla_{\mathbf{x}}^2 + (1-\lambda) V_{\lambda;\sigma}(\mathbf{x}) \right) \psi_\sigma(x)$$

$$S_{\lambda,2}[\psi^\dagger,\psi] = \frac{\lambda}{2}(\psi^\dagger\psi)\cdot U \cdot (\psi^\dagger\psi)$$

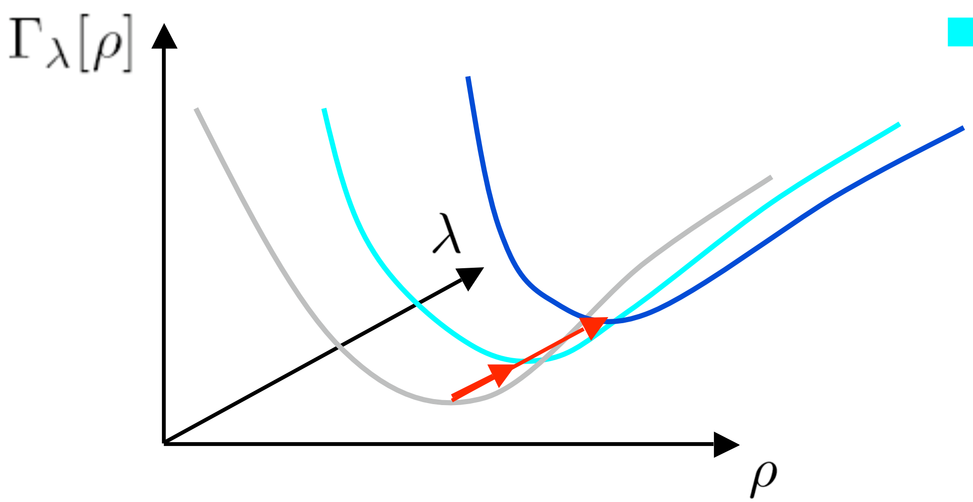
Evolution of the effective action with control parameter

$$\partial_\lambda \Gamma_\lambda[\rho] = \partial_\lambda \left[(1-\lambda)\, V_\lambda\right] \cdot \rho + \frac{1}{2}\, \rho \cdot U \cdot \rho + \frac{1}{2}\, \mathrm{Tr}\left[U \cdot \left(\frac{\delta^2 \Gamma_\lambda[\rho]}{\delta\rho\, \delta\rho} \right)^{-1} \right]$$

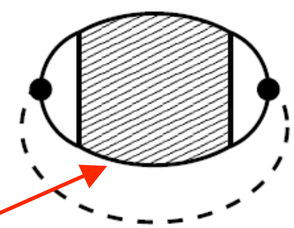
change in: background V   Hartree   exchange-correlations

Expand density functional around evolving gs density

$$\Gamma_\lambda[\rho] = \Gamma[\rho_{\mathrm{gs},\lambda}]^{(0)} + \sum_{n \geqslant 2} \int_{X_1,\ldots,X_n} \frac{1}{n!}\, \Gamma[\rho_{\mathrm{gs},\lambda}]^{(n)}_{X_1,\ldots,X_n} \cdot (\rho - \rho_{\mathrm{gs},\lambda})_{X_1} \cdots (\rho - \rho_{\mathrm{gs},\lambda})_{X_n}$$



Evolution equations for expansion coeff.
(build up many-body correlations)



All exchange-correlations via dressed ph propagator

5) Summary

1. RG removes model dependences from nuclear forces, results in "universal" low-momentum interaction
2. Low-momentum 3N forces become weaker in this regime
   first 3N calculations for A>12 nuclei D. Dean et al., in prep.
3. CC method provides converged results for intermediate-A nuclei
   Results for low-mom. interactions do not require resummations and can be used as many-body test cases
4. Nuclear matter seems perturbative with low-mom. interactions
   ph contributions need further studies
5. Cutoff variation estimates errors + completeness of calculations
   important for extrapolations to extremes, ISAC, FAIR, RIA
6. Low-mom. interactions can provide valuable constraints on DF
   with consistent interaction in ph and pp channel
7. Exciting time to combine progress in nuclear interactions, DFT and exact many-body methods