Atomic Nuclei at Low Resolution

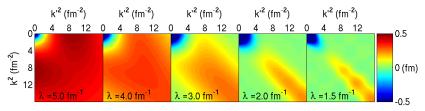
Dick Furnstahl

Department of Physics Ohio State University



EMMI Workshop on Strongly Coupled Systems Happy Birthday, Jochen!

November, 2010



Outline

Overview: Low-energy nuclear physics

Lowering the resolution with RG

Survey of calculations at low resolution

Outlook

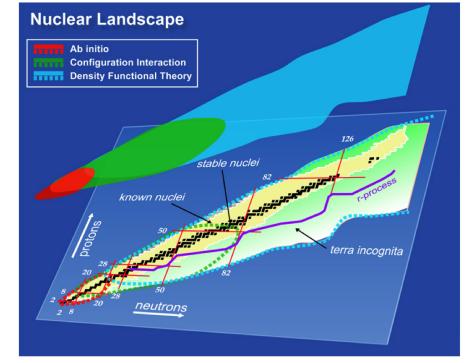
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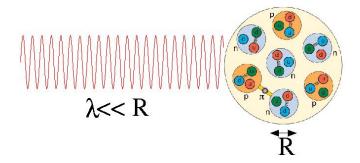


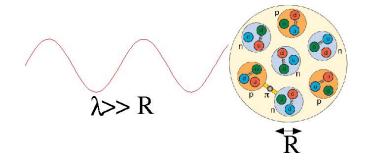
Extremes in low-energy nuclear physics

- Extremes of nuclear existence: driplines, superheavies, ...
- Extremes in the heavens: supernovae, neutron stars, ...
- We want to extrapolate reliably with error estimates, connect to and exploit known microscopic physics
- Shakespeare's Othello (Act 5, Scene 2) I pray you, in your letters, When you shall these unlucky deeds relate, Speak of me as I am; nothing extenuate, Nor set down aught in malice. Then must you speak Of one that lov'd not wisely but too well; Of one not easily jealous, but being wrought, Perplex'd in the extreme . . .

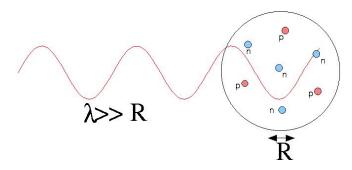


■ To avoid being "perplex'd" ⇒ go to low resolution!

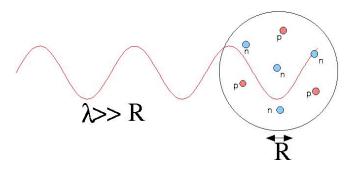




If system is probed at low energies, fine details not resolved



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 - Use low-energy variables for low-energy processes
 - Short-distance structure can be replaced by something simpler without distorting low-energy observables
 - Physics interpretation can change with resolution!
- Could be a model or systematic (e.g., effective field theory)

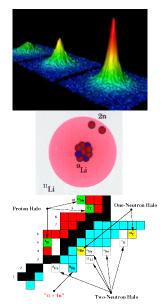


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- Low density ⇔ low interaction energy ⇔ low resolution (?)

Nuclei at very low resolution

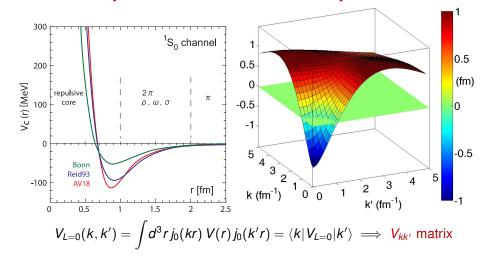
- If separation of scales is sufficient, then EFT with pointlike interactions is efficient (e.g., kR

 1)
- Universal properties (large a_s)
 - connect to cold atom physics
 - low-density neutron matter
 - e.g., Efimov physics
- Pionless EFT
 - e.g., $np \rightarrow d\gamma$ with $E_{\text{typ}} \approx 0.02 \text{--} 0.2 \, \text{MeV}$
- Halo EFT
 - $B_{\text{valence}} \ll B_{\text{core}}, E_{ex}$
 - $n\alpha$ -system (Bedaque et al.) or $\alpha\alpha$ -system (Higa et al.) or ...



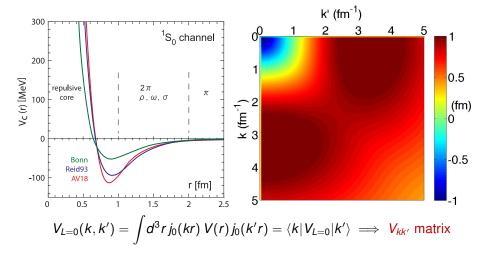
Here: focus on systems where pion exchange is resolved

S-wave NN potential in momentum space



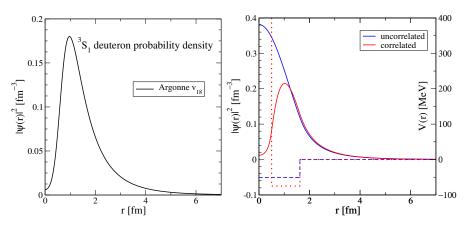
- Momentum units ($\hbar=c=1$): typical relative momentum in large nucleus \approx 1 fm $^{-1}\approx$ 200 MeV but . . .
- Repulsive core \implies large high-k ($\geqslant 2 \, \text{fm}^{-1}$) components

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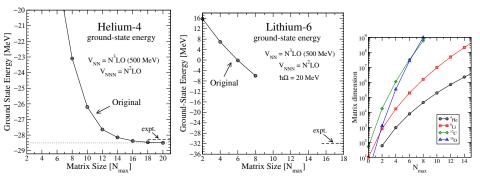
Consequences of a repulsive core



- Probability at short separations suppressed ⇒ "correlations"
- Short-distance structure ⇔ high-momentum components
- Greatly complicates expansion of many-body wave functions

Many short wavelengths ⇒ Large matrices

- ullet Harmonic oscillator basis with N_{max} shells for excitations
- Graphs show convergence for *soft* chiral EFT potential (although not at optimal $\hbar\Omega$ for ⁶Li)



- ullet Factorial growth of basis with $A\Longrightarrow$ limits calculations
- Problem: mismatch of scales/dof's. Solution: use RG.

S. Weinberg on the Renormalization Group

- From "Why the Renormalization Group is a good thing" "The method in its most general form can I think be understood as a way to arrange in various theories that the degrees of freedom that you're talking about are the relevant degrees of freedom for the problem at hand."
- Third Law of Progress in Theoretical Physics: "You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

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- Improving perturbation theory in high-energy physics
 - Mismatch of energy scales can generate large logarithms
 - Shift between couplings and loop integrals to reduce logs
- Universality in critical phenomena
 - Filter out short-distance degrees of freedom
- Simplifying calculations of nuclear structure/reactions
 - Make nuclear physics look more like quantum chemistry!
 - Like other RG applications, can seem like magic

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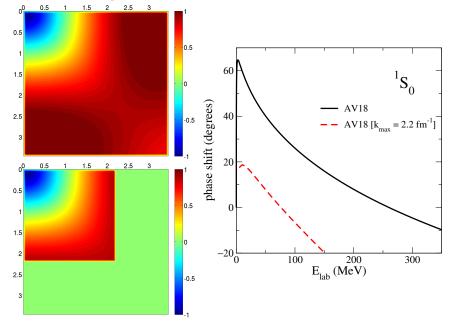
Outlook

Low-pass filter on an image



- Much less information needed
- Long-wavelength info is preserved
- Could also lower resolution by "block spinning"

Effect of low-pass filter on observables



Why did our low-pass filter fail?

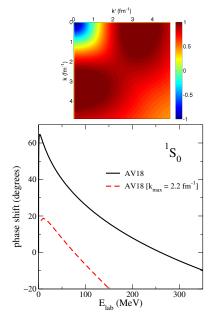
- Basic problem: low k and high k are coupled (wrong dof's!)
- E.g., perturbation theory for (tangent of) phase shift:

$$\langle k|V|k\rangle + \sum_{k'} \frac{\langle k|V|k'\rangle\langle k'|V|k\rangle}{(k^2-k'^2)/m} + \cdots$$

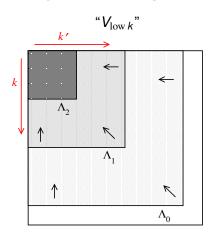
 Solution: Unitary transformation of the H matrix ⇒ decouple!

$$E_{n} = \langle \Psi_{n} | H | \Psi_{n} \rangle \quad U^{\dagger} U = 1$$
$$= (\langle \Psi_{n} | U^{\dagger}) U H U^{\dagger} (U | \Psi_{n} \rangle)$$
$$= \langle \widetilde{\Psi}_{n} | \widetilde{H} | \widetilde{\Psi}_{n} \rangle$$

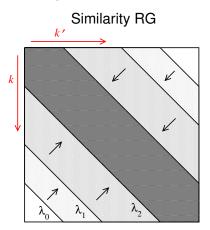
• Here: Decouple using RG



Two ways to decouple with RG equations



• Lower a cutoff Λ_i in k, k', e.g., demand $dT(k, k'; k^2)/d\Lambda = 0$



 Drive the Hamiltonian toward diagonal with "flow equation" [Wegner; Glazek/Wilson (1990's)]

⇒ Both tend toward universal low-momentum interactions!

$$\frac{dV_{\lambda}}{d\lambda}(k,k') \propto -(\epsilon_{k} - \epsilon_{k'})^{2} V_{\lambda}(k,k') + \sum_{q} (\epsilon_{k} + \epsilon_{k'} - 2\epsilon_{q}) V_{\lambda}(k,q) V_{\lambda}(q,k')$$

$${}^{1}S_{0} \quad \lambda = 20.0 \text{ fm}^{-1}$$

$$\frac{dV_{\lambda}}{d\lambda}(k,k') \propto -(\epsilon_{k} - \epsilon_{k'})^{2} V_{\lambda}(k,k') + \sum_{q} (\epsilon_{k} + \epsilon_{k'} - 2\epsilon_{q}) V_{\lambda}(k,q) V_{\lambda}(q,k')$$

$${}^{1}S_{0} \quad \lambda = 15.0 \text{ fm}^{-1}$$

$$\frac{dV_{\lambda}}{d\lambda}(k,k') \propto -(\epsilon_{k} - \epsilon_{k'})^{2} V_{\lambda}(k,k') + \sum_{q} (\epsilon_{k} + \epsilon_{k'} - 2\epsilon_{q}) V_{\lambda}(k,q) V_{\lambda}(q,k')$$

$${}^{1}S_{0} \quad \lambda = 12.0 \text{ fm}^{-1}$$

$$\frac{dV_{\lambda}}{d\lambda}(k,k') \propto -(\epsilon_{k} - \epsilon_{k'})^{2} V_{\lambda}(k,k') + \sum_{q} (\epsilon_{k} + \epsilon_{k'} - 2\epsilon_{q}) V_{\lambda}(k,q) V_{\lambda}(q,k')$$

$${}^{1}S_{0} \quad \lambda = 10.0 \text{ fm}^{-1}$$

$$\frac{dV_{\lambda}}{d\lambda}(k,k') \propto -(\epsilon_{k} - \epsilon_{k'})^{2} V_{\lambda}(k,k') + \sum_{q} (\epsilon_{k} + \epsilon_{k'} - 2\epsilon_{q}) V_{\lambda}(k,q) V_{\lambda}(q,k')$$

$${}^{1}S_{0} \quad \lambda = 6.0 \text{ fm}^{-1}$$

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$${}^{1}S_{0} \quad \lambda = 5.0 \text{ fm}^{-1}$$

$$\frac{dV_{\lambda}}{d\lambda}(k,k') \propto -(\epsilon_{k} - \epsilon_{k'})^{2} V_{\lambda}(k,k') + \sum_{q} (\epsilon_{k} + \epsilon_{k'} - 2\epsilon_{q}) V_{\lambda}(k,q) V_{\lambda}(q,k')$$

$${}^{1}S_{0} \quad \lambda = 4.0 \text{ fm}^{-1}$$

$$\frac{dV_{\lambda}}{d\lambda}(k,k') \propto -(\epsilon_{k} - \epsilon_{k'})^{2} V_{\lambda}(k,k') + \sum_{q} (\epsilon_{k} + \epsilon_{k'} - 2\epsilon_{q}) V_{\lambda}(k,q) V_{\lambda}(q,k')$$

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$${}^{1}S_{0} \quad \lambda = 2.8 \text{ fm}^{-1}$$

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$${}^{1}S_{0} \quad \lambda = 2.2 \text{ fm}^{-1}$$

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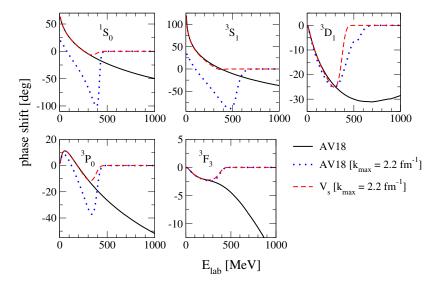
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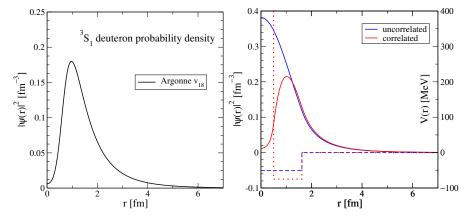
$${}^{0}O_{0.5}$$

Low-Pass Filters Work! [Jurgenson et al., (2008)]

• Phase shifts with $V_s(k, k') = 0$ for $k, k' > k_{max}$

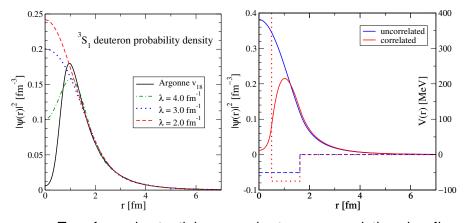


Consequences of a Repulsive Core Revisited



- Probability at short separations suppressed ⇒ "correlations"
- Greatly complicates expansion of many-body wave functions
- Short-distance structure ⇔ high-momentum components

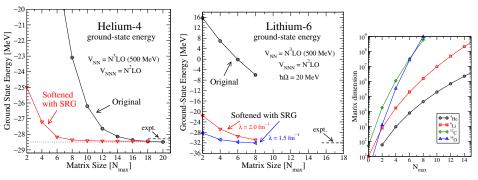
Consequences of a Repulsive Core Revisited



- ullet Transformed potential \Longrightarrow no short-range correlations in wf!
- Potential is now non-local: $V(\mathbf{r})\psi(\mathbf{r}) \longrightarrow \int d^3\mathbf{r}' \ V(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}')$
 - A problem for Green's Function Monte Carlo approach
 - Not a problem for many-body methods using HO matrix elements

Many short wavelengths ⇒ Large matrices

- Harmonic oscillator basis with N_{max} shells for excitations
- Graphs show convergence for soft chiral EFT potential and evolved SRG potentials (including NNN)



■ Better convergence, but rapid growth of basis still a problem
 ⇒ see talk by R. Roth

Basics: SRG flow equations [arXiv:0912.3688]

• Transform an initial hamiltonian, H = T + V:

$$H_s = U_s H U_s^{\dagger} \equiv T + V_s$$
,

where s is the *flow parameter*. Differentiating wrt s:

$$\frac{dH_s}{ds} = [\eta_s, H_s]$$
 with $\eta_s \equiv \frac{dU_s}{ds} U_s^{\dagger} = -\eta_s^{\dagger}$.

• η_s is specified by the commutator with "generator" G_s :

$$\eta_s = [G_s, H_s]$$

which yields the flow equation (T held fixed),

$$\frac{dH_s}{ds} = \frac{dV_s}{ds} = [[G_s, H_s], H_s].$$

• G_s determines flow \Longrightarrow many choices $(T, H_D, H_{BD}, ...)$

Flow in momentum basis with $G_s = T$

• For A = 2, project on rel. momentum states $|k\rangle$, but generic

$$\frac{dV_s}{ds} = [[T_{\rm rel}, V_s], H_s]$$
 with $T_{\rm rel}|k\rangle = \epsilon_k|k\rangle$ and $\lambda^2 = 1/\sqrt{s}$

$$\frac{dV_{\lambda}}{d\lambda}(k,k') \propto -(\epsilon_{k} - \epsilon_{k'})^{2} V_{\lambda}(k,k') + \sum_{q} (\epsilon_{k} + \epsilon_{k'} - 2\epsilon_{q}) V_{\lambda}(k,q) V_{\lambda}(q,k')$$

$$V_{\lambda=3.0}(k,k') \qquad \text{1st term} \qquad \text{2nd term} \qquad V_{\lambda=2.5}(k,k')$$

• First term drives ${}^{1}S_{0}$ V_{λ} toward diagonal:

$$V_{\lambda}(k,k') = V_{\lambda=\infty}(k,k') e^{-\left[\left(\epsilon_k - \epsilon_{k'}\right)/\lambda^2\right]^2} + \cdots$$

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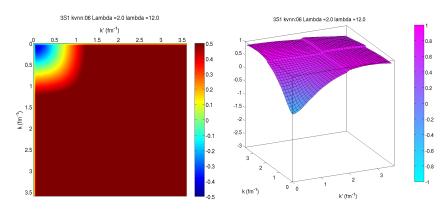
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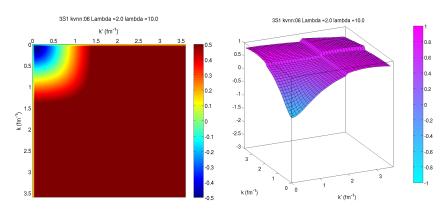
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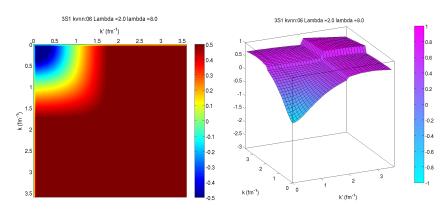
- Can we get a $\Lambda = 2 \, \text{fm}^{-1} \, V_{\text{low } k}$ -like potential with SRG?
- Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$



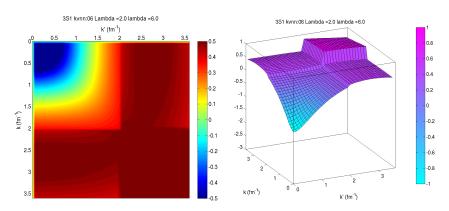
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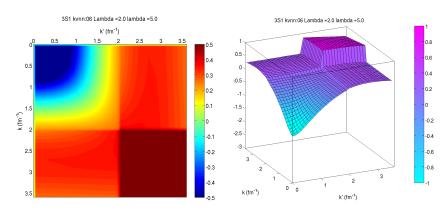
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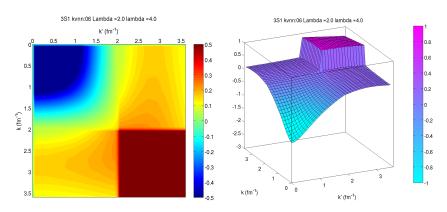
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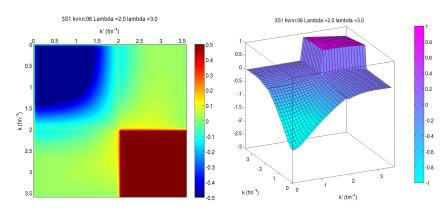
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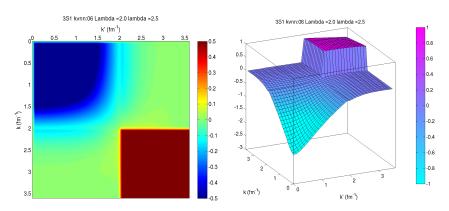
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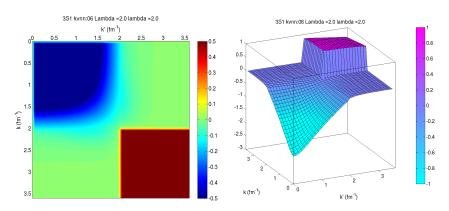
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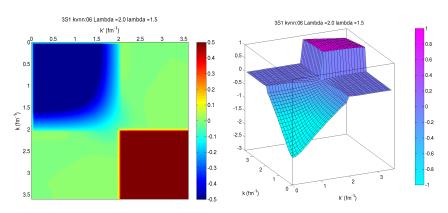
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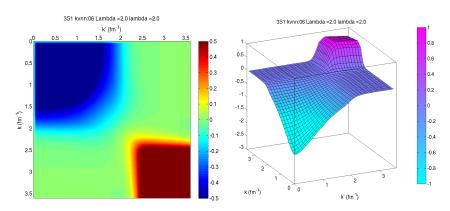
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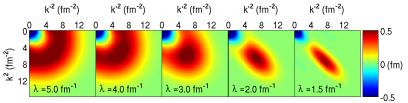


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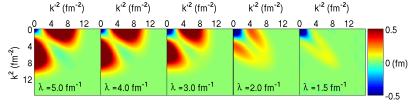


Flow of N³LO chiral EFT potentials

• ¹S₀ from N³LO (500 MeV) of Entem/Machleidt



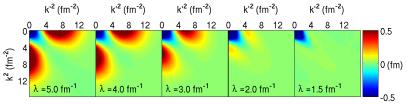
• ${}^{1}S_{0}$ from N³LO (550/600 MeV) of Epelbaum et al.



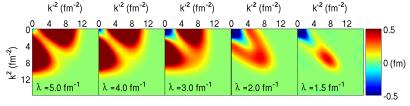
Significant decoupling even for "soft" EFT interaction

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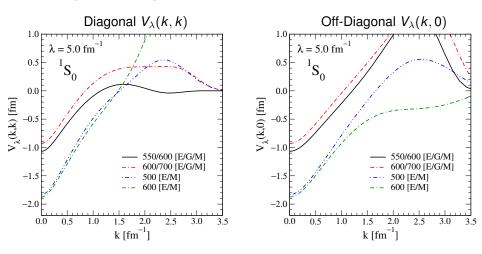
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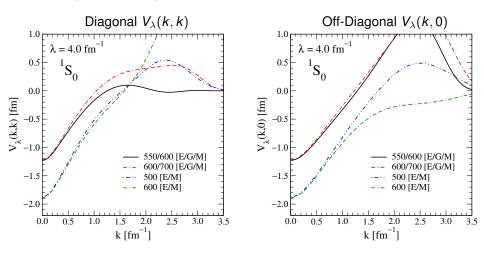
• 3S_1 from N 3 LO (550/600 MeV) of Epelbaum et al.



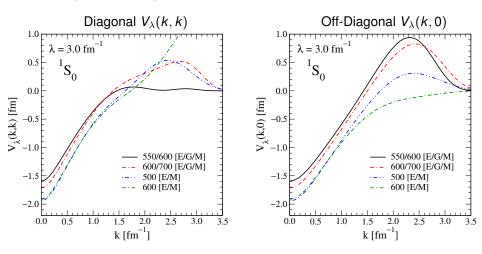
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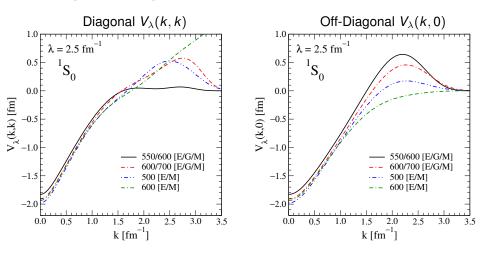
- Consistent with inverse scattering when S-matrices agree
- Will evolved NNN interactions be universal?



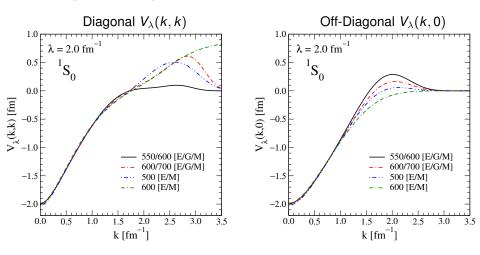
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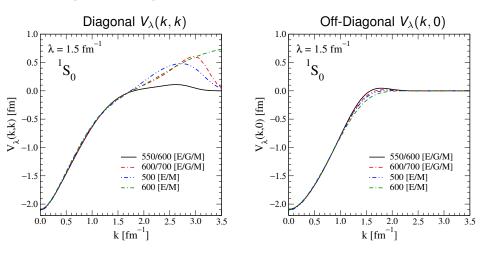
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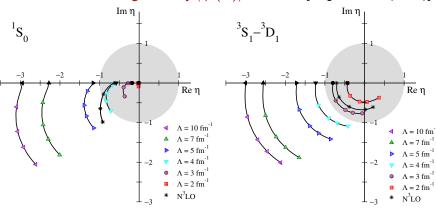
Lowering resolution increases "perturbativeness"

Born Series:
$$T(E) = V + V \frac{1}{E - H_0} V + V \frac{1}{E - H_0} V \frac{1}{E - H_0} V + \cdots$$

• For fixed E, find (complex) eigenvalues $\eta_{\nu}(E)$ [Weinberg]

$$\frac{1}{E-H_0}V|\Gamma_{\nu}\rangle=\eta_{\nu}|\Gamma_{\nu}\rangle \quad \Longrightarrow \quad T(E)|\Gamma_{\nu}\rangle=V|\Gamma_{\nu}\rangle(1+\eta_{\nu}+\eta_{\nu}^2+\cdots)$$

$$\implies$$
 T diverges if any $|\eta_{\nu}(E)| \ge 1$ [Bogner et al. (2006)]

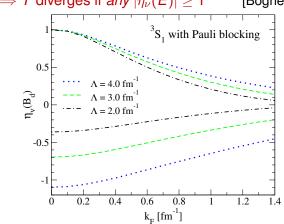


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Flow equations lead to many-body operators

• Consider a's and a^{\dagger} 's wrt s.p. basis and reference state:

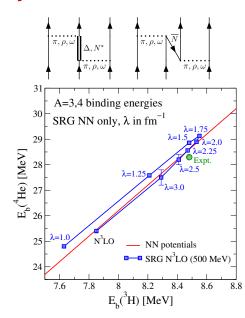
$$\frac{dV_s}{ds} = \left[\left[\sum \underbrace{a^{\dagger}a}_{G_s}, \sum \underbrace{a^{\dagger}a^{\dagger}aa}_{2\text{-body}} \right], \sum \underbrace{a^{\dagger}a^{\dagger}aa}_{2\text{-body}} \right] = \dots + \sum \underbrace{a^{\dagger}a^{\dagger}a^{\dagger}aaa}_{3\text{-body}!} + \dots$$

so there will be A-body forces (and operators) generated

- Is this a problem?
 - Ok if "induced" many-body forces are same size as natural ones
- Nuclear 3-body forces already needed in unevolved potential
 - In fact, there are A-body forces (operators) initially
 - Natural hierarchy from chiral EFT \implies stop flow equations before unnatural or tailor G_s to suppress
 - Still needed: analytic bounds on A-body growth
- SRG is a tractable method to evolve many-body operators
- Alternative: choose a non-vacuum reference state
 in-medium SRG (e.g., HF reference state)

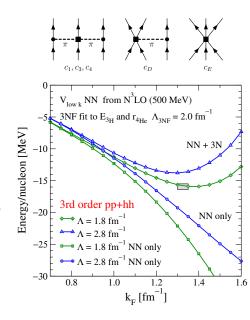
Observations on three-body forces

- Three-body forces arise from eliminating/decoupling dof's
 - excited states of nucleon
 - relativistic effects
 - high-momentum intermediate states
- Omitting 3-body forces leads to model dependence
 - observables depend on Λ/λ
 - cutoff dependence as tool



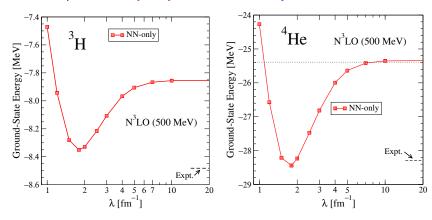
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- Omitting 3-body forces leads to model dependence
 - observables depend on Λ/λ
 - cutoff dependence as tool
- NNN at different Λ/λ must be fit or evolved to χEFT
 - NNN contribution is important at low resolution (e.g., nuclear matter)
 - how large is 4-body?



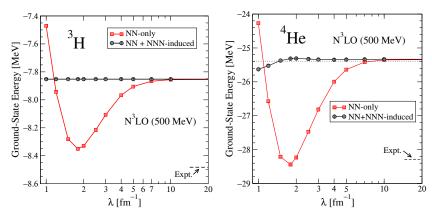
3D SRG evolution with $T_{\rm rel}$ in a Jacobi HO basis

- Evolve in any basis [E. Jurgenson, P. Navrátil, rjf (2009)]
 - Here: use anti-symmetric Jacobi HO basis from NCSM
 - Directly obtain SRG matrix elements in HO basis
 - Separate 3-body evolution not needed
- Compare 2-body only to full 2 + 3-body evolution:



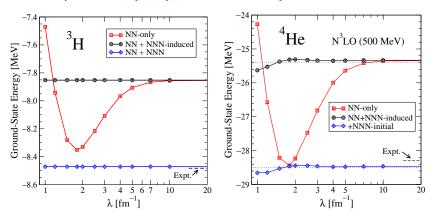
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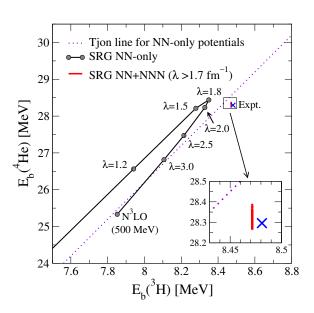


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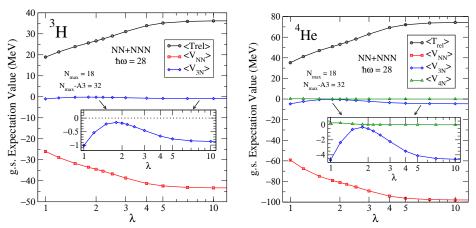


Tjon line revisited



Contributions to the ground-state energy

Look at ground-state matrix elements of KE, NN, 3N, 4N



- Clear hierarchy, but also strong cancellations at NN level
- What about the A dependence? [See R. Roth talk]

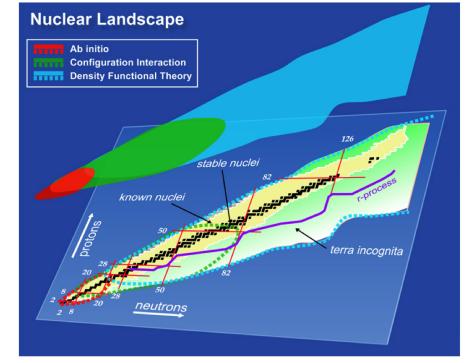
Outline

Overview: Low-energy nuclear physics

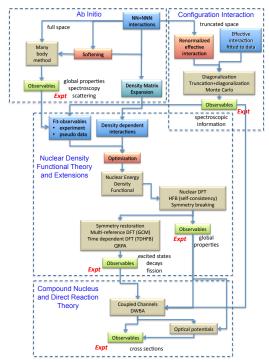
Lowering the resolution with RG

Survey of calculations at low resolution

Outlook



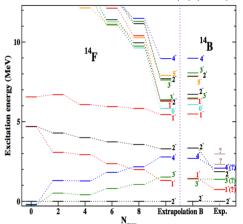
- SciDAC UNEDF project
- Universal Nuclear Energy Density Functional
- Collaboration of physicists, applied mathematicians, and computer scientists
- US funding but international collaborators also
- See unedf.org for highlights



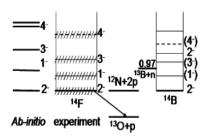
Unstable "proton-dripping" fluorine-14

- Ab initio calculation using low-k inverse-scattering potential
- Theory preceded recent experimental measurement

P. Maris et al., PRC 81, 021301(R) (2010)



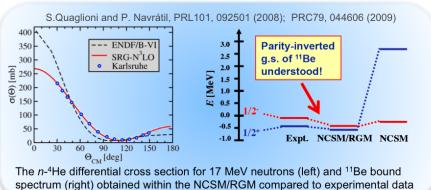
V.Z. Goldberg et al., Phys. Lett. B **692**, 307 (2010)



Matrix dimension 2 × 10⁹,
 2.5 hours on 30,000 cores

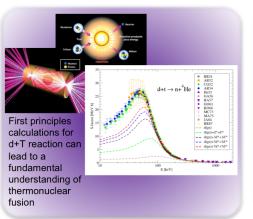
Ab initio approach to light-ion reactions

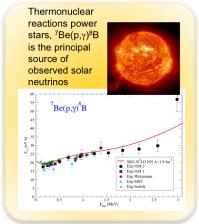
- NCSM/RGM using low momentum SRG NN interactions
- See, e.g., Navrátil, Roth, Quaglioni, PRC 82, 034609 (2010) for nucleon-nucleus scattering



Ab initio approach to light-ion reactions

Applications to fusion energy systems and stellar evolution

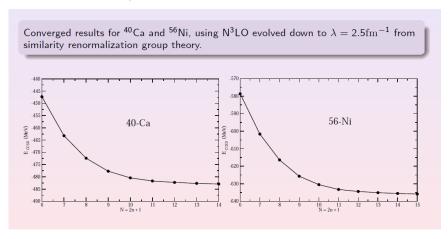




Still to do: including SRG-evolved NNN interactions

More perturbative ⇒ like quantum chemistry

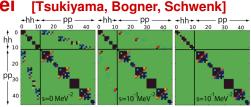
• Powerful coupled cluster method works! (figure from G. Hagen)

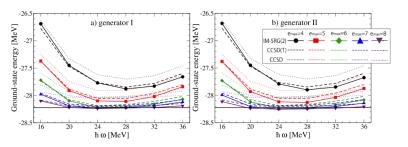


- Improved convergence with low-resolution SRG potentials but also with "bare" chiral EFT potentials [T. Pappenbrock]
- CC extended to 3-body forces by Hagen et al.

In-medium SRG for nuclei

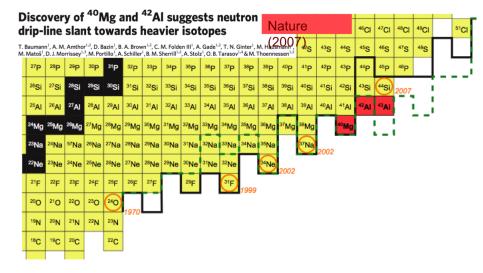
- SRG in A-body system using normal ordering
- Decouple 1p1h, 2p2h, ... sectors from (HF) reference state; approximate N-body





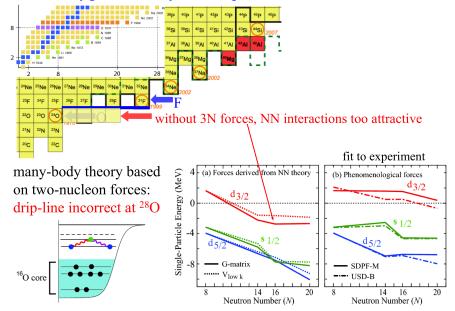
- Promising results for closed-shell nuclei: ⁴He, ¹⁶O, ⁴⁰Ca
- Energies between coupled cluster CCSD and CCSD(T)
- Non-perturbative valence shell-model effective interactions

Finding the "driplines" — limits of existence!



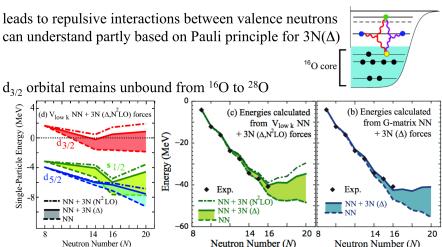
Oxygen-24 is double magic ⇒ Why is it at limit of stability?

The oxygen anomaly - not reproduced without 3N forces



The oxygen anomaly - impact of 3N forces

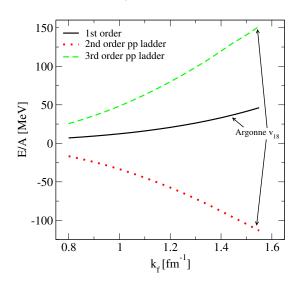
include "normal-ordered" 2-body part of 3N forces (enhanced by core A)



first microscopic explanation of the oxygen anomaly Otsuka, Suzuki, Holt, Schwenk, Akaishi (2010)

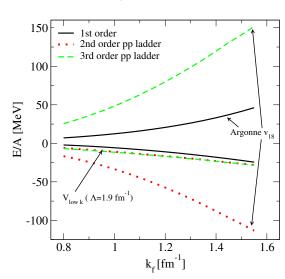
Low resolution \Longrightarrow MBPT is feasible!

- Compare high resolution to low resolution
- MBPT converges!
- R. Roth et al. ⇒ apply to finite nuclei (4NF?)



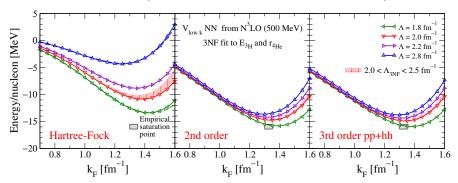
Low resolution \Longrightarrow MBPT is feasible!

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- Need 3-body force for saturation (evolved or fit)



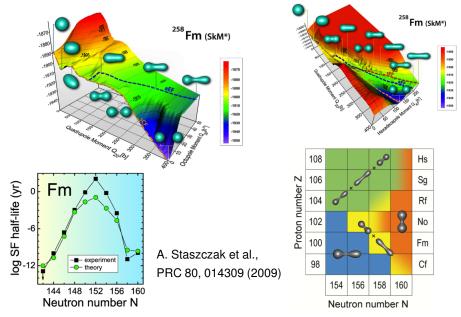
One of the paths to microscopic nuclear DFT

- Construct a chiral EFT to a given order (N³LO at present)
- Evolve Λ down with RG (to $\Lambda \approx 2 \, \text{fm}^{-1}$ for ordinary nuclei)
 - NN interactions fully, NNN interactions approximately
- Generate density functional in MBPT
 - Hartree-Fock plus "≈ second order", use "DME" in k-space



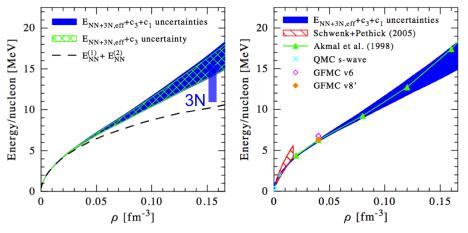
Bogner et al., (2009), Hebeler et al., (2010), Gebremariam et al., (2010)

Spontaneous fission: Energy surfaces from DFT



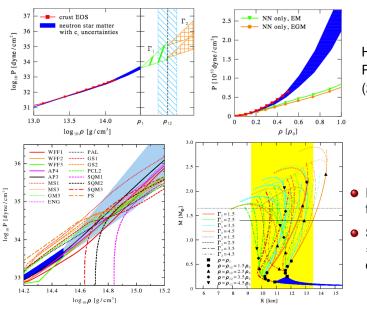
Low resolution calculations of neutron matter

- Evolve NN to low momentum, fit NNN to A = 3, 4
- Neutron matter in perturbation theory [Hebeler, Schwenk (2010)]



- Use cutoff dependence to estimate many-body uncertainty
- Uncertainties from long-range NNN constants are greatest

Constraining neutron stars: R = 9.7-13.9 km for 1.4 M_{sun}



Hebeler, Lattimer, Pethick, Schwenk (2010)

- Extrapolate EOS to higher density
- Solve for M vs. R ⇒ yellow band constrains radius

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Survey of calculations at low resolution

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Summary: Atomic Nuclei at Low Resolution

- Strategy: Lower the resolution and track dependence on it
 - High resolution ⇒ high momenta can be painful!
 ("It hurts when I do this." "Then don't do that.")
 - Correlations in wave functions reduced dramatically
 - Non-local potentials and many-body operators "induced"

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- Flow equations (SRG) achieve low resolution by decoupling
 - Band (or block) diagonalizing Hamiltonian matrix (or ...)
 - Unitary transformations: observables don't change but physics interpretation may change!
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- Applications to nuclei and beyond
 - ullet CI, coupled cluster, HH, ... converge faster \Longrightarrow new possibilities
 - Microscopic shell model ⇒ role of 3-body forces
 - MBPT works ⇒ constructive nuclear density functional theory

Some open questions and issues

- Power counting for evolved many-body interactions
 - Need analytic estimates plus more numerical tests
- Operator issues (SRG evolves operators, too!)
 - Scaling of many-body operators
 - Technical issues (e.g., boosting)
 - Factorization for many-body systems
- Can different choices for G_s ...
 - control the growth of many-body forces?
 - improve convergence in HO basis?
 - drive a non-local potential to local form?
- Use of different basis for SRG evolution
 - Need momentum-space implementation
 - Hyperspherical coordinates? (also for visualization)
- Do many-body interactions flow to universal form?
- Can the SRG help with constructing/analyzing EFT's?

Thanks: collaborators and others at low resolution

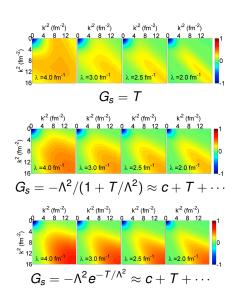
- Darmstadt: R. Roth, A. Schwenk
- INT / Chalmers: L. Platter
- Iowa State: P. Maris, J. Vary
- Michigan State: S. Bogner, H. Hergert
- LLNL: E. Jurgenson, N. Schunck
- Los Alamos: J. Drut
- Ohio State: E. Anderson, M. Bettencourt, W. Li, R. Perry, K. Wendt
- ORNL/UofT: M. Kortelainen, W. Nazarewicz, M. Stoitsov
- TRIUMF: P. Navratil
- UNEDF
- Warsaw: S. Glazek

Flow equations and the SRG: History

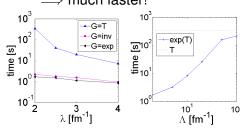
- In the early 1970's, Ken Wilson and Franz Wegner
 critical phenomena and renormalization group (RG)
- Twenty years later, Wilson and Wegner innovate again
 - Unitary RG flow to make many-particle Hamiltonians increasingly energy diagonal
 - Glazek and Wilson, "Renormalization of Hamiltonians" (1993)
 ⇒ SRG for QCD on the light front
 - Wegner, "Flow Equations for Hamiltonians" (1994)

 ⇒ condensed matter problems
- S. Kehrein, "Flow-Equation Approach to Many-Particle Systems"
 - Dissipative quantum systems to correlated electron physics to non-equilibrium problems to . . .
- Particularly well suited for low-energy nuclear physics!
 - Only applied in last few years [arXiv:0912.3688]
 - Technically simpler and more versatile than other methods

Novel generators: $G_s = f(T)$ [Shirley Li, OSU physics major]



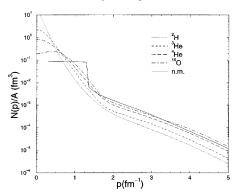
- For Λ = 2 fm⁻¹, low E part of V still decoupled
- Much less evolution at high E
 ⇒ much faster!



- Allows evolution to low λ
- Application to A > 2 evolution
- Other useful generators?

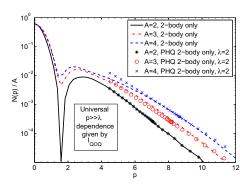
Factorization in few-body nuclei: n(k) at large k

AV14 NN with VMC



From Pieper, Wiringa, and Pandharipande (1992).

 Conventional explanation: Dominance of NN potential and short-range correlations (Frankfurt et al.) A bosons in 1D model



- Alternative: factorization $\int_0^\lambda \int_0^\lambda \ \psi_\lambda^\dagger(k') \left[I_{QOQ} K_\lambda(k') K_\lambda(k) \right] \psi_\lambda(k)$
- universal p dependence from I_{QOQ}
- norm. factor from low-energy m.e.