Effective Field Theory for Density Functional Theory IV

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I. Overview of EFT, RG, DFT for fermion many-body systems

II. EFT/DFT for dilute Fermi systems

III. Refinements: Toward EFT/DFT for nuclei

IV. Loose ends and challenges, Cold atoms, RG/DFT

Outline

Recap of Nuclear DFT/EFT and Challenges

DFT for Cold Atoms with Large Scattering Length

Segue to DFT/RG

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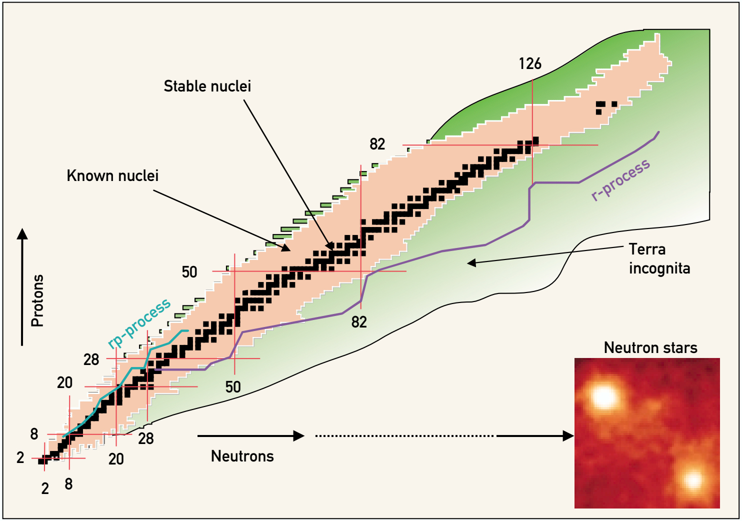


Skyrme Looks Like a Perturbative Functional!

- Skyrme energy density functional (for $N = Z$)

$$E[\rho,\tau,\mathbf{J}] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8}t_0\rho^2 + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)(\boldsymbol{\nabla}\rho)^2 - \frac{3}{4}W_0\rho\boldsymbol{\nabla}\cdot\mathbf{J} + \frac{1}{16}t_3\rho^{2+\alpha} + \cdots \right\}$$

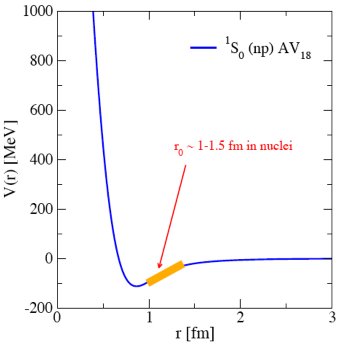
- Dilute $\rho\tau$ energy density functional for $\nu = 4$ ($V_{\mathrm{external}} = 0$)

$$E[\rho,\tau,\mathbf{J}] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8}C_0\rho^2 + \frac{1}{16}(3C_2 + 5C_2')\rho\tau + \frac{1}{64}(9C_2 - 5C_2')(\boldsymbol{\nabla}\rho)^2 - \frac{3}{4}C_2''\rho\boldsymbol{\nabla}\cdot\mathbf{J} + \frac{c_1}{2M}C_0^2\rho^{7/3} + \frac{c_2}{2M}C_0^3\rho^{8/3} + \frac{1}{16}D_0\rho^3 + \cdots \right\}$$

- But isn't nuclear matter very non-perturbative?

Sources of Nonperturbative Physics for NN

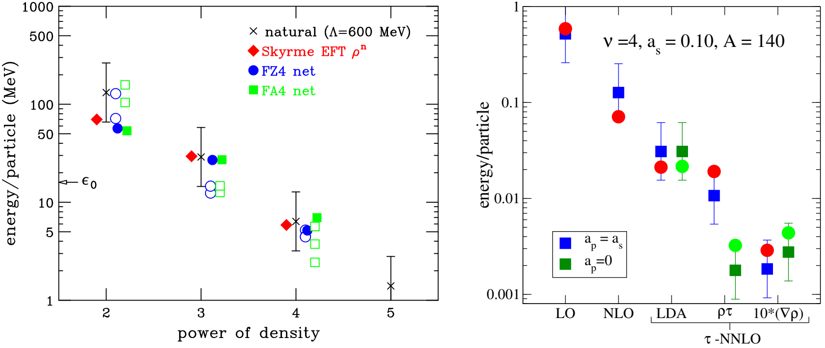
1. Strong short-range repulsion (“hard core”)
2. Iterated tensor (S_{12}) interaction
3. Near zero-energy bound states



- Consequences:
  - In Coulomb DFT, Hartree-Fock gives dominate contribution $\Longrightarrow$ correlations are small corrections $\Longrightarrow$ DFT works!
  - cf. NN interactions $\Longrightarrow$ correlations $\gg$ HF $\Longrightarrow$ DFT fails??
- However . . .
  - the first two depend on the *resolution* $\Longrightarrow$ cutoff dependent
  - third one is affected by Pauli blocking

Comparison to Skyrme

- Same functional as dilute Fermi gas with $t_i \leftrightarrow C_i$
  - equivalent $a_s \approx -2\text{–}3\,\text{fm}$ but $|k_F a_p|,\ |k_F r_s| < 1$ (with $a_p < 0$)
  - missing non-analytic terms
- Skyrme contributions show convergence in density



- Match functional at finite density $\Longrightarrow$ more perturbative?

Questions about DFT and Nuclear Structure

- How do we connect to the free NN$\cdots$N interaction?
  - Chiral EFT $\xrightarrow{RG}$ low-momentum interactions: Power counting?
- How is Kohn-Sham DFT more than “mean field”?
  - Where are the approximations? How do we truncate?
  - How do we include long-range effects (correlations)?
- What about broken symmetries? (translation, rotation, . . .)
- What about UV divergences in DFT pairing?
  - Can we (should we) decouple *pp* and *ph*?
  - Are higher-order contributions important?
- What about the “Dirac sea” in covariant DFT?

Today's Scenario for Microscopic Nuclear DFT

- Construct a chiral EFT to a given order (N^3LO at present)
  - including many-body forces (N^3LO has leading 4-body)
  - increase cutoff regulator Λ until truncation error is minimized
- Evolve Λ down with RG (to $\Lambda \approx 2\,\text{fm}^{-1}$ for ordinary nuclei)
  - *all* interactions
  - *and* other operators
- Generate density functional in effective action form
  - direct construction (e.g., DME++)
  - *or* match to finite-density EFT expansion
  - fine tune with many-body input

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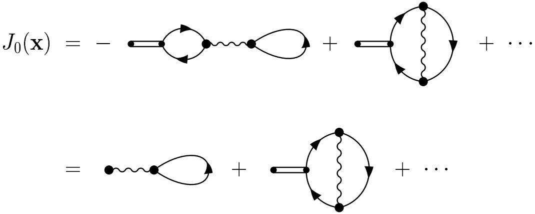
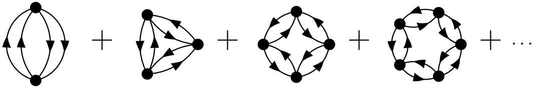
Long-range Effects

- Long-range forces (e.g., pion exchange) $\Longrightarrow$ limits of DME++



- Non-localities from near-on-shell particle-hole excitations

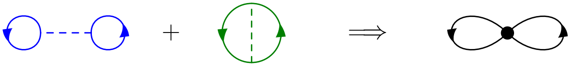


Hartree-Fock Energy using the Density Matrix

- Best single Slater determinant in variational sense

$$|\Psi_{\rm HF}\rangle = \det\{\psi_i(\mathbf{x}), i = 1\cdots A\}\,, \quad \mathbf{x} = (\mathbf{r}, \sigma, \tau)$$

- Hartree-Fock energy (suppress σ, τ):



$$\langle \Psi_{\rm HF}|\widehat{H}|\Psi_{\rm HF}\rangle = \cdots + \frac{1}{2}\sum_{i,j=1}^{A}\int d\mathbf{r}_1 \int d\mathbf{r}_2\, |\psi_i(\mathbf{r}_1)|^2 v(\mathbf{r}_1,\mathbf{r}_2)|\psi_j(\mathbf{r}_2)|^2$$

$$-\frac{1}{2}\sum_{i,j=1}^{A}\int d\mathbf{r}_1 \int d\mathbf{r}_2\, \psi_i^\dagger(\mathbf{r}_1)\psi_i(\mathbf{r}_2)v(\mathbf{r}_1,\mathbf{r}_2)\psi_j^\dagger(\mathbf{r}_2)\psi_j(\mathbf{r}_1)$$

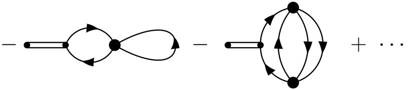
- Express in terms of single-particle density matrix:

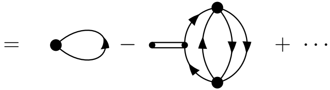
$$\rho(\mathbf{r}_1,\mathbf{r}_2) = \nu \sum_{\epsilon_\alpha \le \epsilon_{\rm F}} \psi_\alpha^\dagger(\mathbf{r}_1)\psi_\alpha(\mathbf{r}_2)$$

Density Matrix Expansion Revisited [Negele/Vautherin]

- Look for alternatives to

$$J_0(\mathbf{x}) = \frac{\delta\Gamma_{\rm int}[\rho]}{\delta\rho(\mathbf{x})} = \int \left(\frac{\delta\rho(\mathbf{x})}{\delta J_0(\mathbf{y})}\right)^{-1} \frac{\delta\Gamma_{\rm int}[\rho]}{\delta J_0(\mathbf{y})} =$$





  with explicit $\rho(\mathbf{x})$ and $\tau(\mathbf{x})$ dependence
- DME: Write one-particle density matrix in Kohn-Sham basis

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \nu \sum_{\epsilon_\alpha \le \epsilon_{\rm F}} \psi_\alpha^\dagger(\mathbf{r}_1)\psi_\alpha(\mathbf{r}_2)$$

- Change to $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ and $\mathbf{s} = \mathbf{r}_1 - \mathbf{r}_2$ and expand in $\mathbf{s}$

$$\rho(\mathbf{R} + \mathbf{s}/2, \mathbf{R} - \mathbf{s}/2) = e^{\mathbf{s}\cdot(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)/2}\, \rho(\mathbf{r}_1, \mathbf{r}_2)|_{\mathbf{s}=0}$$

Density Matrix Expansion (DME)

- Negele and Vautherin result:

$$\rho(\mathbf{r}_1,\mathbf{r}_2) = \frac{3j_1(sk)}{sk}\rho(\mathbf{R}) + \frac{35j_3(sk)}{2sk^3}\left(\frac{1}{4}\nabla^2\rho(\mathbf{R}) - \tau(\mathbf{R}) + \frac{3}{5}k^2\rho(\mathbf{R}) + \cdots\right)$$

  - Now take $\delta/\delta\rho(\mathbf{R})$ and $\delta/\delta\tau(\mathbf{R})$ derivatives directly
  - How to generalize to higher-order diagrams?
- cf. Lee and Parr gaussian: $\rho(\mathbf{r}_1,\mathbf{r}_2) \longrightarrow \rho(\mathbf{R})e^{-s^2\alpha(\mathbf{R})}$
- See also DME applied to ChPT in nuclear medium
  (N. Kaiser et al., nucl-th/0212049, 0313059, 0509040)

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Symmetry Breaking and Zero Modes

- Self-bound systems have no external potential
- The ground-state density is uniform!
- What about breaking of translational, rotational invariance, particle number?
- Little or no guidance from Coulomb DFT
- Effective action $\Longrightarrow$ zero modes
  - cf. soliton zero modes and projection methods
  - Fadeev-Popov games?
- Energy functional for the intrinsic density? [J. Engel]

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UV Divergences in Nonrelativistic and Relativistic Effective Actions

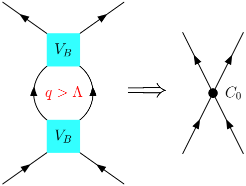
- *All* low-energy effective theories have incorrect UV behavior
- Sensitivity to short-distance physics signalled by divergences
  but finiteness (e.g., with cutoff) doesn't mean not sensitive!
  $\Longrightarrow$ must absorb (and correct) sensitivity by renormalization
- Instances of UV divergences

nonrelativistic	covariant
scattering	scattering
pairing	pairing
	anti-nucleons

Power Counting Lost / Power Counting Regained

- Gasser, Sainio, Svarc $\Longrightarrow$ ChPT for πN with relativistic N's
  - loop and momentum expansions don't agree
    $\Longrightarrow$ systematic power counting lost
  - heavy-baryon EFT restores power counting by $1/M$ expansion
- Hua-Bin Tang (1996) [and with Paul Ellis]:

  "…EFT's permit useful low-energy expansions only if we absorb all of the hard-momentum effects into the parameters of the Lagrangian."



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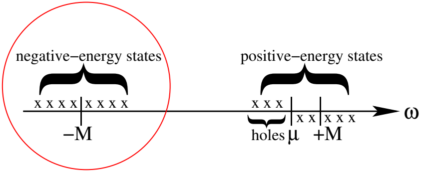


- Becher/Leutwyler IR $\Longrightarrow$ Schindler-Gegelia-Scherer version

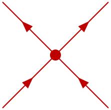
Moving Dirac Sea Physics into Coefficients

- Absorb the “hard” part of a diagram into parameters,
  $\Longrightarrow$ the remaining “soft” part satisfies chiral power counting
  - original πN prescription by H.B. Tang (expand, integrate term-by-term, and resum propagators)
  - systematized for πN by Becher and Leutwyler: “infrared regularization” or IR
  - not unique; e.g., Fuchs et al. additional finite subtractions in DR
- Extension of IR to multiple heavy particles [Lehmann/Prézeau]
  - convenient reformulation by Schindler, Gegelia, Scherer
  - tadpoles, $N\overline{N}$ loops in free space vanish!
  - particle-particle loop reduces to nonrelativistic DR/MS result

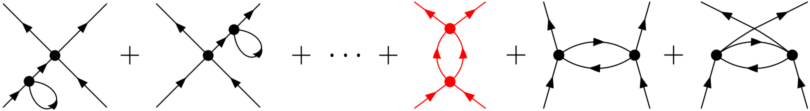
Consequences for Free-Space Natural Fermions

- Tadpoles, $N\overline{N}$ loops in free space vanish!
- Leading order (LO) has scalar, vector, etc. vertices

$$\mathcal{L}_{\rm eft} = \cdots - \frac{C_s}{2}(\overline{\psi}\psi)(\overline{\psi}\psi) - \frac{C_v}{2}(\overline{\psi}\gamma^\mu\psi)(\overline{\psi}\gamma_\mu\psi) + \cdots \Longrightarrow$$



- At NLO, only particle-particle loop survives IR



- Only forward-going nucleons contribute

$\Longrightarrow$ same scattering amplitude as nonrel. DR/MS for small k

Comments on Vacuum Physics

- Unlike QED DFT, “no sea” for nuclear structure is a misnomer
  - include “vacuum physics” in coefficients via renormalization
- Renormalization versus Renormalizability
  - Renormalization is required to account for short-distance behavior but can be implicit
  - Renormalizability at the hadronic level corresponds to making a model for the short-distance behavior
    - not a good model phenomenologically
  - Fixing short-distance behavior is not the same thing as throwing away negative-energy states
- For a long time, searched for *unique* “relativistic effects”; these were largely misguided efforts

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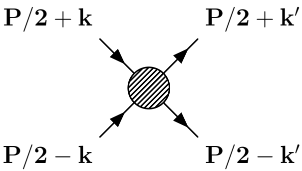
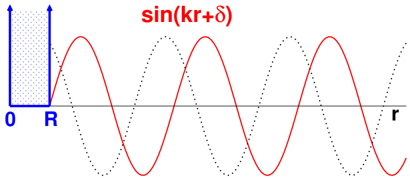
Recap of Nuclear DFT/EFT and Challenges

DFT for Cold Atoms with Large Scattering Length

Segue to DFT/RG

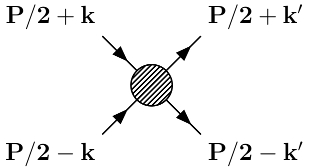
Quick Review of Scattering

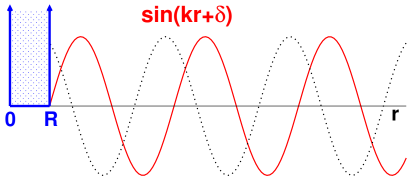




- Relative motion with total $P = 0$: $\psi(r) \xrightarrow{r\to\infty} e^{i\mathbf{k}\cdot\mathbf{r}} + f(k,\theta)\frac{e^{ikr}}{r}$
  where $k^2 = k'^2 = ME_k$ and $\cos\theta = \hat{k}\cdot\hat{k}'$
- Differential cross section is $d\sigma/d\Omega = |f(k,\theta)|^2$

Quick Review of Scattering





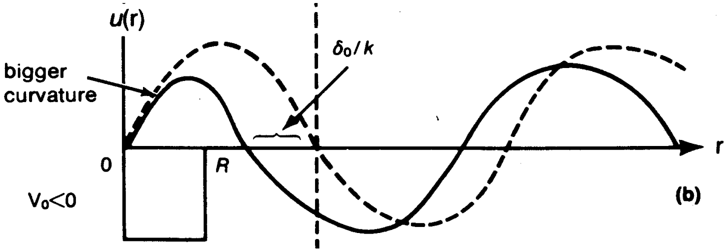
- Relative motion with total $P = 0$: $\psi(r) \overset{r\to\infty}{\longrightarrow} e^{i\mathbf{k}\cdot\mathbf{r}} + f(k,\theta)\frac{e^{ikr}}{r}$
  where $k^2 = k'^2 = ME_k$ and $\cos\theta = \hat{k}\cdot\hat{k}'$
- Differential cross section is $d\sigma/d\Omega = |f(k,\theta)|^2$
- Central $V \implies$ partial waves:
  $f(k,\theta) = \sum_l (2l+1) f_l(k) P_l(\cos\theta)$

$$\text{where} \quad f_l(k) = \frac{e^{i\delta_l(k)}\sin\delta_l(k)}{k} = \frac{1}{k\cot\delta_l(k) - ik}$$

  and the S-wave phase shift is defined by

$$u_0(r) \overset{r\to\infty}{\longrightarrow} sin[kr + \delta_0(k)] \quad \Longrightarrow \quad \delta_0(k) = -kR \text{ for hard sphere}$$

Effective Range Expansion



Total cross section: $$\sigma_{\rm total} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l(k)$$

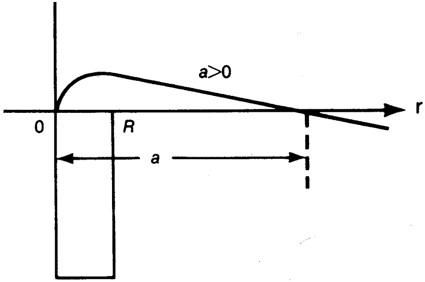
- What happens at low energy ($\lambda = 2\pi/k \gg 1/R$)?

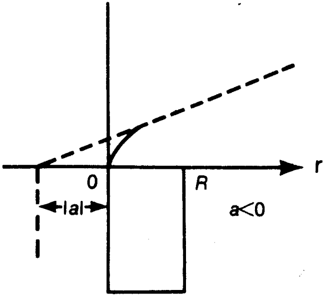
$$k\cot\delta_0(k) \xrightarrow{k\to 0} -\frac{1}{a_0} + \frac{1}{2}r_0 k^2 + \ldots$$

  - a_0 is the “scattering length” and r_0 is the “effective range”

Near-Zero-Energy Bound States

- Bound-state or near-bound state at zero energy
  $\Longrightarrow$ large scattering lengths ($a_0 \to \pm\infty$)





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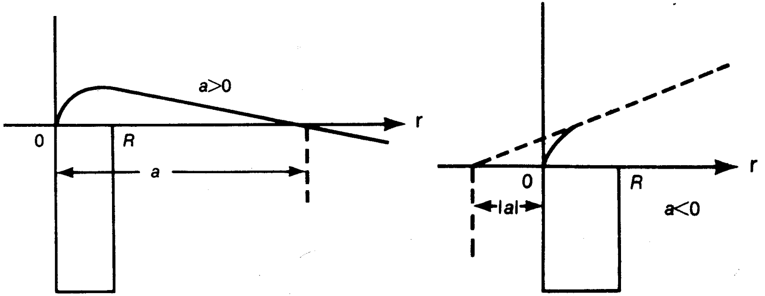
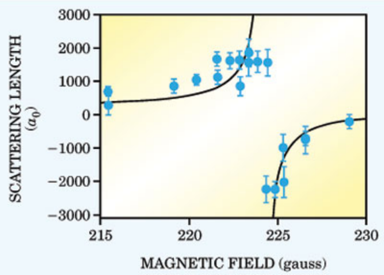


- For $kR \to 0$, the total cross section is

$$\sigma_{\rm total} = \sigma_{l=0} = \frac{4\pi a_0^2}{1+(ka_0)^2} = \begin{cases} 4\pi a_0^2 & \text{for } ka_0 \ll 1 \\ \dfrac{4\pi}{k^2} & \text{for } ka_0 \gg 1 \text{ (unitarity limit)} \end{cases}$$

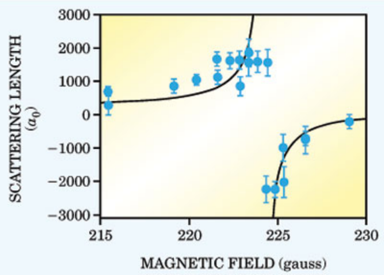
Trapped Fermion Atoms vs. QCD

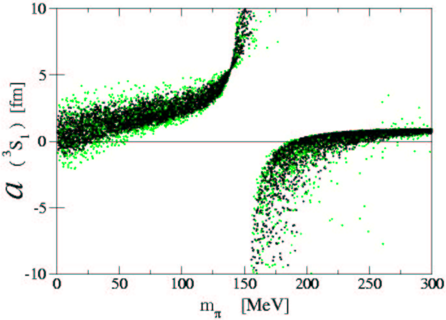
- Atoms: Change magnetic field $\Longrightarrow$ resonant scattering



Trapped Fermion Atoms vs. QCD

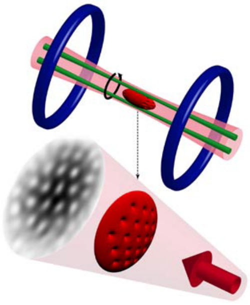
- Atoms: Change magnetic field $\Longrightarrow$ resonant scattering
- QCD: Adjust quark mass theoretically $\Longrightarrow$ m_π changes more

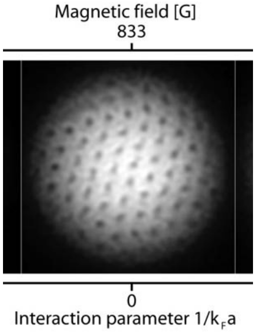


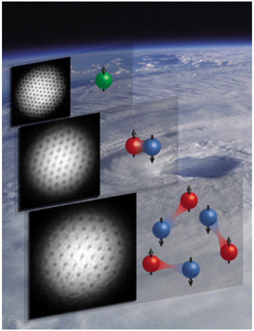


- Universal properties?

Observation of Vortices by W. Ketterle Group (MIT)

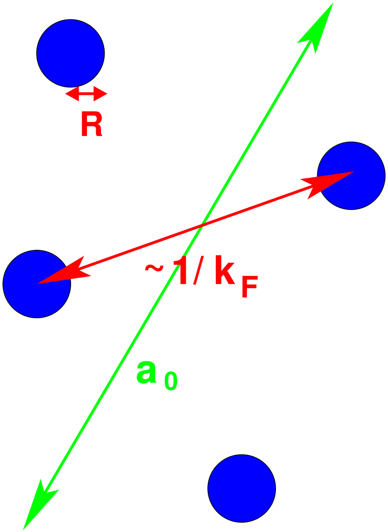




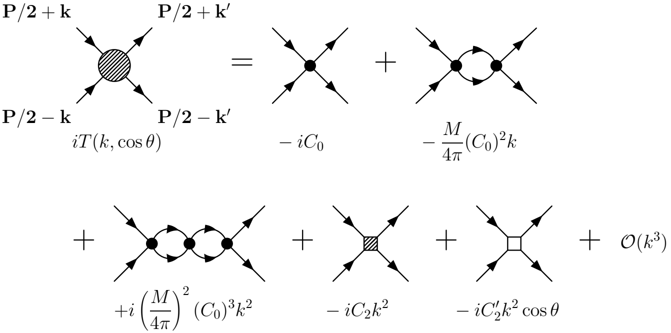


Large Scattering Length Problem

- Attractive with $a_0 \to \infty$
- If $R \ll 1/k_F \ll a_0$, then expect scale invariance
- Energy and gap are pure numbers times $E_{FG} = \frac{3}{5}\frac{k_F^2}{2M}$
- EFT power counting says: sum everything with leading vertices
  - Easy in free space $\Longrightarrow$ geometric sum of bubbles
  - Many more diagrams in the medium



- Dim. reg. + minimal subtraction when $a_0 \to \infty, \quad r_0/a_0 \to 0$

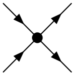


- Before: $C_0 = \frac{4\pi}{M} a_0$ but now $ka_0 \gg 1$ so bubble chains diverge
- Geometric sum $\Longrightarrow f_0(k)$ expansion keeping ka_0 to all orders:

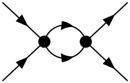
$$f_0(k) \propto \frac{1}{-1/a_0 + r_0 k^2/2 - ik} \longrightarrow \frac{-1}{1/a_0 + ik}\left[1 + \frac{r_0/2}{1/a_0 + ik} k^2 + \cdots\right]$$

Power Counting with Large a_0

- With natural a_0, perturbative expansion since $ka_0 \ll 1$
  - Choose renormalization scheme to reproduce
  - DR/MS (minimal subtraction) particularly convenient
- With large a_0, need new renormalization scheme
  - DR/PDS proposed by Kaplan, Savage, Wise $\Longrightarrow$ count $\mu \sim k$



$$\Longrightarrow \quad C_0(\mu) = \frac{4\pi}{M}\left(\frac{1}{-\mu + 1/a_0}\right) \xrightarrow{a_0\to\infty} -\frac{4\pi}{M\mu}$$



$$\Longrightarrow \quad \int \frac{d^D q}{(2\pi)^3}\frac{1}{k^2 - q^2 + i\epsilon} \xrightarrow{D\to 3} -\frac{\mu + ik}{4\pi}$$

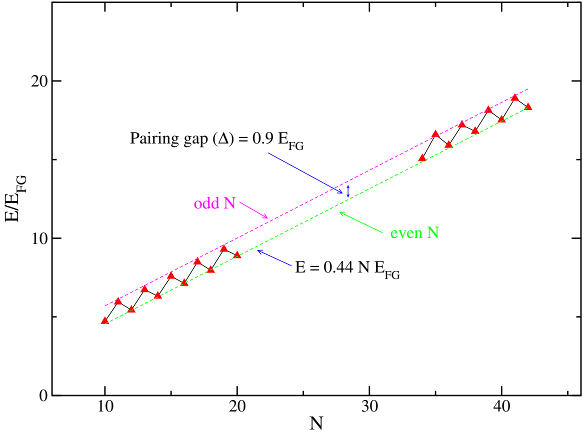
- In medium, each additional C_0 vertex gives a factor

$$C_0(k_{\rm F})\left(\frac{M}{k_{\rm F}^2}\right)^2\left(\frac{k_{\rm F}^5}{M}\right) \sim k_{\rm F}^0$$

$\Longrightarrow$ All C_0 diagrams are leading order!

GFMC Results [J. Carlson et al.]

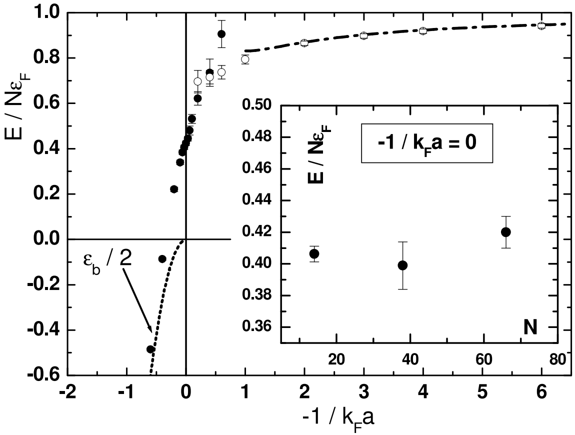
- Extrapolate to large numbers of fermions



- Energy per particle: $E/N = 0.44(1)E_{\rm FG}$

Diffusion MC Results [G.E. Astrakharchik et al.]

- Square-well potential tuned to $a_0 \to \infty$
- Extrapolate to large numbers of fermions



- Energy per particle: $E/N = 0.42(1)E_{\mathrm{FG}}$

Papenbrock DFT for Unitary Regime [cond-mat/0507183]

- Simple, constrained form of the density functional

$$\mathcal{E}[\rho] = \frac{\hbar^2}{m}\left[\frac{m}{2m_{\text{eff}}}\sum_{j=1}^{N}|\nabla\phi_j(r)|^2 + \left(\xi - \frac{m}{m_{\text{eff}}}\right)c\rho^{5/3}\right] + \frac{1}{2}m\omega^2 r^2\rho$$

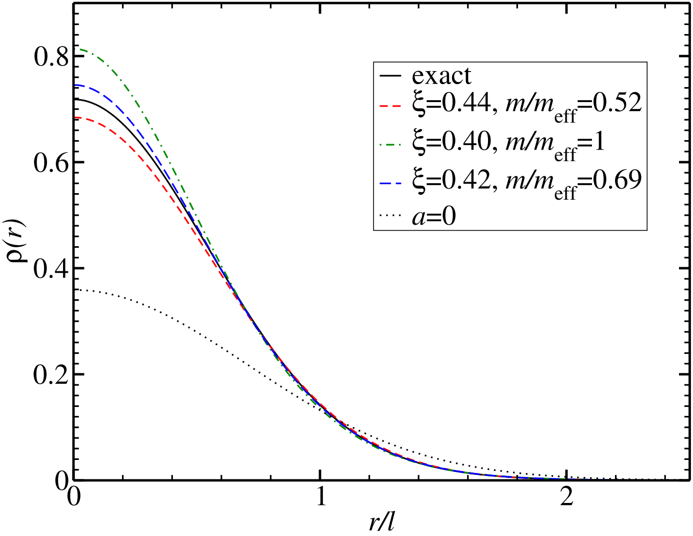
- Non-localities and gradient terms via effective mass
- Fit parameters in $E[\rho] = \int d\mathbf{x}\,\mathcal{E}[\rho(\mathbf{x})]$ for $N = 2$ to exact results for two fermions in harmonic trap [Busch et al (1998)]:

$$\psi_{\text{rel}}(r) = \frac{1}{\sqrt{2^{3/2}\pi l^3}}\frac{l}{r}e^{-r^2/4l^2} \qquad l = \sqrt{\hbar/m\omega}, \quad E = 2\hbar\omega$$

and gaussian COM wave function, which gives

$$\rho_{\text{exact}}(r) = \frac{4}{\pi^{3/2}l^3}\frac{l}{r}e^{-2(r/l)^2}\int_0^r dx\, e^{x^2}$$

Results of Fits



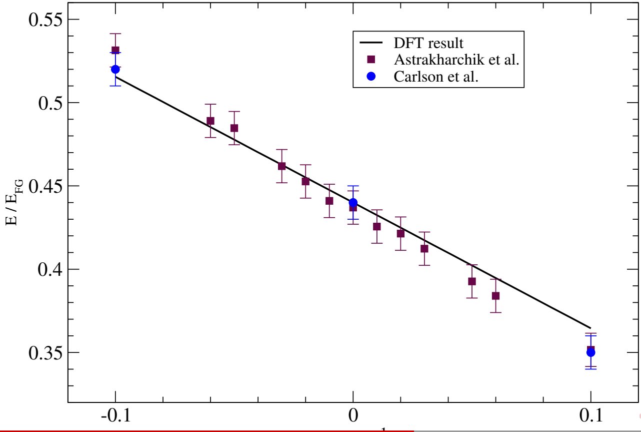
- $\xi = 0.42$, $m/m_{\text{eff}} = 0.69$ from best fit

Corrections [Bhattacharyya/Papenbrock, cond-mat/0602050]

- LDA density functional close to unitary limit

$$\mathcal{E}[\rho] = \mathcal{E}_{\text{FG}} \left(\xi + \frac{c_1}{a\rho^{1/3}} + c_2 r_0 \rho^{1/3} \right)$$

- Fit to harmonically trapped two-fermion system



General Coordinate and Conformal Invariance

[Son/Wingate cond-mat/0509786]

- Is there more than scale invariance for the unitary Fermi gas?
- Expose symmetries by adding background gauge field A_μ and curved space with metric $g_{ij}(t,\mathbf{x})$:

$$S \longrightarrow \int dt\, d\mathbf{x}\, \sqrt{g} \left[\frac{i}{2} \psi^\dagger \overleftrightarrow{\partial}_t \psi - \frac{g^{ij}}{2m} (\partial_i + iA_i)\psi^\dagger (\partial_j - iA_j)\psi \right.$$
$$\left. + (q_0\sigma - A_0)\psi^\dagger\psi - \frac{g^{ij}}{2}\partial_i\sigma\partial_j\sigma - \frac{\sigma^2}{2r_0^2} \right]$$

- More than scale and Galilean invariance!
  - Extra constraint on $\mathcal{L}_{\rm eff}$ at NLO: 5 $\rightarrow$ 3 arbitrary functions
  - For unitary Fermi gas, 3 (*scale*) $\rightarrow$ 2 (*conformal*) constants
- Are there additional constraints on the energy functional?

Outline

Recap of Nuclear DFT/EFT and Challenges

DFT for Cold Atoms with Large Scattering Length

Segue to DFT/RG

Why Use EFT for Energy Functionals

- Eliminating model dependences (no more “minimal” models!)
  - framework for building a “complete” functional
  - renormalization (you’re doing it in any case!)
- Power counting: what to sum at each order in a well-defined expansion
  - naturalness $\Longrightarrow$ estimates of truncation errors
  - robust empirical evidence from Skyrme and RMF functionals
- Similar to conventional “phenomenological” approaches
  - but with a rigorous foundation (DFT from effective action)
  - extendable and can be connected to chiral EFT for NN and few-body
- New insight into analytic structure of functional
  - e.g., logs in low-density expansion in $k_{\rm F}a_0$

(Nuclear) Many-Body Physics: "Old" vs. "New"

One Hamiltonian for all problems and energy/length scales	Infinite # of low-energy potentials; different resolutions $\Longrightarrow$ different dof's and Hamiltonians
Find the "best" potential	There is no best potential $\Longrightarrow$ use a convenient one!
Two-body data may be sufficient; many-body forces as last resort	Many-body data needed and many-body forces inevitable
Avoid divergences	Exploit divergences
Choose diagrams by "art"	Power counting determines diagrams and truncation error

Ab Initio QCD Calculations of Nuclei?

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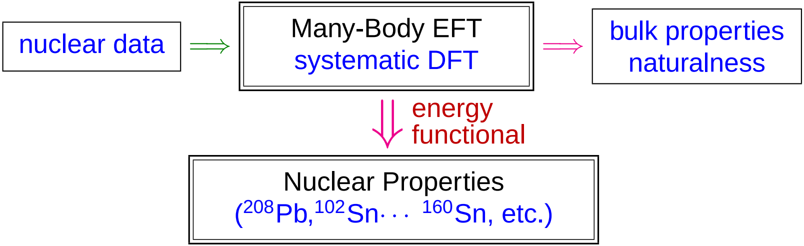
nuclear data $\Longrightarrow$ Many-Body EFT / systematic DFT $\Longrightarrow$ bulk properties / naturalness

Ab Initio QCD Calculations of Nuclei?



Ab Initio QCD Calculations of Nuclei?

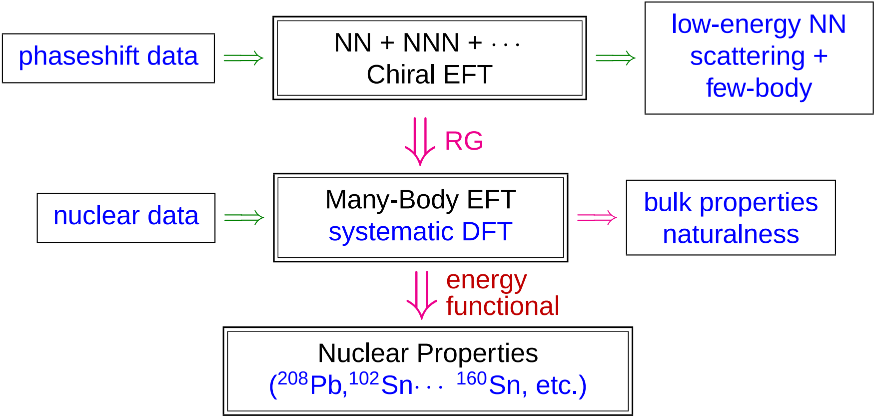
phaseshift data ⟹ NN + NNN + $\cdots$ Chiral EFT ⟹ low-energy NN scattering + few-body

nuclear data ⟹ Many-Body EFT systematic DFT ⟹ bulk properties naturalness

⇓ energy functional

Nuclear Properties (^{208}Pb, ^{102}Sn $\cdots$ ^{160}Sn, etc.)

Ab Initio QCD Calculations of Nuclei?



Ab Initio QCD Calculations of Nuclei?

Nonperturbative Lattice QCD ⟹ f_π, M_n, L_1–L_{10}

phaseshift data ⟹ NN + NNN + $\cdots$ Chiral EFT ⟹ low-energy NN scattering + few-body

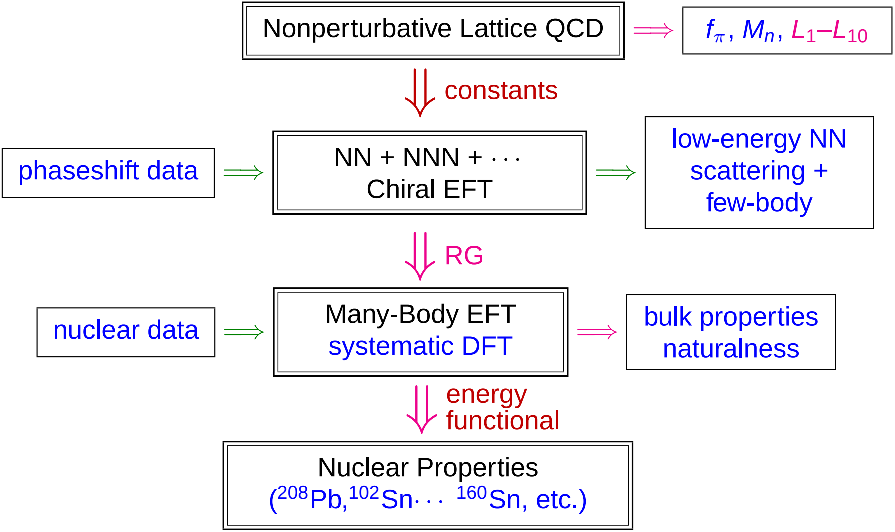
⇓ RG

nuclear data ⟹ Many-Body EFT systematic DFT ⟹ bulk properties naturalness

⇓ energy functional

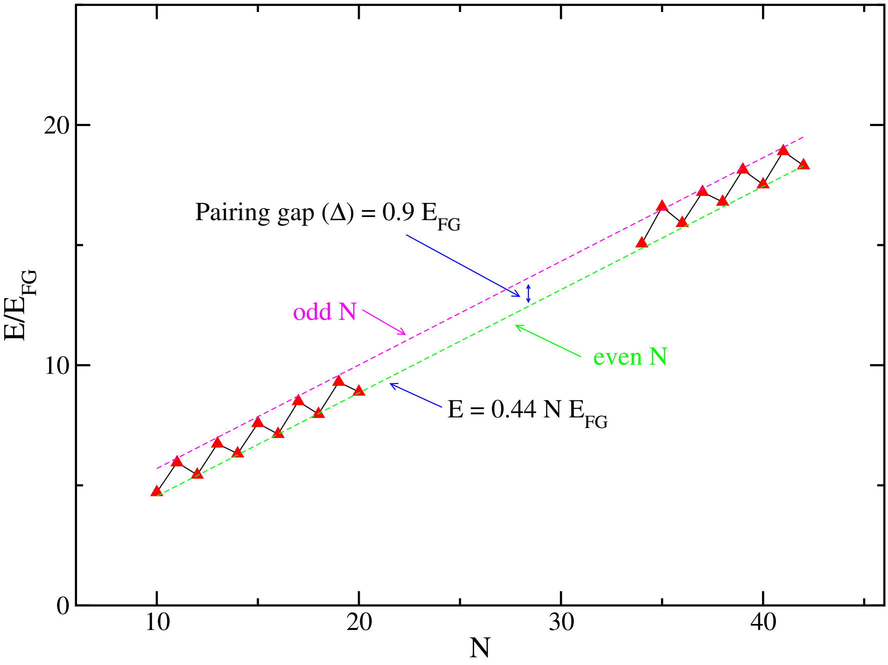
Nuclear Properties (^{208}Pb, ^{102}Sn$\cdots$ ^{160}Sn, etc.)

Ab Initio QCD Calculations of Nuclei?

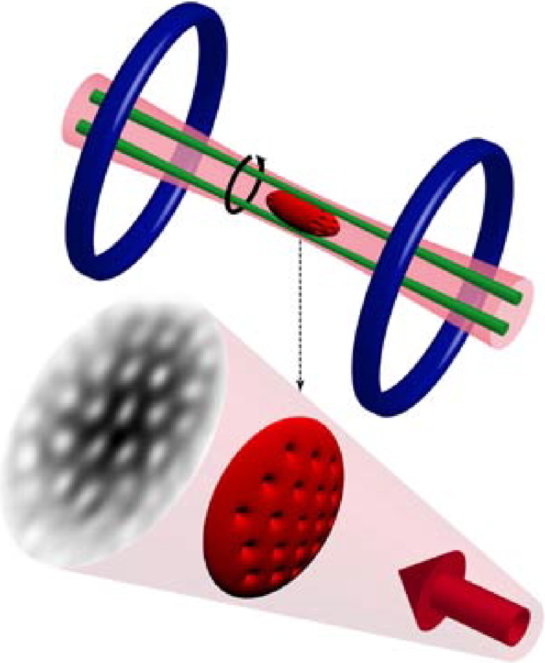


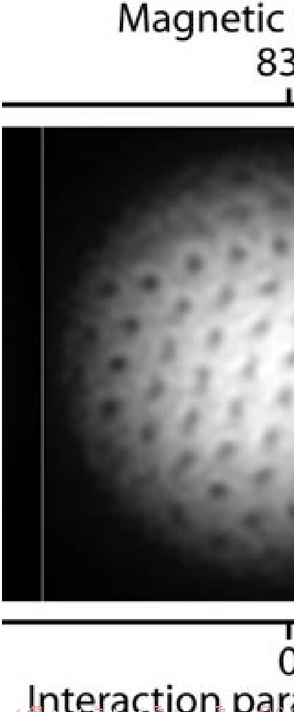
(Some) EFT/DFT Topics Not Covered

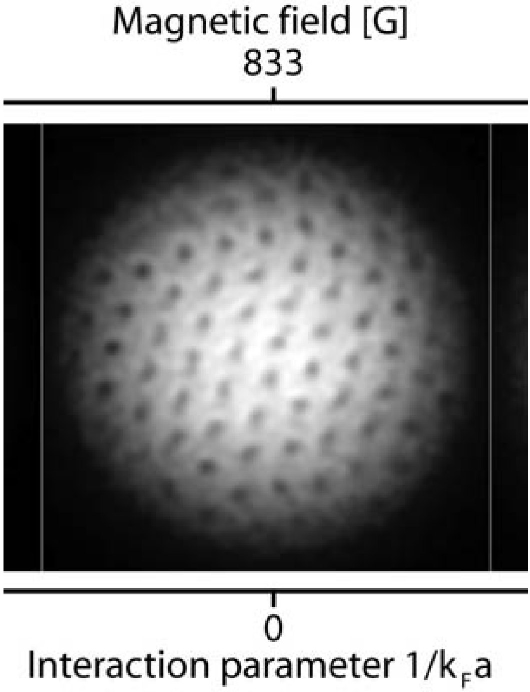
- Chiral perturbation theory in nuclear medium
  - M. Lutz, nucl-th/9906045, 9907078, 0306063
  - N. Kaiser, W. Weise et al., nucl-th/0212049, 0205016, 0412075
- Covariant density functional theory
  - Furnstahl, Serot, nucl-th/0307111, 0205048, 0005072
  - Finelli, Kaiser, Vretenar, Weise, nucl-th/0307069



Pairing gap (Δ) = 0.9 E_{FG}
odd N
even N
E = 0.44 N E_{FG}
E/E_{FG}
N
0
10
20
10
20
30
40




Magnetic
83
0
Interaction


Magnetic field [G]
833
0
Interaction parameter $1/k_F a$