Nuclear Structure and Neutron-Rich Matter

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Pictures have been freely borrowed from online sources; I apologize in advance for any omitted citations. Also, inclusion of particular calculations does not imply that they are the “best”. No animals were harmed in creating this talk.
Nuclear Structure Discussion Questions

1. What is theoretical uncertainty of the $^{208}$Pb neutron skin radius?
2. What is the uncertainty of the neutron skin requested by theory to inform the energy density functional (EDF) in a meaningful way?
3. What part of the above uncertainty comes from the bulk-matter physics and what comes from finite-nuclei physics (e.g., shell effects)?
4. What are additional experiments/calculations that can inform question 3? In particular, are open-shell systems of any interest?
5. There are many correlations between various parameters defining EDF and the neutron skin. What are the independent correlations?
6. What are the complementary quality measurements that can illuminate the question of the neutron skin?
7. Are short-range correlations of any relevance/importance to the question of neutron skin of $^{208}$Pb?
8. Are data for light weakly bound nuclei of any relevance/use to the question of the neutron skin of $^{208}$Pb?
Aspects of Nuclear Structure in Subsequent Talks

- Basic properties of finite nuclei
  - Semi-empirical mass formula (SEMF) ingredients
  - Charge and matter distributions

- Nuclear/neutron matter features and correlations
  - Density dependence of symmetry energy
  - Pairing

- Many-body methods for nuclear structure
  - Microscopic “ab initio” approaches
  - Density functional theory (DFT) [cf. mean-field models]
  - Virial expansion, . . .

- Inter-nucleon interactions $\rightarrow$ Input for structure
  - Boson-exchange (OBE) vs. chiral effective field theory (EFT)
  - Low-momentum potentials: renormalization group $\rightarrow$ “$V_{\text{low } k}$”
  - Three-body forces
Outline

“Just the Facts” About Nuclei

Symmetric and Asymmetric Nuclear Matter

Many-Body Methods

Inter-Nucleon Interactions

Final Thoughts and Prejudices
Outline

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Final Thoughts and Prejudices
Note the hierarchy of energy scales!
- How do we take advantage?
- Note the (collective) dof’s
What Does the Nuclear Potential Look Like?

Textbook answer (for $^1S_0$) — cf. force between atoms:

- Momentum units ($\hbar = c = 1$): typical relative momentum in large nucleus $\approx 1 \text{ fm}^{-1} \approx 200 \text{ MeV}$ \([E_{\text{lab}} \approx 83 \text{ MeV} \cdot \text{fm}^2 k^2_{\text{rel}}]\)
Nuclei are self-bound “liquid drops” (and superfluid!)
Isospin axis is critical in our discussion!
Landscape of Finite Nuclei

Large extrapolations to neutron stars in density and proton fraction!
What Do (Ordinary) Nuclei Look Like?

- Charge densities of magic nuclei (mostly) shown
- Proton density has to be “unfolded” from $\rho_{\text{charge}}(r)$, which comes from elastic electron scattering
- Roughly constant interior density with $R \approx (1.1–1.2 \text{ fm}) \cdot A^{1/3}$
- Roughly constant surface thickness

⇒ Like a liquid drop!
What Do Nuclei Look Like? (figures from Witek)

- Skyrme EDF densities (Energy Density Functional)
- When we have more neutrons than protons, where do the extras go?
- Extreme possibilities:
  - $r_n = r_p$ so $\rho_n > \rho_p$  
    $\implies$ no $(r_n - r_p)$ skin
  - $\rho_n = \rho_p$ so $r_n > r_p$  
    $\implies$ maximal skin
- Reality is in between!
  - What determines the balance?
  - What is it correlated with?
Neutron Skins By One Calculation (from Witek)


- Skyrme HFB SLy4 ("Hartree-Fock Bogolyubov" \(\rightarrow\) pairing)
- Other EDF's (SkX, FSUGold, ...) give different (?) results
- Skyrme vs. RMF (relativistic mean field) EDF's
Semi-Empirical Mass Formula \((A = N + Z)\)

\[
E_B(N, Z) = a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - a_{\text{sym}} \frac{(N - Z)^2}{A} + \Delta
\]

- Many predictions!
- Rough numbers:
  \(a_v \approx 16\) MeV, \(a_s \approx 18\) MeV,
  \(a_c \approx 0.7\) MeV, \(a_{\text{sym}} \approx 28\) MeV
- Pairing \(\Delta \approx \pm \frac{12}{\sqrt{A}}\) MeV
  (even-even/odd-odd) or 0
  [or \(43/A^{3/4}\) MeV or …]
- Surface symmetry energy:
  \(a_{\text{surf sym}}(N - Z)^2/A^{4/3}\)
- Much more sophisticated
  mass formulas include
  shell effects, etc.
- Sometimes \(a_{\text{sym}} \rightarrow a_4\) (or \(\alpha_i\))
Experimental Evidence for Pairing in Nuclei

\[ E_B(N, Z) = \]
\[ \text{(15.6 MeV)} \left[ 1 - 1.5 \left( \frac{N - Z}{A} \right)^2 \right] A \]
\[ - (17.2 \text{ MeV}) A^{2/3} - (0.70 \text{ MeV}) \frac{Z^2}{A^{1/3}} \]
\[ + (6 \text{ MeV}) \left[ (-1)^N + (-1)^Z \right] / A^{1/2} \]

- Odd-even staggering of binding energies (\( S_n \) is plotted)
Experimental Evidence for Pairing in Nuclei

- Odd-even staggering of binding energies \((S_n \text{ is plotted})\)
- Energy gap in spectra of deformed nuclei
- Low-lying \(2^+\) states in even nuclei
- Deformations and moments of inertia (theory requires pairing)

Figure 6.1. Excitation spectra of the \(\text{^{100}Sn}\) isotopes.
Semi-Empirical Mass Formula Per Nucleon

\[ \frac{E_B(N, Z)}{A} = a_v - a_s A^{-1/3} - a_C \frac{Z^2}{A^{4/3}} - a_{\text{sym}} \frac{(N - Z)^2}{A^2} \]

- Divide terms by \( A = N + Z \)
- Rough numbers:
  - \( a_v \approx 16 \text{ MeV}, \ a_s \approx 18 \text{ MeV}, \ a_C \approx 0.7 \text{ MeV}, \ a_{\text{sym}} \approx 28 \text{ MeV} \)
- Surface symmetry energy:
  - \( a_{\text{surf sym}} (N - Z)^2 / A^{7/3} \)
- Now take \( A \to \infty \) with Coulomb \( \to 0 \) and fixed \( N/A, Z/A \)
- Surface terms negligible
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Nuclear and Neutron Matter Energy vs. Density

[Akmal et al. calculations shown]

- Uniform with Coulomb turned off
- Density $n$ (or often $\rho$)
- Fermi momentum $n = (\nu / 6\pi^2)k_F^3$
- Neutron matter ($Z = 0$) has positive pressure
- Symmetric nuclear matter ($N = Z = A/2$) saturates

$$E(n, \alpha) = E(n, 0) + S_2(n)\alpha^2 + S_4(n)\alpha^4 + \cdots \quad \alpha \equiv I = \frac{N - Z}{A}$$

$$E(n, 0) = -a_v + \frac{K_0}{18n_0^2}(n - n_0)^2 + \cdots$$

$$S_2(n) = a_{sym} + \frac{p_0}{n_0^2}(n - n_0) + \frac{\Delta K_0}{18n_0^2}(n - n_0)^2 + \cdots$$
Density Dependence of Symmetry Energy

\[ E(n, \alpha) = E(n, \alpha = 0) + S_2(n)\alpha^2 + \cdots \quad \alpha \equiv I = (N - Z)/A \]

- Or proton fraction \( x = Z/A \)
- Nuclear matter \( \Rightarrow x = 1/2; \) Neutron matter \( \Rightarrow x = 0 \)
- \( S_2(n) \) is not pinned down by past fits to nuclei

FIG. 2. The neutron EOS for 18 Skyrme parameter sets. The filled circles are the Friedman-Pandharipande (FP) variational calculations and the crosses are SkX. The neutron density is in units of neutron/fm\(^3\).
**Neutron Skin in $^{208}$Pb vs. Symmetry Energy**

$$E(n, \alpha) = E(n, 0) + S_2(n)\alpha^2 + S_4(n)\alpha^4 + \cdots \quad \alpha = l = (N - Z)/A$$

$$E(n, 0) = -a_v + \frac{K_0}{18n_0^2}(n - n_0)^2 + \cdots$$

$$S_2(n) = a_{\text{sym}} + \frac{p_0}{n_0^2}(n - n_0) + \frac{\Delta K_0}{18n_0^2}(n - n_0)^2 + \cdots$$
Neutron Skin in $^{208}$Pb vs. Symmetry Energy

$E(n, \alpha) = E(n, 0) + S_2(n)\alpha^2 + S_4(n)\alpha^4 + \cdots \quad \alpha = I = (N - Z)/A$

$E(n, 0) = -a_v + \frac{K_0}{18n_0^2} (n - n_0)^2 + \cdots$

$S_2(n) = a_{sym} + \frac{\rho_0}{n_0^2} (n - n_0) + \frac{\Delta K_0}{18n_0^2} (n - n_0)^2 + \cdots$
Where Does the Symmetry Energy Come From?

Textbook discussion:

- Take $\alpha \equiv (N - Z)/A$ small

- Kinetic energy difference. Use $k_F^{n,p} = k_F(1 \pm \alpha)^{1/3}$ and expand: $\langle T_{\text{sym}}/A \rangle = \frac{1}{3} \frac{\hbar^2 k_F^2}{2M} \alpha^2$

- Average one-body potential $U(k)$ is most attractive for $k = 0$ $\Longrightarrow$ $\frac{1}{6} k_F \left( \frac{\partial U}{\partial k} \right)_k \alpha^2$

- More attraction for $T = 0$ n-p (singlet) than $T = 1$ n-p, p-p, n-n (triplet) and more n-p pairs when $N = Z$ $\Longrightarrow$ $\frac{1}{4} \rho (\tilde{V}_1 - \tilde{V}_0) \alpha^2$

- All cost energy like $\alpha^2$
Symmetry Energy Restoring Force in Nuclei

- Giant dipole resonance: bulk neutrons against protons

- Pygmy resonances: skin against symmetric $N = Z$ core

See Witek’s talk for assessment of correlations
What About at Very Low Densities?

- We can use scattering data directly!
  - If we want model independence, what could be better than using only data?
- EOS for a dilute gas based on virial expansion to 2nd order does this!
  - Controlled expansion in small parameter (fugacity $e^{\mu/T}$) with well-defined range of validity
  - For neutron matter, applies for $n \leq 4 \cdot 10^{11} (T/\text{MeV})^{3/2} \text{g/cm}^3$
  - Virial EOS provides benchmark for all nuclear EOS’s at low density and temperature
- See A. Schwenk’s talk for details (and assumptions)
At Low Energies: Effective Range Expansion

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

- What happens at low energy (\( \lambda = \frac{2\pi}{k} \gg \frac{1}{R} \))?
  \[
  k \cot \delta_0(k) \xrightarrow{k \to 0} -\frac{1}{a_0} + \frac{1}{2} r_0 k^2 + \ldots
  \]

- \( a_0 \) (or \( a_s \)) = “scattering length” and \( r_0 = “\text{effective range}” \)
- While \( r_0 \sim R \), the range of the potential, \( a_0 \) can be anything
  - if \( a_0 \sim R \), it is called “natural”
  - \( |a_0| \gg R \) (unnatural) is particularly interesting
    \( \Rightarrow \) cold atoms and neutrons
Near-Zero-Energy Bound States

- Bound-state or near-bound state at zero energy
  \[ \implies \text{large scattering lengths } (a_0 \to \pm \infty) \]

For \( kR \rightarrow 0 \), the total cross section is

\[
\sigma_{\text{total}} = \sigma_{l=0} = \frac{4\pi a_0^2}{1 + (ka_0)^2} = \begin{cases} 
4\pi a_0^2 & \text{for } ka_0 \ll 1 \\
\frac{4\pi}{k^2} & \text{for } ka_0 \gg 1 \text{ (unitarity limit)}
\end{cases}
\]
GFMC Results for Unitary Gas [J. Carlson et al.]

- Extrapolate to large numbers of fermions

![Graph showing GFMC results for unitary gas](image)

- Energy per particle: $E/N = 0.44(1)E_{FG}$ for $a_0 \to \infty$ and $r_0 \to 0$
- See Joe’s talk for latest neutron matter (finite $a_0$, $r_0$)
When Does Cooper Pairing Occur?

- If there is an attractive interaction at the Fermi surface, back-to-back fermions condense as Cooper pairs.

- The excitation spectrum (energy vs. momentum relation) develops a gap $\Delta$.

- For very dilute fermions, $\Delta \propto e^{-\pi/2k_F|a_0|}$.

$$\epsilon(p) = \sqrt{(p - p_F)^2 + \Delta^2}$$
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Final Thoughts and Prejudices
Given an Interaction, Why Not Just Solve?

Lattice QCD

Exact methods $A \leq 12$
GFMC, NCSM

Coupled Cluster, Shell Model
$A < 100$

Low-mom. interactions

Lattice QCD

Chiral EFT interactions
(low-energy theory of QCD)

QCD Lagrangian

Density Functional Theory $A > 100$
Reach of Microscopic Approaches (from T. Papenbrock)

Microscopic approaches

Entire chart of nuclei: Nuclear density-functional theory
Paths to a Nuclear Energy Functional (EDF)

- Empirical energy functional (Skyrme or RMF)
- Emulate Coulomb DFT: LDA based on precision calculation of uniform system $E[\rho] = \int d\mathbf{r} \mathcal{E}(\rho(\mathbf{r}))$ plus constrained gradient corrections ($\nabla \rho$ factors)

- SLDA (Bulgac et al.)
- Fayans and collaborators (e.g., nucl-th/0009034)
  
  \[
  \mathcal{E}_V = \frac{2}{3} \epsilon_F \rho_0 \left[ a_+^V \frac{1-h_1^V x_+^{1/3}}{1-h_2^V x_+^{1/3}} x_+^2 + a_-^V \frac{1-h_1^V x_-^{1/3}}{1-h_2^V x_-^{1/3}} x_-^2 \right]
  \]

  where $x_\pm = (\rho_n \pm \rho_p)/2\rho_0$

- RG approach (J. Braun, from Polonyi and Schwenk, nucl-th/0403011)
- EDF from perturbative chiral interactions + DME (Kaiser et al.)
- Constructive Kohn-Sham DFT with RG-softened $V_{\chi\text{EFT}}$'s
Hartree-Fock Wave Function

- Best single Slater determinant in variational sense

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

- Hartree-Fock energy:

$$\langle \Psi_{HF}|\hat{H}|\Psi_{HF}\rangle = \sum_{i=1}^{A} \frac{\hbar^2}{2M} \int d\mathbf{x} \nabla \phi_i^* \cdot \nabla \phi_i + \frac{1}{2} \sum_{i,j=1}^{A} \int d\mathbf{x} \int d\mathbf{y} |\phi_i(\mathbf{x})|^2 v(\mathbf{x}, \mathbf{y}) |\phi_j(\mathbf{y})|^2$$

$$- \frac{1}{2} \sum_{i,j=1}^{A} \int d\mathbf{x} \int d\mathbf{y} \phi_i^*(\mathbf{x}) \phi_i(\mathbf{y}) v(\mathbf{x}, \mathbf{y}) \phi_j^*(\mathbf{y}) \phi_j(\mathbf{x}) + \sum_{i=1}^{A} \int d\mathbf{y} v_{ext}(\mathbf{y}) |\phi_j(\mathbf{y})|^2$$

- Determine the $\phi_i$ by varying with fixed normalization:

$$\frac{\delta}{\delta \phi_i^*(\mathbf{x})} \left( \langle \Psi_{HF}|\hat{H}|\Psi_{HF}\rangle - \sum_{j=1}^{A} \epsilon_j \int d\mathbf{y} |\phi_j(\mathbf{y})|^2 \right) = 0$$
Hartree-Fock Wave Function

- Best single Slater determinant in variational sense
  \[ |\psi_{\text{HF}}\rangle = \text{det}\{\phi_i(x), i = 1 \cdots A\}, \quad x = (r, \sigma, \tau) \]
- The \( \phi_i(x) \) satisfy non-local Schrödinger equations:
  \[- \frac{\nabla^2}{2M} \phi_i(x) + \left( V_H(x) + v_{\text{ext}}(x) \right) \phi_i(x) + \int dy \, V_E(x, y) \phi_i(y) = \epsilon_i \phi_i(x)\]

with \( V_H(x) = \int dy \sum_{j=1}^{A} |\phi_j(y)|^2 v(x, y) \), \( V_E(x, y) = -v(x, y) \sum_{j=1}^{A} \phi_j(x) \phi_j^*(y) \)

- Solve self-consistently; non-local unless zero range
- Skyrme HF or RMF have local potentials \( \Rightarrow \) look like DFT
Skyrme Hartree-Fock Energy Functionals

- Skyrme energy density functional (for $N = Z$):
  
  $\mathcal{E}[\rho, \tau, J] = \frac{1}{2M} \tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha} + \frac{1}{16} (3t_1 + 5t_2) \rho \tau$
  
  $+ \frac{1}{64} (9t_1 - 5t_2) (\nabla \rho)^2 - \frac{3}{4} W_0 \rho \nabla \cdot J + \frac{1}{32} (t_1 - t_2) J^2$

- where $\rho(x) = \sum_i |\phi_i(x)|^2$ and $\tau(x) = \sum_i |\nabla \phi_i(x)|^2$ (and $J$)

- Minimize $E = \int dx \, \mathcal{E}[\rho, \tau, J]$ by varying the (normalized) $\phi_i$'s

  \[
  \left( -\nabla \frac{1}{2M^*(x)} \nabla + U(x) + \frac{3}{4} W_0 \nabla \rho \cdot \frac{1}{i} \nabla \times \sigma \right) \phi_i(x) = \epsilon_i \phi_i(x),
  \]

  \[
  U = \frac{3}{4} t_0 \rho + (\frac{3}{16} t_1 + \frac{5}{16} t_2) \tau + \cdots \text{ and } \frac{1}{2M^*(x)} = \frac{1}{2M} + (\frac{3}{16} t_1 + \frac{5}{16} t_2) \rho
  \]

- Iterate until $\phi_i$'s and $\epsilon_i$'s are self-consistent

- In practice: other densities, pairing is very important (HFB), projection needed, \ldots \Rightarrow see Witek's talk for modern status
Density Functional Theory (DFT)

- Hohenberg-Kohn: There exists an energy functional $E_{\text{ext}}[\rho]$ ...

$$E_{\text{ext}}[\rho] = F_{\text{HK}}[\rho] + \int d^3x \, v_{\text{ext}}(x) \rho(x)$$

- $F_{\text{HK}}$ is universal (same for any external $v_{\text{ext}}$) $\implies H_2$ to DNA!

- Introduce orbitals and minimize energy functional $\implies E_{gs}, \rho_{gs}$

- Useful if you can approximate the energy functional

- Construct microscopically or fit a “general” form
Microscopic Nuclear Structure Methods

- Wave function methods (GFMC/AFMC, NCSM/FCI, CC, \ldots)
  - many-body wave functions (in approximate form!)
  - $\Psi(x_1, \ldots, x_A) \implies$ everything (if operators known)
  - limited to $A < 100\text{ or } < 200\text{ or } ? ??$

- Green’s functions (see W. Dickhoff and D. Van Neck text)
  - response of ground state to removing/adding particles
  - single-particle Green’s function $\implies$ expectation value of one-body operators, Hamiltonian
  - energy, densities, single-particle excitations, \ldots

- DFT (see C. Fiolhais et al., *A Primer in Density Functional Theory*)
  - response of energy to perturbations of the density $J(x)\psi^\dagger \psi$
  - natural framework is effective actions for composite operators $\Gamma[\rho] = \Gamma_0[\rho] + \Gamma_{\text{int}}[\rho]$ (e.g., for EFT/DFT) but also consider quantum chemistry MBPT+ approach (Bartlett et al.)
  - energy functional $\implies$ plug in candidate density, get out trial energy, minimize (variational?)
  - energy and densities (TDFT $\implies$ excitations)
Two-Neutron Separation Energies

The diagram illustrates the relationship between neutron number, proton number, and two-neutron separation energy for SkP. The line $N = Z$ and $N = 2Z$ are highlighted, indicating specific energy levels and distributions across different proton and neutron numbers. The two-neutron separation energy (MeV) is shown on the x-axis, while the proton number is on the y-axis, and the neutron number is on the x-axis. The color scale represents energy values from 0 to 30 MeV.
Quadrupole Deformations and $B(E2)$
Fission: Energy Surface from DFT
Problems with Extrapolations

- Mass formulas and energy functionals do well where there is data, but elsewhere . . .
HFB Mass Formula: $\Delta m \sim 1–2 \text{ MeV}$

- Current empirical functionals hit wall at $\sim 1 \text{ MeV}$ (!)
- (cf., expected accuracy of an ab initio functional fit to few-body data)
Issues with Empirical EDF’s

- Density dependencies might be too simplistic
- Isovector components not well constrained
- No (fully) systematic organization of terms in the EDF
- Difficult to estimate theoretical uncertainties
- What’s the connection to many-body forces?
- Pairing part of the EDF not treated on same footing
- and so on . . .

⇒ Turn to microscopic many-body theory for guidance (UNEDF project!)
“Old” View of Relativistic Mean-Field Models

- QHD Lagrangian with one-boson-exchange meson fields
  - Covariant Walecka model + $\phi^3$ and $\phi^4$ terms to get $K_0$

\[
\begin{align*}
+ g_s & + g_v \\
+ g_p & + g_s
\end{align*}
\]

- Mean meson fields $\langle \phi \rangle = \phi_0$, $\langle V_\mu \rangle = \delta_{\mu0} V_0$
- Parameters: $g_s, g_v \approx 10$, $\kappa \approx 5000$ MeV, $\lambda \approx -200$

- Unexplained features:
  - justification of mean-field, “no-sea” approximation
  - how to deal with large couplings and loop corrections
  - truncation at $\phi^4$; why not $V_0^4$?
  - minimal isovector physics (chiral symmetry?)

- Reinterpret as natural covariant density functional
New Terms for Covariant Energy Functionals

- Mueller/Serot $\Rightarrow$ isoscalar ($V_0$) and isovector ($b_0$) vector
  - add $\frac{\zeta}{4!} g^4 V^4_0 + \frac{\xi}{4!} g^4_\rho b^4_0$
  - explore natural size $\zeta$ and $\xi$ impact on EOS $\Rightarrow$ MS$n$ EOS’s

- Horowitz/Piekarewicz et al. $\Rightarrow$ FSUGold
  - add $\frac{\zeta}{4!} g^4 V^4_0 + g^2_\rho b^2_0 [\Lambda^4 g^2_S \phi^2 + \Lambda^v g^2 V^2_0]$
  - knobs for symmetry energy and high-density EOS

- See also Ring et al., DDRMF (density dependent) and G-matrix based covariant EDF’s

- Similar questions
  - Is the energy functional general enough? (E.g., are nonanalytic or nonlocal terms needed?)
  - Can we derive/constrain the functional more microscopically?
  - How can we better constrain parameters?
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Principle of Any Effective Low-Energy Description

If a system is probed at low energies, fine details are not resolved. Use low-energy variables for low-energy processes. Short-distance structure can be replaced by something simpler without distorting low-energy observables. Could be a model or systematic (e.g., effective field theory) physics interpretation can change with resolution!

Low density $\Leftrightarrow$ low interaction energy $\Leftrightarrow$ low resolution

$\lambda \ll R$
Principle of *Any* Effective Low-Energy Description

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- Could be a model or systematic (e.g., effective field theory)
  - physics interpretation can change with resolution!
- Low density \(\Leftrightarrow\) low interaction energy \(\Leftrightarrow\) low resolution
Nucleon-Nucleon Interaction (from T. Papenbrock)

One-pion exchange by Yukawa (1935)

Multi-pions by Taketani (1951)

Repulsive core by Jastrow (1951)

From T. Hatsuda (Oslo 2008)
Nucleon-Nucleon Interaction

- Potential for nonrelativistic many-body Schrödinger equation
- Depends on spins and isospins of nucleons; non-central
  - longest-range part is one-pion-exchange potential

\[ V_\pi(r) \propto (\tau_1 \cdot \tau_2) \left[ (3\sigma_1 \cdot \hat{r}\sigma_2 \cdot \hat{r} - \sigma_1 \cdot \sigma_2)(1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2}) + \sigma_1 \cdot \sigma_2 \right] \frac{e^{-m_\pi r}}{r} \]

- Characterize operator structure of shorter-range potential
- central, spin-spin, non-central tensor and spin-orbit

\[ \{1, \sigma_1 \cdot \sigma_2, S_{12}, L \cdot S, L^2, \sigma_1 \cdot \sigma_2, (L \cdot S)^2\} \otimes \{1, \tau_1 \cdot \tau_2\} \]

- Argonne \nu_{18} is \( V_{EM} + V_\pi + V_{\text{short range}} \) (all cut off at small \( r \))
- Fit to NN scattering data up to 350 MeV (or \( k_{\text{rel}} \leq 2.05 \text{ fm}^{-1} \))
- Alternative characterization is one-boson-exchange
- Systematic treatment: chiral effective field theory (EFT)
Green’s Function Monte Carlo for Light Nuclei

Note the essential role of 3-body forces!
## One-Boson-Exchange Model Scorecard (Machleidt)

<table>
<thead>
<tr>
<th>Coupling</th>
<th>$T = 0$</th>
<th>$T = 1$</th>
<th>Central Spin-Spin</th>
<th>Tensor $S_{12}$</th>
<th>Spin-Orbit $L \cdot S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pseudoscalar</td>
<td>$\eta$</td>
<td>$\pi$</td>
<td>Weak</td>
<td>Strong</td>
<td>—</td>
</tr>
<tr>
<td>Scalar</td>
<td>$\sigma$</td>
<td>$\delta$</td>
<td>Strong</td>
<td>—</td>
<td>Adds to vector</td>
</tr>
<tr>
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<td>$\omega$</td>
<td>$\rho$</td>
<td>Weak, Opposes ps</td>
<td>Opposes ps</td>
<td>Strong, Adds to s</td>
</tr>
<tr>
<td>Tensor</td>
<td>$\omega$</td>
<td>$\rho$</td>
<td>Weak</td>
<td>Opposes ps</td>
<td>—</td>
</tr>
</tbody>
</table>

### Diagrams

**Diagram 1:**
- $V_C$ (potential vs. distance, showing curves for $\eta$, $\pi$, and $\sigma$)

**Diagram 2:**
- $V_T$ (potential vs. distance, showing curves for $\rho$ and $\pi$)
Effective Field Theory Ingredients

See, e.g., “Crossing the Border” [nucl-th/0008064]

1 Use most general $\mathcal{L}$ with low-energy dof’s consistent with the global and local symmetries of the underlying theory

2 Declaration of regularization and renormalization scheme

3 Well-defined power counting $\Rightarrow$ expansion parameters
Effective Field Theory Ingredients: Chiral NN

See, e.g., “Crossing the Border” [nucl-th/0008064]

1 Use most general $L$ with low-energy dof’s consistent with
the global and local symmetries of the underlying theory

- $L_{\text{eft}} = L_{\pi\pi} + L_{\pi N} + L_{NN}$
- chiral symmetry $\implies$ systematic long-distance pion physics

2 Declaration of regularization and renormalization scheme

- momentum cutoff and “Weinberg counting” (still open!)
  $\implies$ define irreducible potential and sum with LS eqn
- use cutoff sensitivity as measure of uncertainties

3 Well-defined power counting $\implies$ expansion parameters

- use the separation of scales $\implies$ $\left\{ \frac{p, m_{\pi}}{\Lambda_{\chi}} \right\}$ with $\Lambda_{\chi} \sim 1 \text{ GeV}$
- chiral symmetry $\implies$ $V_{NN} = \sum_{\nu=\nu_{\text{min}}}^{\infty} c_{\nu} Q^{\nu}$ with $\nu \geq 0$
  ($\nu = 4 - A + 2(L - C) + \sum_i V_i(d_i + f_i/2 - 2)$)
- naturalness: LEC’s are $O(1)$ in appropriate units
Chiral Effective Field Theory for Two Nucleons

- Epelbaum, Meißner, et al.
- Also Entem, Machleidt
- $\mathcal{L}_{\pi N}$ + match at low energy

<table>
<thead>
<tr>
<th>$Q^\nu$</th>
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![Graphs for $1S_0$, $3S_1$, $3P_0$, $1D_2$, $3D_3$, $3G_5$]
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<tbody>
<tr>
<td>$Q^0$</td>
<td>$\cdots\pi\cdots$</td>
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(2)
Chiral Effective Field Theory for Two Nucleons

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<td>$Q^1$</td>
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$\rightarrow \nabla$
Chiral Effective Field Theory for Two Nucleons

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<tr>
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<td>$\pi$</td>
<td>(2)</td>
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<tr>
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<td>$\pi$</td>
<td>$\pi$</td>
<td></td>
</tr>
<tr>
<td>$Q^2$</td>
<td>$\pi$</td>
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<td>(7)</td>
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![Graphs](1S0, 3S1, 3P0, 1D2, 3D3, 3G5)
Chiral Effective Field Theory for Two Nucleons

- Epelbaum, Meißner, et al.
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<td></td>
<td></td>
<td>(7)</td>
</tr>
<tr>
<td>$Q^3$</td>
<td>$\mathcal{L}_{\pi N}$</td>
<td>$\mathcal{L}_{\pi N}$</td>
<td></td>
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Graphs show data for different partial waves:

- $1S_0$
- $3S_1$
- $3P_0$
- $1D_2$
- $3D_3$
- $3G_5$
Chiral Effective Field Theory for Two Nucleons

- Epelbaum, Meißner, et al.
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<tr>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$Q^4$</td>
<td>many</td>
<td>many</td>
<td></td>
</tr>
</tbody>
</table>

(2) $\pi$

(7) $\mathcal{L}_{\pi N}$

(15) $\nabla^4$
Theoretical error estimates from varying cutoff
State of the Art: $N^3$LO (Epelbaum, nucl-th/0509032)

- Theoretical error estimates from varying cutoff
At what orders? $\nu = -4 + 2N + 2L + \sum_i (d_i + n_i/2 - 2)$, so adding a nucleon ($N^{++}$) suppresses by $Q^2/\Lambda^2$.

Power counting confirms $2N \gg 3N > 4N$

$N^2$LO diagrams cancel

3NF vertices may appear in NN and other processes

Fits to the $c_i$'s have sizable error bars
Sample Results with N²LO 3NF

(Epelbaum, nucl-th/0509032)

- \(nd\) scattering at 3, 10, 65 MeV
- \(D\) and \(E\) fixed from triton BE and \(nd\) doublet scattering length
- These are predictions!
- NLO vs. N2LO
- See review for more!
Observations on Three-Body Forces

- Three-body forces arise from eliminating dof’s
  - excited states of nucleon
  - relativistic effects
  - high-momentum intermediate states
- Omitting 3-body forces leads to model dependence
  - but different for each Hamiltonian
- 3-body contributions increase with density
  - uncertain extrapolation if not constrained

Observations on Three-Body Forces

- Three-body forces arise from eliminating dof’s:
  - excited states of nucleon
  - relativistic effects
  - high-momentum intermediate states

- Omitting 3-body forces leads to model dependence
  - but different for each Hamiltonian

- 3-body contributions increase with density
  - uncertain extrapolation if not constrained
Atomic 3-Body Forces: Axilrod-Teller Term (1943)

- Three-body potential for atoms/molecules from triple-dipole mutual polarization (3rd-order perturbation correction)

\[ V(i, j, k) = \nu \left( \frac{1 + 3 \cos \theta_i \cos \theta_j \cos \theta_k}{(r_{ij} r_{ik} r_{jk})^3} \right) \]

- Usually negligible in metals and semiconductors
- Can be important for ground-state energy of solids bound by van der Waals potentials
- Bell and Zuker (1976): 10% of energy in solid xenon
Chiral EFT: Resonance Saturation

[Epelbaum et al. (2002)]

- How is chiral EFT potential related to phenomenological NN potentials based on one-boson exchange?
- Boson exchange $\implies$ model of short-distance physics $\implies$ unresolved in chiral EFT (except for pion) $\implies$ encoded in coefficients of contact terms

\[
\begin{align*}
\frac{g^2}{q^2 + m^2} &\quad \text{treat multiple pion exchanges systematically} \\
\frac{g^2}{m^2} &- \frac{g^2}{m^2} \left( \frac{q^2}{m^2} \right) \\
\end{align*}
\]

- breakdown when $q \approx m$ (how high in density?)
Compare coefficients from phenomenological models to low-energy constants of chiral EFT:

- $C_{1S0}$
- $C_{1S0}$
- $C_{3S1}$
- $C_{3S1}$
- $C_{\varepsilon1}$
- $C_{1P1}$
- $C_{3P0}$
- $C_{3P1}$
- $C_{3P2}$

NLO

NNLO
Chiral EFT: Resonance Saturation (cont.)

- Compare coefficients from phenomenological models to low-energy constants of chiral EFT:

![Graph comparing coefficients C_{1S0}, C_{3S1}, C_{3P1}, C_{3P2} for NLO and NNLO with Bonn-B and NLO data points.](image-url)
Chiral EFT: Resonance Saturation (cont.)

Compare coefficients from phenomenological models to low-energy constants of chiral EFT:

- $C_{1S0}$
- $C_{1S0}$
- $C_{3S1}$
- $C_{3S1}$
- $C_\varepsilon$
- $C_{1P1}$
- $C_{3P0}$
- $C_{3P1}$
- $C_{3P2}$

Graph showing data points for $C_{1S0}$, $C_{1S0}$, $C_{3S1}$, $C_{3S1}$, $C_\varepsilon$, $C_{1P1}$, $C_{3P0}$, $C_{3P1}$, and $C_{3P2}$ with markers for NLO, NNLO, Bonn-B, and CD-Bonn.
Chiral EFT: Resonance Saturation (cont.)

- Compare coefficients from phenomenological models to low-energy constants of chiral EFT:
Naturalness of Coefficients (Epelbaum et al.)

- Georgi-Manohar naive dimensional analysis (NDA):

\[ \mathcal{L}_{\chi \text{eft}} = c_{lmn} \left( \frac{N^\dagger (\cdots) N}{f_\pi^2 \Lambda_\chi} \right)^l \left( \frac{\pi}{f_\pi} \right)^m \left( \frac{\partial ^\mu , m_\pi}{\Lambda_\chi} \right)^n f_\pi^2 \Lambda_\chi^2 \]

- \( f_\pi \sim 100 \text{ MeV} \) and \( \Lambda_\chi \sim 1000 \text{ MeV} \)
- check NLO, NNLO constants from \( \mathcal{L}_{NN} \) (vary cutoff from 500...600 MeV):

<table>
<thead>
<tr>
<th>( f_\pi^2 C_S )</th>
<th>(-1.079 \ldots - 0.953)</th>
<th>( f_\pi^2 C_T )</th>
<th>( 0.002 \ldots 0.040)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f_\pi^2 \Lambda_\chi^2 C_1 )</td>
<td>3.143 \ldots 2.665</td>
<td>( 4 f_\pi^2 \Lambda_\chi^2 C_2 )</td>
<td>2.029 \ldots 2.251</td>
</tr>
<tr>
<td>( f_\pi^2 \Lambda_\chi^2 C_3 )</td>
<td>0.403 \ldots 0.281</td>
<td>( 4 f_\pi^2 \Lambda_\chi^2 C_4 )</td>
<td>(-0.364 \ldots - 0.428)</td>
</tr>
<tr>
<td>( 2 f_\pi^2 \Lambda_\chi^2 C_5 )</td>
<td>2.846 \ldots 3.410</td>
<td>( f_\pi^2 \Lambda_\chi^2 C_6 )</td>
<td>(-0.728 \ldots - 0.668)</td>
</tr>
<tr>
<td>( 4 f_\pi^2 \Lambda_\chi^2 C_7 )</td>
<td>(-1.929 \ldots - 1.681)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- \( 1/3 \lesssim c_{lmn} \lesssim 3 \implies \text{natural!} \implies \text{truncation error estimates} \)
- \( f_\pi^2 C_T \) unnaturally small \implies \text{SU(4) spin-isospin symmetry}
NDA analysis: [Friar et al., rjf et al.]

\[
c \left[ \frac{\psi^\dagger \psi}{f_\pi^2 \Lambda} \right]^l \left[ \frac{\nabla}{\Lambda} \right]^n f_\pi^2 \Lambda^2
\]

\[
\rho \longleftrightarrow \psi^\dagger \psi
\]

\[
\tau \longleftrightarrow \nabla \psi^\dagger \cdot \nabla \psi
\]

\[
J \longleftrightarrow \psi^\dagger \nabla \psi
\]

Density expansion?

\[
\frac{1}{7} \leq \frac{\rho_0}{f_\pi^2 \Lambda} \leq \frac{1}{4}
\]

for $1000 \geq \Lambda \geq 500$
Naive Dimensional Analysis for RMF

- Mass scales in low-energy QCD: [Georgi & Manohar, 1984]
  
  \[ f_\pi \approx 93 \text{ MeV} \], \[ \Lambda \approx 500 \text{ to } 800 \text{ MeV} \]

- NDA rules for a generic term in energy functional:
  
  \[
  c \left[ \frac{f_\pi^2 \Lambda^2}{f_\pi^2 \Lambda} \right] \left[ \left( \frac{\overline{N}N}{f_\pi^2 \Lambda} \right)^{\ell} \frac{1}{m!} \left( \frac{g_\phi}{\Lambda} \right)^m \frac{1}{n!} \left( \frac{gV_0}{\Lambda} \right)^n \left( \frac{\nabla}{\Lambda} \right)^p \right] 
  \]

- "Naturalness" \(\implies\) dimensionless \(c\) is of order unity
- ratio \(\Lambda/f_\pi \rightarrow g \approx 5–10\) is origin of strong couplings

  \(\implies\) \(g_s, g_v \sim g\), \(\kappa \sim g\Lambda\), \(\lambda \sim g^2\)

- Provides expansion parameters at finite density:

  \[
  \frac{g_s \phi}{\Lambda} \approx \frac{g_v V_0}{\Lambda} \approx 1/2, \quad \frac{\rho_s}{f_\pi^2 \Lambda} \approx \frac{\rho_B}{f_\pi^2 \Lambda} \approx 1/5 \at \rho_B^0
  \]
RMF Estimates in Finite Nuclei

\[ \tilde{\rho}_S, \tilde{\rho}_B \rightarrow \langle \rho_B \rangle \frac{f^2}{\Lambda} \]
\[ \tilde{\nabla} \rho_B \rightarrow \langle \nabla \rho_B \rangle \frac{f^2}{\Lambda^2} \]
\[ \tilde{S} \rightarrow \langle S \rangle \frac{f^2}{\Lambda} \]
\[ \tilde{\rho}_3 \rightarrow \frac{Z - N}{2A} \frac{\langle \rho_B \rangle}{f^2} \frac{f^2}{\Lambda} \approx 1 \text{ isovector parameter constrained by energy fit} \]
**Sources of Nonperturbative Physics for NN**

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

**Consequences:**
- In Coulomb DFT, Hartree-Fock gives dominate contribution $\implies$ correlations are small corrections $\implies$ DFT works!
- cf. NN interactions $\implies$ correlations $\gg$ HF $\implies$ DFT fails??
- However . . .
  - the first two depend on the *resolution* $\implies$ changed by RG
  - all three are affected by Pauli blocking

![Graph showing potential energy function $V(r)$ with $1^1S_0 (np)$ AV$_{18}$ and $r_0 \sim 1.5$ fm in nuclei]
S-Wave ($L = 0$) NN Potential in Momentum Space

- Fourier transform in partial waves (Bessel transform)

$$V_{L=0}(k, k') = \int d^3r j_0(kr) V(r) j_0(k'r) = \langle k | V_{L=0} | k' \rangle$$

- Repulsive core $\implies$ big high-$k$ ($\geq 2 \text{ fm}^{-1}$) components
S-Wave \((L = 0)\) NN Potential in Momentum Space

- Fourier transform in partial waves (Bessel transform)

\[
V_{L=0}(k, k') = \int d^3r \, j_0(kr) \, V(r) \, j_0(k'r) = \langle k | V_{L=0} | k' \rangle
\]

- Repulsive core \(\Rightarrow\) big high-\(k\) \((\geq 2\text{ fm}^{-1})\) components
Low-Momentum Interactions from RG \([AV18^{3S_1}]\)

- \(V_{\text{low } k} \longrightarrow \) Lower a cutoff \(\Lambda\) in relative \(k, k'\) [sharp]

\[
\begin{array}{cccccc}
\text{k}^2 (\text{fm}^{-2}) & \text{k}^2 (\text{fm}^{-2}) & \text{k}^2 (\text{fm}^{-2}) & \text{k}^2 (\text{fm}^{-2}) & \text{k}^2 (\text{fm}^{-2}) \\
0 & 4 & 8 & 12 & 0 & 4 & 8 & 12 & 0 & 4 & 8 & 12 & 0 & 4 & 8 & 12 \\
\end{array}
\]

- \(\Lambda = 5.0 \text{ fm}^{-1}\) \(\Lambda = 4.0 \text{ fm}^{-1}\) \(\Lambda = 3.0 \text{ fm}^{-1}\) \(\Lambda = 2.0 \text{ fm}^{-1}\) \(\Lambda = 1.5 \text{ fm}^{-1}\)

- SRG \(\longrightarrow\) Drive the Hamiltonian toward diagonal \([\lambda \equiv 1/s^{1/4}]\)

\[
\begin{array}{cccccc}
\text{k}^2 (\text{fm}^{-2}) & \text{k}^2 (\text{fm}^{-2}) & \text{k}^2 (\text{fm}^{-2}) & \text{k}^2 (\text{fm}^{-2}) & \text{k}^2 (\text{fm}^{-2}) \\
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- Other transformations also decouple (e.g., UCOM)

- Isn’t chiral EFT already soft? Or why not use a lower cutoff? [e.g., E/G/M: 450 MeV, E/M: N3LOW (400 MeV)]
Probability at short separations suppressed $\Rightarrow$ "correlations"

- Greatly complicates expansion of many-body wave functions
- Short-distance structure $\Leftrightarrow$ high-momentum components
Repulsive Core Before and After

\( ^3S_1 \) deuteron probability density

- Transformed potential \( \rightarrow \) no short-range correlations in \( \psi \)
- Potential is now non-local: \( V(r)\psi(r) \rightarrow \int d^3r' \, V(r, r')\psi(r') \)
  - Also few-body forces. Problems for many-body methods? \( \rightarrow \) For some yes, for others no!
What are the measurable quantities?

- True observables do not change under field redefinitions or unitary transformations in low-energy effective theories.
  - Examples: cross sections, conserved quantities like charge.
- Many useful quantities are extracted from measurements via a convolution (e.g., using some type of factorization).
  - But these will vary with the convention used.
  - E.g., parton distributions.
- Conventions are renormalization prescriptions, cutoffs, 
  - Different potentials reflect different conventions.
- Unitary transformation \((U^\dagger U = 1)\) of \(H\) and other operators
  \(\implies\) choose \(U\) to decouple!

\[
E_n = \langle \psi_n | H | \psi_n \rangle = (\langle \psi_n | U^\dagger \rangle U H U^\dagger (U | \psi_n \rangle) = \langle \tilde{\psi}_n | \tilde{H} | \tilde{\psi}_n \rangle
\]

- The convention for the long-range part of NN\( \cdots \)N potentials is agreed to be (local) pion exchange, but differs widely for the short-range part. (Note: \(V_{\text{low } k}\) preserves long-distance part.)
Quantities that vary with convention

→ *not* observables

- deuteron D-state probability
  [Friar, PRC 20 (1979)]
- off-shell effects
  [Fearing/Scherer]
- occupation numbers
  [Hammer/Furnstahl]
- wound integrals
- short-range part of wave functions
- short-range potentials; e.g., contribution of short-range 3-body forces
Short-Term Roadmap for Microscopic Nuclear DFT

- Use a chiral EFT to a given order (e.g., E/M $N^3$LO below)
- Soften with RG (evolve to $\Lambda \approx 2 \text{ fm}^{-1}$ for ordinary nuclei)
  - NN interactions fully, NNN interactions (3NF) approximately
- Generate density functional using DME in $k$-space

**Graph:**

- $V_{\text{low } k \text{ NN}}$ from $N^3$LO (500 MeV)
- 3NF fit to $E_3^H$ and $r_4^He$ (Nogga)
- $2.0 < \Lambda_{3NF} < 2.5 \text{ fm}^{-1}$

**Hartree-Fock:**

- $\Lambda = 1.8 \text{ fm}^{-1}$
- $\Lambda = 2.0 \text{ fm}^{-1}$
- $\Lambda = 2.2 \text{ fm}^{-1}$

**pp ladders**

- $\Lambda = 1.8 \text{ fm}^{-1}$
- $\Lambda = 2.0 \text{ fm}^{-1}$
- $\Lambda = 2.2 \text{ fm}^{-1}$
Outline

“Just the Facts” About Nuclei

Symmetric and Asymmetric Nuclear Matter

Many-Body Methods

Inter-Nucleon Interactions

Final Thoughts and Prejudices
Universal Nuclear Energy Density Functional
Collaboration of physicists, applied mathematicians, and computer scientists

Funding in US but international collaborators also
Goals of SciDAC 2 Project: Building a Universal Nuclear Energy Density Functional

- Understand nuclear properties “for element formation, for properties of stars, and for present and future energy and defense applications”
- Scope is all nuclei (there are more than 5000!), with particular interest in reliable calculations of unstable nuclei and in reactions
  \[ \rightarrow \text{Density functional theory (DFT) is method of choice} \]
- Order of magnitude improvement over present capabilities
  \[ \rightarrow \text{precision calculations of masses, . . .} \]
- Connected to the best microscopic physics
- Maximum predictive power with well-quantified uncertainties

[See http://www.scidacreview.org/0704/html/unedf.html by Bertsch, Dean, and Nazarewicz]
Major UNEDF Research Areas

- **Ab initio structure** — Nuclear wf’s from microscopic NN···N
  - NCSM/NCFC, CC, GFMC/AFMC
  - AV18/ILx, chiral EFT $\rightarrow V_{\text{low } k}$

- **Ab initio energy functionals** — DFT from microscopic N···N
  - Cold atoms — superfluid LDA+ as prototype for nuclear DFT
  - $\chi$EFT $\rightarrow V_{\text{low } k} \rightarrow \text{MBPT} \rightarrow \text{DME}$

- **DFT applications** — Technology to calculate observables
  - Skyrme HFB+ for all nuclei (solvers)
  - Fitting the functional to data (e.g., correlation analysis)

- **DFT extensions** — Long-range correlations, excited states
  - LACM, GCM, TDDFT, QRPA, CI

- **Reactions** — Low-energy reactions, fission, . . .
<table>
<thead>
<tr>
<th>(Nuclear) Many-Body Physics: “Old” vs. “New”</th>
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<tbody>
<tr>
<td>One Hamiltonian for all problems and energy/length scales</td>
</tr>
<tr>
<td>Find the “best” potential</td>
</tr>
<tr>
<td>Two-body data may be sufficient; many-body forces as last resort</td>
</tr>
<tr>
<td>Avoid (hide) divergences (e.g., with form factors)</td>
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<tr>
<td>Choose diagrams by “art”</td>
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<tr>
<td>Test models only by comparison to experiment</td>
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Plan: Use DOF’s to Simplify and Make Efficient

- Weinberg’s 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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- There’s an old vaudeville joke about a doctor and patient . . .
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Patient: Doctor, doctor, it hurts when I do this!
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- There’s an old vaudeville joke about a doctor and patient . . .

Patient: Doctor, doctor, it hurts when I do this!
Doctor: Then don’t do that.