# I) Motivation for Microscopically-based EDFs

## a.) Successes of EDF (Skyrme etc.)

* Computational simplicity (mass tables in a day, global studies a-la PH Heenen's talk fission barriers/energy surfaces, etc.)
* rms error ~ 1 MeV (versus $\frac{1\,\mathrm{MeV}}{A}$ for ab-initio in limited medium mass)
* Access open shell/deformed nuclei
* Show figures?

## b) Failures/Shortcomings => (why insights from ab-initio might help)

* Stuck @ ~ 1MeV brick wall despite influx of sophisticated optimization methods
* performance for spectroscopy not as solid
* poorly constrained isovector + t-odd couplings

* Loss of predictive power away from mass region /observables fitted to (show, e.g., $S_{2n}$ figure in Sn)

** $E[\rho]$ too simple!

* Why only bilinear in $\rho$'s w/ the lone $\rho^{2+\alpha}$ term?

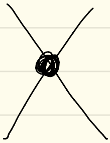
e.g., 3NF play big role in ab-initio (=> tri-linear, at least)

e.g., Even toy model systems (e.g., dilute gas of fermions in a trap interacting w/ short-range forces) where one can constructively build $F_{HK}[\rho]$ has multiple non-analytic (non-integer) terms of the form $\rho^\alpha$

* In PME, even @ HF level see non-analytic behavior due to finite range

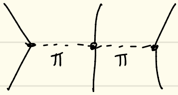
# E[ρ] too simple (cont'd)

* ab-initio (show SM + GFMC plots) calculations => 2 very different sources of LS physics

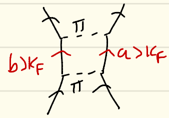


Short-range NN LS-force

long-range 3NF




iterated π-exchange

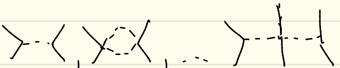



Consistent w/ Skyrme

$i W_0 (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k}' \times \delta(\vec{r}_1 - \vec{r}_2) \vec{k}$

How can zero range Skyrme capture this?

* Pion-exchanges (



, etc) have very rich spin/isospin/space dependence. Where are they in Skyrme? Could putting them in solve/ameliorate the poorly constrained isovector & t-odd couplings?

* **Aesthetics**: Can we at least have indirect link to QCD? χ-EFT theory of forces has this link. [* show EFT figure]

=> Can we connect E[ρ] to χ-EFT 2- & 3N interactions?

## Thoughts on Coulomb DFT (see Perdew reference posted)

**LDA**: Do ab-initio calc. of the electron gas over wide range of $\rho$

* extract $\Rightarrow \dfrac{E_{xc}^{gas}}{A} \equiv \varepsilon_{xc}(\rho)$   parameterize dep. on $\rho$.

* treat finite IHG system like it's a chunk of $e^-$ gas locally (LDA)

$$\Rightarrow E_{xc}^{LDA} = \int d^3r' \, \rho(\vec{r}') \, \varepsilon_{xc}(\rho(\vec{r}'))$$

$$v_{xc}^{LDA}(\vec{r}) = \frac{\delta E_{xc}^{LDA}}{\delta \rho(\vec{r})} = \varepsilon_{xc}(\rho(\vec{r})) + \rho(\vec{r}) \frac{\partial \varepsilon_{xc}(\rho(\vec{r}))}{\partial \rho}$$

### * Gradient corrections

* early attempts using linear response failed (corrections made things worse)

$\Downarrow$

$$E_\nabla[\rho] \sim \int d^3r \, C \, |\nabla \rho(\vec{r})|^2$$

huge correction.

* Generalized Gradient Approx (GGA)
  - empirical form w/ eg., resummed gradients in denominator

$$\text{e.g.,} \quad \int d^3r \, \rho(\vec{r}) \varepsilon_c(\rho) \left[ 1 - \frac{\beta |\nabla \rho|^2}{\nu \rho \, \varepsilon_c(\rho)} \right]^{-\nu} \quad \text{(Ma-Brueckner)}$$

$\nu$ = fit parameter

* later versions by Perdew et al: choose complicated forms; impose sum rule + general scaling relations

Perdew et. al.: Non-empirical GGA functionals

* start w/ some ansatz for re-summed gradients
* impose exact relations (sum rules, scaling properties, etc) to essentially eliminate any fit parameters in the ansatz

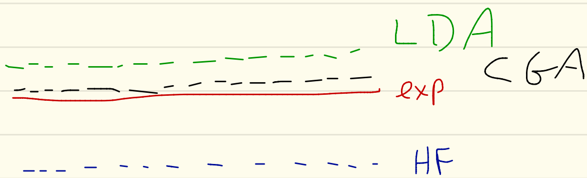
Comment: To my knowledge, these constraints using exact relations follow from the simplicity of $V_{coulomb}$.

Probably can't do the same in nuclear physics do to extreme complexity of $V_{NN} + V_{3N}$.

However, see eg. the work of Dobaczewski using gauge-invariance etc. to find relations between couplings.

Question: Does Coulomb DFT work so well in part because XC effects small?

e.g., HF is good starting point




With soft EFT + RG-evolved 2N + 3N interactions, HF becomes a not crazy (still not quantitative) starting point, w/ bulk of correlation energy coming in low order MBPT / BHP type correlations

## II) Skryme from BHF

* BHF crash review

{ upshot, eqns. look like HF

$$E^{BHF} = \sum_{i=1}^{A} \langle i|t|i\rangle + \frac{1}{2}\sum_{ij=1}^{A} \langle ij|G(\omega=\varepsilon_i+\varepsilon_j)|ij\rangle$$

$$G(\omega) = V + V\frac{Q}{\omega - t}G \qquad Q = \sum_{ab}|ab\rangle\langle ab| + \sum_{ai}|ai\rangle\langle ai|$$

$$\varepsilon_i = t_{ii} + \sum_j G_{ijij}(\omega=\varepsilon_i+\varepsilon_j)$$

* In practice to make BHF as much as possible,

① $G(\omega=\varepsilon_i+\varepsilon_j) \Rightarrow G(\varepsilon_{av})$ $\quad \sum_{ij}\langle ij|G(\varepsilon_{av})|ij\rangle$ in $\rho$-matrices

② $\langle \vec r_1\vec r_2|G|\vec r_3\vec r_4\rangle = \delta(\vec R-\vec R')\,G^{|\vec R|}(\vec r,\vec r') \approx \delta(\vec R-\vec R')\delta(\vec r-\vec r')\,G^{|\vec R|}(\vec r)$

$$\Rightarrow E^{BHF}_{int} \sim \iint d\vec R\, d\vec r\; \rho^2\!\left(\vec R+\frac{\vec r}{2}, \vec R-\frac{\vec r}{2}\right) G(\vec r)$$

* Skyrme $\neq$ zero range exp. of $G(r)$

* what sets falloff of $\rho(\vec R+\frac{\vec r}{2}, \vec R-\frac{\vec r}{2})$? $\Big\langle$ NM example / HO example $\Big]$ $k_F(R)$ does.

# Crash Course on BHF

HF: $\Psi(1,\dots A) \approx \mathcal{A}(\phi_i(1)\phi_j(2)\cdots\cdots)$  HF orbitals

BHF:


Naive HF won't even bind due to S.R. repulsion

- however, as Peter said, nuclei sit here
- likewise $\lambda_{MFP} \sim$ size of nucleus

Nucleus is "dilute"

=> suggests the next level of approx, BHF or Indep. Pair Approx.

$$\Psi(1,2,\dots A) \simeq N \sum_{k\ell} \mathcal{A}\Big(\underbrace{\psi_{k\ell}(1,2)}_{\text{correlated pair}}\, \phi_m(3) \cdots \phi_n(A)\Big)$$

$$\big(\underbrace{T(i)+U_{MF}(i)}_{H_0(i)}\big)\phi_q(i) = \varepsilon_q \phi_q(i)$$

Correlated pair: $(H_0(1)+H_0(2)+V_{12})\psi_{k\ell}(1,2) = e_{k\ell}\,\psi_{k\ell}(1,2)$

expand: $|\psi_{k\ell}\rangle = |\phi_k\phi_\ell\rangle + \sum_{a,b>\epsilon_F} |\phi_a\phi_b\rangle\langle\phi_a\phi_b|\psi_{k\ell}\rangle$

(add'l $|\phi_a\phi_\ell\rangle$, $|\phi_k\phi_a\rangle$ terms infinite nuclei, but I ignore them)

$$\boxed{|\psi_{k\ell}\rangle = |\phi_k\phi_\ell\rangle + \frac{Q}{e_{k\ell}-H_0}\, v\, |\psi_{k\ell}\rangle} \qquad Q = \sum_{ab>\epsilon_F} |\phi_a\phi_b\rangle\langle\phi_a\phi_b|$$

Bethe-Goldstone eqn (Pauli-Blocked Lippmann Schwinger)

<u>G-matrix</u>: Just like $\hat{V}|\psi\rangle = \hat{T}|\phi\rangle$ in LS eqn in Scattering theory,

<u>Def</u>
$$\boxed{\hat{V}|\psi_{k\ell}\rangle \equiv G(\omega = e_{k\ell})|\phi_k\phi_\ell\rangle}$$

$\Rightarrow$ Bethe Goldstone eqn then gives
$$\boxed{G(\omega) = v + v\frac{Q}{\omega - H_0}G(\omega)}$$

<u>Can show w/ these definitions</u>

$$E^{BHF} = \sum_{i=1}^{A}\langle\phi_i|T|\phi_i\rangle + \frac{1}{2}\sum_{ij=1}^{A}\langle\phi_i\phi_j|G(\varepsilon_i+\varepsilon_j)|\phi_i\phi_j\rangle$$

$$\varepsilon_i = \langle\phi_i|T|\phi_i\rangle + \sum_{j=1}^{A}\langle\phi_i\phi_j|G(\varepsilon_i+\varepsilon_j)|\phi_i\phi_j\rangle$$

<u>Comments</u>: (1) looks like HF $V \to G(\varepsilon_i+\varepsilon_j)$ [Doubly self-consistent though]

(2) Even if $\langle\vec{r}_1\vec{r}_2|V|\vec{r}_3\vec{r}_4\rangle = \delta(\vec{r}_1-\vec{r}_3)\delta(\vec{r}_2-\vec{r}_4)V(\vec{r})$,
$= \delta(\vec{R}_{12}-\vec{R}_{34})\delta(\vec{r}_{12}-\vec{r}_{34})V(\vec{r}_{12})$ Local

$$\langle\vec{r}_1\vec{r}_2|G|\vec{r}_3\vec{r}_4\rangle = \delta(\vec{R}_{12}-\vec{R}_{34})\underbrace{G^{\vec{R}_{12}}(\vec{r}_{12},\vec{r}_{34})}$$

Non-local, parametric (weak) COM dependence

(3) Energy dependence prevents from writing $E_{BHF}$ in terms of $\rho(\vec{r}_1,\vec{r}_2)$, $\rho(\vec{r})$.

## Comments (Cont'd):

4. BHF replaced by more sophisticated theories in practice (CC, IMSRG, ...) but all such methods dominated by BHF-type correlations

5. Notice no prescription given for how to compute $\varepsilon_q > \varepsilon_F$
Technical point: different prescriptions exist. Using old fashioned "hard" V results can be very sensitive. Claim this goes away w/ softer interactions now in vogue.

## Making BHF look more like HF

1.) avg out E-dependence, e.g. $G(\varepsilon_i + \varepsilon_j) \rightarrow G(\bar{\varepsilon}_{pair})$

2.) avg out non-locality & COM dep $\Rightarrow$ $G^{\vec{R}}(\vec{r}_{12}, \vec{r}_{34}; \varepsilon) \longrightarrow \delta(\vec{r}_{12} - \vec{r}_{34})\, G(\vec{r}_{12})$

$\Downarrow$

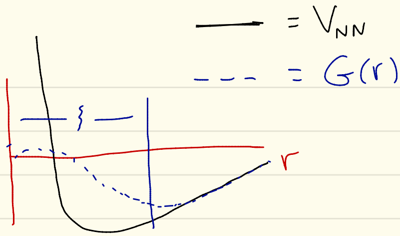
Then,

$$\boxed{\begin{aligned} E_{BHF} &\sim \frac{1}{2} \sum_{ij} \langle ij | G(r) | ij \rangle \\ &\sim \frac{1}{2} \iint d\vec{R}\, d\vec{r}\; \rho(R + \tfrac{r}{2})\, \rho(R - \tfrac{r}{2})\, G(r) \\ &\quad - \frac{1}{2} \iint d\vec{R}\, d\vec{r}\; \rho^2(\vec{R} + \tfrac{\vec{r}}{2}, \vec{R} - \tfrac{\vec{r}}{2})\, G(r) \end{aligned}}$$

[reminder, $G(r)$ is $\rho$-dependent!]

# Final point Re: BHF

Correlations are "short-range"




$\xi$ = "healing distance"

$\sim \dfrac{\pi}{k_F}$

Crudely speaking: $\boxed{G(r) \sim \Theta(r-\xi)\, V(r) + \Theta(\xi - r)\left[C_0\, \delta(\vec{r}) + C_2 \nabla^2 \delta(\vec{r}) + \cdots\right]}$

Will make use of this later on...

* $\hat{v}_{\text{Skyrme}}$ is NOT a zero-range expansion of $V_{NN}(r)$ (or $G_{NN}(r)$)

* It is sometimes incorrectly said that $\hat{v}_{SK}$ is a zero-range approx. to $V_{NN}/G_{NN}$, which are said to be "short ranged"

- Range of NN-force controlled by $m_\pi$; i.e., $V(r) \sim \frac{g\, e^{-m_\pi r}}{r}$

- Under what conditions can we take $V(r) \sim C_0 \delta(\vec{r}) + C_2 \nabla^2 \delta(\vec{r}) + \cdots$ like $\hat{v}_{SK}$?

- Go over to momentum space: $\tilde{V}(\vec{q}) = \int \frac{d^3 r}{(2\pi)^3} e^{i\vec{q}\cdot\vec{r}}\, V(r)$

$$\propto \frac{g}{\vec{q}^{\,2} + m_\pi^2}$$

* at $q \lesssim m_\pi$: $\tilde{V}(\vec{q}) \approx C_0 + C_2 q^2 + \cdots$

$$\Downarrow \text{ FT back to } r\text{-space}$$

$$V(r) \approx C_0 \delta^{(3)}(\vec{r}) + C_2 \nabla^2 \delta^{(3)}(\vec{r}) + \cdots$$

$\Rightarrow$ Can approximate $V(r) \sim$ zero-range only for cases where you probe momenta $q \lesssim m_\pi$

$\Downarrow$

But $E^{HF}_{int} \sim \sum_{ij=1}^{A} \langle ij | V | ij \rangle$

$E^{BHF}_{int} \sim \sum_{ij=1}^{A} \langle ij | G | ij \rangle$

probe momenta $\mathcal{O}(k_F)$

$k_F \sim 1\text{-}1.3\ \text{fm}^{-1}$

$m_\pi \sim .7\ \text{fm}^{-1}$

$\Rightarrow$ Misleading to say $V_{SK} \sim$ zero range expansion of $V_{NN}(r)/G_{NN}(r)$

<u>Remark</u>: Approximating $V(\vec{r}) \sim C_0\delta(\vec{r}) + C_2\nabla^2\delta(\vec{r}) + \cdots$ equivalent to doing Taylor expansion about the diagonal of the density matrix

<u>ex</u>: $E_x = \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2\, \rho^2(\vec{r}_1,\vec{r}_2)\, V(\vec{r}_1-\vec{r}_2) = \frac{1}{2}\int d\vec{R}\, d\vec{r}\, \rho^2(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2})\, V(r)$

let $\rho(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}) \sim \rho(\vec{R},\vec{R}) + \underbrace{r_i\nabla_i\, \rho(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2})\Big|_{r=0}}_{\text{0 in even-even by T-reversal}} + \frac{1}{2} r_i r_j \nabla_i\nabla_j\, \rho(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2})\Big|_{\vec{r}=0} + \cdots$

eg: LO term $\frac{1}{2}\int d\vec{R}\, d\vec{r}\, \rho^2(R)\, V(r) = \frac{1}{2}\int d\vec{R}\, \rho^2(R) \underbrace{\int d\vec{r}\, V(r)}_{\vec{q}=0 \text{ term of } \tilde{V}(\vec{q})}$

from expanding DM

(i.e., 1st term in taylor expanding $\tilde{V}(\vec{q}) \simeq \tilde{V}(0) + \cdots$)

* You can verify the $\vec{r}\cdot\vec{\nabla}\rho$ term vanishes in even-even system due to time reversal, while the cross-terms $\rho(R)\,\frac{1}{2}\,\vec{r}\cdot\vec{\nabla}\,\vec{r}\cdot\vec{\nabla}\,\rho(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2})\Big|_{r=0}$ give the same term as for the $2^{nd}$ term of expanding $\tilde{V}(q) \simeq \tilde{V}(0) + q^2\,\tilde{V}'(q^2=0)$

<u>Question</u>: Might it be possible to find a resummed taylor expansion that "factorizes" the non-locality ($r$-dependence) of density matrix?

$$\rho(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}) \approx \sum_n \Pi_{2n}(r)\,\nabla^{2n}\rho(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2})\Big|_{\vec{r}=0}$$

all we require at this point is that $\Pi_{2n}(r)$ has correct small-$r$ behavior to match Taylor exp.

$\Rightarrow$ Non-local Fock energy calculated w/ a realistic NN pot. then has a form that resembles what $V_{Skyrme}$ gives

$$E_x = \frac{1}{2}\iint d\vec{R}\,d\vec{r}\; V(r)\,\rho^2\!\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right) \overset{?}{\approx} \frac{1}{2}\sum_{n,m}\int d\vec{R}\,\underbrace{\left(\nabla^{2n}\rho(\vec{R})\right)\nabla^{2m}\rho(\vec{R})}_{\text{local densities + their gradients}} \times \underbrace{\int d\vec{r}\;\Pi_{2n}(r)\,\Pi_{2m}(r)\,V(r)}_{\text{coupling from underlying NN}}$$

$$= \int d\vec{R}\left[\rho^2(R)\,g_{00} + \rho(R)\nabla^2\rho(R)\,g_{02} + \cdots\right]$$

* OK, so we see that "factorizing" the non-locality (i.e, r-dependence) of $\rho(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2})$ allows us to map non-local Fock-energy into a local Skyrme-like EDF!

* We call this expansion the "Density matrix expansion" (DME). I haven't told you <u>how</u> to do this yet (Moreover, there is no 1 unique prescription), but this gives us a hint that the Skyrme EDF can be understood as performing the DME on a microscopic HF/BHF calculation

$$\begin{array}{c}\text{Microscopic}\\ \text{HF/BHF}\\ \text{w/ "realistic"}\\ V_{NN}\end{array} \xRightarrow{\text{DME}} \begin{array}{c}\text{Skyrme}\\ \text{phenomenology}\end{array}$$

* Before we go over a couple recipes for the DME, need to understand what sets the scale for the falloff in r-direction of $\rho(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2})$

<u>ex1</u>: infinite homogenous matter; HF sp wf's = plane waves $\phi_{\vec{k}}(\vec{r}_0) = \dfrac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\chi_\sigma$

$$\rho(\vec{r}_1,\vec{r}_2) = 2\sum_{\vec{k}<k_F}\phi^*_{\vec{k}}(\vec{r}_2)\phi_{\vec{k}}(\vec{r}_1) = \frac{2}{V}\sum_{\vec{k}<k_F} e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)} \xrightarrow[V\to\infty]{} 2\int_0^{k_F}\frac{d^3k}{(2\pi)}\,e^{i\vec{k}\cdot\vec{r}}$$

$$\Rightarrow \rho_{NM}\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right) = \frac{2\cdot 4\pi}{(2\pi)^3}\int_0^{k_F} k^2 dk\, j_0(kr) = \frac{1}{\pi^2} k_F^3 \int_0^1 \bar{k}^2 d\bar{k}\, j_0(\bar{k}\bar{r})$$

$\bar{k} = \frac{k}{k_F}$

$\bar{r} = r k_F$

$\frac{1}{3\pi^2} k_F^3 = \rho \Rightarrow$

$$= 3\rho \int_0^1 \bar{k}^2 d\bar{k}\, j_0(\bar{k}\bar{r})$$

$$= 3\rho \frac{j_1(k_F r)}{k_F r}$$

$$\boxed{\begin{aligned} \rho_{NM}\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right) &= \rho\, \rho_{SL}(k_F r) \\ \rho_{SL}(k_F r) &= \frac{3 j_1(k_F r)}{k_F r} \end{aligned}}$$

i.e., $k_F$ controls falloff in $r$.

<u>Comment</u>: The Slater Approximation mentioned by Nicolas for treating Coulomb exchange in Skyrme calculations derived by taking
$\rho\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right) \approx \rho(\vec{R})\, \rho_{SL}(k_F(R)\, r)$ ("local density approx" or LDA)

# Phase-Space Averaging (PSA) Formulation of DME (Gebremariam, SKB/Duguet)

* Start w/ spin/isospin decomposition of density matrix

$$\underset{\sim}{\rho}(\vec{r}_1,\vec{r}_2) = \frac{1}{4}\sum_{\mu}\sum_{\nu} \rho_{\mu\nu}(\vec{r}_1,\vec{r}_2)\,\hat{\sigma}_\mu\,\hat{\tau}_\nu \qquad \hat{\sigma}_\mu = (\mathbb{I}, \vec{\sigma})$$

matrix in
$\sigma\tau$ space

$$\rho_{\mu\nu}(\vec{r}_1,\vec{r}_2) = \mathrm{Tr}_\sigma \mathrm{Tr}_\tau\, \underset{\sim}{\rho}(\vec{r}_1,\vec{r}_2)\,\hat{\sigma}_\mu\,\hat{\tau}_\nu$$

* Formally expand out the non-locality of $\rho_{\mu\nu}(\vec{r}_1,\vec{r}_2) = \rho_{\mu\nu}(\vec{R}+\frac{\vec{r}}{2}, \vec{R}-\frac{\vec{r}}{2})$

$$\rho_{\mu\nu}(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}) = e^{\frac{\vec{r}}{2}\cdot\vec{\nabla}_r}\rho(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2})\Big|_{\vec{r}=0} = e^{\vec{r}\cdot\left(\frac{\vec{\nabla}_1-\vec{\nabla}_2}{2}\right)}\rho(\vec{r}_1,\vec{r}_2)\Big|_{\vec{r}_1=\vec{r}_2=\vec{R}}$$

* Multiply by $1 = e^{i\vec{r}\cdot\vec{k}}\,e^{-i\vec{r}\cdot\vec{k}} \Rightarrow$

$$\rho_{\mu\nu}(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}) = e^{i\vec{r}\cdot\vec{k}}\, e^{\vec{r}\cdot\left[\frac{\vec{\nabla}_1-\vec{\nabla}_2}{2} - i\vec{k}\right]}\rho_{\mu\nu}(\vec{r}_1,\vec{r}_2)\Big|_{\vec{r}_1=\vec{r}_2=\vec{R}}$$

$$\approx e^{i\vec{r}\cdot\vec{k}}\left[1 + \vec{r}\cdot\left(\frac{\vec{\nabla}_{12}}{2} - i\vec{k}\right) + \frac{1}{2}\left(\vec{r}\cdot\left(\frac{\vec{\nabla}_{12}}{2} - i\vec{k}\right)\right)^2\right]\rho_{\mu\nu}(\vec{r}_1,\vec{r}_2)\Big|_{\vec{R}} \qquad \otimes$$

* physically, $\vec{k}$ ~ some avg. rel momentum in nucleus

* Assume we have some model local momentum distribution $g(\vec{R},\vec{k})$

$\Rightarrow$ Want to average $\otimes$ over $g(\vec{R},\vec{k})$

Def: $\Pi_n(\vec{r},\vec{R}) = \dfrac{\int d\vec{k}\, e^{i\vec{r}\cdot\vec{k}}\,(\vec{r}\cdot\vec{k})^n\, g(\vec{R},\vec{k})}{\int d\vec{k}\, g(\vec{R},\vec{k})}$

$$\vec{j}_{\mu\nu}(\vec{R}) = -\frac{i}{2}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right)\rho_{\mu\nu}(\vec{r}_1,\vec{r}_2)\Big|_{\vec{r}_1=\vec{r}_2=\vec{R}}$$

$$\tau_{ab,\mu\nu}(\vec{R}) = \vec{\nabla}_1^a\, \vec{\nabla}_2^b\, \rho_{\mu\nu}(\vec{r}_1,\vec{r}_2)\Big|_{\vec{r}_1=\vec{r}_2=\vec{R}}$$

Spatial indices (KE Tensor density)

$$\boxed{\begin{aligned}\Rightarrow \rho_{\mu\nu}(\vec{r}_1,\vec{r}_2) \approx{}& \left[\Pi_0 - i\Pi_1 - \frac{\Pi_2}{2}\right]\rho_{\mu\nu}(\vec{R}) + i\left[\Pi_0 - i\Pi_1\right]\sum_{a=1}^{3} r_a\, j_{a,\mu\nu}(\vec{R}) \\ &+ \frac{\Pi_0}{2}\sum_{a,b=1}^{3} r_a r_b\left[\frac{1}{4}\nabla_a\nabla_b\,\rho_{\mu\nu}(\vec{R}) - \tau_{ab,\mu\nu}(\vec{R})\right]\end{aligned}} \qquad \otimes$$

*Eg: $g(\vec{R},\vec{k}) = \Theta(k_F(R) - |\vec{k}|)$ (Phase Space of $\infty$-matter)

$$\Rightarrow \Pi_0(k_F r) = \frac{3 j_1(k_F r)}{k_F r} = \rho_{SL}(k_F r) \approx 1 + \mathcal{O}(k_F r)^2$$

$$\Pi_1(k_F r) = -i3 j_0(k_F r) + i9\,\frac{j_1(k_F r)}{k_F r} \approx i\,\frac{(k_F r)^2}{5} + \mathcal{O}\left((k_F r)^4\right)$$

$$\Pi_2(k_F r) = 15 j_0 - 36\,\frac{j_1}{k_F r} - 3\cos k_F r \approx \frac{(k_F r)^2}{5} + \mathcal{O}(k_F r)^4$$

*We further re-order $\otimes$ by counting $k_F \sim \nabla$

$$\Rightarrow \rho_{\mu\nu}(\vec{r}_1,\vec{r}_2) \approx \Pi_0(k_F r)\,\rho_{\mu\nu}(\vec{R}) + i\,\Pi_0 \sum_{a=1}^{3} r_a\, j_{a,\mu\nu}(\vec{R}) + \frac{\Pi_0(k_F r)}{2}\sum_{a,b} r_a r_b\left[\frac{1}{4}\nabla_a\nabla_b\,\rho_{\mu\nu}(R) - \tau_{ab,\mu\nu}(R) + \delta_{ab}\frac{k_F^2}{5}\rho_{\mu\nu}(R)\right]$$

$$\equiv \Pi_0(k_F r)\,\rho_{\mu\nu}(\vec{R}) + i\,\Pi_1(k_F r)\sum_{a=1}^{3} r_a\, j_{a,\mu\nu}(\vec{R}) + \frac{\Pi_2}{2}\sum_{a,b} r_a r_b\left[\frac{1}{4}\nabla_a\nabla_b\,\rho_{\mu\nu} + \dots\right]$$

$\Downarrow$ Even-Even & integrate over $\int d\hat{r}$

$$\boxed{\begin{aligned}&\rho_t\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right) \simeq \Pi_0(k_F r)\,\rho_t(\vec{R}) + \frac{r^2}{6}\Pi_2(k_F r)\left[\frac{1}{4}\nabla^2\rho_t(\vec{R}) - \tau_t(\vec{R}) + \frac{3}{5}k_F^2\rho_t(\vec{R})\right]\\ &k_F = k_F(\vec{R}) = \left[\frac{3\pi^2}{2}\rho(\vec{R})\right]^{1/3}\end{aligned}}$$

$$\boxed{\vec{S}_t\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right) \simeq -\frac{i}{2}\Pi_1(k_F r)\,\vec{r}\times\vec{J}_t(\vec{R})}$$

PSA-DME ($w/\ g(R,k) = \Theta(k_F - k)$)

$$\Pi_0 = \Pi_1 = \Pi_2 = \frac{3 j_1(k_F r)}{k_F r} = \rho_{SL}(k_F r)$$

Negele-Vautherin DME

$$\Pi_0 = \rho_{SL}(k_F r) \qquad \Pi_2 = 105\,\frac{j_3(k_F r)}{(k_F r)^3}$$

$$\Pi_1 = j_0(k_F r)$$

# HF energy for realistic (e.g., chiral EFT) interactions

$$E^{HF}_{int} = \frac{1}{2}\sum_{\substack{\sigma_1\cdots\sigma_4\\ \tau_1\cdots\tau_4}} \prod_{i=1}^{4} d\vec{r}_i \, (\vec{r}_1\sigma_1\tau_1\,\vec{r}_2\sigma_2\tau_2|\hat{V}\mathcal{A}_{12}|\vec{r}_3\sigma_3\tau_3\,\vec{r}_4\sigma_4\tau_4)\,\rho(\vec{r}_3\sigma_3\tau_3,\vec{r}_1\sigma_1\tau_1)\,\rho(\vec{r}_4\sigma_4\tau_4,\vec{r}_2\sigma_2\tau_2)$$

$$= \frac{1}{2}\mathrm{Tr}^{(1)}_{\sigma\tau}\mathrm{Tr}^{(2)}_{\sigma\tau}\int\prod_{i=1}^{4} d\vec{r}_i\,(\vec{r}_1\vec{r}_2|\hat{\underset{\sim}{\mathcal{V}}}^{1\otimes 2}|\vec{r}_3\vec{r}_4)\,\underset{\sim}{\rho}^{(1)}(\vec{r}_3,\vec{r}_1)\,\underset{\sim}{\rho}^{(2)}(\vec{r}_4,\vec{r}_2)$$

$\left(\hat{\underset{\sim}{\mathcal{V}}} = \hat{V}\hat{\mathcal{A}}_{12}\right)$

Matrix on spin/isospin space $1\otimes 2$

Matrix in spin/isospin space of particle 1

Matrix in spin/isospin space of particle ②

* hereafter drop $1\otimes 2$ + particle ① + ② labels unless absolutely needed

Now, $(\vec{r}_1\vec{r}_2|\hat{\underset{\sim}{\mathcal{V}}}|\vec{r}_3\vec{r}_4) = \delta(\vec{R}-\vec{R}')\,\langle\vec{r}|\hat{\underset{\sim}{\mathcal{V}}}|\vec{r}\,'\rangle$

$$\boxed{\Rightarrow E^{HF}_{int} = \frac{1}{2}\mathrm{Tr}^{(1)}_{\sigma\tau}\mathrm{Tr}^{(2)}_{\sigma\tau}\int d\vec{R}\,d\vec{r}\,d\vec{r}\,'\,\langle\vec{r}|\hat{\underset{\sim}{\mathcal{V}}}|\vec{r}\,'\rangle\,\underset{\sim}{\rho}\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}+\tfrac{\vec{r}\,'}{2}\right)\underset{\sim}{\rho}\left(\vec{R}-\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}\,'}{2}\right)}$$

* Where A.S. potential in coordinate space given as

$$\langle\vec{r}|\hat{\underset{\sim}{\mathcal{V}}}|\vec{r}\,'\rangle = \int\frac{d\vec{p}\,d\vec{p}\,'}{(2\pi)^3(2\pi)^3}\,e^{i\vec{p}\cdot\vec{r}\,'}\,e^{-i\vec{p}\,'\cdot\vec{r}}\,\langle\vec{p}\,'|\hat{V}(1-P_\sigma P_\tau P_r)|\vec{p}\rangle$$

$$= \int\frac{d\vec{p}\,d\vec{p}\,'}{(2\pi)^6}\,e^{i\vec{p}\cdot\vec{r}\,'-i\vec{p}\,'\cdot\vec{r}}\left(\langle\vec{p}\,'|\hat{V}|\vec{p}\rangle - \langle\vec{p}\,'|\hat{V}P_\sigma P_\tau|-\vec{p}\rangle\right)$$

Note: Why bother w/ $\vec{p}$-space? Because modern chiral EFT potentials most naturally given in momentum space.

## General form of $\hat{V}$ as in, say, chiral EFT

$$\langle \vec{p}'|\hat{V}|\vec{p}\rangle = \left[V_c + \tau_1\cdot\tau_2 W_c\right] + \left[V_s + \tau_1\cdot\tau_2 W_s\right]\vec{\sigma}_1\cdot\vec{\sigma}_2 + \left[V_T + \cdots\right]\vec{\sigma}_1\cdot\vec{q}\,\sigma_2\cdot\vec{q}$$

$$+\left[\tilde{V}_c + \tau_1\tau_2\tilde{W}_c\right] + \left[\tilde{V}_s + \cdots\cdots\right]\vec{\sigma}_1\cdot\vec{\sigma}_2 + \left[\tilde{V}_T + \cdots\right]\vec{\sigma}_1\cdot\vec{K}\,\sigma_2\cdot\vec{K}$$

$$+\left[V_{LS} + \tau_1\tau_2 W_{LS}\right]\frac{i}{2}(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{q}\times\vec{K}$$

where $\vec{q} = \vec{p}' - \vec{p}$ and $\{V_c, W_c, \ldots\}$ depend on $\vec{q}$ only

$\vec{K} = \dfrac{\vec{p}+\vec{p}'}{2}$ $\quad\{\tilde{V}_c, \tilde{W}_c, \ldots\}$ depend on $\vec{K}$ only

If this is obscure to you, think of a term in the Minnesota potential without a $P_r$ factor

e.g. $V(r)$ $\quad \langle\vec{p}'|V|\vec{p}\rangle = \int d\vec{r}\, V(r)\, e^{i\vec{r}\cdot(\vec{p}-\vec{p}')}$ only depends on $\vec{q}$

* Now consider a term $V(r)P_r$: $\langle\vec{p}'|VP_r|\vec{p}\rangle = \int d\vec{r}\,\langle\vec{p}'|\vec{r}\rangle V(r)\langle\vec{r}|P_r|\vec{p}\rangle = \int d\vec{r}\,\langle\vec{p}'|\vec{r}\rangle V(r)\langle-\vec{r}|\vec{p}\rangle$

$$= \int d\vec{r}\, e^{-i\vec{r}\cdot(\vec{p}+\vec{p}')}\, V(r)$$ only depends on $\vec{K} = \vec{p}+\vec{p}'$

* Likewise, you can expand

$$\langle\vec{p}'|\hat{V}P_\sigma P_\tau|-\vec{p}\rangle = \left[V_c^x + \cdots\right] + \cdots + \left[V_T^x + \tau_1\cdot\tau_2 W_T^x\right]\vec{\sigma}_1\cdot\vec{K}\,\vec{\sigma}_2\cdot\vec{K}$$

$$+\left[\tilde{V}_c^x + \cdots\right] + \cdots + \left[\tilde{V}_T^x + \cdots\cdots\right]\vec{\sigma}_1\cdot\vec{q}\,\sigma_2\cdot\vec{q}$$

where $\{V_c^x, \cdots V_T^x\}$ depend only on $\vec{K} = \dfrac{\vec{p}'+\vec{p}}{2}$

$\{\tilde{V}_c^x \cdots \hat{V}_T^x\}$ depend only on $\vec{q} = \vec{p}' - \vec{p}$

Note: The $\{V_i^x, W_i^x, \tilde{V}_i^x, \tilde{W}_i^x\}$ can be expressed as linear combos of the $\{V_i, W_i, \tilde{V}_i, \tilde{W}_i\}$

Claim: Making use of the above components of NN-interaction, plus the following

$$\rho_0(\vec{r}_1,\vec{r}_2) \equiv \mathrm{Tr}_{\sigma\tau}\, \underset{\sim}{\rho}(\vec{r}_1,\vec{r}_2)$$
$$\rho_1(\vec{r}_1,\vec{r}_2) \equiv \mathrm{Tr}_{\sigma\tau}\left[\underset{\sim}{\rho}(\vec{r}_1,\vec{r}_2)\tau_z\right]$$
$$\vec{S}_0(\vec{r}_1,\vec{r}_2) = \mathrm{Tr}_{\sigma\tau}\left[\underset{\sim}{\rho}(\vec{r}_1,\vec{r}_2)\vec{\sigma}\right]$$
$$\vec{S}_1(\vec{r}_1,\vec{r}_2) = \mathrm{Tr}_{\sigma\tau}\left[\underset{\sim}{\rho}(\vec{r}_1,\vec{r}_2)\vec{\sigma}\tau_z\right]$$

For even-even Nuclei for Simplicity

$$\boxed{\begin{aligned} E_H &= \frac{1}{2}\sum_{t=0,1}\int d\vec{R}\,d\vec{r}\left[\rho_t\left(\vec{R}+\frac{\vec{r}}{2}\right)\rho_t\left(\vec{R}-\frac{\vec{r}}{2}\right)\Gamma_C^t(r) + \vec{r}\cdot\vec{J}_t\left(\vec{R}+\frac{\vec{r}}{2}\right)\rho_t\left(\vec{R}-\frac{\vec{r}}{2}\right)\Gamma_{LS}^t(r)\right] \\ E_F &= -\frac{1}{2}\sum_{t=0,1}\Bigg[\int d\vec{R}\,d\vec{r}\Big[\rho_t^2\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right)\Gamma_C^{xt}(\vec{r}) - \vec{S}_t^{\,2}\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right)\Gamma_S^{xt} \\ &\quad + S_t^\alpha\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right)S_t^\beta\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right)\nabla_\alpha\nabla_\beta\,\Gamma_T^{xt}(\vec{r}) \\ &\quad + i\,\Gamma_{LS}^{xt}(r)\,\vec{S}_t\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right)\cdot\left(\vec{r}\times\vec{\nabla}_{12}\right)\rho_t(\vec{r}_1,\vec{r}_2)\Big]\end{aligned}}$$

where:

$$\boxed{\begin{aligned} \Gamma_i^t(r) &\equiv V_i(\vec{r}) - \tilde{V}_i^x(\vec{r}) \quad t=0 & \Gamma_i^{xt}(\vec{r}) &\equiv V_i^x(\vec{r}) - \tilde{V}_i(\vec{r}) \quad t=0 \\ &\equiv W_i(\vec{r}) - \tilde{W}_i^x(\vec{r}) \quad t=1 & &\equiv W_i^x(\vec{r}) - \tilde{W}_i(\vec{r}) \quad t=1 \end{aligned}}$$

and $$V_i(r) \equiv \int \frac{d\vec{q}}{(2\pi)^3} e^{i\vec{q}\cdot\vec{r}} V_i(\vec{q}) \qquad i = C, S, T$$

$$\equiv \frac{i}{r^2} \int \frac{d\vec{q}}{(2\pi)^3} e^{i\vec{q}\cdot\vec{r}} (\vec{q}\cdot\vec{r}) V_i(\vec{q}) \qquad i = LS$$

(Ditto for $W_i(r)$)

[See arXiv:1003.5210 for the gory details! I merely sketch the development here so

1) You can use my DME notebooks to generate EDF for Minnesota potential neutron drops

2) You can appreciate the complicated space, spin, & isospin structures that are being built into the EDF

$\chi$-EFT NN interactions thru $N^2LO$ [* Show figure w/ eqns?]

$$E_x^{DME} = \int d\vec{R} \sum_{t=0,1} \left[ C_t^{\rho^2}(u)\, \rho_t^2(R) + C_t^{\rho\tau}(u)\, \rho_t(R)\tau_t(R) + C_t^{\rho\Delta\rho}(u)\, \rho_t \nabla^2 \rho_t + C_t^{J^2}(u)\, J_t^2 \right]$$

$$u \equiv \frac{k_F(R)}{m_\pi}$$

each coupling function has skeleton form

$$C_t^g(u) = \sum_{n=0}^{2} C_{t,n}^g(u)$$

$\begin{bmatrix} n=0 & \text{LO EFT} \\ 1 & \text{NLO } '' \\ 2 & N^2\text{LO } '' \end{bmatrix}$

$g \in \{\rho\rho, \rho\tau, \rho\Delta\rho, \ldots\}$

$$C_{t,n}^g(u) = \sum_{j=0}^{2} \alpha_j^g(n,t,u)\, F_j(n,u)$$

$$C_t^g(u) = \sum_{n=0}^{2} C_{t,n}^g(u) \qquad g \in \{ \rho\rho, \rho\tau, \rho\Delta\rho, .. \}$$

$$C_{t,n}^g(u) = \alpha_0^g(n,t,u) + \sum_{j=1}^{2} \alpha_j^g(n,t,u)\, \mathcal{F}_j(n,u)$$

rational polynomial in $u$

Non-analytic in $u$ due to finite range

e.g.: LO ($1\pi$-exchange):

$$\mathcal{F}_1(0,u) = \log(1+4u^2)$$

$$\mathcal{F}_2(0,u) = \mathrm{Arctan}\, 2u$$

NLO ($2\pi$-exchange):

$$\mathcal{F}_1(1,u) = \left[\log\left(1+2u^2+2u\sqrt{1+u^2}\right)\right]^2$$

$$\mathcal{F}_2(1,u) = \sqrt{1+u^2}\,\log\left(1+2u^2+2u\sqrt{1+u^2}\right)$$