Recap from last time: DME to get rid of non-locality

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

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

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

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

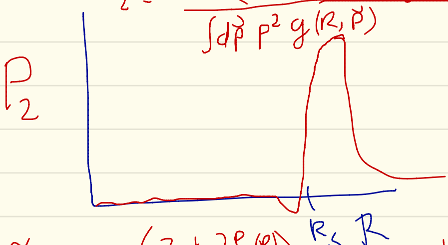
both ρ + $\vec{S}$ good

$\Updownarrow$

build in surface physics,

namely $g(R_0,\vec{k}) \neq$ spherical

$$P_2 \doteq \frac{\int d\vec{p}\,\left(3(\vec{p}\cdot\hat{r})^2 - p^2\right) g(\vec{R},\vec{p})}{\int d\vec{p}\ p^2\, g(R,\vec{p})}$$



$$\tilde{k}_F(R) \equiv \left(\frac{2+2P_2(R)}{2-2P_2(R)}\right) k_F(R)$$ to include these eff.

Negele-Vautherin DME

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

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

Scalar ρ good
Vector $\vec{S}$ bad

e.g.: $E_F = \frac{1}{2}\int d\vec{R}\int d\vec{r}\, V(r)\, \rho^2(R+\frac{r}{2}, R-\frac{r}{2})$

$$\simeq \int d\vec{R}\left[C^{\rho\rho}(\rho)\cdot\rho^2(R) + C^{\rho\tau}\rho\tau + C^{\rho\nabla^2\rho}(\rho)\cdot\rho\nabla^2\rho + \dots\right]$$

eg: $C^{\rho\rho}(\rho) = \int d\vec{r}\, V(r)\left[\Pi_0^2(k_F r) + \frac{1}{5}\Pi_0\Pi_2\, k_F^2 r^2\right]$ etc...

Finite range physics mapped into density-dependent couplings

* Longer range $V \Rightarrow$ stronger ρ-dep.

e.g., $V_{1\pi}$ gives couplings of the form

$$C^i(\rho) = \alpha_1^i(u) + \alpha_2^i(u)\log(1+4u^2) + \alpha_3^i(u)\,\mathrm{Arctan}\,2u \qquad u \equiv \frac{k_F(R)}{m_\pi}$$

i ranges over ρ_*^2, $\rho_*\tau_*$, etc.

2 Strategies to use this DME to build EDFs

1.) Purely ab-initio :- Apply DME to averaged G-matrix $G(r)$ w/no adjustment
- obviously limited by level/accuracy of the ab-initio H and MB method (BHF)

2.) Improve existing Skyrme Phenomenology (or, Adding π's to Skyrme)

$$G(r) \approx \underbrace{\Theta(r-\xi)V(r)}_{\text{long-range tail of } V_{bare}} + \underbrace{\Theta(\xi-r)\left[C_0\delta(\vec{r}) + C_2\nabla^2\delta(\vec{r}) + \dots\right]}_{\text{already Skyrme-like give local } E[\rho]} \quad \text{(healing property)}$$

(strongest non-loc. $\Leftrightarrow$ density dep.)

=> 1) Calculate DME contributions in HF of long-range V_{2N}, V_{3N}
(same types would arise in BHF calc or CCSD. or...) due to healing property

- Parameter free
- fixed by long-distance physics (best understood, QCD connection via χ-symm.)
- Novel ρ-dep.

2) Add these to existing Skyrme EDF's, but re-fit Skyrme constants (t_0, t_3, x_0, α, etc..)

$$E[\rho] = \int d\vec{R} \sum_{t=0,1} \left[C_t^{\rho^2}(\rho)\, \rho_t^2(R) + C_t^{\rho\tau}(\rho)\, \rho\tau + \ldots \right]$$

each $C_t^i(\rho) = \underbrace{C^i_{t,SK}}_{\text{Coupling constant}} + \underbrace{C^i_{t,DME}(\rho)}_{\text{Coupling function}}$

(encodes SR physics + bulk correlations) adjusted to data

- encodes π-physics
- no free params.

"KS"-eqns: $h^\tau \phi_i(\vec{r}\tau) = E_{i\tau}\, \phi_i(\vec{r}\tau)$ $\qquad \phi_i(\vec{r}\tau) = \begin{pmatrix} \phi_i(\vec{r}\,\sigma = +\tfrac{1}{2}, \tau) \\ \phi_i(\vec{r}\,\sigma = -\tfrac{1}{2}, \tau) \end{pmatrix}$

$$h^\tau = -\vec{\nabla}\cdot B_\tau \vec{\nabla} + U_\tau(\vec{r}) - i\,\vec{W}_r \cdot \vec{\nabla}\times\vec{\sigma}$$

$$B_\tau(r) = \frac{\delta E}{\delta \tau_\tau} \qquad \vec{W}_\tau(r) = \frac{\delta E}{\delta \vec{J}_\tau}$$

$$U_\tau(r) = \frac{\delta E}{\delta \rho_\tau}$$

(Need to modify Skyrme codes where sp fields hard-coded, to take into account $\frac{\delta}{\delta\rho}(C\rho^2) = 2C\rho + \frac{\delta C}{\delta \rho}\rho^2$

Speculative thought: It would be interesting to see if Nuclei "know" about m_π (a-la phase shift analysis of NN) if you let it float in the refit.

Sketch of how it looks for χ-EFT V_{2N}:

$$V = \sum_{i=C,S,T,LS} \left(\hat{V}_i + \tau_1\tau_2 \hat{W}_i\right)\hat{O}_i$$

$$O_C = 1,\quad O_S = \sigma_1\cdot\sigma_2$$

HF energy for Realistic (e.g., Chiral EFT) interactions

$$O_T = \vec{\sigma}_1\cdot\vec{r}\,\vec{\sigma}_2\cdot\vec{r} \quad \text{etc}$$

* Trivially evaluate E_{HF} using:

$$\rho_0(\vec{r}_1,\vec{r}_2) \equiv \mathrm{Tr}_{\sigma\tau}\, \underset{\sim}{\rho}(\vec{r}_1,\vec{r}_2)$$

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

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

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

and $\underset{\sim}{\hat{V}} = \underset{\sim}{\hat{V}}^D + \underset{\sim}{\hat{V}}^E P_r$

even-even ....

$$E_H = \frac{1}{2}\sum_{t=0,1}\int d\vec{R}\,d\vec{r}\left[\rho_t\left(\vec{R}+\frac{\vec{r}}{2}\right)\rho_t\left(\vec{R}-\frac{\vec{r}}{2}\right)V_C^{Dt}(r) + \vec{r}\cdot\vec{J}_t\left(\vec{R}+\frac{\vec{r}}{2}\right)\rho_t\left(\vec{R}-\frac{\vec{r}}{2}\right)V_{LS}^{Dt}(r)\right]$$

$$\begin{aligned}E_F = -\frac{1}{2}\sum_{t=0,1}\Bigg[\int d\vec{R}\,d\vec{r}\Big[&\rho_t^2\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right)V_C^{Et}(\vec{r}) - \vec{S}_t^2\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right)V_S^{Et}(r)\\ &+ S_t^\alpha\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right)S_t^\beta\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right)\nabla_\alpha\nabla_\beta V_T^{Et}(\vec{r})\\ &+ i\,V_{LS}^{Et}(r)\,\vec{S}_t\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right)\cdot\left(\vec{r}\times\vec{\nabla}_{12}\right)\rho_t(\vec{r}_1,\vec{r}_2)\Big]\end{aligned}$$

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

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

(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

<u>χ-EFT NN interactions thru N^2LO</u> [* Show figure w/ eqns?]

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

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

each coupling <u>function</u> has skeleton form

$$C_t^g(u) = \sum_{n=0}^{2} C_{t,n}^g(u) \qquad \left[\begin{array}{ll} n=0 & \text{LO EFT} \\ 1 & \text{NLO } '' \\ 2 & N^2\text{LO } '' \end{array} \right] \quad g \in \{\rho\rho, \rho\tau, \rho\Delta\rho, \ldots\}$$

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

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

$$C_{t,n}^g(u) = \underbrace{\alpha_0^g(n,t,u)}_{} + \sum_{j=1}^{2} \underbrace{\alpha_j^g(n,t,u)}_{\text{rational polynomial in } u} \underbrace{F_j(n,u)}_{\text{Non-analytic in } u \text{ due to finite range}}$$

rational polynomial in u

Non-analytic in u due to finite range

e.g.: LO (1π-exchange): $\quad F_1(0,u) = \log(1+4u^2)$

$$F_2(0,u) = \text{Arctan}\, 2u$$

NLO (2π-exchange): $\quad F_1(1,u) = \left[\log\left(1+2u^2+2u\sqrt{1+u^2}\right)\right]^2$

$$F_2(1,u) = \sqrt{1+u^2}\,\log\left(1+2u^2+2u\sqrt{1+u^2}\right)$$

Simpler example: Minnesota pot. in ND

$$\hat{\underset{\sim}{V}} = \hat{V}^D + \hat{V}^E P_r \qquad \hat{V}^D = \hat{V}^E = \frac{1}{2}(V_R+V_S)(1-P_\sigma)$$

$$= \frac{1}{2}(V_R+V_S)\left(\frac{1-\sigma_1\cdot\sigma_2}{2}\right)$$

$$= \frac{1}{4}(V_R+V_S) - \frac{1}{4}(V_R+V_S)\,\sigma_1\cdot\sigma_2$$

$$\underset{\sim}{V}^{E,D} \equiv f(r) - f(r)\,\sigma_1\cdot\sigma_2$$

$$\Rightarrow E_{HF} = \frac{1}{2}\,\mathrm{Tr}_\sigma^{(1)}\mathrm{Tr}_\sigma^{(2)} \int d\vec{R}\,d\vec{r}\;\underset{\sim}{\hat{V}}(r)\,\underset{\sim}{\rho}^{(1)}\!\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right)\underset{\sim}{\rho}^{(2)}\!\left(\vec{R}-\tfrac{\vec{r}}{2},\vec{R}+\tfrac{\vec{r}}{2}\right)$$

$$= \frac{1}{2}\,\mathrm{Tr}^{(1)}\mathrm{Tr}^{(2)} \int d\vec{R}\,d\vec{r}\;f(r)\left(1-\sigma_1\cdot\sigma_2\right)\underset{\sim}{\rho}^{(1)}\!\left(\vec{R}+\tfrac{\vec{r}}{2}\right)\underset{\sim}{\rho}^{(2)}\!\left(\vec{R}-\tfrac{\vec{r}}{2}\right) = E_H$$

$$-\frac{1}{2}\,\mathrm{Tr}^{1}\mathrm{Tr}^{2} \int d\vec{R}\,d\vec{r}\;f(r)\left(1-\sigma_1\cdot\sigma_2\right)\underset{\sim}{\rho}^{(1)}\!\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right)\underset{\sim}{\rho}^{(2)}\!\left(\vec{R}-\tfrac{\vec{r}}{2},\vec{R}+\tfrac{\vec{r}}{2}\right) = E_F$$

$\cancel{E_F}$ Use $\underset{\sim}{\rho}\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right) = \frac{1}{2}\left[\rho\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right)\mathbb{1} + \vec{S}(r_1,r_2)\cdot\vec{\sigma}\right]$

$$\mathrm{Tr}\,\sigma_x\sigma_y = \delta_{xy} \text{ etc.} \Rightarrow \rho = \mathrm{Tr}\,\underset{\sim}{\rho}, \quad \vec{S} = \mathrm{Tr}\,\underset{\sim}{\rho}\,\vec{\sigma}$$

$$\Rightarrow \boxed{E_F = -\frac{1}{2}\int d\vec{R}\,d\vec{r}\;f(r)\,\rho^2\!\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right)} + \cancel{\frac{1}{2}\int d\vec{R}\,d\vec{r}\;f(r)\,\vec{S}\!\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right)\cdot\vec{S}\!\left(\vec{R}-\tfrac{\vec{r}}{2},\vec{R}+\tfrac{\vec{r}}{2}\right)}$$

0 spins saturated

plug in

$$\rho_t\!\left(\vec{R}+\tfrac{\vec{r}}{2},\vec{R}-\tfrac{\vec{r}}{2}\right) \simeq \Pi_0(k_F r)\,\rho_t(\vec{R}) + \frac{r^2}{6}\Pi_2(k_F r)\left[\frac{1}{4}\nabla^2\rho_t(\vec{R}) - \tau_t(\vec{R}) + \frac{3}{5}k_F^2\rho_t(\vec{R})\right]$$

$$k_F = k_F(\vec{R}) = \left[\frac{3\pi^2}{2}\rho(\vec{R})\right]^{1/3}$$

and group terms accordingly (only keep terms to 2nd order, where the [ ] in DME is 2nd order)

Voila, you have a local EDF to compare against your exact HF!

$h(R)$ local, most naturally solved in r-space as PDE

$\Downarrow$

however, you can easily adopt your HF code to this task

$$h(R) \to \langle n\ell jm | h | n'\ell jm \rangle$$

* Show examples 1.) Neutron Drop (explain diff approxs) $\Rightarrow$ (PSA > NV when though not probed !!)

2.) Preoptimization for χ-EFT] meant to check if things work

72 Even Even

8 OEM diffs