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Skyrme EDF and Naturalness

The Skyrme energy density functional (EDF) approach has been used to calculate the entire mass table of nuclei
 ⇒ try every N and Z and see if a bound solution is found
 ⇒ gives estimate of proton and neutron driplines, as well as limits of superheavies

Motivate form of a Skyrme calculation by returning to Hartree-Fock specialized to a contact interaction
 ⇒ $V(\vec{x}, \vec{y}) = C_0 \delta^3(\vec{x} - \vec{y})$

Then

$$\begin{aligned} \langle \Psi_{HF} | \hat{H} | \Psi_{HF} \rangle &= \int d\vec{x} \frac{1}{2m} \sum_{i=1}^A \nabla \phi_i^* \cdot \nabla \phi_i + \frac{1}{2} \int d\vec{x} \int d\vec{y} \sum_i |\phi_i(\vec{x})|^2 C_0 \delta^3(\vec{x} - \vec{y}) \sum_j |\phi_j(\vec{y})|^2 \\ &\quad - \frac{1}{2} \int d\vec{x} \int d\vec{y} \sum_{i=1}^A \phi_i^*(\vec{x}) \phi_i(\vec{y}) C_0 \delta^3(\vec{x} - \vec{y}) \sum_j \phi_j^*(\vec{y}) \phi_j(\vec{x}) \\ &= \int d\vec{x} \left[\frac{1}{2m} \left(\sum_{i=1}^A \nabla \phi_i^* \cdot \nabla \phi_i \right) + \frac{1}{2} \left(1 - \frac{1}{2} \right) C_0 \left(\sum_i |\phi_i(\vec{x})|^2 \right)^2 \right] \\ &= \int d\vec{x} \left[\frac{1}{2m} \rho(\vec{x}) + \frac{1}{2} \left(1 - \frac{1}{2} \right) C_0 \rho(\vec{x})^2 \right] \equiv E[\rho, \rho] \quad \text{energy functional!} \end{aligned}$$

(Recall that a functional takes functions as input, in this case $\rho(\vec{x})$ and $\rho(\vec{x})$, and outputs a number, here a real energy.)

The equations for $\phi_i(\vec{x})$ follow from

$$\frac{\delta}{\delta \phi_i^*(\vec{x})} \left(E[\rho, \rho] - \sum_j \epsilon_j \int d\vec{y} |\phi_j(\vec{y})|^2 \right) = 0$$

$$\Rightarrow -\frac{\hbar^2}{2m} \nabla^2 \phi_i(\vec{x}) + \left[\left(1 - \frac{1}{2} \right) C_0 \rho(\vec{x}) \right] \phi_i(\vec{x}) = \epsilon_i \phi_i(\vec{x})$$

Procedure: i) Guess $\rho(\vec{x}), \rho(\vec{x})$ ii) find $\{\phi_i, \epsilon_i\}$ iii) evaluate $E[\rho, \rho]$
 iv) stop if self-consistent (ϵ_i 's stable) v) go to ii)

• Look at some slides from TALENT_dft.pdf.

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Skyrme EDF as traditionally formulated has a more general form for V_2 that looks like a low-momentum (pionless) EFT expansion:

$$\langle \vec{k} | V_2^{\text{Skyrme}} | \vec{k}' \rangle = t_0 + \frac{1}{2} t_1 (\vec{k}^2 + \vec{k}'^2) + t_2 (\vec{k} \cdot \vec{k}') + i W_0 (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot (\vec{k} \times \vec{k}')$$

which generalizes the equation for ϕ_i to

$$\left(-\vec{\nabla} \cdot \frac{1}{2m^*(x)} \vec{\nabla} + U(x) + \frac{3}{4} W_0 \vec{\nabla} \rho \cdot \frac{1}{\nabla \times \vec{\sigma}} \right) \phi_i(\vec{x}) = \epsilon_i \phi_i(\vec{x})$$

$$\text{with } U = \frac{3}{4} t_0 \rho + \left(\frac{3}{16} t_1 + \frac{5}{16} t_2 \right) \rho^2 + \dots; \quad \frac{1}{2m^*(x)} = \frac{1}{2m} + \left(\frac{3}{16} t_1 + \frac{5}{16} t_2 \right) \rho$$

• Historically viewed as a mean-field approximation (that is, neglecting correlations) for an effective interaction that was an expansion of the G-matrix (in-medium T matrix)

• Modern view: The functional itself is more fundamental. View Skyrme as a parametrization of the energy functional that density functional theory (DFT) promises should exist (more below)

$$\Rightarrow E_{\text{Skyrme}}[\rho, \uparrow, \vec{J}, \dots] = \int d\vec{x} \mathcal{E}[\rho(\vec{x}), \uparrow(\vec{x}), \vec{J}(\vec{x}), \dots] \quad (\text{here for } N=Z)$$

$$\mathcal{E}[\rho, \uparrow, \vec{J}] = \frac{1}{2m} \rho^2 + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_2 \rho^{2+\alpha} + \frac{1}{16} (3t_1 + 5t_2) \rho^{\uparrow} + \frac{1}{16} (9t_1 - 5t_2) (\nabla \rho)^2 - \frac{3}{4} W_0 \rho \vec{\nabla} \cdot \vec{J} + \frac{1}{32} (t_1 - t_2) \vec{J}^2$$

$$\text{where } \rho(\vec{x}) = \sum_{i=1}^N |\phi_i(\vec{x})|^2, \quad \uparrow(\vec{x}) = \sum_{i=1}^N |\nabla \phi_i(\vec{x})|^2, \quad \dots$$

• In practice: There are additional densities, pairing is very important (Hartree-Fock Bogoliubov or HFB), projection is needed for good numbers,

• Looks like a pionless $\rho \uparrow \vec{J}$ perturbative EDF for $\rho \ll \rho_0$, but with many missing terms (not complete).

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Do Skyrme functions fit to nuclear data know about chiral physics?

Refs: "Skyrme energy functional and naturalness", Jf, J.C. Hackett, PRC 56, 2875 (1997)

"Natural units for nuclear energy density functional theory",
M. Kortelainen, Jf, W. Nazarewicz, M.V. Stoitsov, PRC 82, 011304 (2010)

⇒ Look for signatures of chiral physics in Skyrme functionals, even though there are no explicit pions

* Apply Georgi-Manohar naive dimensional analysis (NDA) to the functional. Recall how it works for a low-energy strong interaction Lagrangian without pions: Scale each term by factors of $f_\pi = 93 \text{ MeV}$ and $\Lambda_\chi \sim 500 - 1000 \text{ MeV}$ according to

$$c \left[\frac{m_\pi^2}{f_\pi^2 \Lambda_\chi} \right]^n \left[\frac{1}{\Lambda_\chi} \right]^n f_\pi^2 \Lambda_\chi^2$$

"Natural" means the left-over dimensionless coefficient c is $\mathcal{O}(1)$

Typical case: Skyrme 3 from Ring and Schuck's many-body book
 $t_0 = -1128.8 \text{ MeV fm}^3$, $t_1 = 395 \text{ MeV fm}^5$, $t_2 = -95 \text{ MeV fm}^9$, $t_3 = 14000 \text{ MeV fm}^6$,
 $W_0 = 120 \text{ MeV fm}^3$.

Clearly these units don't reveal natural scales!

The rescaled $\mathcal{H}(\vec{r})$ [where $E(\rho, \tau, \vec{j}) = \int d^3r \mathcal{H}(\vec{r})$] takes the form

$$\mathcal{H}(\vec{r}) = C_1 \frac{\rho}{\Lambda} + C_2 \frac{\rho^2}{f_\pi^2} + C_3 \frac{\rho^3}{f_\pi^2 \Lambda} + C_4 \frac{\rho \tau}{f_\pi^2 \Lambda^2} + C_5 \frac{(\vec{j} \cdot \vec{j})^2}{f_\pi^2 \Lambda^2} + C_6 \frac{\rho \vec{j} \cdot \vec{j}}{f_\pi^2 \Lambda^3} + C_7 \frac{\vec{j}^2}{f_\pi^2 \Lambda^3}$$

Skyrme 3 ⇒ $C_1 = 0.5$, $C_2 = -0.48$, $C_3 = 1.05$, $C_4 = 1.14$, $C_5 = 1.62$, $C_6 = -2.31$, $C_7 = 0.39$
 ⇒ pretty natural! (disclaimer: limited range of l)

Claim: scaling by M_N or m_π or m_ρ or ... does not work.
 (should revisit this!)

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A large-scale study in 2010 examined all Skyrme EDFs and found that the best (i.e., most successful phenomenologically) functions are consistent with naturalness

- see plot on triumf_2014_funstabl.pdf slides (29)
- strong deviations from naturalness were associated with known deficiencies in fitting the functionals
- when Λ_π determined by most natural (close to 1 couplings), Λ_π found to be about 700 MeV.

If we arrange the first four terms like

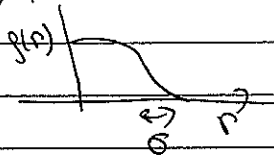
$$T(\vec{r}) = \frac{\rho}{\Lambda} (c_2 + c_4 \frac{\rho}{\Lambda^3}) + \frac{\rho^2}{\Lambda^2} (c_3 + c_5 \frac{\rho}{\Lambda^3}) + \dots$$

then we have an implied density expansion with expansion parameter

$$\left(\frac{\rho}{\Lambda^3} \right) \sim (0.17 \text{ fm}^{-3}) (197.33 \text{ MeV} \cdot \text{fm})^3 / [(93 \text{ MeV})^3 (700 \text{ MeV})] \sim \frac{1}{5}$$

\Rightarrow not a bad expansion parameter! (could be $1/4 - 1/7$ in general!)

There is also a gradient expansion. A relevant scale for derivatives (of density) in nuclei nuclei is the surface thickness δ (which is a constant)



$\Rightarrow \frac{\delta}{\Lambda} \lesssim \frac{1}{5}$ is the expansion parameter.


The same analysis indicates relativistic mean field models are also natural, with a greater density range.

Summary: While not definitive, this suggests that nuclei know about chiral symmetry.

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What is Density Functional Theory?

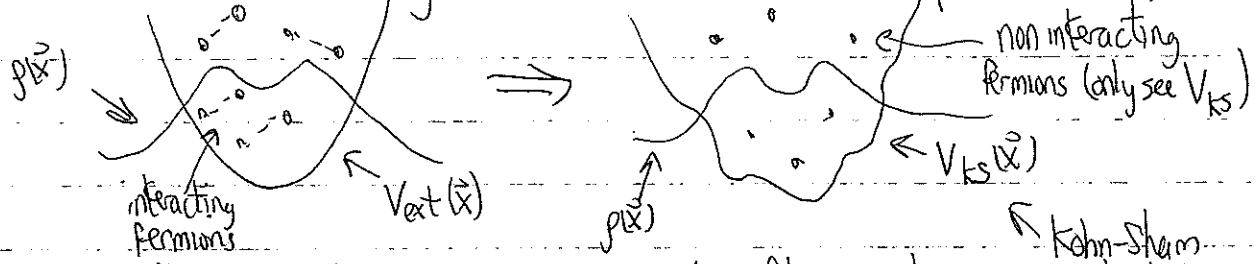
- Skyrme functionals are often regarded as DFT functionals. What is the background?
- Hohenberg and Kohn formulated an existence proof for an energy functional: $E_{\text{ext}}[\rho] = F_{\text{HK}}[\rho] + \int d\vec{x} V_{\text{ext}}(\vec{x}) \rho(\vec{x}) \Rightarrow E_{\text{gs}}, \rho_{\text{gs}}$
 - $\rho(\vec{x})$ is the density  $\langle \psi(\vec{x}) | \psi(\vec{x}) \rangle$ ground state = GS or gs
 - but we'll extend it to mean other local densities (same \vec{x}) such as the kinetic energy density $\langle \nabla^2 \psi(\vec{x}) | \nabla^2 \psi(\vec{x}) \rangle \equiv T(\vec{x})$
- V_{ext} is an external potential and F_{HK} is universal (independent of V_{ext})
 - most applications have in mind that V_{ext} is the Coulomb potential due to the nuclei in an atom or molecule, and the goal is to find the energy and density distribution of electrons. \rightarrow in nuclear case, $V_{\text{ext}} = 0!$

not constructive, just an existence proof

Kohn-Sham (KS) DFT introduces orbitals to calculate $\rho(\vec{x})$

Kohn, Sham

Let's think of interacting fermions in a harmonic trap



"true" system

Kohn-Sham system (reference system)

Kohn-Sham potential

*** \Rightarrow same density $\rho(\vec{x})$ in both

• Solve for orbitals $\{\psi_i(\vec{x})\}$ ($i=1, \dots, A$) in local potential $V_{\text{KS}}(\vec{x})$

$$\Rightarrow \left(-\frac{\nabla^2}{2m} + V_{\text{KS}}(\vec{x}) \right) \psi_i(\vec{x}) = \epsilon_i \psi_i(\vec{x})$$

Then the density $\rho(\vec{x}) = \sum_{i=1}^A |\psi_i(\vec{x})|^2$ is easily found.

• Find Kohn-Sham potential $V_{\text{KS}}[\rho, \vec{x}]$ from response of energy to local changes in density: $\delta E_{\text{interacting}}[\rho] / \delta \rho(\vec{x}) \rightarrow V_{\text{KS}}(\vec{x})$

• Solve self-consistently: first one, then the other, until they stop changing to some tolerance

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Unraveling the magic of DFT [Kutzelnigg (2008)]

• Wavefunction based methods take an anti-symmetric N -body $|\Psi\rangle$ and find $E_{\text{ground state}} = \underset{\text{all } |\Psi\rangle\text{'s}}{\text{minimum}} \langle \Psi | \hat{H} | \Psi \rangle$

• For example, the NCSM uses a single-particle basis of harmonic oscillators to build \hat{H} and then diagonalizes it to find $|\Psi\rangle$.

• In DFT, the fermion densities are the basic variables.

• Common (but misleading) statements:

"All information about a quantum mechanical ground state is contained in its (electron) density ρ ."

"The energy is completely expressible in terms of the density alone."

• These would seem at odds with the kinetic and interaction energies needing the $(1, 2, \dots)$ -particle density matrices

• eg. exchange term in HF needs $\rho(x_1, x_2)$, not just $\rho(x)$

• Key difference: The WF formulation deals with a single, fixed Hamiltonian. In this case, E is stationary to density matrix (or $|\Psi\rangle$) variations, not just $\rho(x)$.

But in DFT we consider a family of Hamiltonians $\hat{H}[v] \rightarrow E[v]$

$$\Rightarrow F_{HK}[\rho] = \min_v \{ E[v] - \int dx v(x) \rho(x) \}$$

and

$$E[\rho] = \min_p \{ F[\rho] + \int dx v(x) \rho(x) \} = \min_p \{ E_v[\rho] \}$$

external source potential

For each v , we know the ground state energy

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Wave function vs. Green's function methods.

- In the WF approach, the full many-body wavefunction is the object under consideration.
- With the Green's function, one considers the response of the ground state to adding or removing particles.
- Underlying idea is that knowing the most general response of the ground state (or the partition function in the presence of the most general sources) gives a complete specification of the many-body problem.
- The sources for DFT are more limited: $V(\vec{x})$ and μ like. Instead of non-local sources that individually create particles in one place and destroy them elsewhere, for DFT the perturbation by the source is a local shift in density.
 - ⇒ more limited response means more limited observables probed
 - but includes ground-state energy

* Not a mean-field approximation but an organization that takes a mean-field state as a reference state.

- Includes, if solved completely, all many-body correlations.
- The real issue is how much correlation is included in a given approximation to the exact functional.

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DFT as Thermodynamic Legendre transform (average)

zero temperature
↓

- Recall ordinary thermodynamics with $N = \langle \hat{N} \rangle$ particles at $T=0$
 \Rightarrow grand canonical ensemble (but $T=0$ limit)
 (not T and V as independent variables plus chemical potential)

- Use a chemical potential μ as a source to change $\langle \hat{N} \rangle$:
 $\Omega(\mu) = -kT \ln Z(\mu)$ and $N = - \left(\frac{\partial \Omega}{\partial \mu} \right)_{TV} \Rightarrow N(\mu)$
 $\frac{1}{\beta}$ partition function

because Ω is convex
 \downarrow
 N is monotonically increasing function of μ

- We can invert $N(\mu)$ to find $\mu(N)$ [why is this possible?]
 and then Legendre transform to the free energy $F(N)$:
 $F(N) = \Omega(\mu(N)) + \mu(N)N$ [check that the thermodynamic derivative relations work]

\rightarrow this is our ^(free) energy function of the particle number.

[actually, since V_{ext} is typically given rather than eliminated, a closer analogy is to define $\Omega_{\mu}(N) \equiv F(N) - \mu N$, which depends explicitly on both N and μ . This gives the grand potential when minimized with respect to N]

- Now generalize to a spatially dependent chemical potential $J(\vec{x})$, then
 $Z(\mu) \rightarrow Z[J(\vec{x})]$ and $\mu N = \mu \int \psi^\dagger \psi \rightarrow \int J(\vec{x}) \psi^\dagger \psi(\vec{x})$

- Now Legendre transform from $\ln Z[J(\vec{x})]$ to $\Gamma[\rho(\vec{x})]$ where
 $\rho = \langle \psi^\dagger \psi \rangle_J$ (density in presence of source J)

- Two paths to ab initio functional from microscopic forces!
 (i) effective action for composite local operators \leftarrow my favorite! (see references on first slide)
 (ii) MBPT

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MBPT construction:

- Recall that we introduce a single-particle potential $U(\vec{x})$ and divide H into (with V_{ext} as well)

$$H = (T + U) + (V - U + V_{\text{ext}})$$

- If we can choose $U = V_{\text{KS}}$ then we get DFT
 - criterion: order-by-order require density to be unchanged
 - need a perturbative expansion
 - \Rightarrow use a low-momentum interaction

Challenges:

- essential role of pairing

- need for symmetry restoration in finite, self-bound systems

- to derive the Kohn-Sham equations, we need to take

functional derivatives with respect to densities $\rho = \sum_{i=1}^A |\phi_i(\vec{x})|^2$

but beyond LO the many body contributions do not have explicit densities (but explicit $\phi_i(\vec{x})$ dependence and eigenvalue dependence),

\Rightarrow need to apply a chain rule (or equivalent)

[see reference 1 for details]

- alternative: use an approximation that casts the contributions directly into functionals of density (for example) \Rightarrow density matrix expansion (DME)

reference state
✓ breaks symmetry
(eg. translational)

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Hartree-Fock energy using the density matrix

From before $\odot - \ominus + \ominus \Rightarrow \odot \odot$

$$\begin{aligned} \Rightarrow \langle \Psi_{HF} | A | \Psi_{HF} \rangle = \dots + \frac{1}{2} \sum_{i,j=1}^A \int d\vec{r}_1 \int d\vec{r}_2 |\psi_i(\vec{r}_1)|^2 V(\vec{r}_1, \vec{r}_2) |\psi_j(\vec{r}_2)|^2 \\ - \frac{1}{2} \sum_{i,j=1}^A \int d\vec{r}_1 \int d\vec{r}_2 \psi_i^\dagger(\vec{r}_1) \psi_j(\vec{r}_2) V(\vec{r}_1, \vec{r}_2) \psi_j^\dagger(\vec{r}_2) \psi_i(\vec{r}_1) \end{aligned}$$

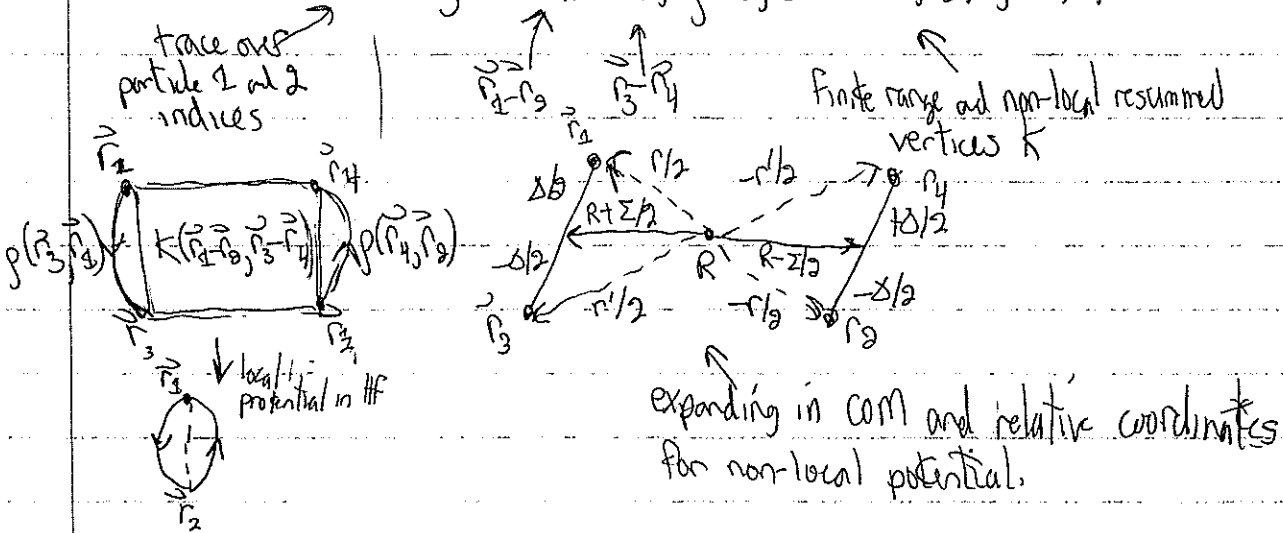
$\underbrace{\psi_i^\dagger(\vec{r}_1) \psi_j(\vec{r}_2)}_{\propto \rho(\vec{r}_1, \vec{r}_2)} \quad \underbrace{\psi_j^\dagger(\vec{r}_2) \psi_i(\vec{r}_1)}_{\propto \rho(\vec{r}_2, \vec{r}_1)}$

\Rightarrow express in terms of single-particle density matrix:

$$\rho(\vec{r}_1, \vec{r}_2) = \nu \sum_{\alpha \in \text{occ}} \psi_\alpha^\dagger(\vec{r}_1) \psi_\alpha(\vec{r}_2)$$

In general, the dominant MBPT contributions take the form:

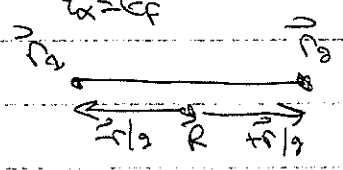
$$\langle V \rangle \sim \text{Tr}_1 \text{Tr}_2 \int d\vec{R} \int d\vec{r}_{12} \int d\vec{r}_{34} \rho(\vec{r}_1, \vec{r}_2) K(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4) \rho(\vec{r}_3, \vec{r}_4) + \text{NNN} + \dots$$



Density Matrix Expansion (DME): Expand KS density matrix in local operators with factored non-locality

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$$g(\vec{r}_1, \vec{r}_2) = \sum_{\epsilon_\alpha \leq \epsilon_F} \psi_\alpha^\dagger(\vec{r}_1) \psi_\alpha(\vec{r}_2) = \sum_n \pi_n(\vec{r}) \langle \hat{O}_n(\vec{R}) \rangle$$



different prescriptions for these functions

with $\langle \hat{O}_n(\vec{R}) \rangle = \{ \rho(\vec{R}), \nabla^2 \rho(\vec{R}), \tau(\vec{R}), \dots \}$

⇒ maps $\langle V \rangle$ to Skyrme-like EDF! But now coefficients, instead of being constants, are known functions of density,

- adds density dependences missing in Skyrme
- Original OME expands about nuclear matter ⇒ includes long-range effects
 - improved version (Gambhir et al.) uses phase-space averaging for finite nuclei
 - applied to long-range interactions ⇒ pion exchange in NN and NNN from chiral effective field theory (χEFT)

* See slides for details and references for generalizations and extensions

In its simplest form:

$$g(\vec{R} + \frac{\vec{r}}{2}, \vec{R} - \frac{\vec{r}}{2}) \sim g_{SL}(k_F(\vec{R})r) \rho(\vec{R}) + n^0 g(k_F(\vec{R})r) \times [\frac{1}{4} \nabla^2 \rho(\vec{R}) - \tau(\vec{R}) + \frac{2}{5} k_F(\vec{R})^2 \rho(\vec{R})]$$

where $k_F(\vec{R}) = (\frac{3\pi^2}{2} \rho(\vec{R}))^{1/3}$ or some other local density approximation

and

$$g_{SL}(x) \equiv \frac{3j_1(x)}{x}, \quad g(x) \equiv \frac{35j_3(x)}{2x^3}$$

* Not a short-range expansion because $\frac{k_F}{m_\pi}$ is not $\ll 1$. Instead, an expansion about the exact nuclear matter density matrix (first term).