

7/19/13

Lecture F3b: From Forces to Density Functionals

slides ① Overview: Skyrme Hartree-Fock as ^{an} example EDF
 • Pseudo data: from neutron drops \Rightarrow guidance from ab initio

② Looking for chiral physics: NDA, naturalness and Skyrme parametrizations.

③ Density Functional Theory (DFT)
 • standard definition
 • DFT as Legendre transformation

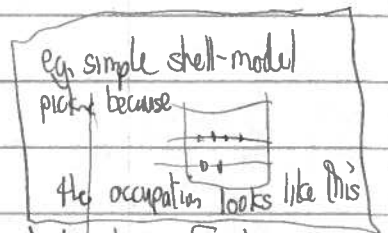
④ From MBPT to DFT via the density matrix expansion (DME)
 • hybrid approach: incorporating long range pion physics
 • current status - neutron drops

⑤ UNEDF and NUCLEI projects

① Overview - look at some slides.

We've heard about Skyrme or Gogny (Bogoliubov) Hartree-Fock (also relativistic mean field models) which have traditionally been interpreted as mean-field approximations (i.e., neglecting correlations) for effective interactions. Alternative: interpret as approximate DFT (which can have all correlations in principle)

• Here: Impact of forces on existing versions and working toward more general version with ab initio input through density functional theory.



change \vec{x}, \vec{y} to \vec{x}_1, \vec{x}_2

M36-5

7/15/13

Aside: Standard Hartree-Fock discussion for local $V(\vec{x}, \vec{y}) \rightarrow V(\vec{x}=\vec{y})$

• Best Slater determinant in a variational sense ↑ ↑
not relative coordinates here
 $|\Psi_{HF}\rangle = \det \{ \phi_i(\vec{x}), i=1 \dots A \}$ $\vec{x} = (\vec{r}, \sigma, \tau)$

$\langle \Psi_{HF} | \hat{H} | \Psi_{HF} \rangle = \sum_{i=1}^A \frac{1}{2m} \int d\vec{x} \nabla \phi_i^* \cdot \nabla \phi_i$ Feynman diagrams in coordinate space:

local potential
(later will need non-local)
⇒ more integrations

$+ \frac{1}{2} \sum_{i,j=1}^A \int d\vec{x} \int d\vec{y} |\phi_i(\vec{x})|^2 V(\vec{x}, \vec{y}) |\phi_j(\vec{y})|^2$ direct (Hartree)

$- \frac{1}{2} \sum_{i,j=1}^A \int d\vec{x} \int d\vec{y} \phi_i^*(\vec{x}) \phi_i(\vec{y}) V(\vec{x}, \vec{y}) \phi_j^*(\vec{y}) \phi_j(\vec{x})$ exchange (Fock)

$\sum_i \phi_i^*(\vec{x}) \phi_i(\vec{y}) \rightarrow$ one particle density matrix $\rho(\vec{y}, \vec{x})$

• Determine the ϕ_i by varying with fixed normalization

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

⇒ standard Hartree-Fock equation. * Fill the lowest A orbitals (for closed shell)

• If $V(\vec{x}, \vec{y}) = C_0 \delta^3(\vec{x} - \vec{y})$, and $\phi_i(\vec{x}) \rightarrow \frac{1}{\sqrt{V}} e^{i\vec{k}_i \cdot \vec{x}} \chi_{\alpha}$, we recover our alternative results, [exercise]

non-local potential

• zero range
 • more generally (still with local): $\left\{ -\frac{\hbar^2}{2m} \nabla^2 + V_H(\vec{x}) \right\} \phi_i(\vec{x}) + \int d\vec{y} V(\vec{x}, \vec{y}) \phi_i(\vec{y}) = \epsilon_i \phi_i(\vec{x})$

solve self-consistently
(potentials depend on ϕ_i 's)

where $V_H(\vec{x}) = \int d\vec{y} V(\vec{x}, \vec{y}) \sum_{j=1}^A |\phi_j(\vec{y})|^2 = \int d\vec{y} V(\vec{x}, \vec{y}) \rho(\vec{y})$

$V_F(\vec{x}, \vec{y}) = -V(\vec{x}, \vec{y}) \sum_{j=1}^A \phi_j^*(\vec{y}) \phi_j(\vec{x}) = -V(\vec{x}, \vec{y}) \rho(\vec{x}, \vec{y})$

• more complicated with non-local potential density matrix

7/19/13

(F3b-2)

Recall from (M3b-5) the standard discussion of Hartree Fock, but specialize to a contact interaction $V(\vec{x}, \vec{y}) = C_0 \delta^3(\vec{x} - \vec{y})$

$$\begin{aligned} \text{Then } \langle \Psi_{\text{HF}} | \hat{H} | \Psi_{\text{HF}} \rangle &= \int d\vec{x} \frac{1}{2m} \sum_{i=1}^A \nabla \phi_i^* \cdot \nabla \phi_i + \frac{1}{2} \int d\vec{x} d\vec{y} \sum_i |\phi_i(\vec{x})|^2 C_0 \delta^3(\vec{x} - \vec{y}) \sum_j |\phi_j(\vec{y})|^2 \\ &\quad - \frac{1}{2} \int d\vec{x} \int d\vec{y} \sum_{i,j} \phi_i^*(\vec{x}) \phi_j(\vec{y}) C_0 \delta^3(\vec{x} - \vec{y}) \sum_j \phi_j^*(\vec{y}) \phi_j(\vec{x}) \\ &= \int d\vec{x} \left[\frac{1}{2m} \left(\sum_{i=1}^A \nabla \phi_i^* \cdot \nabla \phi_i \right) + \frac{1}{2} \left(1 - \frac{4}{\nu} \right) C_0 \left(\sum_i |\phi_i(\vec{x})|^2 \right)^2 \right] \\ &= \int d\vec{x} \left[\frac{1}{2m} \tau(\vec{x}) + \frac{1}{2} \left(1 - \frac{4}{\nu} \right) C_0 \rho(\vec{x})^2 \right] = E[\tau, \rho] \quad \text{energy functional!} \end{aligned}$$

- The equations for $\phi_i(\vec{x})$ reduce to [easiest to do $\frac{\delta}{\delta \phi_i(\vec{x})} (E[\tau, \rho] - \sum_j \epsilon_j \int d\vec{y} |\phi_j(\vec{y})|^2) = 0$]
- $$-\frac{\hbar^2}{2m} \nabla^2 \phi_i(\vec{x}) + \left[\left(1 - \frac{4}{\nu} \right) C_0 \rho(\vec{x}) \right] \phi_i(\vec{x}) = \epsilon_i \phi_i(\vec{x})$$

⇒ looks like a Hartree calculation or Kohn-Shan DFT!

⇒ reinterpret "Skyrme Hartree Fock" as doing DFT with a nonless EFT-like expansion of the density functional!

Conventional Skyrme story has $\langle \vec{k} | V_2^{\text{Skyrme}} | \vec{k}' \rangle = t_0 + \frac{1}{2} t_1 (k^2 + k'^2) + t_2 k \cdot k' + i W_0 (k_1 + k'_1)$

generalize

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

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

shift focus from V^{Skyrme} to functionals

7/19/13 Do Skyrme functionals fit to nuclear data know about chiral physics? F3b-3

"Skyrme energy functional and naturalness," *nj*, J.C. Haddock, PRC 56, 2875 (1997),

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

• Looking for signatures of chiral physics in Skyrme functionals, even though there are no explicit pions.

• Consider the textbook version of Skyrme (eg., Ring+Schuck's text)
[in practice, isovector terms, pairing, ...]

$$E[\rho, \tau, \vec{J}] = \int d^3r H(\vec{r}) = \int d^3r \frac{1}{2m} \tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^3 + \frac{1}{16} (3t_1 + 5t_2) \rho \tau + \frac{1}{64} (9t_2 - 5t_3) (\nabla \rho)^2 - \frac{3}{4} W_0 \rho^2 \vec{J} \cdot \vec{J} + \frac{1}{32} (t_1 t_2) \vec{J} \cdot \vec{J}$$

• $\rho(\vec{r})$ is the nuclear density, $\tau(\vec{r})$ is the kinetic energy density, $\vec{J}(\vec{r})$ is the spin-orbit density.

• Recall Georg-Manohar naive dimensional analysis (NDA):
scale each term in the low-energy Lagrangian by factors of $F_\pi = 93 \text{ MeV}$ and $\Lambda_\chi \sim 500-1000 \text{ MeV}$ according to:

$$c \left[\frac{4+4}{F_\pi^2 \Lambda} \right] \left[\frac{1}{\Lambda} \right]^n F_\pi^2 \Lambda^2$$

"Natural" means the left-over dimensionless coefficient c is $O(1)$.

• here: apply directly to Skyrme functional, assuming explicit pions would only lead to order unity changes, ↙ as if a Lagrangian/Hamiltonian

7/19/13

F3b-4

Typical case: Skyrme 3 in Ring and Schuck

$$t_0 = -1128.8 \text{ MeV fm}^3, t_1 = 395 \text{ MeV fm}^3, t_2 = -95 \text{ MeV fm}^5, t_3 = 1400 \text{ MeV fm}^6, \\ w_0 = 120 \text{ MeV fm}^3, \text{ these units don't reveal natural scales!}$$

Rescaled $H(\vec{r})$ takes the form

$$H(\vec{r}) = c_1 \frac{\rho}{\Lambda} + c_2 \frac{\rho^2}{f_{\pi}^2} + c_3 \frac{\rho^3}{f_{\pi}^4 \Lambda} + c_4 \frac{\rho^4}{f_{\pi}^2 \Lambda^2} + c_5 \frac{(\nabla \rho)^2}{f_{\pi}^2 \Lambda^2} + c_6 \frac{\rho \nabla^2 \rho}{f_{\pi}^2 \Lambda^2} + c_7 \frac{\rho^3}{f_{\pi}^2 \Lambda^2}$$

Skyrme 3

$$\Rightarrow c_1 = 0.5, c_2 = -0.48, c_3 = 1.05, c_4 = 1.14, c_5 = 1.62, c_6 = -2.31, c_7 = 0.39$$

→ pretty natural! (Although limited range of density dependence)
 scaling by m_N or m_{π} or ... does not work.

• Large-scale study in 2010 examined all Skyrmes and found that the best functionals are consistent with naturalness and strong deviations were associated with known deficiencies in fitting the functional.

• If Λ_x was determined by the most natural (close to 1 couplings), Λ_x came out to be about 700 MeV.

• We can arrange the first four terms as:

$$H(\vec{r}) = \frac{\rho}{\Lambda} (c_1 + c_4 \frac{\rho}{f_{\pi}^2 \Lambda}) + \frac{\rho^2}{f_{\pi}^2} (c_2 + c_3 \frac{\rho}{f_{\pi}^2 \Lambda}) + \dots$$

which implies a density expansion with expansion parameter $(\rho / f_{\pi}^2 \Lambda) \sim (0.17 \text{ fm}^{-3}) (197.33 \text{ MeV fm})^3 / [(93 \text{ MeV})^2 (700 \text{ MeV})] \sim 1/5$

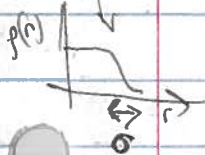
⇒ not a bad expansion parameter! (maybe $1/4 - 1/7$ in general)

• There is also a gradient expansion. The relevant scale ^{for derivatives} in

nuclei is the surface thickness $\sigma \Rightarrow 1/15 \approx 1/5$ is the expansion parameter

• The same analysis shows relativistic mean field models are also natural.
 • Summary: not definitive, but suggestive that nuclei know about chiral symmetry!

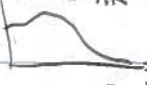
~ constant surface thickness



7/19/13 Turn now to the main question: can we reinterpret Skyrme as DFT?

What is Density Functional Theory?

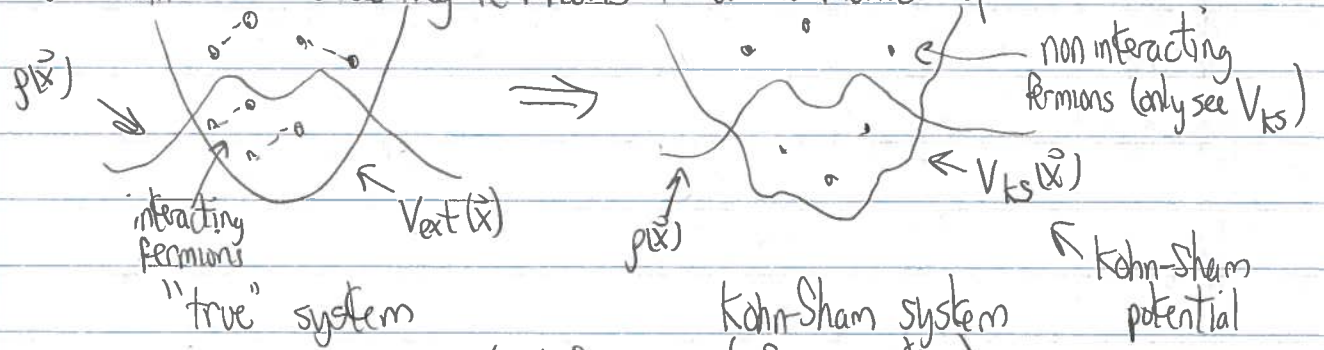
- Skyrme functionals are often regarded as DFT functionals. What is the background?
- Hohenberg and Kohn formulated an existence proof for an energy functional $E_{\text{ext}}[\rho] = F_{\text{HK}}[\rho] + \int d\vec{x} V_{\text{ext}}(\vec{x}) \rho(\vec{x}) \Rightarrow E_{\text{gs}}, \rho_{\text{gs}}$ minimize

• $\rho(\vec{x})$ is the density  $\langle \psi(\vec{x}) | \psi(\vec{x}) \rangle$ ground state = GS or gs but we'll extend it to mean over local densities (same \vec{x}) such as the kinetic energy density $\langle \psi(\vec{x}) | -\nabla^2 \psi(\vec{x}) \rangle \equiv \tau(\vec{x})$

- 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's potential due to the nuclei in an atom or molecule, and the goal is to find the energy and density distribution of electrons.

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

• Let's think of interacting fermions in a harmonic trap



\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: $\delta E_{\text{interacting}}[\rho] / \delta \rho(\vec{x}) \rightarrow V_{\text{KS}}$
- Solve self-consistently: first one, then the other, until they stop changing to some tolerance

not constructive, just an existence proof

7/19/13

F36-6

Unraveling the magic of DFT [Kutzelnigg (2008)]

• Wavefunction based methods take an anti-symmetric Ψ 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 $|\Psi\rangle$ and 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 $\hat{H}[v] \rightarrow E[v]$

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

and

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

external source potential
↓

For each v , we know the ground state energy

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F3b-7

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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F3b-8

DFT as Thermodynamic Legendre transform

zero temperature

(average)

- Recall ordinary thermodynamics with $N = \langle \hat{N} \rangle$ particles at $T=0$
 \Rightarrow grand canonical ensemble (but $T=0$ limit)

(want T and V as independent variables plus chemical potential)

- Use a chemical potential μ as a source to change $\langle \hat{N} \rangle$:

$$\Omega(\mu) = -kT \ln Z(\mu) \quad \text{and} \quad N = - \left(\frac{\partial \Omega}{\partial \mu} \right)_{TV} \Rightarrow N(\mu)$$

$\frac{1}{\beta}$ 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 $F(N)$:

$$F(N) = \Omega(\mu(N)) + \mu(N) N \quad [\text{check that the thermodynamic derivative relations work}]$$

\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 operator \leftarrow my favorite! (see references on first slide)
- ii) MBPT

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F3b-9

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
 - ⇒ 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),

⇒ 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) ⇒ density matrix expansion (DME)

7/19/13

Hartree-Fock energy using the density matrix

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

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

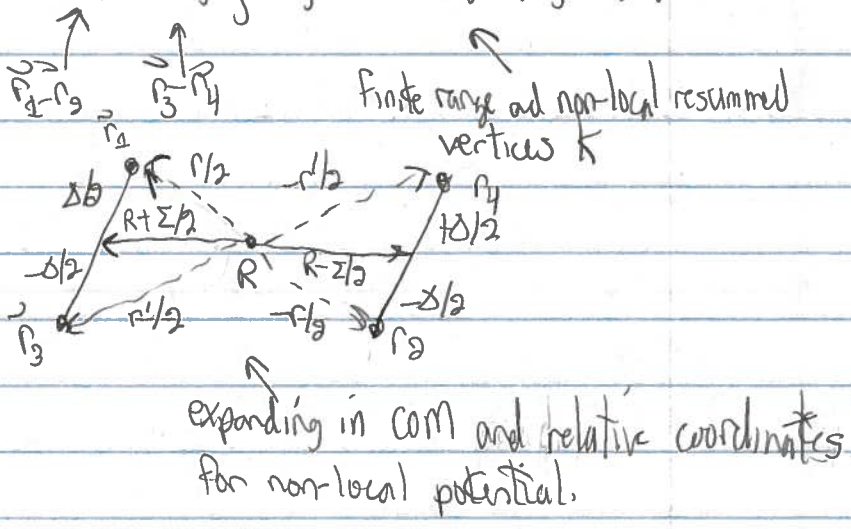
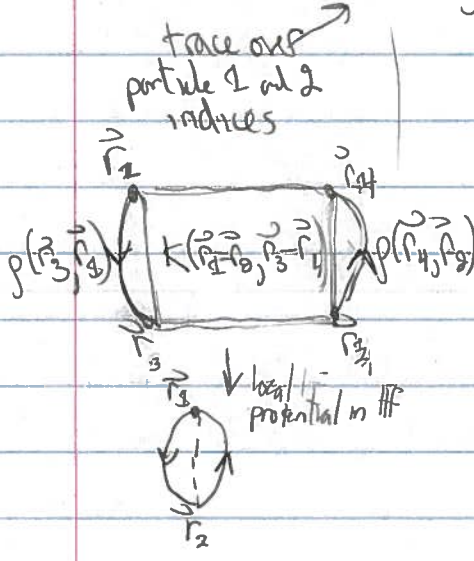
$\underbrace{\psi_i^\dagger(\vec{r}_1) \psi_j(\vec{r}_2)}_{\propto \rho(\vec{r}_1, \vec{r}_2)} \quad \underbrace{\psi_j^\dagger(\vec{r}_2) \psi_i(\vec{r}_1)}_{\propto \rho(\vec{r}_2, \vec{r}_1)}$

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

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

In general, the dominant MBPT contributions take the form:

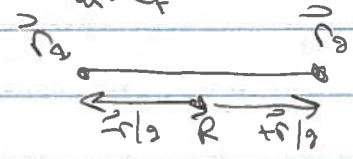
$$\langle V \rangle \sim \text{Tr}_1 \text{Tr}_2 \int d\vec{R} \int d\vec{r}_1 \int d\vec{r}_2 \rho(\vec{r}_1, \vec{r}_2) K(\vec{r}_1, \vec{r}_2) \rho(\vec{r}_2, \vec{r}_1) + \text{NNN} \dots$$



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

7/19/13

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



different prescriptions for these functions

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

⇒ 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 DME expands about nuclear matter ⇒ includes long-range effects
 - improved version (Gobromarian 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:

$$g(\vec{R} + \frac{\vec{r}}{2}, \vec{R} - \frac{\vec{r}}{2}) \approx f_{sk}(k_F(\vec{R})r) \rho(\vec{R}) + \tau^2 g(k_F(\vec{R})r) \times [\frac{1}{4} \nabla^2 \rho(\vec{R}) - \tau(\vec{R}) + \frac{2}{5} k_F(\vec{R})^2 \rho(\vec{R})]$$

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

and

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

* 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).