Density Functional Theory for Nuclei: Old Ideas and New Questions

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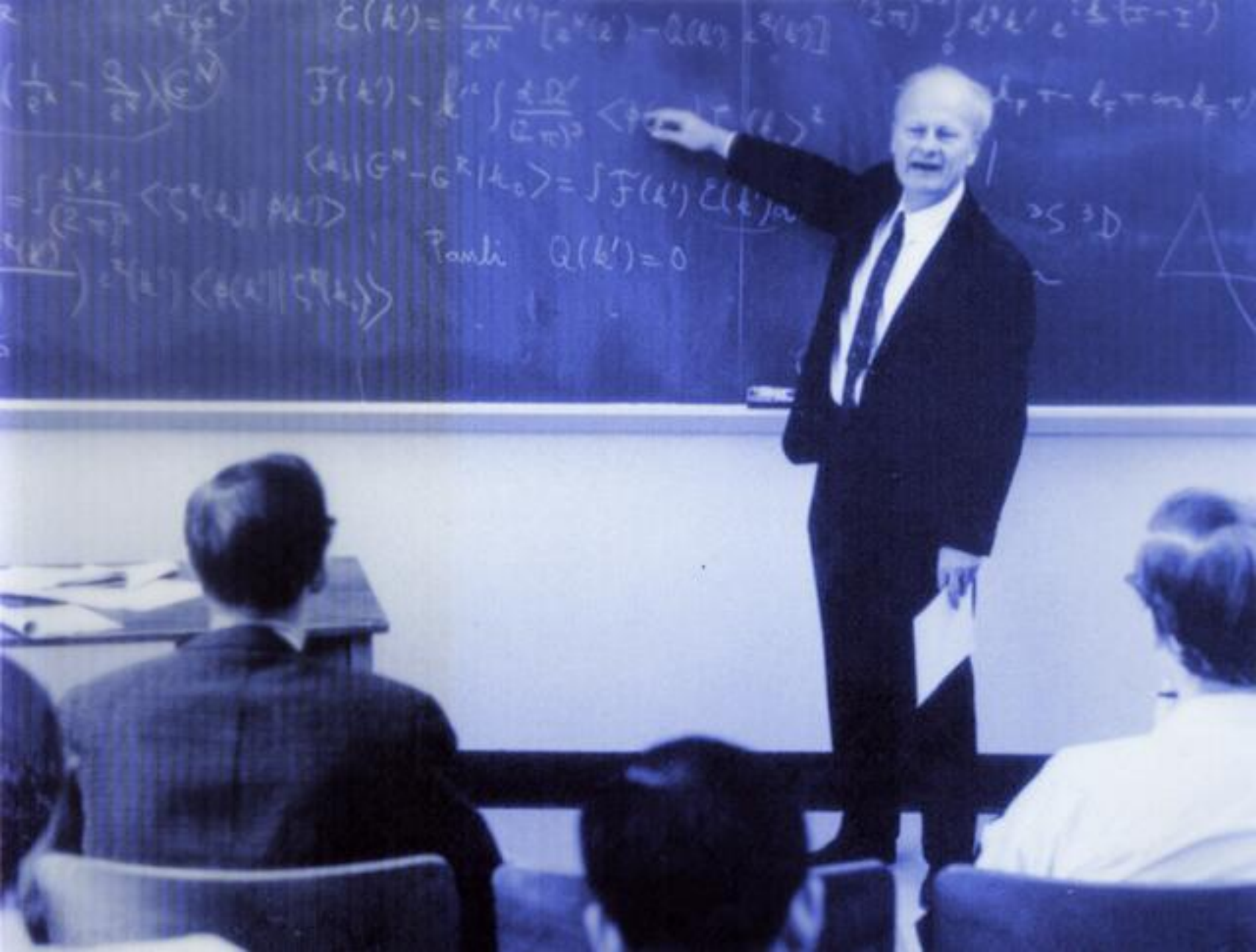
INT Workshop 9/26/05

Outline

- Caveats
- Context - Nonrelativistic Many Body Theory
- Density Functionals
  - Hohenberg Kohn
  - Density Matrix Expansion
  - Effective Potential
  - Two Body Density Matrix
- Issues and Questions


Pomtli Q(k')=0

NON RELATIVISTIC MANY BODY THEORY WITH STATIC POTENTIAL

POTENTIAL

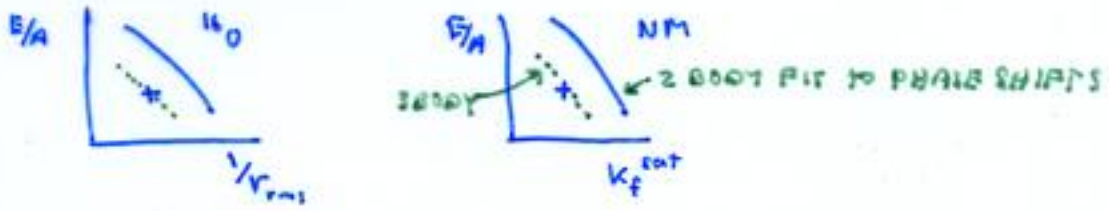
LONG RANGE : PION EXCHANGE

TENSOR FORCE

SHORT RANGE : FIT PHASE SHIFTS

3-BODY - BINDING ENERGY IN NUCLEI, NUCLEAR MATTER

CONSISTENT WITH EFT



VALUABLE TO REALLY SOLVE THIS MANY-BODY PROBLEM

FEASIBLE

COUPLED CLUSTER

LLNL BLUE GENE 1/3 PETAFLOPS

HOMEWORK PROBLEM - V_{18} POTENTIAL FOR LIGHT NUCLEI

SAME RESULTS IN GFMC & COUPLED CLUSTER

SEPARATE MANY BODY APPROXIMATIONS FROM

AMBIGUITIES IN INTERACTION

COMPARE DENSITY FUNCTIONAL APPROACH TO

"EXACT" SOLUTIONS

SCIDAC PROJECT ??

HOHENBERG & KOHN DENSITY FUNCTIONAL (1964)

IN MODERN NOTATION, CONSIDER ADDING 1-BODY POTENTIAL TO MANY BODY PROBLEM AS EXTERNAL SOURCE

$$H = T\psi^*\psi + U(r_1 - r_2)\psi^*(r_1)\psi^*(r_2)\psi(r_2)\psi(r_1) + J(r)\psi^*(r)\psi(r)$$

DEFINE $n(r) = \langle \Psi | \psi^*(r)\psi(r) | \Psi \rangle$ FOR GROUND STATE $|\Psi\rangle$

$n(r)$ IS FUNCTIONAL OF $J(r)$

SHOW $J(r)$ IS UNIQUE FUNCTIONAL OF $n(r)$ BY VARIATIONAL ARGUMENT (ASSUME DIFFERENT $J'(r) \Rightarrow$ CONTRADICTION)

DEFINE $F[n(r)] \equiv \langle \Psi | T+V | \Psi \rangle$ ($|\Psi\rangle$ IS FUNCTIONAL OF $n(r)$)

UNIVERSAL FUNCTIONAL - CENTRAL OBJECT

CONSIDER $E_J[n] \equiv \int dr\, J(r)\, n(r) + F[n]$

MINIMIZATION W.R.T. $n(r) \Rightarrow$ GROUND STATE

NOTE: COULD DO SAME FOR OTHER SOURCES

E.G. $J(r r')\,\psi^*(r)\psi(r') \Rightarrow$ DENSITY MATRIX $n(r, r')$

ISSUE IS CONSTRUCTING $F[n(r)]$

NO GUIDANCE FROM THIS DERIVATION

TYPICALLY USE LOCAL DENSITY APPROXIMATION

FOR NUCLEAR PHYSICS, STRONG MOTIVATION TO USE DENSITY MATRIX

ILLUSTRATIVE CASE : SPIN-ISOSPIN SATURATED NUCLEI

$$\frac{1}{4}\sum_{\xi\chi}\langle MN|V|MN-NM\rangle = \langle mn|\underbrace{\tfrac{3}{8}v_{ev}+\tfrac{5}{8}v_{odd}}_{v_{dir}}|mn\rangle + \langle mn|\underbrace{\tfrac{3}{8}v_{ev}-\tfrac{5}{8}v_{odd}}_{v_{exch}}|nm\rangle$$

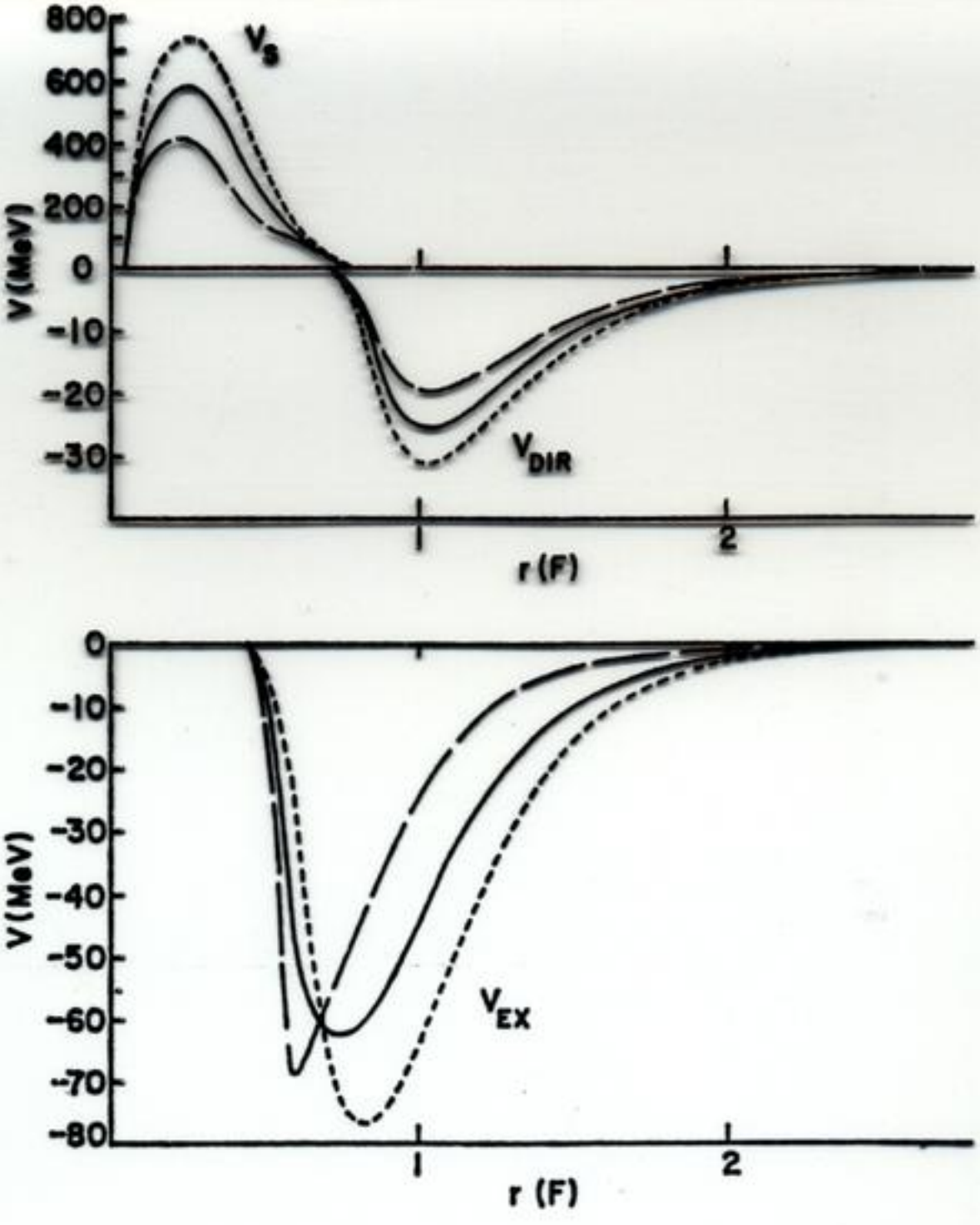
$$= \int dr_1 dr_2\, \rho(r_1)\, v_{dir}(r_1-r_2)\, \rho(r_2) + \int dr_1 dr_2\, \rho(r_1,r_2)\, v_{exch}(r_1-r_2)\, \rho(r_2,r_1)$$

where $\rho(r) = \sum_n \phi_n^*(r)\,\phi_n(r)$ $\qquad$ $\rho(r_1,r_2) = \sum_n \phi_n^*(r_1)\,\phi_n(r_2)$

SIMPLEST IMPLEMENTATION OF K-S :

USE $\rho(r_1,r_2) = \rho\left(\frac{r_1+r_2}{2}\right)\underbrace{\rho_{SL}(r_1-r_2)}_{\frac{3\tilde{j}_1(k_{F_n}|r_1-r_2|)}{k_{F_n}|r_1-r_2|}}$

COMPARE v_{dir} & v_{exch} $\qquad$ (JN 1970)


800
600
400
200
0
-10
-20
-30
V(MeV)
V_S
V_{DIR}
1
2
r (F)
0
-10
-20
-30
-40
-50
-60
-70
-80
V(MeV)
V_{EX}
1
2
r (F)

DENSITY MATRIX EXPANSION

J.N. & D. VAUTHERIN

OBJECTIVES:

GENERALIZE DENSITY FUNCTIONAL THEORY TO INCLUDE LEADING OFF-DIAGONAL BEHAVIOR OF DENSITY MATRIX

CALCULATE FUNCTIONAL IN TERMS OF EFFECTIVE INTERACTION

MAKE CONTACT WITH SKYRME INTERACTION

BASIC IDEA:

$$\rho\left(R+\frac{s}{2}, R-\frac{s}{2}\right) = e^{\frac{\vec{s}}{2}\cdot(\vec{\nabla}_1-\vec{\nabla}_2)} \sum_a \phi_a^*(R_1)\,\phi_a(R_2)\Big|_R$$

THROUGH 2nd ORDER, $\int \frac{d\Omega}{4\pi}\,\rho^2 = \left[\int \frac{d\Omega}{4\pi}\,\rho\right]^2$

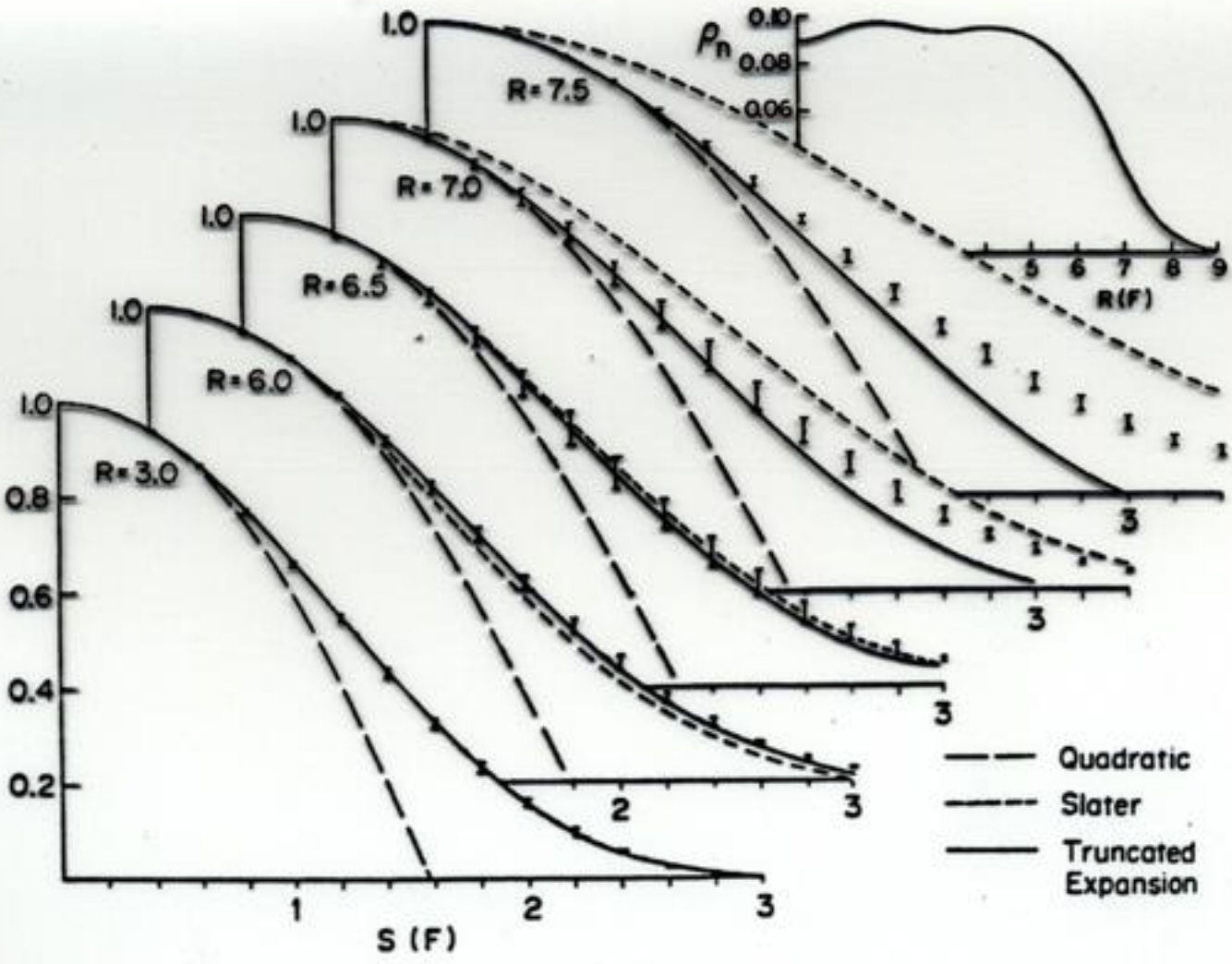
$$\int \frac{d\Omega}{4\pi}\,\rho\left(R+\tfrac{s}{2}, R-\tfrac{s}{2}\right) = \frac{1}{k_F}\sum_n (4n+3)\, j_{2n+1}(sk_F)\, Q_n\left(\frac{\nabla_1-\nabla_2}{2k_F}\right)^2 \rho(R_1,R_2)$$

$$= \rho_{SL}(sk_F)\,\rho(R) + \frac{35}{2sk_F^3}\, j_3(sk_F)\left[\frac{1}{4}\nabla^2\rho(R) - \tau(R) + \frac{3}{5}k_F^2\,\rho(R)\right] + \cdots$$

$$\rho(R) = \sum |\phi_a(R)|^2, \quad \tau(R) = \sum |\nabla\phi_a(R)|^2, \quad \rho_{SL} = \frac{3j_1(sk_F)}{sk_F}$$

NOTE: GROUPED $k_F, \frac{1}{k_F}$ TO OBTAIN ρ_{SL} AND MAKE EACH TERM VANISH IN NUCLEAR MATTER

OBTAIN GOOD APPROXIMATION TO NEUTRON DENSITY MATRIX IN ^{208}Pb


1.0
R=7.5
1.0
R=7.0
1.0
R=6.5
1.0
R=6.0
1.0
R=3.0
0.8
0.6
0.4
0.2
1
2
3
S (F)
ρ_n
0.10
0.08
0.06
5
6
7
8
9
R(F)
Quadratic
Slater
Truncated
Expansion

DENSITY FUNCTIONAL H(R)

$$\langle V \rangle = \frac{1}{2}\int d^3r_1 d^3r_2 \Big\{ \Big[\rho_p(r_1)\rho_p(r_2) + \rho_n(r_1)\rho_n(r_2)\Big] \Big[G^{SE}(r_{12}) \; G^{TE}(r_{12}) \; G^{SO}(r_{12}) \; G^{TO}(r_{12}) \Big]$$

$$\Big[\tfrac{1}{4} \quad 0 \quad 0 \quad \tfrac{3}{4} \Big]$$

$$+ \; 2\rho_p(r_1)\rho_n(r_2) \qquad \Big[\tfrac{3}{8} \quad \tfrac{1}{8} \quad \tfrac{3}{8} \quad \tfrac{1}{8} \Big]$$

$$+ \Big[\rho_p^2(r_1 r_2) + \rho_n^2(r_1 r_2)\Big] \Big[\tfrac{1}{4} \quad 0 \quad 0 \quad -\tfrac{3}{4} \Big]$$

$$+ \; 2\rho_p(r_1 r_2)\rho_n(r_1 r_2) \qquad \Big[\tfrac{3}{8} \quad \tfrac{1}{8} \quad -\tfrac{3}{8} \quad -\tfrac{1}{8} \Big] \Big\}$$

DME YIELDS:

$$H(R) = \frac{\hbar^2}{2m}\left[\tau_n + \tau_p\right]$$
$$+ A\,(\rho_n \rho_p)$$
$$+ B\,(\rho_p \rho_n)\,\tau_p + B\,(\rho_n \rho_p)\,\tau_n$$
$$+ C\,(\rho_n \rho_p)\,|\nabla\rho_n|^2 + C\,(\rho_p \rho_n)\,|\nabla\rho_p|^2$$
$$+ D\,(\rho_n \rho_p)\;\vec{\nabla}\rho_n \cdot \vec{\nabla}\rho_p$$

SKYRME INTERACTION:

PARAMETERIZES A, B, C, D WITH t_0, t_1, t_2, t_3, x_0 + POWERS OF ρ

QUANTITATIVE AGREEMENT IN INTERIOR

DIFFERENT IN SURFACE

CONSIDERABLE DENSITY DEPENDENCE IN DME - MAY NEED IT FOR QUANTITATIVE CALCULATION

EFFECTIVE POTENTIAL

GENERAL LANGUAGE FOR MANY-BODY OR FIELD THEORY

RECALL GENERATING FUNCTION $\mathcal{Z}$ FOR GREENS FUNCTIONS:

$$\mathcal{Z}(J^*_\alpha(\tau) J_\alpha(\tau)) = \frac{1}{\mathcal{Z}} \int \mathcal{D}\psi^*\psi\, e^{-\int d\tau [\underbrace{\psi^*_\alpha(\tau)(\partial_\tau - \mu)\psi_\alpha(\tau) + H(\psi^*_\alpha(\tau)\psi_\alpha(\tau))}_{\mathcal{L}} + J^*_\alpha(\tau)\psi_\alpha(\tau) + \psi^*_\alpha(\tau) J_\alpha(\tau)]}$$

$$\mathcal{Z}(J^* J) = \frac{1}{\mathcal{Z}} \int \mathcal{D}\psi^*\psi\, e^{-S[\mathcal{L} + J^*\psi + \psi^* J]} \equiv e^{W(J^*, J)}$$

$\frac{\delta^{2n} \mathcal{Z}(J^*J)}{\delta J^*_1 \cdots \delta J^*_n \delta J_{n'} \cdots \delta J_{1'}}$ = n body G.F. $\qquad$ $\frac{\delta^{2n} W(J^*J)}{\delta J^*_1 \cdots \delta J^*_n \delta J_{n'} \cdots \delta J_{1'}}$ = n body connected G.F.

SPIN EXAMPLE: $F(H)$ = FREE ENERGY IN MAGNETIC FIELD H

$G(M)$ = EFFECTIVE POTENTIAL FOR MAGNETIZATION M

$$\mathrm{Tr}\, e^{-(\beta \mathcal{H}(S_i) - H \sum_i S_i)} \equiv e^{-\beta F(H)}$$

$$\langle S \rangle_H \equiv M = -\frac{\partial F(H)}{\partial H}$$

$M(H) \Rightarrow H(M)$ Legendre transf.

$$G(M) = F(H(M)) + M\, H(M)$$

$$\frac{\partial G}{\partial M} = \frac{\partial F}{\partial H}\frac{\partial H}{\partial M} + H + M\frac{\partial H}{\partial M} = H$$

H	$\leftrightarrow$ $-J$
F	$\leftrightarrow$ $-W$
S	$\leftrightarrow$ ψ
M	$\leftrightarrow$ ϕ
G	$\leftrightarrow$ Γ

SPIN EXAMPLE

$$\mathrm{Tr}\, e^{-\beta H - HS} = e^{-\beta F(H)}$$

$$\langle S \rangle_H = M = -\frac{\partial F(H)}{\partial H}$$

$$M(H) \rightarrow H(M)$$

$$G(M) = F(H(M)) + M H(M)$$

$$\frac{\partial G}{\partial M} = H$$

GENERATING FUNCTION

$$\frac{1}{Z}\int \mathcal{D}\psi^*\psi\, e^{-\int dx\,[\mathcal{L} + J_\alpha^* \psi_\alpha + \psi_\alpha^* J_\alpha]} = e^{W(J^*J)}$$

$$\langle \psi_\alpha \rangle_{J^*J} \equiv \phi_\alpha = -\frac{\partial W(J_\alpha^* J_\alpha)}{\partial J_\alpha^*} \qquad \phi_\alpha^* = -\frac{\partial W}{\partial J_\alpha}$$

$$\{\phi_\alpha(J_\alpha^* J_\alpha),\ \phi_\alpha^*(J_\alpha^* J_\alpha)\} \Rightarrow \{J_\alpha(\phi_\alpha^* \phi_\alpha),\ J_\alpha^*(\phi_\alpha^* \phi_\alpha)\}$$

$$\Gamma[\phi_\alpha^* \phi_\alpha] = -W[J_\alpha^*, J_\alpha] - \int dx\,[\phi_\alpha^* J_\alpha + J_\alpha^* \phi_\alpha]$$

$$\frac{\partial \Gamma}{\partial \phi_\alpha^*} = -J_\alpha \qquad \frac{\partial \Gamma}{\partial \phi_\alpha} = -J_\alpha^*$$

- WHEN EXTERNAL SOURCES J_α J_α^* ZERO, Γ STATIONARY

- RELATE TO DENSITY FUNCTIONALS BY CONSIDERING A VARIETY OF SOURCES

  FUKUDA
  VALIBU & FERNANDO
  FURNSTAHL
  ...

LOCAL DENSITY

$$\frac{1}{Z}\int d\psi^* \psi \; e^{-\int [\mathcal{L} + J(x)\psi^*(x)\psi(x)]} = e^{W(J)}$$

$$\langle \psi^*(x)\psi(x)\rangle = \rho(x) = -\frac{\partial W}{\partial J(x)}$$

$$\Gamma(\rho(x)) = -W(J) - \int J(x)\,\psi^*(x)\psi(x)$$

$$\frac{\partial \Gamma}{\partial \rho(x)} = J(x) \to 0 \quad \text{for ground state}$$

$\Gamma(\rho(x))$ is Hohenberg Kohn functional

ONE BODY DENSITY MATRIX

$$\int [\mathcal{L} + J(x,x')\,\psi^*(x)\psi(x')$$

$$\langle \psi^*(x)\,\psi(x')\rangle = \rho(x,x') = -\frac{\partial W}{\partial J(x,x')}$$

$$\Gamma(\rho(x,x'))$$

DIAGONAL + FIRST DERIVATIVE OF DENSITY MATRIX (ρ & τ)

$$\int [\mathcal{L} + J_\rho(x)\,\psi^*(x)\psi(x) + J_\tau(x)\,\nabla\psi^*(x)\nabla\psi(x)]$$

$$\langle \psi^*(x)\psi(x)\rangle = \rho(x) = -\frac{\partial W}{\partial J_\rho(x)} \qquad \langle \nabla\psi^*(x)\nabla\psi(x)\rangle = \tau(x) = -\frac{\partial W}{\partial J_\tau(x)}$$

$\Gamma(\rho,\tau)$ or DME FORM

$$\int \mathcal{L} + J_\rho \psi^*\psi + J_\tau \nabla\psi^*\nabla\psi \text{ contains } \psi^*\left[-\nabla\underbrace{\left(\frac{1}{2m} + J_\tau(x)\right)}_{\frac{1}{2M_{eff}}}\nabla + \underbrace{U(x) + J_\rho(x)}_{U_{eff}}\right]\psi$$

BCS

$$\int [\mathcal{L} + J_{Pairing}(x)\,(\psi^*(x)\psi^*(x) + \psi(x)\psi(x))]$$

$$\langle \psi^*(x)\psi^*(x) + \psi(x)\psi(x)\rangle = \Delta(x) = -\frac{\partial W}{\partial J_{pairing}(x)}$$

HFB

$$\int [\mathcal{L} + J(x,x')\,\psi^*(x)\psi(x') + J_{pairing}(x)\,(\psi^*(x)\psi^*(x) + \psi(x)\psi(x))]$$

COMMENTS

- HUGE AMOUNT OF FREEDOM = MANY ALTERNATIVES!
- PURE (EMPTY?) FORMALISM
- PHYSICAL CRITERION FOR "BEST" FORMULATION
- HOW TO CALCULATE $\Gamma(\rho(x))$, $\Gamma(\rho(x,x'))$, $\Gamma(\rho,\tau)$, $\Gamma(\rho(x,x'),\Delta(x))$?

  DIAGRAM EXPANSION - NO EASIER THAN SOLVING MANY BODY PROB.

  EFT - FURNSTAHL, BHATTACHARYYA

  VIABLE TRUNCATION SCHEME FOR SELF BOUND SYSTEM?

TWO-PARTICLE DENSITY MATRIX

CSANYI, GOEDECKER, ARIAS (02)

$$\gamma(x_1 x_2 x_1' x_2') = \langle \Psi | \psi^\dagger(x_1') \psi^\dagger(x_2') \psi(x_2) \psi(x_1) | \Psi \rangle$$

TENSOR PRODUCT EXPANSION:

$$\gamma = \sum_i g_i \otimes h_i$$

I: $g(x_1 x_1') h(x_2 x_2')$

II: $g(x_1 x_2) h(x_2' x_1')$

III: $g(x_1 x_2') h(x_2 x_1')$

HARTREE: $\hat{\gamma}_H = \frac{1}{2} \hat{n} \underset{I}{\otimes} \hat{n}$

HARTREE FOCK $\hat{\gamma}_{HF} = \frac{1}{2} (\hat{n} \underset{I}{\otimes} \hat{n} - \hat{n} \underset{III}{\otimes} \hat{n})$

CONSTRAINTS: HERMITICITY

PERMUTATION SYMMETRY

FERMION ANTISYMMETRY

SUM RULE: $\int dx_2 \, \gamma(x_1 x_2 : x_1' x_2) = \frac{N-1}{2} n(x_1 x_1')$

CORRECTED HARTREE: $\hat{\gamma}_{CH} = \hat{\gamma}_H - \frac{1}{2} \sqrt{\hat{n}} \underset{III}{\otimes} \sqrt{\hat{n}}$

CORRECTED HF: $\hat{\gamma}_{CHF} = \gamma_{HF} - \frac{1}{2} (\sqrt{\hat{n}(1-\hat{n})} \underset{III}{\otimes} \sqrt{\hat{n}(1-\hat{n})}$

NEW CORR. HF: $\gamma_{NEW} = \frac{1}{2} (\hat{n} \underset{I}{\otimes} \hat{n}) - \frac{1}{4} \left[\hat{n} \underset{III}{\times} \hat{n} + \sqrt{\hat{n}(1-\hat{n})} \underset{III}{\times} \sqrt{\hat{n}(1-\hat{n})} \right]$

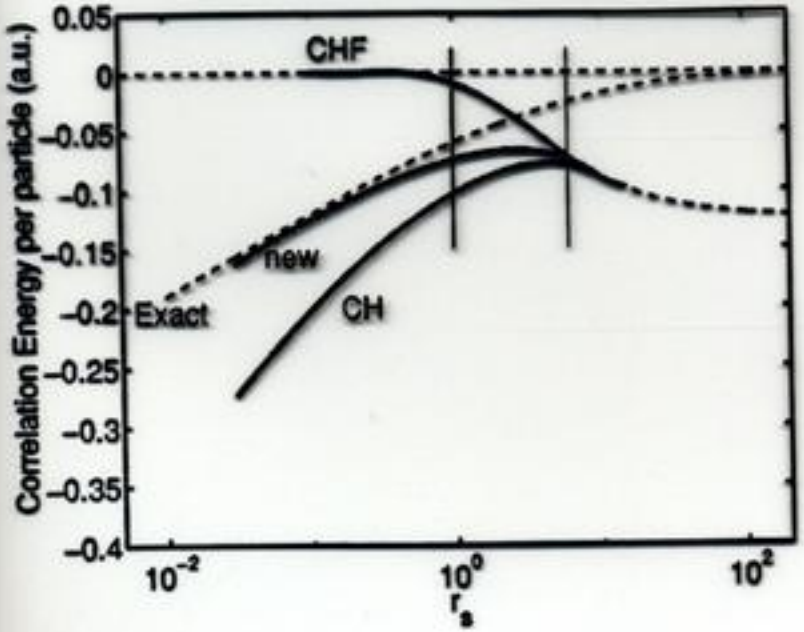
EXCELLENT FOR DENSE ELECTRON GAS

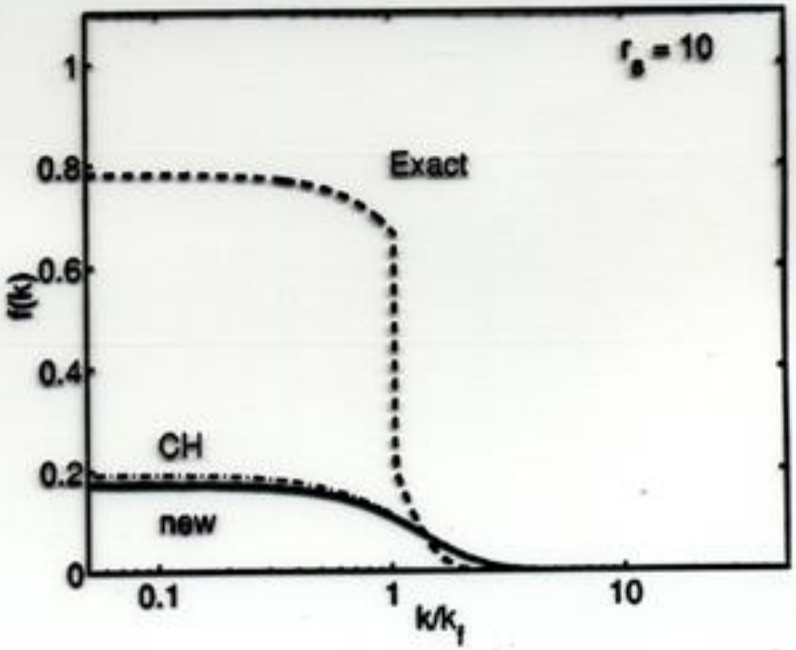
OVERCORRELATED AT LOW DENSITY

DEPLETED MOMENTUM FRACTION

GENERIC FEATURE OF SINGLE TERM

GOOD FOR ATOMS He - O^{4+}


Correlation Energy per particle (a.u.)
0.05
0
−0.05
−0.1
−0.15
−0.2
−0.25
−0.3
−0.35
−0.4
CHF
new
Exact
CH
10^{-2}
10^{0}
10^{2}
r_s


$r_s = 10$
f(k)
1
0.8
0.6
0.4
0.2
0
Exact
CH
new
0.1
1
10
k/k_f

ISSUES and QUESTIONS

GOALS

QUANTITATIVE UNDERSTANDING OF NUCLEI

PREDICTIVE POWER

NUCLEAR ASTROPHYSICS

NEW PHENOMENA, EXTREME STATES

IS DENSITY FUNCTIONAL BEST APPROACH ?

POTENTIAL THEORY

HOW ACCURATELY CAN WE SOLVE COUPLED CLUSTER FOR "REALISTIC" POTENTIAL ?

CAN WE USE IT FOR QUANTITATIVE TEST OF DENSITY FUNCTIONAL THEORY ?

CAN WE ADD 3-BODY TERMS TO GET ACCURATE AGREEMENT WITH EXPT ?

IS THERE CLEAR EVIDENCE OF MISSING ESSENTIAL D.O.F. ?
MESONS, QUARKS ?

HOW TO FORMULATE A TEST ?

EFFECTIVE FIELD THEORY

NO SCALE SEPARATION (HEAVY QUARK PHYSICS BUSY)

$r_{PROTON} \sim 1$ fm $\quad r_{NUCLEI} \sim$ SEVERAL fm

HOW CLOSE ARE WE TO CONTROLLED EXPANSION FOR SELF BOUND SYSTEM ? (TRAPS LESS DEMANDING)

ESSENTIAL DIFFERENCES BETWEEN POTENTIAL THEORY AND MESON-NUCLEON FIELD THEORY ?

NONLOCAL EFFECTIVE THEORY ?

ISSUES and QUESTIONS (CONT.)

DENSITY FUNCTIONAL THEORY

TO WHAT EXTENT ARE WE GOING BEYOND MEAN FIELD?

WHAT IS (ARE) OPTIMAL DENSITY (DENSITIES)?

$\rho(r)$, $\rho(r,r')$, $\tau(r)$, $\Delta(r)$ ...

HOW USEFUL IS PAIRING APPROXIMATION?

SIZE OF NUCLEON VS COOPER PAIR

$S=0, T=1$ MATRIX ELEMENTS

ROLE OF EXPERIMENTAL INPUT

GIVEN LIMITED ABILITY TO CALCULATE MEASURED NUCLEI,

HOW DO NEW ISOTOPES HELP?