Many-Body Theory of Nuclei and Nuclear Matter

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Lecture I : Introduction and Realistic Models of Nuclear Forces

- Basic assumptions of nuclear many-body theory.
- Basic assumptions in Urbana-Argonne models of nuclear forces.
- The one-pion exchange NN potential.
- Two-pion exchange NN and NNN potentials.
- Three-pion exchange NNN potential.
- The phenomenological short-range parts.
- Momentum dependent interactions.
- Comments on Boson-exchange models and effective field theories.

Lecture II : Deuteron and Variational Wave Functions

Lecture III : Quantum Monte Carlo Calculations

Lecture IV : Nuclear and Neutron Matter

I.1 : Basic assumptions of Nuclear Many-Body Theory

Nucleus is a bound state of A nucleons : $i = 1, A$

Nucleon i has

position $\mathbf{r}_i$, **spin** $\sigma_i : \uparrow, \downarrow$ & **isospin** τ_i : p (proton),n (neutron)

$\mathbf{x}_i = \mathbf{r}_i,\ \sigma_i,\ \tau_i$

$\mathbf{X} = \mathbf{x}_1,\ \mathbf{x}_2,\ ...\mathbf{x}_A$

$\mathbf{R} = \mathbf{r}_1,\ \mathbf{r}_2,\ ...\mathbf{r}_A$ *Configuration Vector in* $3A$ *Dimensions*

$|\alpha\rangle$: *Spin − Isospin States*

Example : $|\uparrow p, \downarrow p, \uparrow n\rangle$ *is one of the* 24 *spin − isospin states in* ^3He

$\alpha = 1$ *to* Max; $\quad Max = 2^A \dfrac{A!}{N!Z!}$; $\quad Max(^3He) = 2^3 \dfrac{3!}{1!2!} = 24$

Nuclear Hamiltonian

$$H = \sum_i -\frac{1}{2m}\nabla_i^2 + \sum_{i<j} v(ij) + \sum_{i<j<k} V(ijk) + ...$$

Neglect : *Four − Nucleon and Higher Interactions*

Problem : Solve the many-body Schrödinger Equation

$$H|\Psi_i(\mathbf{X})\rangle = E_i|\Psi_i(\mathbf{X})\rangle$$

General Representations of $\Psi(\mathbf{X})$

$$\Psi(\mathbf{X}) = \sum_{I=1,\infty} \beta_I \Phi_I(\mathbf{X}) \quad \textit{No Core Shell Model}$$

$$\Psi(\mathbf{X}) = \sum_{\alpha=1,Max} \psi_\alpha(\mathbf{R})|\alpha\rangle \quad \textit{Quantum Monte Carlo}$$

Why Use Potentials ?

The Energy of a collection of static particles, either elementary or composite can always be expressed as a sum of potentials

Let A particles (without spin or isospin for simplicity) be in a configuration $\mathbf{R}$. All the fields and internal states of these particles are in their lowest energy state. Let the system have energy $E(\mathbf{R})$. **We define**

$$E(\mathbf{R}) = E_0 + \sum_{i<j} v(\mathbf{r}_{ij}) + \sum_{i<j<k} V(\mathbf{r}_{ij}, \mathbf{r}_{jk}, \mathbf{r}_{ki}) + \sum_{i<j<k<l} \mathcal{V}_{ijkl} + \ldots$$

E_0 is the energy of noninteracting particles; v, V, $\mathcal{V}_{ijkl}$, .. denote 2-, 3-, 4-, .. body potentials. This is generally possible; **BUT** is useful only when:

$$\sum_{i<j} v(\mathbf{r}_{ij}) > \sum_{i<j<k} V(\mathbf{r}_{ij}, \mathbf{r}_{jk}, \mathbf{r}_{ki}) > \sum_{i<j<k<l} \mathrm{V}_{ijkl} > \ldots$$

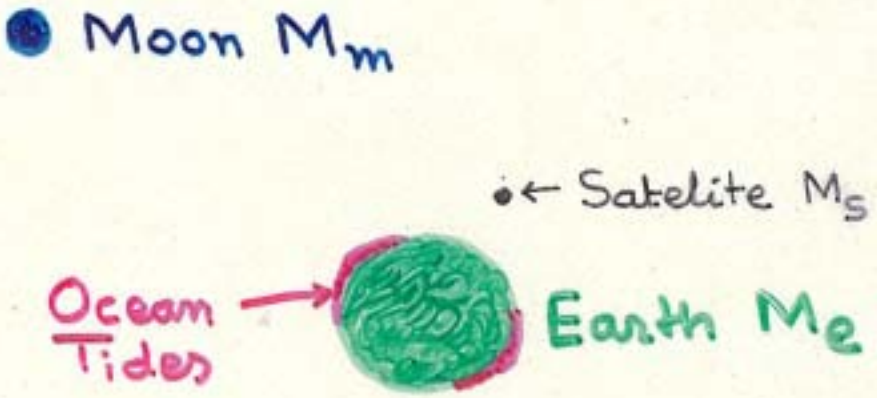
We can then truncate the series and consider only potentials with few particles. In nuclei we find that this series is convergent and omit terms with 4- and higher-body potentials.

When the particles are elementary only the fields coupled to these particles depend on $\mathbf{R}$. When they are composite, *i.e.* they have internal degrees of freedom, their internal state also depends on $\mathbf{R}$

Classical mechanics : Earth, moon satelite for example

In quantum mechanics it is called the **Born Oppenheimer** approximation, which becomes exact when the "particles" (in their case atoms) are stationary.

Gravitational Interactions Between Earth, Moon and Satalite



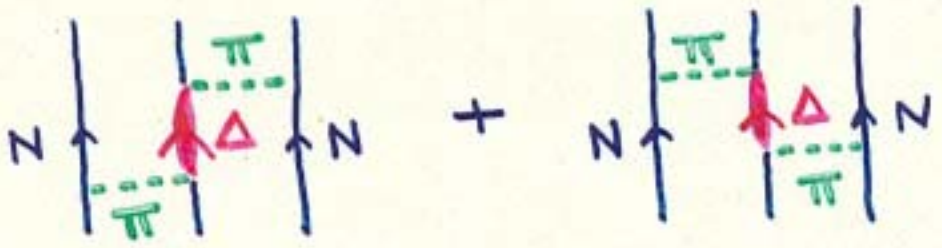
$$Grav.\ Pot.\ Energy = -G_N\left(\frac{M_m M_e}{r_{me}} + \Delta(r_{me}) + \frac{M_m M_s}{r_{ms}} + \frac{M_e M_s}{r_{es}}\right) + V_{ems}(r_{me}, r_{es}, r_{sm})$$

Fujita-Miyazawa Three-Nucleon Interaction

The pion fields of nucleons (1 and 3) polarize nucleon (2). The interaction of (2) with (1 and 3) then has a term that depends upon positions, spins and iso-spins of all the three nucleons (1, 2 and 3).

spin-isospin of quarks in nucleon 2 polarized by pion fields of nucleons 1 & 3.

Feynman Diagrams



I.2 : Basic Assumptions in Urbana-Argonne Models of Nuclear Forces

Assumption I (is implicit in all models)

Based on : pion is the lightest meson : $m_\pi \sim 138$ MeV

Other nonstrange meson masses :

$m_\eta = 547 \quad m_\rho = 769 \quad m_\omega = 783$ MeV : larger than $4m_\pi$

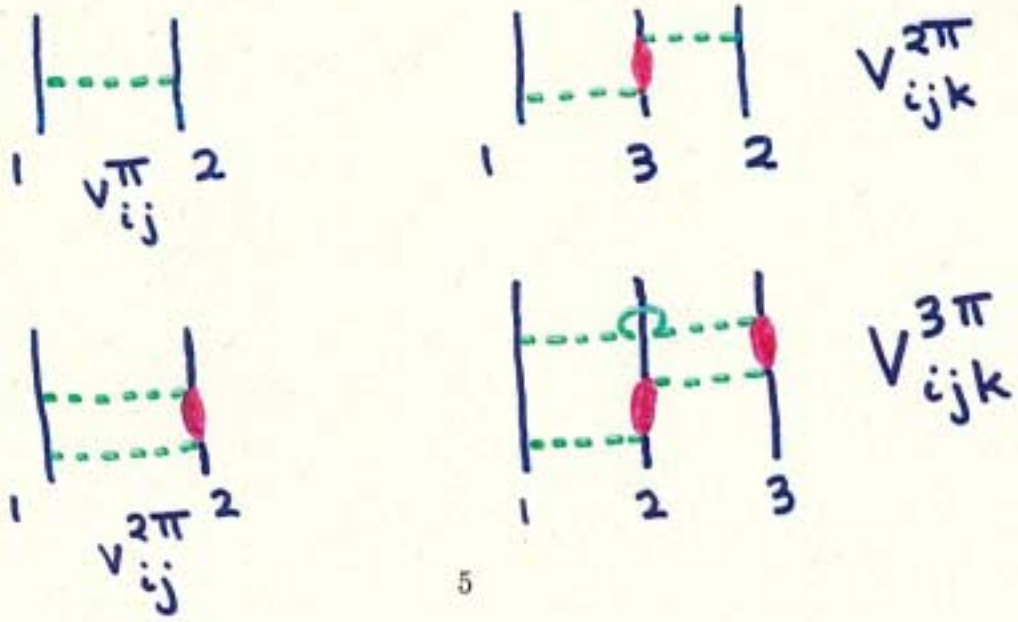
We can assume that:

1. The longest-range part is given by one-pion exchange : v^π
2. Next is a part with the range of two-pion exchange : $v^{2\pi}$
3. Finally there is a short-range core v^R due to heavy mesons, quarks, etc.

$$v_{ij} = v_{ij}^\pi + v_{ij}^{2\pi} + v_{ij}^R$$

Similarly

$$V_{ijk} = V_{ijk}^{2\pi} + V_{ijk}^{3\pi} + V_{ijk}^R$$



Assumption II (is not made in all models)

Based on the observation that velocities of Nucleons in Nuclei are small:

Density of matter at the center of a large nucleus, $\rho_0 \sim 0.16$ fm^{-3}

Fermi momentum $k_F \sim 1.3$ fm^{-1} : $\rho = \frac{4}{6\pi^2} k_F^3$

This gives (Fermi velocity)^2 $\left(\frac{k_F}{m}\right)^2 \sim .07$

However correlations increase the kinetic energy of nucleons in nuclei to $\sim$ 50 MeV per nucleon. This gives (average velocity)$^2 \sim 0.11$.

Velocity $\sim$ 0.3 is not very small.

$$v_{ij} = v_{ij}^{static} + v_{ij}^{ls} + v_{ij}^{quadratic}$$

$$v_{ij}^{static} = \sum_{p=1,6} v_p(r_{ij}) O_{ij}^p$$

$$O_{ij}^{p=1,6} = [1,\ \sigma_i \cdot \sigma_j,\ S_{ij}] \otimes [1,\ \tau_i \cdot \tau_j]$$

$$S_{ij} = 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} \ - \ \sigma_i \cdot \sigma_j \quad \textit{The Tensor Operator}$$

$$v_{ij}^{ls} = \sum_{p=7,8} v_p(r_{ij}) O_{ij}^p$$

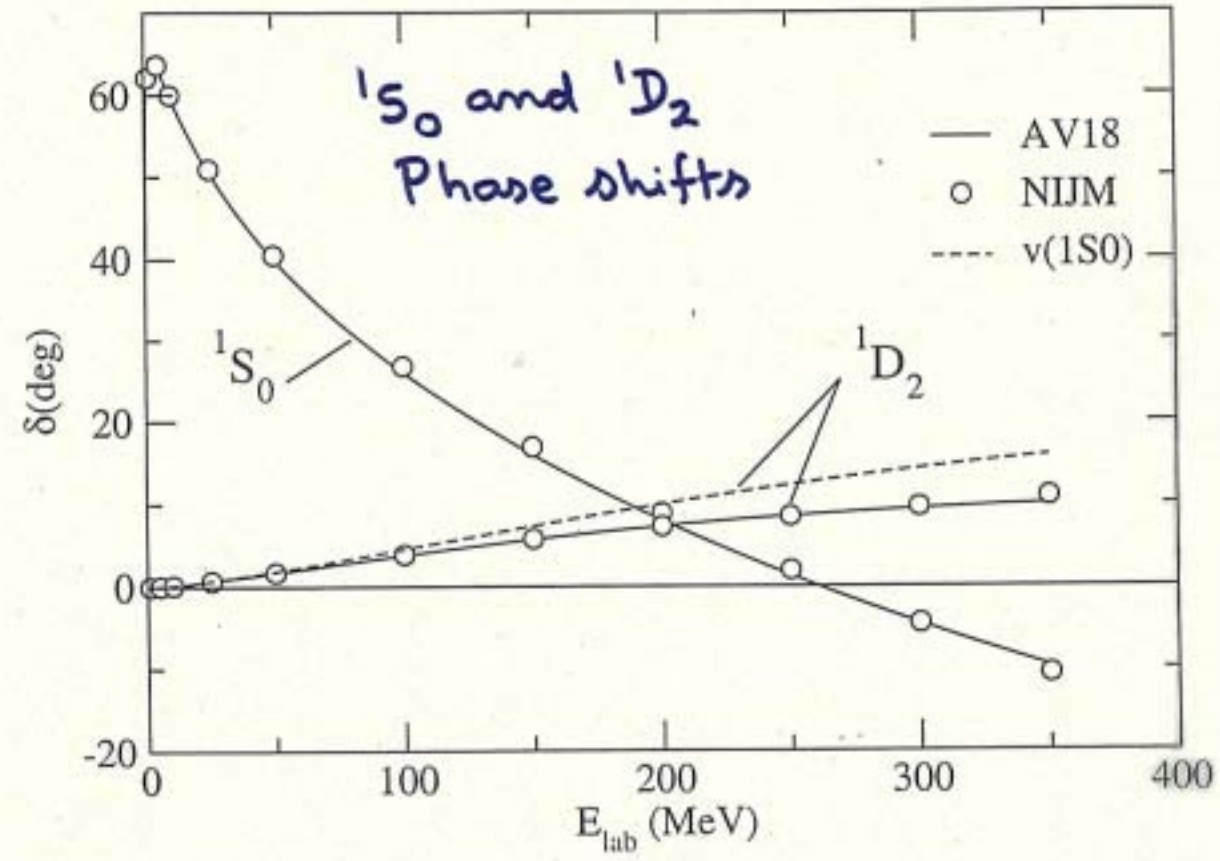
$$O_{ij}^{p=7,8} = (\mathbf{L} \cdot \mathbf{S})_{ij} \otimes [1,\ \tau_i \cdot \tau_j]$$

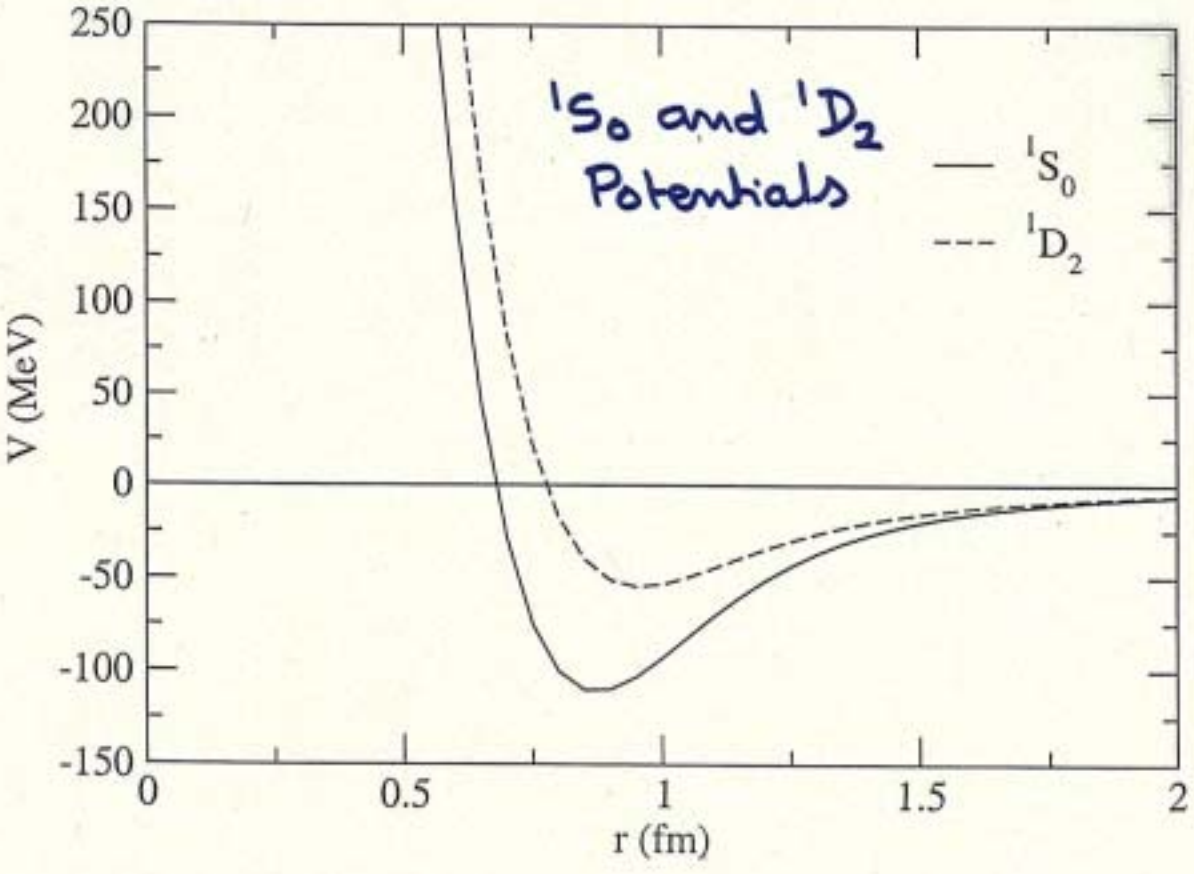
The above v^{static} and v^{ls} contain all terms independent of momenta and linear in momenta

The Interaction $v_8(ij) \equiv v^{static} + v^{ls} = \sum_{p=1,8} v_p(r_{ij}) O_{ij}^p$

is the most general interaction with static + linear velocity dependence.

It can explain all S- and P-wave NN phase shifts


$^1S_0$ and $^1D_2$
Phase shifts
AV18
NIJM
v(1S0)
$^1S_0$
$^1D_2$
δ(deg)
60
40
20
0
-20
0
100
200
300
400
E_{lab} (MeV)


$^1S_0$ and $^1D_2$
Potentials
$^1S_0$
$^1D_2$
V (MeV)
250
200
150
100
50
0
-50
-100
-150
0
0.5
1
1.5
2
r (fm)

Need For Quadratic Terms in v_{ij} in $P_{ij} = 0$ (center of mass) Frame

The NN phase shifts in S- and D-waves, and in P- and F-waves can not be fit simultaniously with any v_8 potential.

Example : $^1S_0$ and $^1D_2$ Phase shifts

Both these partial waves have total spin $S = 0$ and isospin $T = 1$. For any v_8 interaction the potentials in these waves are the same: In spin zero states the tensor and $\mathbf{L} \cdot \mathbf{S}$ interactions absent.

$$v_8(in\ S = 0\ states) = v_c(r) + v_\tau(r)\tau_i \cdot \tau_j + v_\sigma(r)\sigma_i \cdot \sigma_j + v_{\sigma\tau}(r)\sigma_i \cdot \sigma_j \tau_i \cdot \tau_j$$

In $S = 0$ state $\sigma_i \cdot \sigma_j = -3$ and in $T = 1$ state $\tau_i \cdot \tau_j = 1$

$$v(^1S_0) = v(^1D_2) = v_c(r) + v_\tau(r) - 3v_\sigma(r) - 3v_{\sigma\tau}(r)$$

Experimental Data Says : $v(^1S_0) \neq v(^1D_2)$

Problem : There are many quadratic operators

- $[\mathbf{L}^2, (\sigma_i \cdot \sigma_j)\mathbf{L}^2] \otimes [1, \tau_i \cdot \tau_j]$. — 4 terms
- $[\mathbf{p}^2, (\sigma_i \cdot \sigma_j)\mathbf{p}^2] \otimes [1, \tau_i \cdot \tau_j]$. — 4 "
- $\{\sigma_i \cdot \mathbf{L}, \sigma_j \cdot \mathbf{L}\} \otimes [1, \tau_i \cdot \tau_j]$. — 2 "
- $\{\sigma_i \cdot \mathbf{p}, \sigma_j \cdot \mathbf{p}\} \otimes [1, \tau_i \cdot \tau_j]$. — 2 "
- and more with S_{ij} and $\mathbf{L}^2$ and $\mathbf{p}^2$

and not enough data to determine the associated potentials

In Urbana-Argonne v_{14} models we choose :

$$v_{ij}^{quadratic} = \sum_{p=9,14} v_p(r_{ij}) O_{ij}^p$$
$$O_{ij}^{p=9,14} = [\mathbf{L}^2, (\sigma_i \cdot \sigma_j)\mathbf{L}^2, (\mathbf{L}\cdot\mathbf{S})^2] \otimes [1, \tau_i \cdot \tau_j] \ ,$$

- All the NN scattering data (E < 350 MeV) can be explained
- We can define a v_8'-interaction such that

$$v_{14} - v_8' = 0 \ \ in\ all\ L = 0\ and\ 1\ states$$

- Treat $(v_{14} - v_8')$ in first order perturbation theory

Recent Test

Construct a $v_{14,pq}$ model in which we choose:

Note $\mathbf{p}^2 = -\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{\mathbf{L}^2}{r^2}$

$$O_{ij}^{p=9,14} = [\mathbf{p}^2, (\sigma_i \cdot \sigma_j)\mathbf{p}^2, Q_{ij}^2] \otimes [1, \tau_i \cdot \tau_j] \ ,$$
$$Q_{ij} = \frac{3}{2}\{\sigma_i \cdot \mathbf{L}, \sigma_j \cdot \mathbf{L}\} - \sigma_i \cdot \sigma_j \mathbf{L}^2$$

- Field theoretical, (ω, σ)-meson exchange models favour $v_{14,pq}$.
- It can also explain the scattering data.
- The results it gives for $A = 3$ and 4 nuclei are very similar to v_{14} results.
- Can not treat $v_{14,pq} - v_8'$ in first order.

We will return to meson exchange models later.

Total : $P_{ij} \neq 0$

Relativistic Boost Interaction : A Part of Quadratic Terms

The interaction v_{ij} depends upon the momenta $\mathbf{p}_i$ and $\mathbf{p}_j$ of i and j.

We define relative and total momenta:

$$\mathbf{p}_{ij} = \frac{1}{2}(\mathbf{p}_i - \mathbf{p}_j) \quad and \quad \mathbf{P}_{ij} = \mathbf{p}_i + \mathbf{p}_j$$

Example : the momentum dependent interaction between two equal charges

$$-\frac{Q^2}{r_{ij}}\frac{\mathbf{p}_i \cdot \mathbf{p}_j}{2m^2} = \frac{Q^2}{r_{ij}}\left(\frac{p_{ij}^2}{2m^2} - \frac{P_{ij}^2}{8m^2}\right)$$

The p_{ij}^2-term is included in the center of mass frame interaction denoted by v_{ij} in nuclear theory. The P_{ij}^2-term is the **BOOST** interaction denoted by $\delta v(\mathbf{P}_{ij})$. Including it we get the Hamiltonian:

$$H = \sum \frac{p_i^2}{2m} + \sum (v_{ij} + \delta v(\mathbf{P}_{ij})) + \sum V_{ijk} + \cdots,$$

The $\delta v(\mathbf{P}_{ij})$ is related to v_{ij} by the Foldy-Friar Eq.

$$\delta v(\mathbf{P}) = -\frac{P^2}{8m^2}v^{stat} + \frac{1}{8m^2}[\mathbf{P}\cdot\mathbf{r}\,\mathbf{P}\cdot\nabla, v^{stat}] + \frac{1}{8m^2}[(\sigma_i - \sigma_j)\times\mathbf{P}\cdot\nabla, v^{stat}].$$

Up to order P^2/m^2

It is included in Relativistic Mean Field Theory,

but often neglected in nuclear many-body theory.

Examples of effects of $\delta v(\mathbf{P}_{ij})$ in nuclei

1. $\langle \delta v(\mathbf{P}_{ij}) \rangle$ in ^{4}He ~ 1.9 MeV *i. e.* ~ 7 % of E_0 but $< 2\%$ of $\langle v_{ij} \rangle$

2. Nuclear matter equilibrium $\rho_0 = 0.30$ fm^{-3} $E_0 = -18.2$ MeV without

$= 0.22$ $\quad = -14.1$ with $\delta v(\mathbf{P}_{ij})$

Calculations of $A = 3, 4$ nuclei using the Hamiltonian

$$H_R = \sum_i (\sqrt{m^2 + p_i^2} - m) + \sum_{i<j} [\tilde{v}_{ij} + \delta v(\mathbf{P}_{ij})] + \sum_{i<j<k} V_{ijk},$$

$$\tilde{v}_{ij} = \frac{m}{\sqrt{m^2 + p^2}} \; v_{ij}^{\pi} \; \frac{m}{\sqrt{m^2 + p^2}} + v_{ij}^{2\pi} + v_{ij}^{R}$$

Suggest that terms with $p^{n \geq 4}$ in the nuclear H have small effect.

– Stop at quadratic –

Assuming the v_{14} operator structure

$$v_{ij} = \sum_{p=1,14} v_p(r_{ij}) O_{ij}^p$$

$$v_p(r_{ij}) = v_p^{\pi}(r_{ij}) + v_p^{2\pi}(r_{ij}) + v_p^{R}(r_{ij})$$

Our next task is to determine these functions of r

- We can calculate only the one-pion exchange potential v^{π}.
- We **model** $v^{2\pi}$ and v^R. Model parameters are determined from data.
- Fortunately $\langle v^{\pi} \rangle > \langle v^{2\pi} + v^R \rangle$ in nuclei : Good
- **But** there is a large cancellation between $\langle v^{2\pi} \rangle$ and $\langle v^R \rangle$
- In 1993 the Nijmegen group produced a multienergy partial-wave analysis of elastic NN data below $T_{lab} = 350$ MeV (PWA93) that was able to reproduce over 4300 data points with a χ^2/datum ~ 1.
- Models which fit these 4300 data with χ^2/datum ~ 1 are "successful". They include : Nijm I, Nijm II, Reid93, Argonne v_{18} and CD Bonn.
- However all except Argonne v_{18}, are all adjusted partial-wave by partial-wave; they do not represent v_{ij} as a local operator.

The one pion exchange potential

Pions are pseudoscalar mesons with spin parity 0^-, and isospin 1.

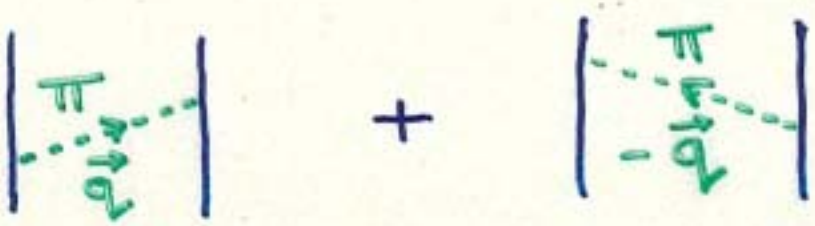
The pion field operator $\Phi(\mathbf{r})$ is a vector in isospin space.

The interaction of the pion field with a nonrelativistic nucleon at position $\mathbf{r}$ is described by the interaction Hamiltonian:

$$H_{\pi NN} = -\frac{f_{\pi NN}}{\mu}\sigma \cdot (\nabla\Phi(\mathbf{r}) \cdot \tau) = -\frac{f_{\pi NN}}{\mu}\sigma_i \cdot (\nabla_i\Phi_a(\mathbf{r}) \cdot \tau_a),$$

$f_{\pi NN}$ is the pion-nucleon coupling constant and μ the pion mass.

The one pion exchange potential in momentum space is obtained as:



$$v^\pi(\mathbf{q}) = -\frac{f^2_{\pi NN}}{\mu^2}\ \tau_1 \cdot \tau_2\ \ \sigma_1 \cdot \mathbf{q}\ \sigma_2 \cdot \mathbf{q}\ \ \frac{1}{(q^2+\mu^2)}\ \ e^{-i\mathbf{q}\cdot\mathbf{r}}$$

In Configuration Space

$$\begin{aligned} v^\pi(\mathbf{r}) &= -\frac{f^2_{\pi NN}}{\mu^2}\ \int \frac{d^3q}{(2\pi)^3}\ \tau_1 \cdot \tau_2\ \ \sigma_1 \cdot \mathbf{q}\ \sigma_2 \cdot \mathbf{q}\ \ \frac{1}{(q^2+\mu^2)}\ \ e^{-i\mathbf{q}\cdot\mathbf{r}}, \\ &= \frac{f^2_{\pi NN}}{\mu^2}\tau_1 \cdot \tau_2\ \ \sigma_1 \cdot \nabla\ \sigma_2 \cdot \nabla\ \ \int \frac{d^3q}{(2\pi)^3}\frac{1}{(q^2+\mu^2)}e^{-i\mathbf{q}\cdot\mathbf{r}}, \\ &= \frac{f^2_{\pi NN}}{4\pi\ \mu^2}\tau_1 \cdot \tau_2\ \ \sigma_1 \cdot \nabla\ \sigma_2 \cdot \nabla\ \ \frac{e^{-\mu r}}{r}. \end{aligned}$$

After evaluating the gradients we get:

$$v^\pi(\mathbf{r}) = \frac{1}{3}\frac{f^2_{\pi NN}}{4\pi}\ \mu\ \tau_1\cdot\tau_2\ \ \left[T_\pi(r)S_{12} + \left(Y_\pi(r) - \frac{4\pi}{\mu^3}\delta(\mathbf{r})\right)\sigma_1\cdot\sigma_2\right],$$

$$Y_\pi(r) = \frac{e^{-\mu r}}{\mu r},$$

$$T_\pi(r) = \left(1 + \frac{3}{\mu r} + \frac{3}{\mu^2 r^2}\right) Y_\pi(r),$$

$$S_{12} = 3\ \sigma_1\cdot\hat{\mathbf{r}}\ \sigma_2\cdot\hat{\mathbf{r}} - \sigma_1\cdot\sigma_2,$$

Here $Y_\pi(r)$ and $T_\pi(r)$ are dimensionless functions of μr,

S_{12} is the tensor operator,

The part of v^π containing $T_\pi(r)S_{12}$ is called the tensor force.

The part containing $Y_\pi(r)\sigma_1\cdot\sigma_2$ is called the Yukawa.

Within the range of v^π, $\mu r < 1$, and $T_\pi(r) > Y_\pi(r)$ by a factor > 7.

The tensor part of the v^π is therefore much larger than the Yukawa part.

The $\delta(\mathbf{r})$ part of v^π must be taken together with other short range interactions included in v^R. We omit it from v^π redefined as:

$$v^\pi(\mathbf{r}) = \frac{1}{3}\frac{f^2_{\pi NN}}{4\pi}\ \mu\ \tau_1\cdot\tau_2\ \ \mathbf{X}_{ij}$$

$$\mathbf{X}_{ij} = T_\pi(r)S_{12} + Y_\pi(r)\sigma_1\cdot\sigma_2,$$

The $1/r$ and $1/r^3$ singular behaviors of $Y_\pi(r)$ and $T_\pi(r)$ are cut off due to finite nucleon size. For example, in Urbana-Argonne models

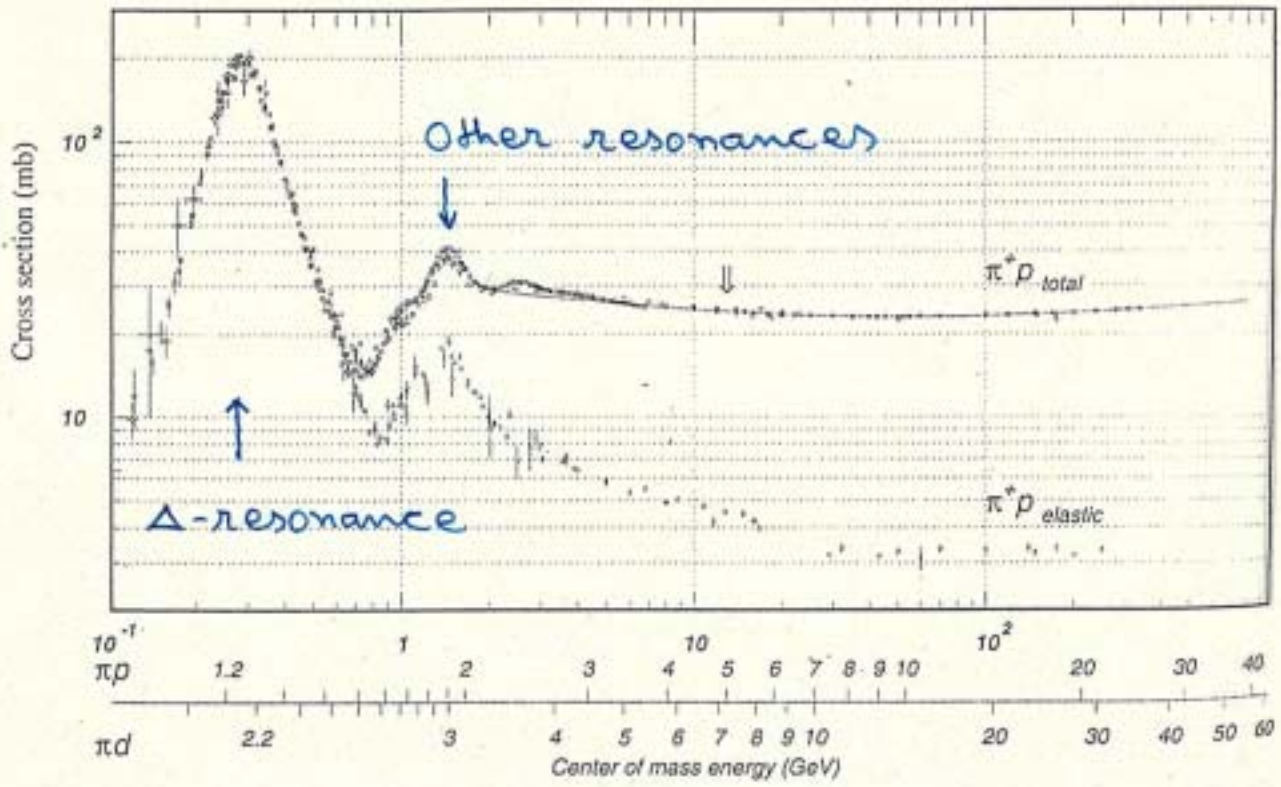
$$Y_\pi(r) = \frac{e^{-\mu r}}{\mu r}\left(1 - e^{-cr^2}\right)$$

$$T_\pi(r) = \left(1 + \frac{3}{\mu r} + \frac{3}{\mu^2 r^2}\right)\frac{e^{-\mu r}}{\mu r}\left(1 - e^{-cr^2}\right)^2$$

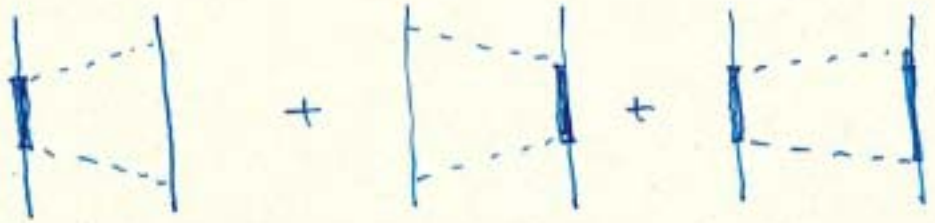
Note: $Y_\pi(r \to 0) = T_\pi(r \to 0) = 0$; **all short range parts in** v^R

we will return to cut offs

$\pi^{\pm} p$ Scattering cross-section



Two pion exchange forces via resonances



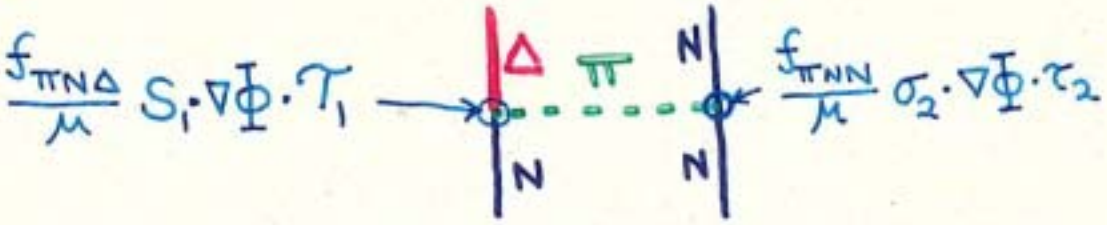
+ many other

Modeling of the two-pion exchange interaction

Assume $v_{ij}^{2\pi}$ is dominated by the internal excitations of nucleons

π-N Scatt.

The $NN \to N\Delta$ Transition Potentials



$$v_{NN\to N\Delta}^{\pi} = \frac{1}{3}\frac{f_{\pi N\Delta} f_{\pi NN}}{4\pi}\ \mu\ \mathcal{T}_1 \cdot \tau_2\ \left[T_\pi(r) S_{12}^I + Y_\pi(r)\mathcal{S}_1 \cdot \sigma_2\right],$$

$$S_{12}^I = 3\ \mathcal{S}_1 \cdot \hat{\mathbf{r}}\ \sigma_2 \cdot \hat{\mathbf{r}} - \mathcal{S}_1 \cdot \sigma_2,$$

$\mathcal{S}$ and $\mathcal{T}$ are transition spin and isospin operators. They convert $N \to \Delta$.

Consider: **One of the terms in the $v^{2\pi}$**

In the closure approximation it will give a contribution:

$$\begin{aligned} v^{(2\pi,\Delta N)} &= \frac{1}{(m_N - m_\Delta)} v_{\Delta N\to NN}^{\pi} v_{NN\to N\Delta}^{\pi} \\ &= \frac{1}{(m_N - m_\Delta)}\left[\frac{1}{3}\frac{f_{\pi N\Delta} f_{\pi NN}}{4\pi}\ \mu\right]^2 \\ &\times T_\pi^2(r)\left[8 + \frac{8}{3}\tau_i \cdot \tau_j - \frac{4}{3}\sigma_i \cdot \sigma_j - \frac{4}{9}\sigma_i \cdot \sigma_j \tau_i \cdot \tau_j + \frac{4}{3}S_{ij} + \frac{4}{9}S_{ij}\tau_i \cdot \tau_j\right] + \ldots \\ &= \sum_{p=1,6} I_p^{\Delta N} T_\pi^2(r) O_{ij}^p + \textit{smaller terms with } T_\pi Y_\pi \textit{ and } Y_\pi^2 \end{aligned}$$

The complete $v^{2\pi}$ will have contributions from many process such as:

$$NN \to \Delta\Delta \to NN,\ NN \to RN \to NN \text{ etc}$$

We can write: Note: R denotes any $\pi - N$ P-wave resonance

$$\begin{aligned} v^{2\pi} &= \sum_{p=1,6} \sum_{RR' \neq NN} I_p^{RR'} T_\pi^2(r) O_{ij}^p \ + \ \ldots \\ &= \sum_{p=1,6} I_p T_\pi^2(r) O_{ij}^p + \textit{smaller terms with } T_\pi Y_\pi \textit{ and } Y_\pi^2 \end{aligned}$$

It is all **static** because of the closure approximation

- We do not know all the $I_p^{RR' \neq NN}$.
- Closure approximation is not accurate.

Urbana-Argonne Approximation

$$v^{2\pi} = \sum_{p=1,14} I_p T_\pi^2(r) O_{ij}^p$$

Obtain the 14 strengths I_p by fitting the NN scattering data

Fits with $\chi^2 \sim 1$ are obtained.

Present data not accurate enough to determine the smaller terms from experiment.

- Need more accurate data - difficult
- Fit data at $E_{Lab} > 350$ MeV

correct for inelasticity & relativity

Seattle : Fall 2003

this semester

Modeling the v^R

Radial shape of v^R_{ij} is basically unknown; we assume

$$v^R_{ij} = \sum_p \left[P_p + \mu r Q_p + (\mu r)^2 R_p\right] W(r) O^p_{ij}$$

$$W(r) = \left[1 + e^{(r-r_0)/a}\right]^{-1} \quad : \quad \text{Woods Saxon}$$

This completes the description of the NN interaction, **recall**

$$v_{ij} = v^\pi_{ij} + v^{2\pi}_{ij} + v^R_{ij}$$

It has 3 shape parameters: $c = 2.1$ fm^{-2}, $r_0 = 0.5$ fm and $a = 0.2$ fm.

All the $v^{2\pi}_{ij}$ strengths I_p are obtained by fitting the data.

One of the three parameters : P_p, Q_p and R_p is obtained from the $r = 0$ limits:

$$v_p(r = 0) = 0 \quad : \quad \textit{for tensor potentials}$$

$$\frac{\partial v_p(r)}{\partial r}(r = 0) = 0 \quad : \quad \textit{for other potentials}$$

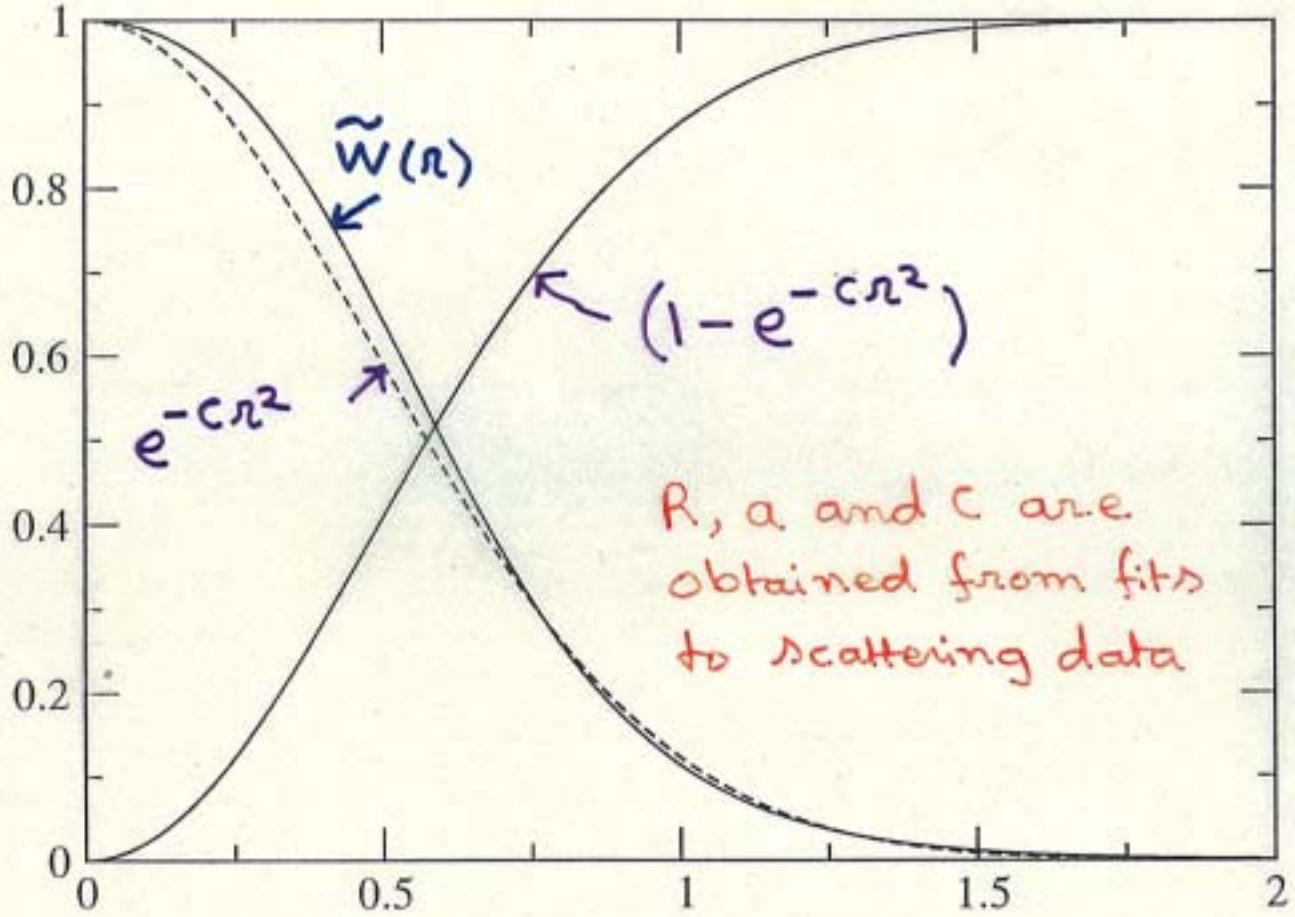
Other two are obtained by fitting scattering data

Shape parameters seem to be related.

$$\tilde{W}(r) = \frac{1 + (1 + \frac{r}{a}) e^{-R/a}}{1 + e^{(r-R)/a}} \quad ; \quad \left.\frac{\partial \tilde{W}(r)}{\partial r}\right|_{r=0} = 0$$

Normalized: $\tilde{W}(r=0) = 1$

$$\frac{d}{dr}\tilde{W}(r)\Big|_{r=0} = 0$$



In Urbana-Argonne models the core size and v^{π} cutoff seem to be related

WHY ?

Need For Three-Nucleon Interaction V_{ijk}

$$H = \sum_i -\frac{1}{2m}\nabla_i^2 + \sum_{i<j} v(ij) \qquad \textit{leads to :}$$

Problem I : Light Nuclei are underbound

^{3}H Energy

-8.48 MeV : Experiment

-7.62 MeV : Reid 93; Nijm II and Argonne V18 - Faddeev

-7.72 MeV : Nijm I - Faddeev

-8.00 MeV : CD-Bonn - Faddeev

Problem II : Nuclear Matter is overbound and dense

Energy	Density	
-16 MeV	0.16 fm^{-3}	: Empirical values
-18 MeV	0.27 fm^{-3}	: Nijm II and Argonne V18 LOBT results
-19 MeV	0.28 fm^{-3}	: Reid 93 LOBT results
-20 MeV	0.31 fm^{-3}	: Nijm I LOBT results
-23 MeV	0.37 fm^{-3}	: CD Bonn LOBT results

- All the above calculations do not include boost correction $\delta v(\mathbf{P}_{ij})$
- $\delta v(\mathbf{P}_{ij})$ increases ^{3}H energy by 0.4 MeV (away from experiment)
- $\delta v(\mathbf{P}_{ij})$ decreases nuclear matter density to ~ 0.2 fm^{-3} : Variational AV18
- $\delta v(\mathbf{P}_{ij})$ decreases nuclear matter energy to ~ -14 MeV : Variational AV18
- CD Bonn is more different from other models, we discuss why ?

$$V_{ijk}^{(2\pi,PW)} = \sum_{cyclic} \frac{1}{(m_N - m_\Delta)} (v_{\Delta N\to NN}^{\pi}(jk) v_{NN\to N\Delta}^{\pi}(ij) + v_{\Delta N\to NN}^{\pi}(ji) v_{NN\to N\Delta}^{\pi}(kj)) .$$

It is convenient to use the $\mathbf{X}_{ij}$ operators in v^π to express this interaction in a convenient form:

$$\begin{aligned} V_{ijk}^{(2\pi,PW)} &= \sum_{cyclic} A_{2\pi,PW}\{\mathbf{X}_{ij}, \mathbf{X}_{jk}\}\{\tau_i \cdot \tau_j, \tau_j \cdot \tau_k\} \\ &\quad + C_{2\pi,PW}[\mathbf{X}_{ij}, \mathbf{X}_{jk}][\tau_i \cdot \tau_j, \tau_j \cdot \tau_k], \\ A_{2\pi,PW} &= -\frac{\mu^2 f_{\pi N\Delta}^2 f_{\pi NN}^2}{(m_\Delta - m_N)(12\pi)^2} \frac{2}{9}, \\ C_{2\pi,PW} &= \frac{1}{4} A_{2\pi,PW}. \end{aligned}$$

The above equation gives an estimate of $A_{2\pi,PW} = -0.04$ MeV for the strength of the anticommutator part of the FM potential.

This estimate could be too large due to use of closure approximation

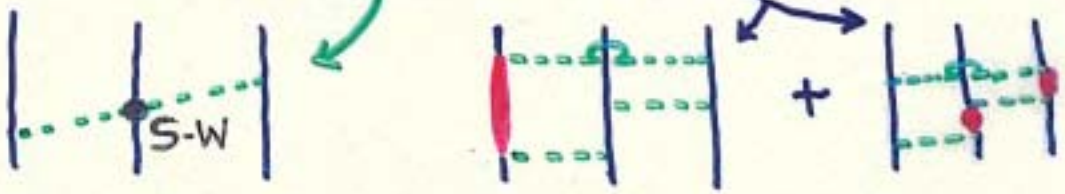
It could be too small because we include only the Δ resonance

bottomline : Get $A_{2\pi,PW}$ from experiment

We rewrite: $V_{ijk}^{(2\pi,PW)} = A_{2\pi,PW} O_{ijk}^{2\pi,PW}$ = strength × operator

$$O_{ijk}^{2\pi,PW} = \sum_{cyclic} \{\mathbf{X}_{ij}, \mathbf{X}_{jk}\}\{\tau_i \cdot \tau_j, \tau_j \cdot \tau_k\} + \frac{1}{4}[\mathbf{X}_{ij}, \mathbf{X}_{jk}][\tau_i \cdot \tau_j, \tau_j \cdot \tau_k],$$

We also calculate the $2\pi, SW$ and $3\pi, 1\Delta$ interactions using closure.



The realistic V_{ijk} is assumed to be:

$$V_{ijk} = A_{2\pi,PW} O_{ijk}^{2\pi,PW} + A_{2\pi,SW} O_{ijk}^{2\pi,SW} + A_{3\pi,1\Delta} O_{ijk}^{3\pi,1\Delta} + A_R O_{ijk}^R$$

$$O_{ijk}^R = \sum_{cyclic} T_\pi^2(r_{ij}) T_\pi^2(r_{jk}) \quad : \textit{The phenomenological term}$$

A repulsive $V_{ijk}^R = A_R O_{ijk}^R$ interaction is necessary to stabilize matter.

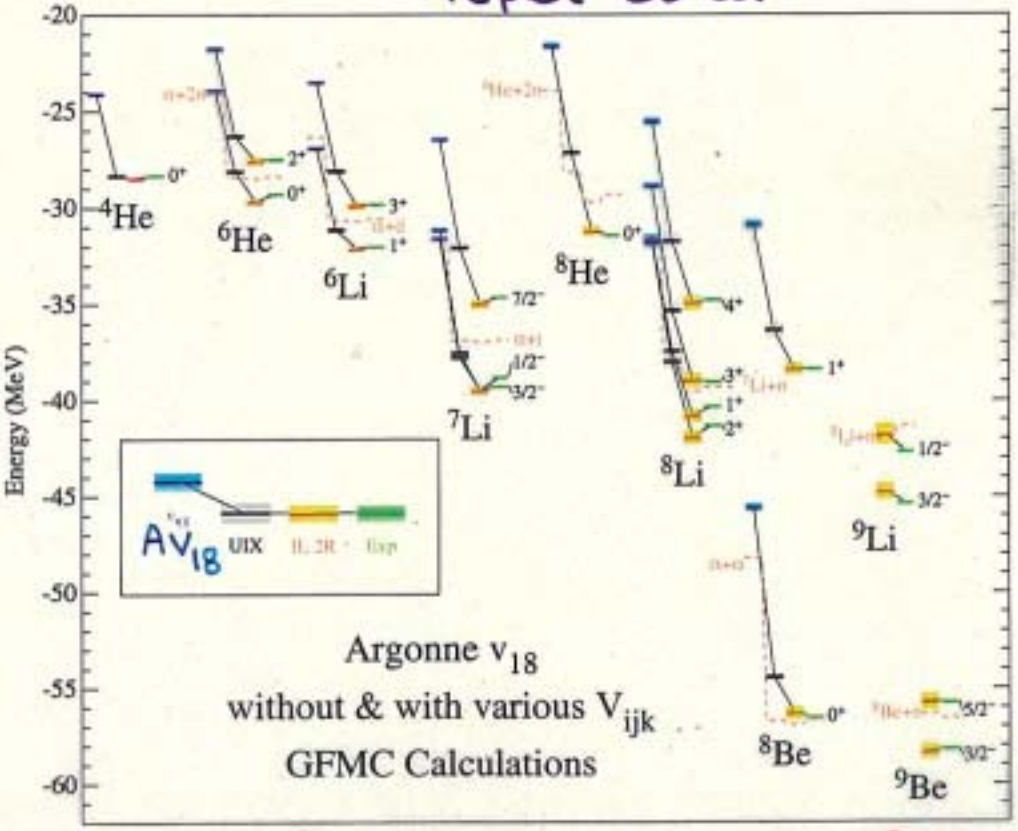
- Urbana IX (U-IX) $V_{ijk} = A_{2\pi,PW} O_{ijk}^{2\pi,PW} + A_R O_{ijk}^R$ with strengths obtained from ^{4}He energy and nuclear matter density.

- Illinois 2 and 4 (IL-2 and 4) models have all four terms. The strengths : $A^{2\pi,PW}$, $A^{3\pi,1\Delta}$ and A^R are obtained by fitting the energies of all $A \leq 8$ bound states. A range of A_R values is possible. Need nuclear matter calculations to fix A_R.

- The $V_{ijk}^{2\pi,SW}$ is very small : We take $A^{2\pi,SW}$ from effective field theory.

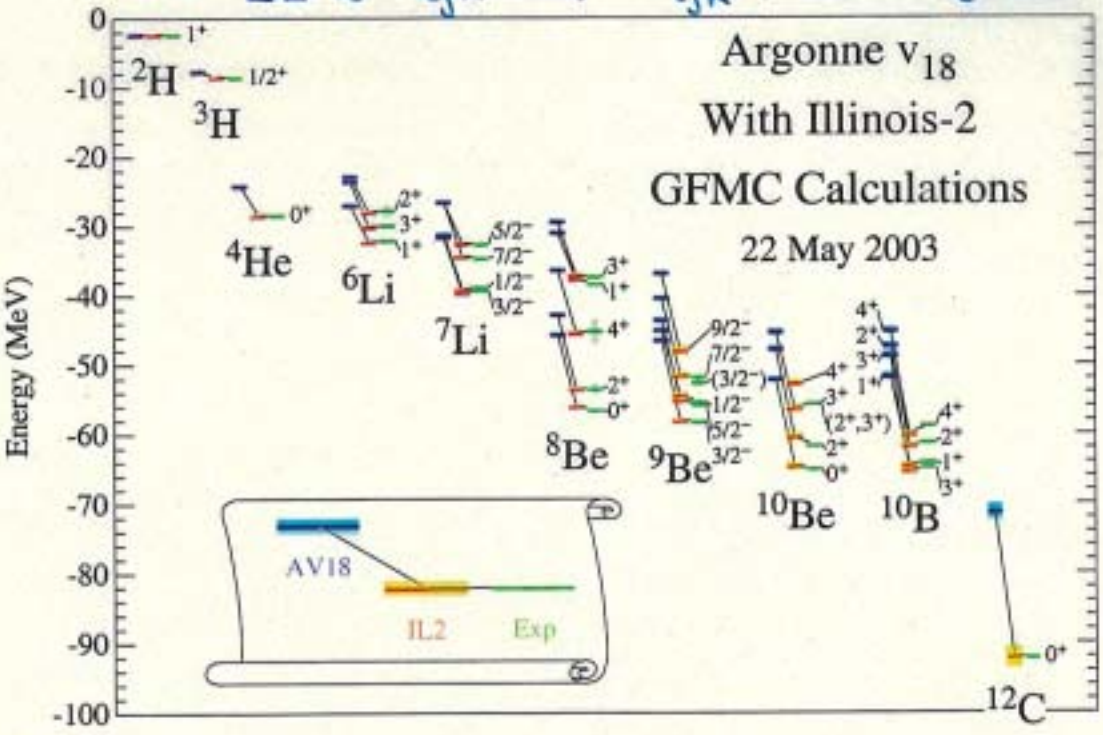
The spectrum of light nuclei

Pieper et al.



Problems with UIX : ^{8}He

IL-2 V_{ijk} has $V_{ijk}^{3\pi}$: looks good



Estimated error in GFMC < 2%

- The AV18 (NN) + Illinois (NNN) Interactions give encouraging results.
- **BUT** These models are not perfect.
- They do not explain all the available $N-d$ scattering data.
- AV18 explains NN data up to 350 MeV (Lab). Improved model is being constructed to fit data up to 500 MeV.
- New models of V_{ijk} should also be constructed to fit the nuclear binding energies and $N-d$ scattering.

In the next three lectures we discuss how to solve the nuclear Schrödinger equation with these potentials

Hierarchy of Many-Body Hamiltonians

- $v_{ij} = v^c(r_{ij})$; $V_{ijk} = 0$: the simplest & most unrealistic.
- $v_{ij} = v^c_{ij} + v^\pi_{ij}$, $V_{ijk} = 0$: the basic "v_6" nuclear many-body problem
- $v_{ij} = v^c_{ij} + v^{static}_{ij} + v^{ls}_{ij}$, $V_{ijk} = 0$: the "v_8" problem
- $v_{ij} = v^c_{ij} + v^{static}_{ij} + v^{ls}_{ij} + V_{ijk}$: the "present" problem
- $(v_{18} - v'_8)$ and $\delta v(\mathbf{P}_{ij})$: "quadratic terms" treated as a perturbation

The general expression for v^π

Dyson, Sugawara, Okubo, Friar ····→ Forest Phys. Rev. C 61, 034007 (2000)
(1948) (1960) (1977)

$$v^\pi(\mu,\vec{p}',\vec{p}) = -\frac{f^2_{\pi NN}}{m^2_\pi}\frac{\tau_1\cdot\tau_2}{(m^2_\pi+q^2)}\frac{m}{E}\frac{m}{E'}\left[\vec{\sigma}_1\cdot\vec{q}\,\vec{\sigma}_2\cdot\vec{q}+\mu(E'-E)\left\{\frac{\vec{\sigma}_1\cdot\vec{p}'\,\vec{\sigma}_2\cdot\vec{p}'}{E'+m}-\frac{\vec{\sigma}_1\cdot\vec{p}\,\vec{\sigma}_2\cdot\vec{p}}{E+m}\right\}\right]$$

$E=\sqrt{m^2+p^2}$ $\quad \vec{q}=\vec{p}'-\vec{p}$

- μ is a theoretical parameter associated with Dyson transformation
- Changing μ corrasponds to making unitary transformations
- Results are independent of μ when V_{ijk} & $\vec{J}_{ij}$ induced by the unitary transformation are included: varified for deuteron

CD-Bonn has $\mu=-1$; Urbana-Argonne-Nijmegan $\mu=0$

"minimal nonlocality"

V_{ijk} with CD-Bonn will be less attractive in light nuclei

BUT More repulsive in Nuclear Matter

L, S, J dependance of coupling constants in CD-Bonn v_{ij}

TABLE VII. Parameters of the scalar isoscalar bosons σ_1 and σ_2, for the pp $T=1$ potential. An asterisk denotes the default which is the $^1S_0$ parameters. The boson masses m_{σ_1} and m_{σ_2} are in units of MeV. A blank indicates that the σ_2 contribution is not considered.

	$g^2_{\sigma_1}/4\pi$ (m_{σ_1})	$g^2_{\sigma_2}/4\pi$ (m_{σ_2})
$^1S_0$	4.24591 (452)	17.61 (1225)
$^3P_0$	7.866 (560)	* (*)
$^3P_1$	2.303 (424)	* (*)
$^3P_2$	4.166 (470)	24.80 (*)
$^1D_2$	2.225 (400)	190.7 (*)
$^3F_2$, $^3F_3$	1.5 (*)	56.21, 74.44 (793)
$^3F_4$, $^3H_4$	3.8 (*)	* (*)
$^1G_4$	* (*)	
$^3H_5$	* (*)	

TABLE IX. Parameters of the scalar isoscalar bosons, σ_1 and σ_2, for the $T=0$ np potential. An asterisk denotes the default which is the $^3S_1$ parameters. The boson masses m_{σ_1} and m_{σ_2} are in units of MeV. A blank indicates that the σ_2 contribution is not considered.

	$g^2_{\sigma_1}/4\pi$ (m_{σ_1})	$g^2_{\sigma_2}/4\pi$ (m_{σ_2})
$^3S_1$	0.51673 (350)	14.01164 (793)
$^1P_1$, $^3D_2$	0.81, 0.53 (*)	71.5, 154.5 (1225)
$^3D_1$	0.575 (*)	
$^3D_3$	3.4 (452)	
$^1F_3$	0.73 (*)	
$^3G_3$	0.29 (*)	
$^3G_4$	0.62 (*)	
$^3G_5$, $^3I_5$	0.96 (*)	
$^1H_5$	* (*)	

One-boson exchange models of v_{ij} have "problems"

III. REFERENCES FOR ADDITIONAL READING

1. R. A. M. Klomp, V. G. J. Stoks and J. J. de Swart; Phys. Rev. C 44, R1258 (1991)

Evidance for v^π in NN interaction and the πNN coupling constant.

2. V. G. J. Stoks, R. A. M. Klomp, M. C. M. Rentmeester and J. J. de Swart, Phys. Rev. C 48, 792 (1993)

Partial wave analysis of all NN scattering data.

3. R. B. Wiringa, V. G. J. Stoks and R. Schiavilla, Phys. Rev. C 51, 38 (1995).

The Argonne v_{18} interaction + references for Argonne v_{14} and Urbana v_{14}.

4. R. B. Wiringa, A. Arriaga and V. R. Pandharipande, Quadratic Momentum Dependence in the Nucleon-Nucleon Interaction, preprint (2003)

Compares potentials assuming $\mathbf{L}^2$ and $\mathbf{p}^2$ dependence.

5. S. C. Pieper, V. R. Pandharipande, R. B. Wiringa and J. Carlson, Phys. Rev. C 64, 014001 (2001)

Illinois three-nucleon interaction models + references for Urbana models.

6. J. L. Forest, V. R. Pandharipane and A. Arriaga, Phys. Rev. C 60, 014002 (1999)

Relativistic effects in light nuclei

III. THE DEUTERON DENSITY DISTRIBUTION

The structure of the deuteron and the mixing of its S- and D-waves is most obvious in the nucleon density distribution $\rho_d^M(r',\theta)$ which gives the probability to find a nucleon at position $\mathbf{r}'$ in the deuteron center of mass frame. It depends upon the projection M of the total deuteron angular momentum, the distance r' from the deuteron center of mass, and the polar angle θ of $\mathbf{r}'$; it is independent of the azimuthal angle ϕ.

Note : The interparticle distance $\mathbf{r} = 2\mathbf{r}'$, and the $\rho_d^M(r',\theta)$ has :

$$Normalization \quad : \quad \int d^3\mathbf{r}' \; \rho_d^{M_d}(\mathbf{r}') = 2,$$

$$\int d^3\mathbf{r} \Psi_d^{M\dagger}(\mathbf{r}) \Psi_d^M(\mathbf{r}) = 1$$

and $d^3\mathbf{r} = 8\; d^3\mathbf{r}'$. Therefore

$$\rho_d^M(\mathbf{r}') = 16 \Psi_d^{M\dagger}(2\mathbf{r}') \Psi_d^M(2\mathbf{r}') = 16 \sum_\alpha \psi_{d,\alpha}^{M*}(2\vec{r}') \psi_{d,\alpha}^{M}(2\vec{r}')$$

$$\rho_d^0(\mathbf{r}') = \frac{4}{\pi} \left[C_0(2r') - 2C_2(2r') \; P_2(cos\theta) \right] \; ,$$

$$\rho_d^{\pm 1}(\mathbf{r}') = \frac{4}{\pi} \left[C_0(2r') + C_2(2r') \; P_2(cos\theta) \right] \; ,$$

$$C_0(r) = \frac{1}{r^2} \left(u^2(r) + w^2(r) \right) \; ,$$

$$C_2(r) = \frac{\sqrt{2}}{r^2} \; u(r) \; w(r) - \frac{1}{2r^2} w^2(r) \; .$$

Note that these density distributions are symmetic about $\theta = \pi/2$,

do not depend on ϕ

$$\rho_d^0(r', \theta = \pi/2) = \rho_d^{\pm 1}(r', \theta = 0) = \frac{4}{\pi} \left[C_0(2r') + C_2(2r') \right] \; .$$

Many-Body Theory of Nuclei and Nuclear Matter

Vijay Pandharipande

(September 2003)

Lecture II Deuteron and Variational Monte Carlo

2.1 The two nucleon Schrödinger eq.

2.2 The deuteron wave function and density distribution

2.3 Variational wave functions for A=2,3,4 nuclei

2.4 Variational wave functions for nuclear matter

2.5 Variational Monte Carlo Calculations

2.6 Results for nuclei with A=2,3,4

2.7 Results for nuclei with A up to 8

2.8 Pair distribution functions

2.9 Cluster distribution functions

2.10 Quasi-hole orbitals

2.11 Elastic scattering form factors

2.12 Radiative Decay Rates

2.11 Radiative Capture Reactions

2.13 Shapes of nuclei

2.14 References for additional reading

I. THE TWO NUCLEON SCHRÖDINGER EQUATION

Nuclear Hamiltonian

$$H = \sum_i -\frac{1}{2m}\nabla_i^2 + \sum_{i<j} v_{14}(ij) + \sum_{i<j<k} V(ijk)$$

$V(ijk)$ does not appear in the two nucleon Schrödinger Eq.

Quantum Numbers of Two Nucleon States

Total Isospin $T = 0, 1$ **Total Spin** $S = 0, 1$

Total Angular Momentum $J = 0, 1, 2...$ **Parity** $\pi = \pm 1 = (-1)^L$

Orbital Angular Momentum $L = J$ when $S = 0$

& $L = J,\ J \pm 1$ when $S = 1$

Single Channels : $J = L,\ S = 0, 1$, and ${}^3P_0$ (an exception)

In ${}^{2S+1}L_J$ Notation : ${}^1S_0,\ {}^3P_0,\ {}^1P_1,\ {}^1D_2,\ {}^3D_2,\ ...$

Coupled Channels : $L = J \pm 1,\ S = 1$ Mixed by the Tensor Force

Examples : $({}^3S_1 - {}^3D_1),\ ({}^3P_2 - {}^3F_2),\ ({}^3D_3 - {}^3G_3),\ ...$

have same T, S, J

Allowed antisymmetric states have : $(S + T + L)$ odd.

Representation of Eigenfunctions

$$Single\ \ Channels\ \ :\ \ \Psi = R_{JLS}(r)\mathcal{Y}^M_{JLS} = \frac{1}{r}u_{JLS}(r)\mathcal{Y}^M_{JLS}$$

Coupled Channels :

$$\begin{aligned}\Psi &= R_{J(L=J-1)S}(r)\mathcal{Y}^M_{J(L=J-1)S} + R_{J(J=L+1)S}(r)\mathcal{Y}^M_{J(J=L+1)S} \\ &= \frac{1}{r}\left[u_{J(L=J-1)S}(r)\mathcal{Y}^M_{J(L=J-1)S} + w_{J(J=L+1)S}(r)\mathcal{Y}^M_{J(J=L+1)S}\right]\end{aligned}$$

The Spin-angle functions $\mathcal{Y}^M_{JLS}$ are obtained by:

Couple $\sigma_i + \sigma_j$ to total spin $\mathbf{S}$, Next Couple $\mathbf{S} + \mathbf{L}$ to total J with $J_z = M$.

Channel Potentials : Definition

$$v_{JLS}(r) = \frac{L(L+1)}{mr^2} + \langle \mathcal{Y}^M_{JLS} | v_{14}(r) | \mathcal{Y}^M_{JLS} \rangle$$

These include the centrifugal potential for convenience.

NOTATION

$v^c,\ v^\sigma,\ v^t,\ v^{ls}\ , v^{l2},\ v^{l2\sigma}$ and v^{ls2}

denote potentials associated with operators

$1,\ \sigma_i \cdot \sigma_j,\ S_{ij},\ \mathbf{L}\cdot\mathbf{S},\ \mathbf{L}^2,\ \mathbf{L}^2\sigma_i\cdot\sigma_j$ and $(\mathbf{L}\cdot\mathbf{S})^2$

$v^\tau,\ v^{\sigma\tau},\ v^{t\tau},\ v^{ls\tau}\ , v^{l2\tau},\ v^{l2\sigma\tau}$ and $v^{ls2\tau}$

are those with above operators $\times\ \tau_i \cdot \tau_j$

In this notation we find, for example :

$$v(^1S_0) = v_{000}(r) = v^c(r) + v^\tau(r) - 3v^\sigma(r) - 3v^{\sigma\tau}(r)$$

$$v(^3S_1) = v_{101}(r) = v^c(r) - 3v^\tau(r) + v^\sigma(r) - 3v^{\sigma\tau}(r)$$

$$\begin{aligned} v(^3D_1) = v_{121}(r) = {} & \frac{6}{mr^2} + v^c(r) - 3v^\tau(r) + v^\sigma(r) - 3v^{\sigma\tau}(r) \\ & - 2v^t(r) + 6v^{t\tau}(r) - 3v^{ls} + 9v^{ls\tau}(r) + 6v^{l2}(r) - 18v^{l2\tau}(r) \\ & + 6v^{l2\sigma}(r) - 18v^{l2\sigma\tau}(r) + 9v^{ls2}(r) - 27v^{ls2\tau}(r) \end{aligned}$$

NOTE : In v_8' the v^{1-8} are redefiend such that the potentials in $^1S_0$, $^3S_1$, $^1P_0$, $^3P_{0,1,2}$ and the $^3D_1$ channels, and the channel coupling tensors, $v^t_{T=0,1}$, are the same as in v_{14}.

Single Channel Schrödinger Equation

$$-\frac{1}{m}\frac{d^2u}{dr^2} + v_{JLS}(r)u(r) = Eu(r)$$

$E > 0$: No bound states in single channels

Schrödinger Equation for the Deuteron

$$\begin{aligned} -\frac{1}{m}\frac{d^2u}{dr^2} + v_{101}(r)u(r) + v^t_{T=0}(r)\sqrt{8}w(r) &= E_d u(r) \,, \\ -\frac{1}{m}\frac{d^2w}{dr^2} + v_{121}(r)w(r) + v^t_{T=0}(r)\sqrt{8}u(r) &= E_d w(r). \end{aligned}$$

Channel Coupling Tensor Potentials

$$v^t_{T=0}(r) = v^t(r) - 3v^{t\tau}(r)$$

$$v^t_{T=1}(r) = v^t(r) + v^{t\tau}(r)$$

II. THE DEUTERON WAVE FUNCTION

In order to see the structure of the deuteron we have to write the deuteron wave fuction:

$$\Psi_d^M = \frac{1}{r}\left(u(r)\mathcal{Y}_{101}^M + w(r)\mathcal{Y}_{121}^M\right)\frac{1}{\sqrt{2}}\left(|p_1 n_2\rangle - |n_1 p_2\rangle\right) .$$

as a function of $\mathbf{r} = r, \theta, \phi$ in the spin states:

$$|S, M_S\rangle \ : \ |1,1\rangle, \ \ |1,0\rangle, \ \ |1,-1\rangle$$

Ignoring the isospin factor $\frac{1}{\sqrt{2}}\left(|p_1 n_2\rangle - |n_1 p_2\rangle\right)$ for brevity we get:

$$\Psi_d^{M=1} = \frac{1}{\sqrt{4\pi}}\frac{1}{r}\Big[\left(u(r) + \frac{1}{\sqrt{8}}(3\,cos^2\theta - 1)w(r)\right)|1,1\rangle + \frac{3}{2}cos\theta\ sin\theta\ e^{i\phi}w(r)|1,0\rangle + \frac{3}{\sqrt{8}}sin^2\theta\ e^{2i\phi}w(r)|1,-1\rangle\Big] ,$$

$$\Psi_d^{M=0} = \frac{1}{\sqrt{4\pi}}\frac{1}{r}\Big[\left(u(r) + \frac{1}{\sqrt{2}}(3\,cos^2\theta - 1)w(r)\right)|1,0\rangle + \frac{3}{2}cos\theta\ sin\theta\ e^{-i\phi}w(r)|1,1\rangle - \frac{3}{2}cos\theta\ sin\theta\ e^{i\phi}w(r)|1,-1\rangle\Big] ,$$

$$\Psi_d^{M=-1} = \frac{1}{\sqrt{4\pi}}\frac{1}{r}\Big[\left(u(r) + \frac{1}{\sqrt{8}}(3\,cos^2\theta - 1)w(r)\right)|1,-1\rangle - \frac{3}{2}cos\theta\ sin\theta\ e^{-i\phi}w(r)|1,0\rangle + \frac{3}{\sqrt{8}}sin^2\theta\ e^{-2i\phi}w(r)|1,1\rangle\Big] .$$

Our QMC notation

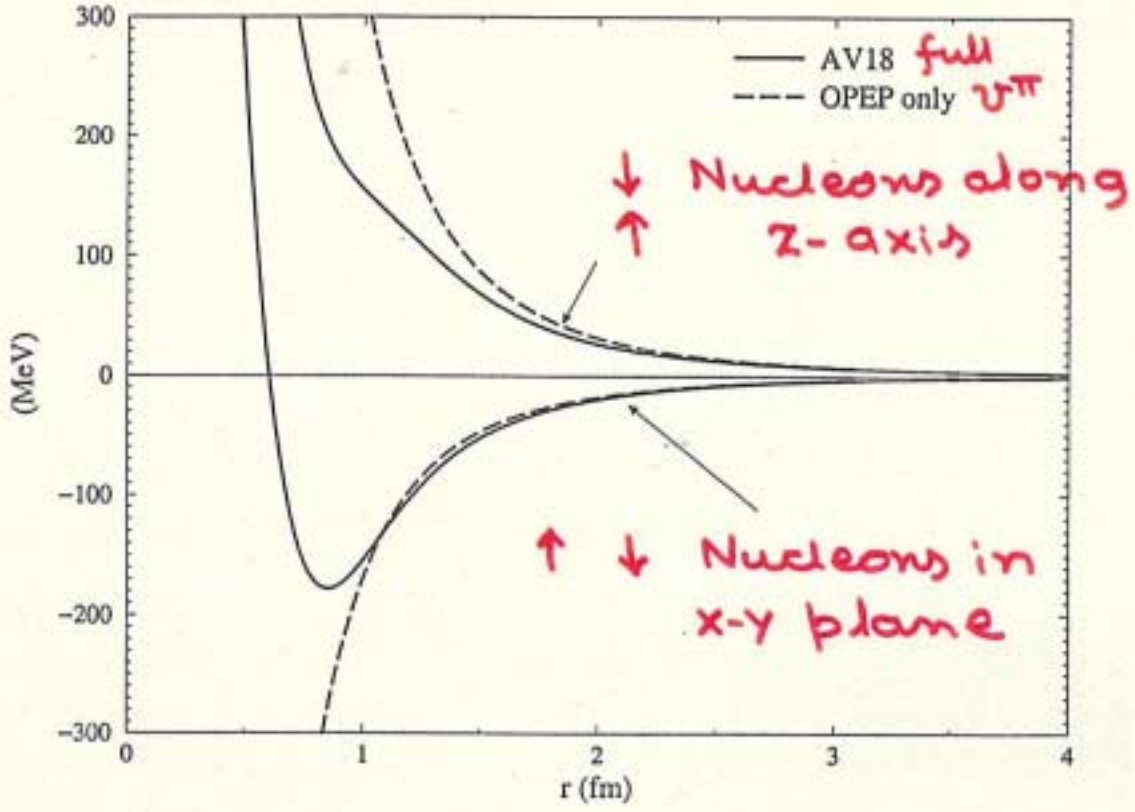
$$\Psi_d^M(X) = \sum_\alpha \psi_{d,\alpha}^M(\vec{R})\,|\alpha\rangle$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$\vec{R} = \vec{r}_1 \quad \vec{r}_2$$

Deuteron Structure : A Stringent test of v_{ij}

The static (without spin-orbit) potential in deuteron, spin projection M=0 state (similar to potential of magnetic dipoles)

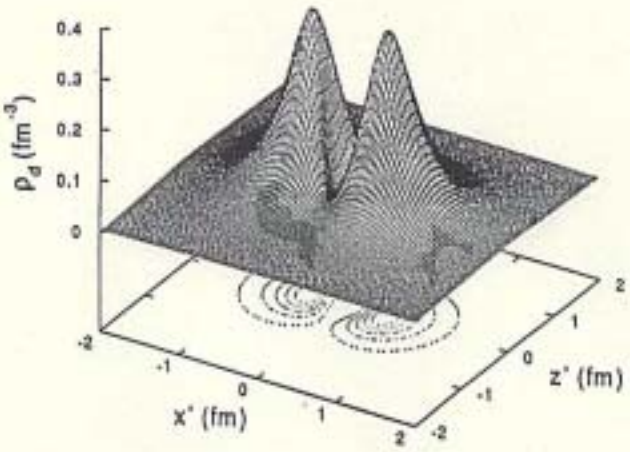


3-D Equidensity surfaces at

$\rho = 0.24\ fm^{-3}$

M = ±1 M = 0

Cross section of $\rho(\vec{r})$ for M=0 in x-z plane



IV. THE STATIC POTENTIAL IN THE DEUTERON

Ignore all momentum dependent terms in the NN interaction

$$v_d^{static}(\mathbf{r}) = v_{101}(r) + v_{T=0}^t(r)[3\sigma_i \cdot \hat{\mathbf{r}}\sigma_j \cdot \hat{\mathbf{r}} - \sigma_i \cdot \sigma_j]$$

This potential is anistropic : makes the deuteron anistropic

It depends upon the value of M_S

$$\langle 1, M_S = 0|v_d^{static}|1, M_S = 0\rangle = v_{101}(r) - 4v_{T=0}^t(r)P_2(cos\theta)$$

$$\langle 1, M_S = \pm 1|v_d^{static}|1, M_S = \pm 1\rangle = v_{101}(r) + 2v_{T=0}^t(r)P_2(cos\theta)$$

It is like the interaction between magnetic dipoles

CONCLUSIONS

1. The D-state of the deuteron is close to maximum value at $r < 2$ fm.
2. The deuteron is the smallest toroid known : 0.5 fm radius.
3. Realistic NN potentials give a quantitative description of NN interaction at $r >\sim 0.7$ fm
4. At $r < 0.7$ fm the nuclear wave function is small.

V. VARIATIONAL WAVE FUNCTIONS FOR A=2,3,4 NUCLEI

The state: $\Phi_d^{M=1} = (\uparrow p \uparrow n - \uparrow n \uparrow p) = \mathcal{Y}_{101}^{M=1}(|p_1 n_2\rangle - |n_1 p_2\rangle)$

describes two **uncorrelated** nucleons in $J = 1$, $M = 1$, $S = 1$ and $T = 0$ state with the deuteron quantum numbers.

We can write

$$\Psi_d^M = \left(R_S(r)\mathcal{Y}_{101}^M + R_D(r)\mathcal{Y}_{121}^M\right)\left(|p_1 n_2\rangle - |n_1 p_2\rangle\right) .$$
$$= (f_d^c(r) + f_d^t(r)S_{ij})\Phi_d^M = \mathcal{CO}\Phi_d^M$$

with

$$f_d^c(r) = R_S(r) \;\; and \;\; f_d^t(r) = \frac{1}{\sqrt{8}}R_D(r)$$

Note : $S_{ij}\mathcal{Y}_{101}^M = \sqrt{8}\mathcal{Y}_{121}^M$

In general we can write $\Psi = \mathcal{CO}\Phi$ to obtain the correlated eigenstates of H from uncorrelated states with appropriate quantum numbers. An exact calculation of the correlation operator $\mathcal{CO}$ is as difficult as solving the many body Schrödinger equation. In the variational method we approximate the Φ and $\mathcal{CO}$ by simple forms with few parameters and determine them using the variational principle:

$$\delta\langle H\rangle = \delta\left(\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}\right) = 0$$

Our approximations will give us the deuteron exactly, but not nuclei having $A > 2$.

The uncorrelated states Φ

The $A = 3$ nuclei have only one bound state with $T = \frac{1}{2}$ and $J = \frac{1}{2}$. The uncorrelated states with $T_z = \pm\frac{1}{2}$ and $J_z = \pm\frac{1}{2}$ are uniquely given by:

$$\Phi_3 = \mathcal{A}[\uparrow p \downarrow p \uparrow n],\ \mathcal{A}[\uparrow p \downarrow p \downarrow n],\ \mathcal{A}[\uparrow p \uparrow n \downarrow n],\ \mathcal{A}[\downarrow p \uparrow n \downarrow n]$$

$\mathcal{A}$ is the Antisymmetrizer; All Φ are antisymmetric

The $A = 4$ (^{4}He) has only one bound state with $J = 0$ and $T = 0$. The uncorrelated state with these quantum numbers is:

$$\Phi_4 = \mathcal{A}[\uparrow p \downarrow p \uparrow n \downarrow n]$$

$\Phi_{A>4}$ must have $\vec{R}$ dependence

The State of Uncorrelated Nuclear Matter

$A \to \infty$

Is Noninteracting Fermi Gas

$$\Phi_{SNM} = \mathcal{A}\left[\prod_{k\le k_F}\prod_{n=1,4} e^{i\mathbf{k}\cdot\mathbf{r}_i}\chi_n(i)\right]$$

$$\Phi_{PNM} = \mathcal{A}\left[\prod_{k\le k_F}\prod_{n=1,2} e^{i\mathbf{k}\cdot\mathbf{r}_i}\chi_n(i)\right]$$

$\chi_{n=1,4} : \uparrow n,\ \downarrow n,\ \uparrow p,\ \downarrow p$

SNM : Symmetric Nuclear Matter $N = Z = \frac{A}{2}$ and degeneracy $d = 4$

PNM : Pure Neutron Matter $N = A,\ Z = 0$ (Neutron Stars) and $d = 2$

Use Shell-Model type wave functions for uncorrelated bound states of $A > 4$ Nuclei

$A = 2, 3, 4$ & ∞ is "Simple"

Generalized Jastrow Approximation for $\mathcal{CO}$

$$\mathcal{CO} = \mathcal{S}\left[\prod_{i<j<A} \mathcal{F}_{ij}\right]$$

$$\mathcal{F}_{6,ij} = \sum_{p=1,6} f_p(r_{ij}) O_{ij}^p \; : \; static$$ used in QMC

$$\mathcal{F}_{8,ij} = \sum_{p=1,8} f_p(r_{ij}) O_{ij}^p \; : \; static + spin-orbit$$ used in cluster expansions

Recall: $O_{ij}^{p=1,8} = 1,\ \tau_i \cdot \tau_j,\ \sigma_i \cdot \sigma_j\ , \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j,\ S_{ij},\ S_{ij}\tau_i \cdot \tau_j,\ \mathbf{L}\cdot\mathbf{S},\ \mathbf{L}\cdot\mathbf{S}\tau_i \cdot \tau_j$

$\mathcal{S}$ is the symmetrizer; $\mathcal{F}_{ij}$ do not commute with $\mathcal{F}_{jk}$.

The General Assumption

We can always write the exact $\mathcal{CO}$ for a nucleus as:

$$\mathcal{CO} = \mathcal{F}_{ijk...A}... \; \mathcal{S}\left[\prod_{i<j<k<A} \mathcal{F}_{ijk}\right] \; \mathcal{S}\left[\prod_{i<j<A} \mathcal{F}_{ij}\right]$$

← included in light-nuclei, not in A→∞ matter

$\mathcal{F}_{ijk...A}$ is an A-body operator

Assume Convergence

$$(1 - \mathcal{F}_{ijk...A}) < .. < \left(1 - \mathcal{S}\left[\prod_{i<j<k<A} \mathcal{F}_{ijk}\right]\right) < \left(1 - \mathcal{S}\left[\prod_{i<j<A} \mathcal{F}_{ij}\right]\right)$$

1. $\mathcal{F}_6$ is used in all Monte Carlo Calculations
2. $\mathcal{F}_8$ in most calculations using cluster expansions
3. Monte Carlo calculations also include approximate three-body $\mathcal{F}_{ijk}$

The equations for $\mathcal{F}$

The eight $f_{p=1,8}(r)$ are to be obtained by minimizing the $\langle H \rangle$

This is difficult because the $\langle H \rangle$ is very sensitive to the f_p's at small r, where the interaction is strong.

We can assume that $\mathcal{F}$ obeys a Schrödinger like equation:

$$\left(-\frac{1}{m}\nabla^2 + v_{ij} - \Lambda_{ij}\right)\mathcal{F}_{ij} = 0$$

$$\Lambda_{ij} = \sum_{p=1,8} \lambda_p(r_{ij}) O^p_{ij}$$

and vary the Λ_{ij} to minimize $\langle H \rangle$. This is always possible and is much simpler because some parts of λ_p's can be calculated from the condition on $f_p(r \to \infty)$, and the rest approximated with rather simple **smooth** functions of r.

The $\mathcal{F}$ and v_{14} commute with the total spin S and isospin T. The equations for the 8 f_p's breakup into 4 sets:

1 & 2 : $S = 0$ single channel Eq. for $f_{c,S=0,T=0,1}$

3 & 4 : $S = 1$ coupled channel Eq. for $f_{c,S=1,T=0,1}$, $f_{t,T=0,1}$ and $f_{ls,T=0,1}$

The $\mathcal{F}$ operator is constructed from these 8 functions

For the equations see:

I.E.Lagaris and VRP Nucl. Phys. A359, 349 (1981)-Nuclear matter

and R.B.Wiringa Phys. Rev. C 43, 1585 (1991)-light nuclei

VI. REPRESENTATION OF NUCLEAR WAVE FUNCTION IN QUANTUM MONTE CARLO

Nucleus is a bound state of A nucleons : $i = 1, A$

Nucleon i has

position r_i, **spin** σ_i :$\uparrow, \downarrow$ & **isospin** τ_i : p (proton),n (neutron)

Any nuclear state can be represented by

$$\Psi(\mathbf{R}) = \sum_{\alpha=1,Max} \psi_\alpha(\mathbf{R})|\alpha\rangle$$

$$\mathbf{R} = \mathbf{r}_1,\ \mathbf{r}_2,\ ...\mathbf{r}_A$$

$|\alpha = 1, Max\rangle$: are **spin-isospin states**

For example an $|\alpha\rangle$ in ^{3}H is $|p\uparrow\ n\uparrow\ n\uparrow\rangle$

^{3}H has 24 spin-isopsin states : $Max = 24$:

$$(pnn\ \ npn\ \ nnp) \otimes (\uparrow\uparrow\uparrow\ \ \uparrow\uparrow\downarrow\ \ \uparrow\downarrow\uparrow\ \ \uparrow\downarrow\downarrow\ \ \downarrow\uparrow\uparrow\ \ \downarrow\uparrow\downarrow\ \ \downarrow\downarrow\uparrow\ \ \downarrow\downarrow\downarrow)$$

In General $Max = 2^A \dfrac{A!}{N!\ Z!}$

Z and N are the number of protons and neutrons : $A = Z + N$

$Max = 96$ in ^{4}He; $\sim 4 \times 10^6$ in ^{12}C; $\sim 8 \times 10^8$ in ^{16}O

We can reduce Max by a factor of $\sim$ 4 to 10 by using symmetries and isospin conservation.

Present range of quantum Monte Carlo: Nuclei up to ^{12}C and 14 neutrons

The static operators $O_{ij}^{p=1,6}$ are built from

$$\sigma_i \cdot \sigma_j, \ \ \tau_i \cdot \tau_j, \ \text{ and } \sigma_i \cdot \mathbf{r}_{ij}$$

We use

$$\sigma_i \cdot \sigma_j = 2P_{ij}^{\sigma} - 1; \qquad P_{ij}^{\sigma} \ : \ \textit{spin exchange operator}$$

$$\tau_i \cdot \tau_j = 2P_{ij}^{\tau} - 1; \qquad P_{ij}^{\tau} \ : \ \textit{isospin exchange operator}$$

$$\sigma_i \cdot \mathbf{r} = \sigma_i^Z z + \sigma_i^+ (x - iy) + \sigma_i^- (x + iy)$$

Let these operate on a 3-nucleon spin-isospin state for example

$$\sigma_1 \cdot \sigma_2 | \uparrow n \ \downarrow \ p \uparrow n\rangle = 2|\downarrow n \ \uparrow p \ \uparrow n\rangle - |\uparrow n \ \downarrow p \ \uparrow n\rangle$$

$$\tau_1 \cdot \tau_2 | \uparrow n \ \downarrow \ p \uparrow n\rangle = 2|\uparrow p \ \downarrow n \ \uparrow n\rangle - |\uparrow n \ \downarrow p \ \uparrow n\rangle$$

$$\sigma_1 \cdot \mathbf{r} | \uparrow n \ \downarrow \ p \uparrow n\rangle = (x + iy)|\downarrow n \ \downarrow p \ \uparrow n\rangle + z|\uparrow n \ \downarrow p \ \uparrow n\rangle$$

With above equations we represent each $v_{6,ij}$ and $\mathcal{F}_{ij}$ by a $Max \times Max$ matrix function of $\mathbf{R}$. In practice we teach the computer how to do it.

WE MUST KEEP ALL THE Max STATES

$\langle \alpha' | H | \alpha \rangle \neq 0$ even when $\alpha' \neq \alpha$

This makes the nuclear many-body problem exceptionally challenging

If $v_6(ij)$ were to be spin-isospin independent $v_c(r_{ij})$ like the Coulomb potential we can keep only one of the possible $|\alpha\rangle$ states because in that case $\langle \alpha' | H | \alpha \rangle = 0$ when $\alpha' \neq \alpha$

VARIATIONAL MONTE CARLO (VMC)

$$Define \ : \ \mathcal{S}\left[\prod_{i<j}\mathcal{F}_{ij}\right] = \sum_{\beta}\prod_{\beta}\mathcal{F}_{ij}$$

$$\prod_{\beta}\mathcal{F}_{ij} \ : \ Product\ of\ \mathcal{F}_{ij}\ in\ the\ order\ specified\ by\ \beta$$

$$\langle H\rangle = \frac{\Sigma_{\beta,\,\gamma}\int d\mathbf{R}\Phi_V^{\dagger}(\mathbf{R})[\Pi_{\beta}\mathcal{F}_{ij}]H[\Pi_{\gamma}\mathcal{F}_{ij}]\Phi_V(\mathbf{R})}{\Sigma_{\beta,\,\gamma}\int d\mathbf{R}\Phi_V^{\dagger}(\mathbf{R})[\Pi_{\beta}\mathcal{F}_{ij}][\Pi_{\gamma}\mathcal{F}_{ij}]\Phi_V(\mathbf{R})}$$

In VMC the $\int d\mathbf{R}$ and the sums over $\beta,\ \gamma$ are carried out with the Monte Carlo method

Central Limit Theorem

$$\begin{aligned}\int d\mathbf{R}G(\mathbf{R}) &= \int d\mathbf{R}\frac{G(\mathbf{R})}{W(\mathbf{R})}W(\mathbf{R}) \\ &= \left[\frac{1}{N}\sum_{i=1,N}\frac{G(\mathbf{R}_i)}{W(\mathbf{R}_i)}\right]\int d\mathbf{R}W(\mathbf{R})\end{aligned}$$

1. $W(\mathbf{R})$ real positive normalizable probability distribution, also called the weight function

2. The density of configurations $\mathbf{R}_i$ at $\mathbf{R}$ is proportional to $W(\mathbf{R})$; *i.e.* $\mathbf{R}_i$ are distributed with probability $W(\mathbf{R})$.

3. The number of configurations $N \to \infty$

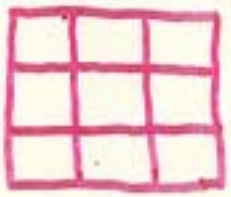
Generalize to include discret sums

$$\sum_{\beta}\int d\mathbf{R}G(\mathbf{R},\beta) = \left[\frac{1}{N}\sum_{i=1,N}\frac{G(\mathbf{R}_i,\beta_i)}{W(\mathbf{R}_i,\beta_i)}\right]\left[\sum_{\beta}\int d\mathbf{R}W(\mathbf{R},\beta)\right]$$

Monte Carlo Integration

$$\int dR\, G(R) = \sum_{\alpha} \Delta V\, G(R_\alpha)$$

Divide integration volume in many bins of volume ΔV



Take $\mathcal{N}$ samples distributed with weight $W(R)$

Number of samples N_α in bin α

$$N_\alpha = \frac{\Delta V\, W(R_\alpha)}{\int dR\, W(R)}\, \mathcal{N}$$

$$\frac{1}{\mathcal{N}} \sum_i \frac{G(R_i)}{W(R_i)} = \frac{1}{\mathcal{N}} \sum_\alpha \frac{N_\alpha\, G(R_\alpha)}{W(R_\alpha)}$$

$$= \sum_\alpha \frac{\Delta V\, G(R_\alpha)}{\left[\int dR\, W(R)\right]} = \frac{\int dR\, G(R)}{\int dR\, W(R)}$$

In quantum mechanics we need:

$$\frac{\int \Psi^\dagger(R)\, \hat{O}\, \Psi(R)\, dR}{\int \Psi^\dagger(R)\, \Psi(R)\, dR}$$

Ratio's of integrals

We do not need $\int dR\, W(R)$

Sample $\mathbf{R},\ \beta,\ \gamma$ using weight function:

$$W(\mathbf{R},\ \beta,\ \gamma) = |\Phi_V^\dagger(\mathbf{R})[\prod_\beta F_{ij}][\prod_\gamma F_{ij}]\Phi_V(\mathbf{R})|$$

Sampling means getting N configurations $\mathbf{R}_k,\ \beta_k,\ \gamma_k$ distributed with probability $W(\mathbf{R},\beta,\gamma)$. We will discuss Metropolis sampling shortly. Now assume that we have the samples.

$$\langle H\rangle = \frac{\Sigma_{\beta,\ \gamma}\int d\mathbf{R}\Phi_V^\dagger(\mathbf{R})[\Pi_\beta \mathcal{F}_{ij}]H[\Pi_\gamma \mathcal{F}_{ij}]\Phi_V(\mathbf{R})}{\Sigma_{\beta,\ \gamma}\int d\mathbf{R}\Phi_V^\dagger(\mathbf{R})[\Pi_\beta \mathcal{F}_{ij}][\Pi_\gamma \mathcal{F}_{ij}]\Phi_V(\mathbf{R})} = \frac{\mathcal{N}}{\mathcal{D}}$$

$$\mathcal{N} = \frac{1}{N}\sum_{k=1,N}\frac{\Phi_V^\dagger(\mathbf{R}_k)[\Pi_{\beta_k}\mathcal{F}_{ij}]H[\Pi_{\gamma_k}\mathcal{F}_{ij}]\Phi_V(\mathbf{R}_k)}{|\Phi_V^\dagger(\mathbf{R}_k)[\Pi_{\beta_k}F_{ij}][\Pi_{\gamma_k}F_{ij}]\Phi_V(\mathbf{R}_k)|}$$

$$\mathcal{D} = \frac{1}{N}\sum_{k=1,N}\frac{\Phi_V^\dagger(\mathbf{R}_k)[\Pi_{\beta_k}\mathcal{F}_{ij}][\Pi_{\gamma_k}\mathcal{F}_{ij}]\Phi_V(\mathbf{R}_k)}{|\Phi_V^\dagger(\mathbf{R}_k)[\Pi_{\beta_k}F_{ij}][\Pi_{\gamma_k}F_{ij}]\Phi_V(\mathbf{R}_k)|}$$

Metropolis Sampling of $W(\mathbf{X})$

Based on principle of detailed balance

$\rho_C(\mathbf{X})$ = density of configuration $\mathbf{X}_i$ at $\mathbf{X}$

If these configurations are allowed to move with the transition probability $T(\mathbf{X}\to\mathbf{X}')$ then the condition for dynamical equilibrium: ؛ن

$$\rho_C(\mathbf{X}')T(\mathbf{X}'\to\mathbf{X}) = \rho_C(\mathbf{X})T(\mathbf{X}\to\mathbf{X}')$$

$$we\ want\ :\ \frac{W(\mathbf{X})}{W(\mathbf{X}')} = \frac{\rho_C(\mathbf{X})}{\rho_C(\mathbf{X}')} = \frac{T(\mathbf{X}'\to\mathbf{X})}{T(\mathbf{X}\to\mathbf{X}')}$$

$$\textbf{Metropolis Solution} \quad T(\mathbf{X}' \to \mathbf{X}) = min\left[1,\ \frac{W(\mathbf{X})}{W(\mathbf{X}')}\right]$$

$$If \quad W(\mathbf{X}) > W(\mathbf{X}') \quad then \quad T(\mathbf{X}' \to \mathbf{X}) = 1 \quad and \quad T(\mathbf{X} \to \mathbf{X}') = \frac{W(\mathbf{X}')}{W(\mathbf{X})}$$

The Metropolis algorithm is implemented by sequentially obtaining the configurations $\mathbf{X}_k = \mathbf{R}_k,\ \beta_k,\ \gamma_k$ in a random walk.

To obtain $\mathbf{X}_{k+1}$ make a random step from $\mathbf{X}_k$: $\mathbf{X}' = \mathbf{X}_k + \Delta\mathbf{X}$

and accept it with probability : $T(\mathbf{X}_k \to \mathbf{X}') = min\left[1,\ \frac{W(\mathbf{X}')}{W(\mathbf{X})}\right]$

If accepted $\mathbf{X}_{k+1} = \mathbf{X}'$ If rejected $\mathbf{X}_{k+1} = \mathbf{X}_k$

NOTE The configurations generated in a Metropolis walk are correlated

If you want N configurations make nN steps and take every nth $\mathbf{X}$

Typically $n \sim 10$ to 20

It is all done with random numbers

1. Use a new random number η distributed between 0 and 1 each time
2. In a step each $x_i' = x_i + (\eta - 0.5)\ell$

   there are $3A$ componants x_i of $\mathbf{R}$

   ℓ is chosen to accept $\sim$ half the steps
3. β' and γ' are picked randomly from all orders of $\Pi\,\mathcal{F}_{ij}$
4. If $T(\mathbf{X}_k \to \mathbf{X}') = 1$ then **accept**
5. If $T(\mathbf{X}_k \to \mathbf{X}') < 1$ then **accept** if $\eta < T(\mathbf{X}_k \to \mathbf{X}')$

   reject if $\eta > T(\mathbf{X}_k \to \mathbf{X}')$

In VMC $\langle H \rangle$ is calculated by Metropolis sampling

The simplest way to calculate the statistical sampling error is to divide the N configurations in B blocks; each block has N/B configurations.

Let E_i be the $\langle H \rangle$ calculated from configurations in block i, $i = 1, B$

$$\bar{E} = \frac{1}{B} \sum_{i=1,B} E_i$$
$$\langle H \rangle = \bar{E} \pm \frac{\sigma_B}{\sqrt{B}}$$
$$\sigma_B^2 = \frac{1}{B} \sum_{i=1,B} (E_i - \bar{E})^2$$

Minimize $\langle H \rangle$ by varying Λ in $\mathcal{F}$ equations

$\langle \mathcal{O} \rangle$ are calculated like $\langle H \rangle$

Nondiagonal Matrix Elements

$$\mathcal{O}_{IJ} = \frac{\int d\mathbf{R} \Psi_I^\dagger(\mathbf{R}) \mathcal{O} \Psi_J(\mathbf{R})}{\sqrt{[\int d\mathbf{R} \Psi_I^\dagger(\mathbf{R}) \Psi_I(\mathbf{R})][\int d\mathbf{R} \Psi_J^\dagger(\mathbf{R}) \Psi_J(\mathbf{R})]}}$$
$$= \frac{\int d\mathbf{R} \Psi_I^\dagger(\mathbf{R}) \mathcal{O} \Psi_J(\mathbf{R})}{\int d\mathbf{R} \Psi_I^\dagger(\mathbf{R}) \Psi_I(\mathbf{R})} \times \sqrt{\frac{\int d\mathbf{R} \Psi_I^\dagger(\mathbf{R}) \Psi_I(\mathbf{R})}{\int d\mathbf{R} \Psi_J^\dagger(\mathbf{R}) \Psi_J(\mathbf{R})]}}$$

Calculate both the factors using $W(\mathbf{R}) = \Psi_I^\dagger(\mathbf{R}) \Psi_I(\mathbf{R})$

We can calculate electro-weak transition rates and radiative capture cross sections from $\mathcal{O}_{IJ}$

Overlaps between Ψ_I and Ψ_J are also calculated in a similar way;

set $\mathcal{O} = 1$

Results for A=3,4

PRC 52, 2362 (1995)

TABLE IV. Binding energy in MeV for ^{3}H with old and new correlations.

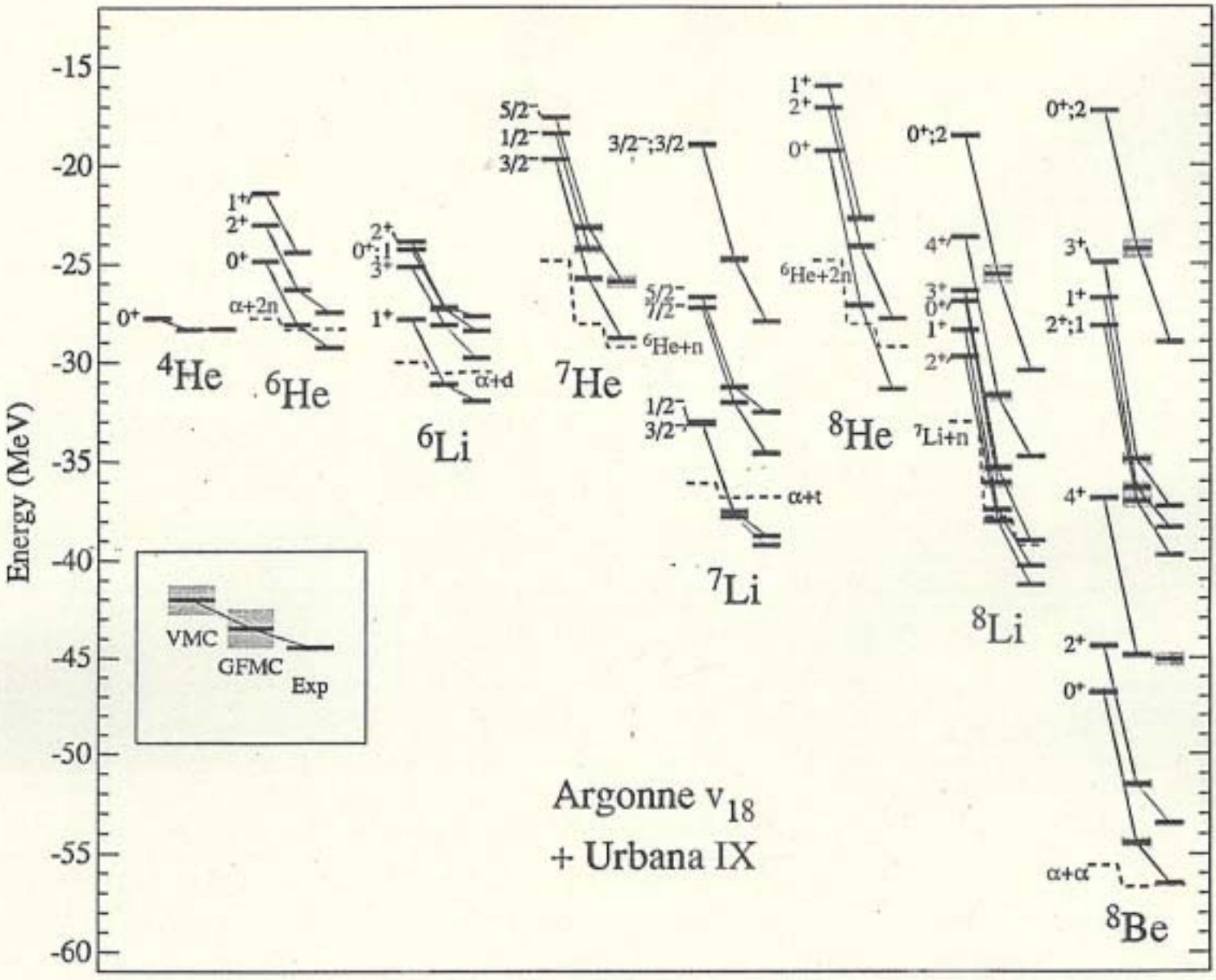
Hamiltonian	Reid v_8	Argonne v_{14}	Argonne v_{14} + Tucson	Argonne v_{14} + Urbana VII	Argonne v_{14} + Urbana VIII
Old[a]	7.31 (2)	7.45 (1)	8.80 (3)	8.79 (1)	8.21 (2)
New	7.44 (3)	7.53 (2)	9.05 (2)	8.95 (1)	8.35 (1)
Faddeev	7.59 (2)	7.70 (1)	9.33 (2)	9.05 (1)	8.49 (1)

TABLE V. Binding energy in MeV for ^{4}He with old and new correlations.

Hamiltonian	Reid v_8	Argonne v_{14}	Argonne v_{14} + Tucson	Argonne v_{14} + Urbana VII	Argonne v_{14} + Urbana VIII
Old[a]	23.62(6)	23.54(4)	30.64(9)	30.51(4)	27.23(6)
New	24.01(8)	23.80(6)	31.69(9)	30.79(5)	27.63(5)
FY[b]		23.90			
CHH[c]		23.93			27.48
GFMC[d]	24.55(13)	24.2(2)			28.3(2)

VMC in P-Shell

PRC 62, 014001 (2000)



VMC becomes less accurate as A increases

Spin-orbit correlations?

Other problems?

Applications

→ Pair distributions

Studies of Cluster Distributions in Nuclei

Example : α-d Distributions in ^{6}Li :

$$\Psi_I(\mathbf{R}) = \Psi_V(^6Li, M_J; \mathbf{R})$$

$$\Psi_J(\mathbf{R}) = \Psi_V(\alpha; \mathbf{R}_\alpha)\Psi_d(d, M_d, \mathbf{R}_d)\delta(\mathbf{r}_{\alpha d} - \mathbf{R}_\alpha^{cm} + \mathbf{R}_d^{cm})$$

Calculate for $\mathcal{O} = 1$:

$$\mathcal{O}_{IJ} = \frac{\int d\mathbf{R}\Psi_I^\dagger(\mathbf{R})\mathcal{O}\Psi_J(\mathbf{R})}{\sqrt{[\int d\mathbf{R}\Psi_I^\dagger(\mathbf{R})\Psi_I(\mathbf{R})][\int d\mathbf{R}\Psi_J^\dagger(\mathbf{R})\Psi_J(\mathbf{R})]}}$$

→ Form factors.

Nucleon Momentum Distributions

One-body density matrix : $\rho_1(\mathbf{r}_1, \mathbf{r}_1')$

Momentum distribution : $n(\mathbf{k}) = \int \rho_1(\mathbf{r}_1, \mathbf{r}_1')e^{i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_1')}d\mathbf{r}_1 d\mathbf{r}_1'$

In VMC it is simpler to calculate

$$\rho_1(\mathbf{x}) = \frac{\int d\mathbf{R}\Psi_V^\dagger(\mathbf{R}_+)\Psi_V(\mathbf{R}_-)}{\int d\mathbf{R}\Psi_V^\dagger(\mathbf{R})\Psi_V(\mathbf{R})} \quad with \quad \mathbf{R}_\pm = (\mathbf{r}_1 \pm \frac{1}{2}\mathbf{x}),\ \mathbf{r}_2,\ ...\mathbf{r}_A$$

Quasi-hole Orbitals in ^{7}Li for Example

$$\psi_{0,3/2}(k) = \langle \Psi_V(^6He, J = 0)\psi(p_{3/2}, k)|\Psi_V(^7Li, M)\rangle$$

Gives the probability to find in the ^{7}Li ground state : a proton in the $p_{3/2}$ state and ^{6}He in its ground state.

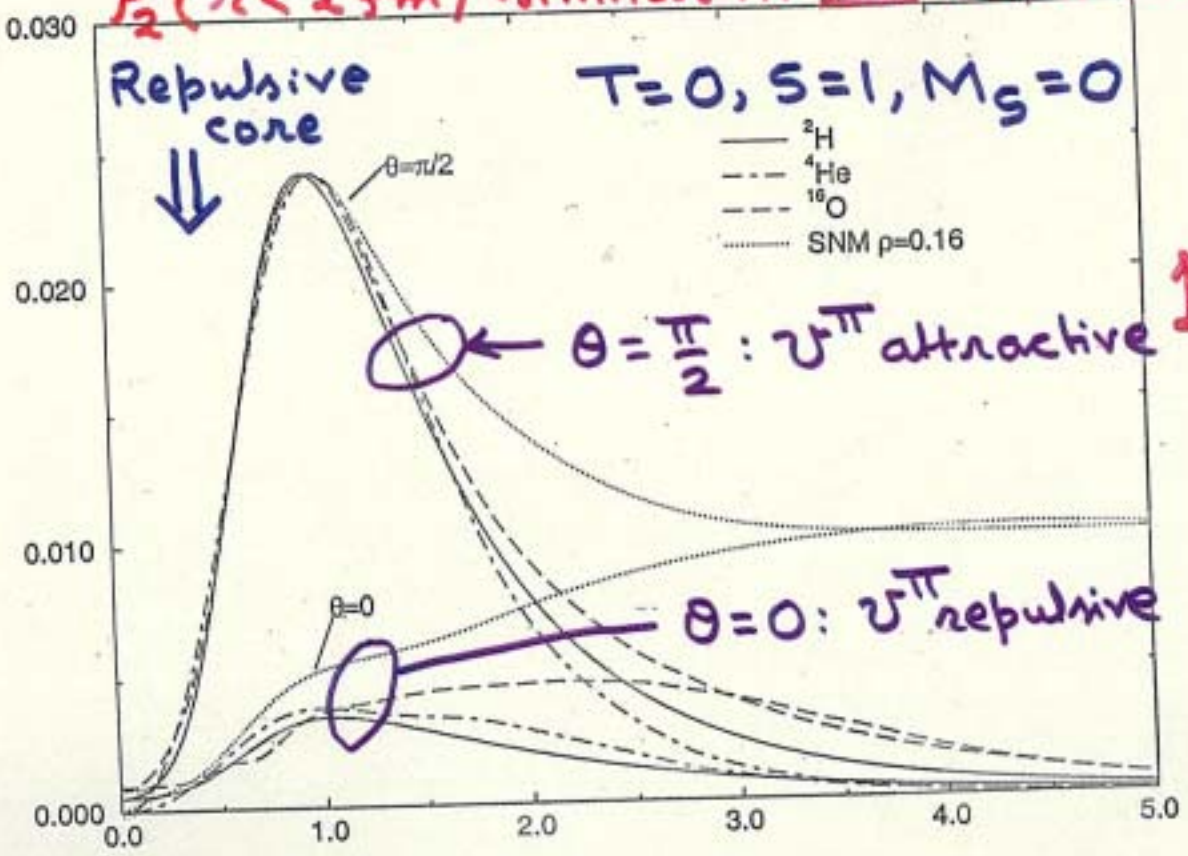
→ Electro weak transitions + captures.

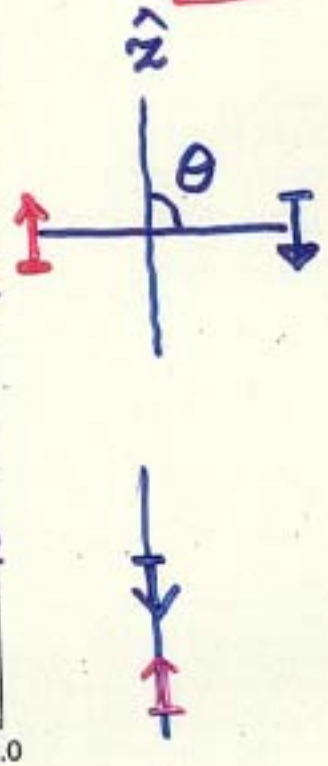
→ shapes of nuclei

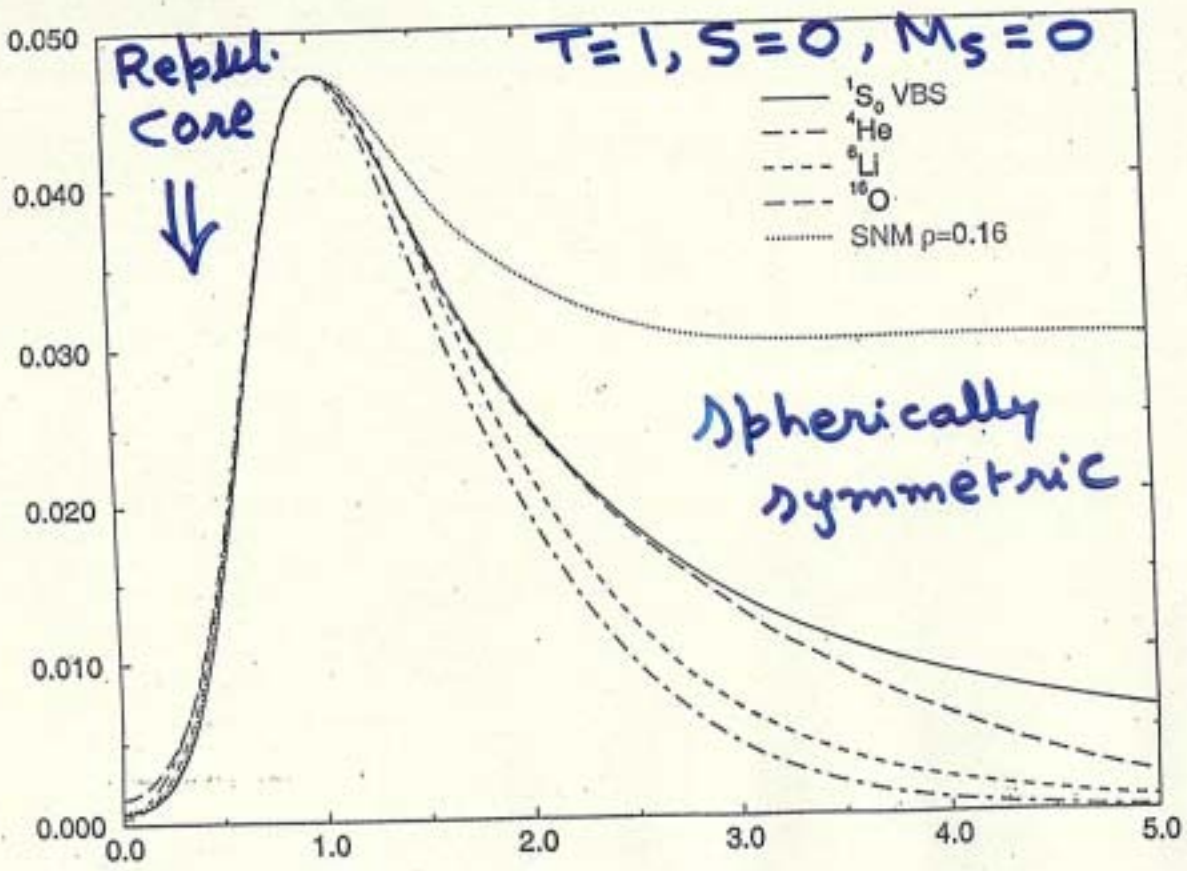
$\rho_2(\vec{r})$: Two nucleon distribution functions

→ Give probability to find 2-N's $\vec{r}$ apart

$\rho_2(r<2\,fm)$ similar in all nuclei - Normalized at peak







Studies of cluster structure in ^{4}He : d+d

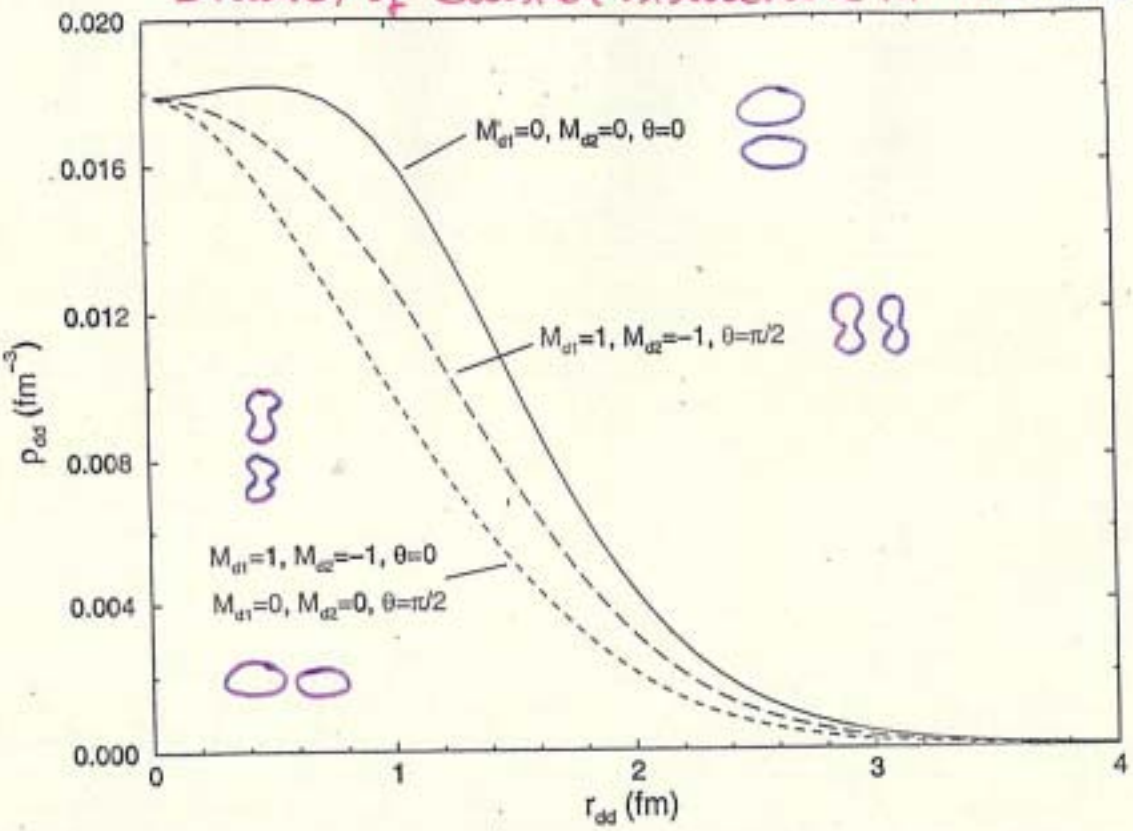


FIG. 19. Density distribution of $\vec{d}\vec{d}$ clusters in ^{4}He in parallel (θ=0) and transverse ($\theta=\pi/2$) directions.

Cluster structure in ^{6}Li : α+d

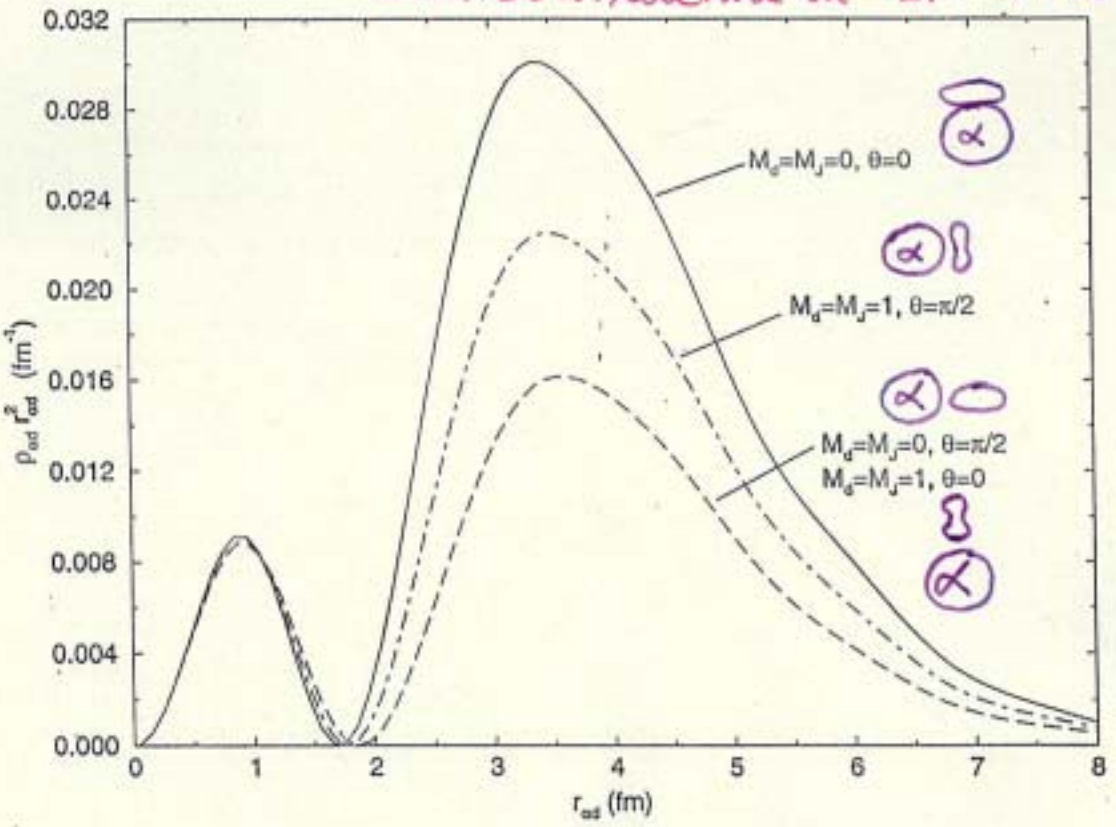
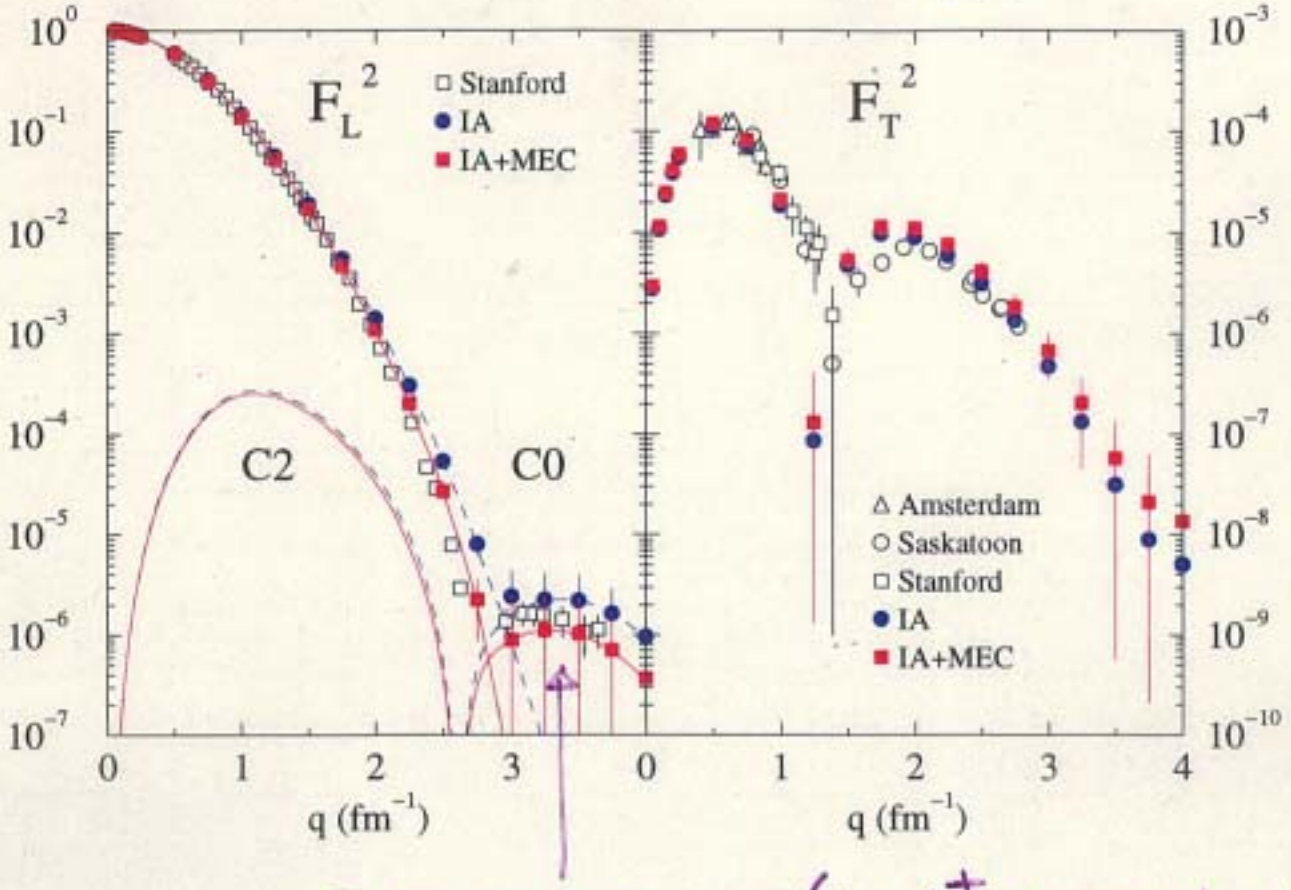


FIG. 22. Density distribution of $\alpha\vec{d}$ clusters in ^{6}Li in parallel (θ=0) and transverse ($\theta=\pi/2$) directions.

Fig.1 Wiringa & Schiavilla

^{6}Li : Elastic electron scattering form factors



Due to L=2 in ^{6}Li 1^+ ground state

: in M = 0 State 

^{6}Li Inelastic form factors are also good

Need more data on ^{6}Li & ^{7}Li

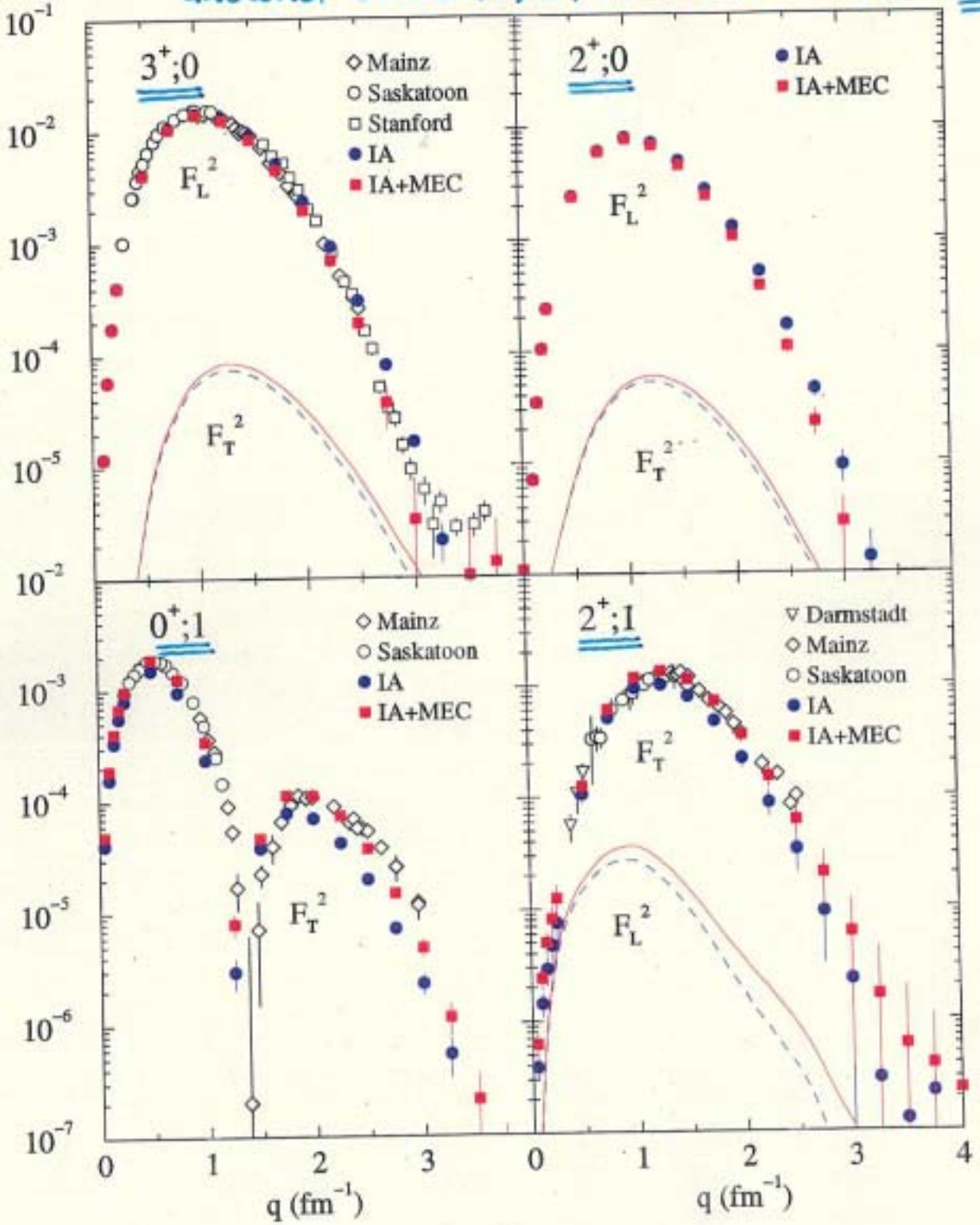
Elastic & Inelastic form factors.

Bare charges

^{6}Li: Inelastic electron scattering form factors

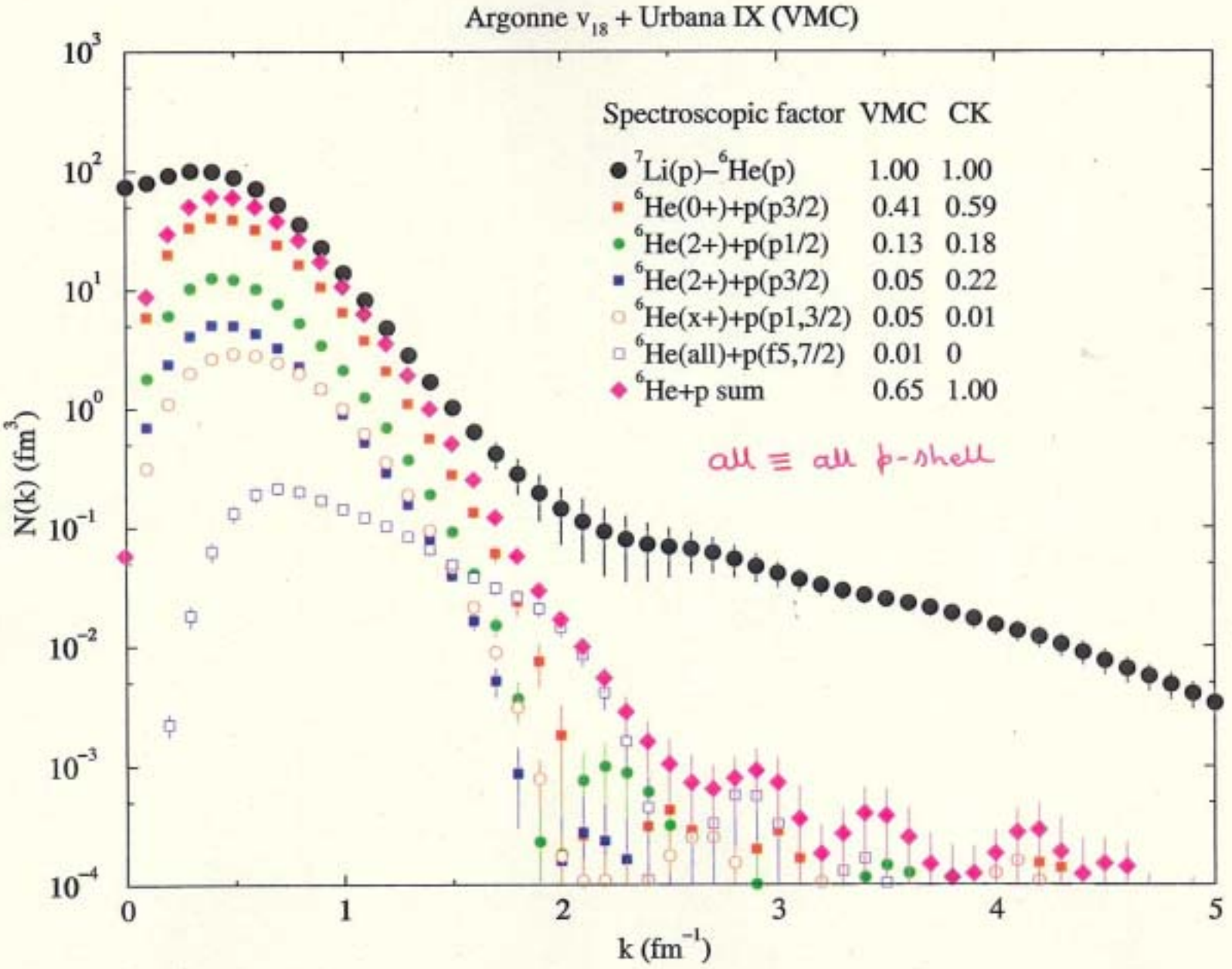
Fig.2 Wiringa & Schiavilla

Ground State $(1^+;0) \Rightarrow$ excited state $(J^\pi;T)$



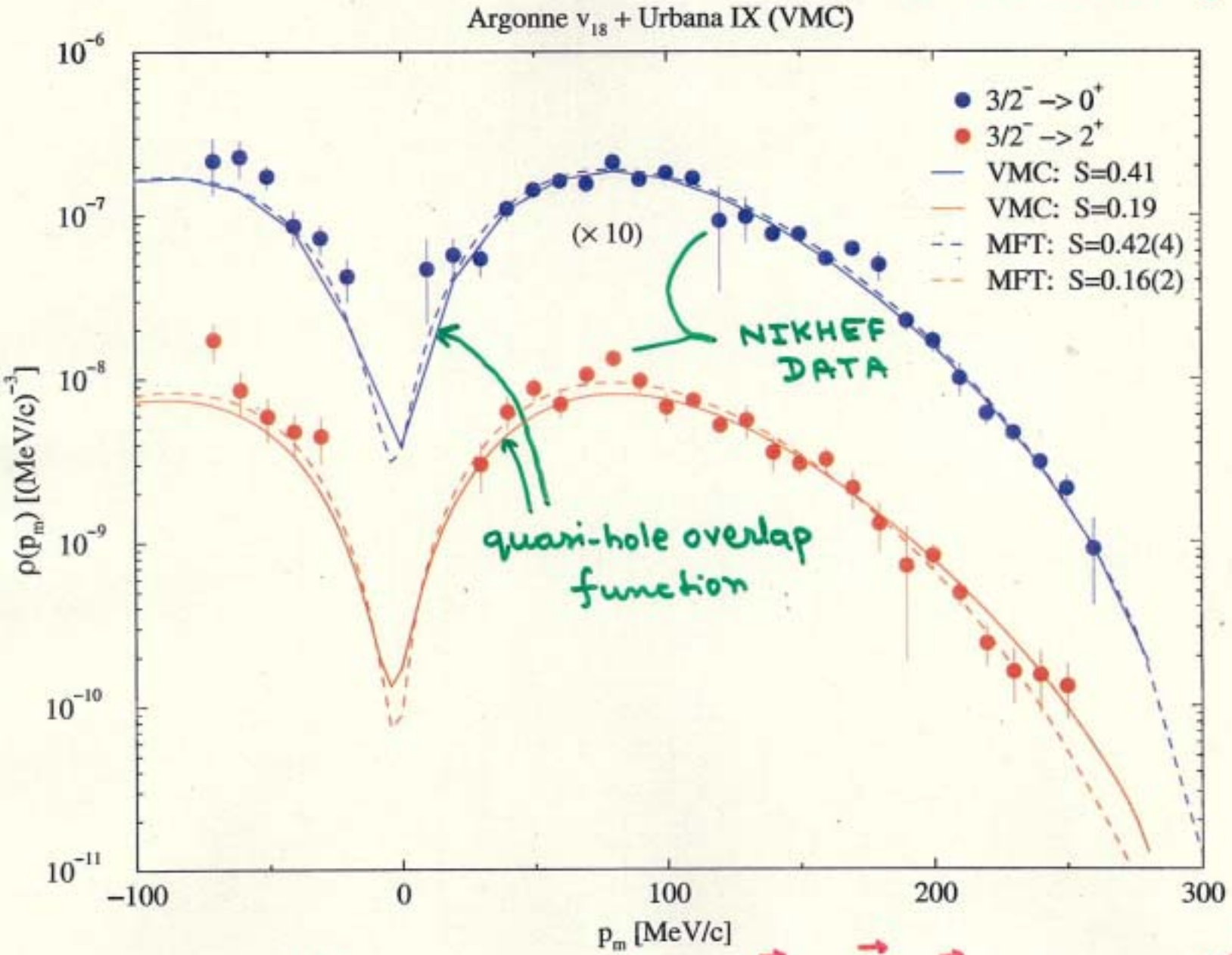
With bare charges

Momentum distributions for ^{7}Li

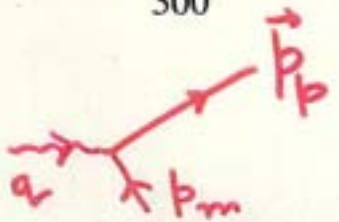


^{7}Li(e,e'p)^{6}He

Lapikás, Wesseling & Wiringa



Missing momentum $\vec{p}_m = \vec{p}_p - \vec{q}$



β-decay Gamow-Teller Matrix Elements

VMC GT Matrix Elements

Argonne v_{18} + Urbana IX

fitted

		I.A.	+ M.E.C.	Expt	
$^3H(\beta^-)^3He$	FIT	0.929(1)	0.957(1)	0.957(3)	exact
$^6He(\beta^-)^6Li$		2.248(4)	2.277(7)	2.173(4)	
$^7Be(\epsilon)^7Li$		2.356(2)	2.435(4)	2.599	
$^7Be(\epsilon)^7Li^*$		2.142(2)	2.201(7)	2.323	
$^7Li^*/^7Li$		10.15%	10.23%	10.52%	
$^8Li(\beta^-)^8Be^*$		0.085(4)	0.094(6)	0.22	

VMC Approx

Suppressed Wigner Symmetry

Can GFMC fix this?

VMC B(E2), Argonne v_{18} + Urbana IX

Electric quadrupole transitions

	B(E2)	Γ(E2) (eV)	
	e^2 fm^4	Computed	Expt.
$^6Li(3^+\rightarrow1^+)$	8.5(3)	$3.5(1)\times10^{-4}$	$4.4(4)\times10^{-4}$
$^6Li(2^+\rightarrow1^+)$	7.0(2)	$8.7(3)\times10^{-3}$	$5.4(3)\times10^{-3}$
$^7Li(\frac{1}{2}^-\rightarrow\frac{3}{2}^-)$	11.8(3)	$2.42(7)\times10^{-7}$	$2.8(2)\times10^{-7}$
$^7Li(\frac{7}{2}^-\rightarrow\frac{3}{2}^-)$	6.8(1)	$1.08(4)\times10^{-2}$	6.3×10^{-3}
$^9Be(\frac{5}{2}^-\rightarrow\frac{3}{2}^-)$	17.3(9)	$1.2(1)\times10^{-3}$	$1.9(1)\times10^{-3}$
$^9Be(\frac{7}{2}^-\rightarrow\frac{3}{2}^-)$	7.0(4)	$6.0(4)\times10^{-2}$	$8.(4.)\times10^{-2}$

VMC Approx

CAN GFMC FIX THESE?

^{2}H$(\alpha,\gamma)^6$Li Capture Reaction

U. of Chicago thesis work of K. Nollett

A primordial nuclear synthesis reaction

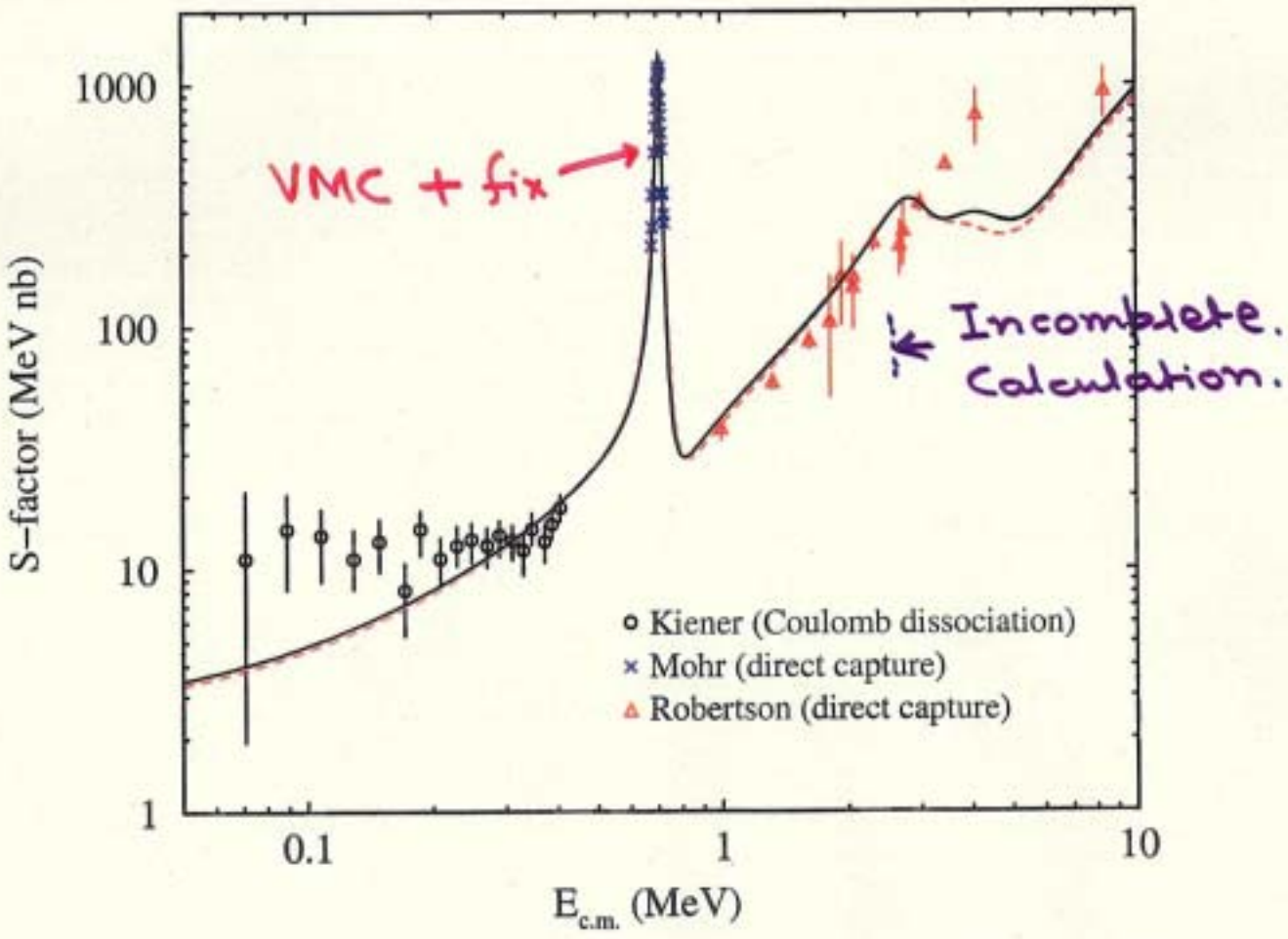
Astrophysically important region is 20−200 keV.

No direct capture data in this region

Full 6-nucleon calculation with variational wave functions

^{6}Li Variational wave function has proper α−d cluster form.

^{3}H$(\alpha,\gamma)^7$Li & ^{3}He$(\alpha,\gamma)^7$Be also being done



^{3}H$(\alpha,\gamma)^7$Li & ^{3}He$(\alpha,\gamma)^7$Be Capture Reactions

U. of Chicago thesis work of K. Nollett

Source of ^{7}Li in the big bang

- Astrophysically important region is 20−500 keV.

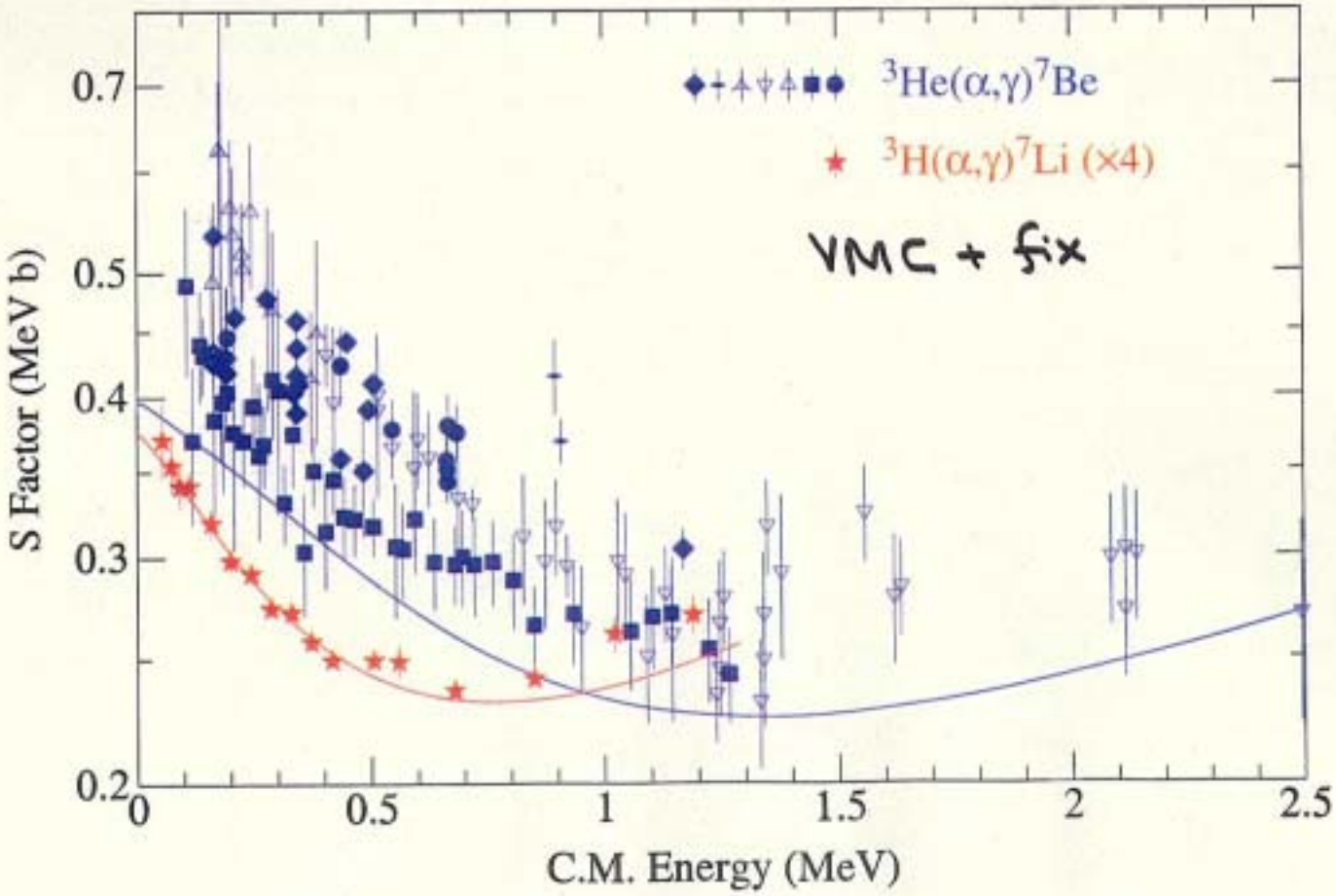
^{7}Be reaction also source of solar neutrinos

- Astrophysically important region is 20 keV.
- No data in this region

Full 7-nucleon calculation with variational wave functions

- $A = 7$ wave functions have proper 3+4 cluster form.

^{2}H$(\alpha,\gamma)^6$Li also done



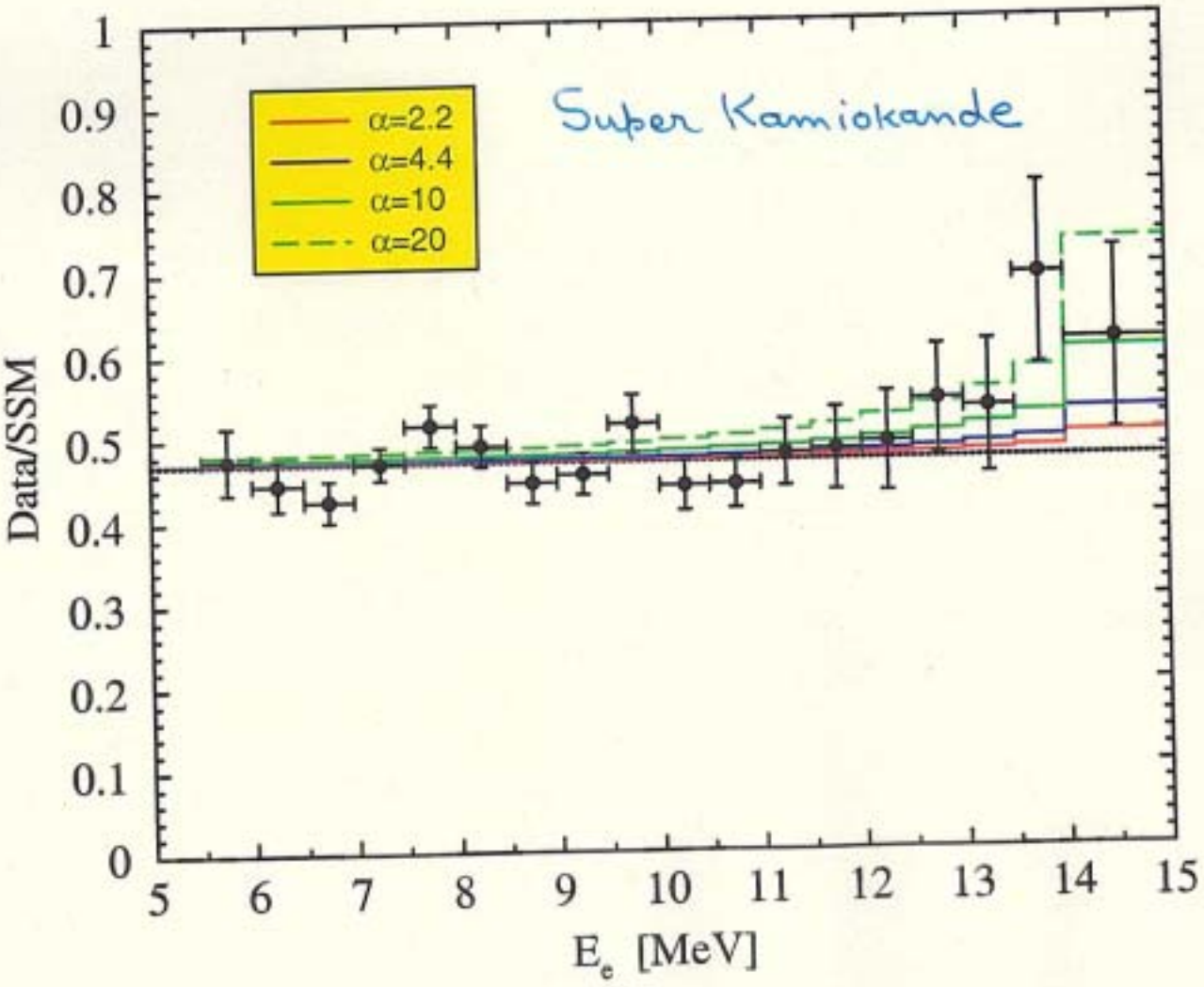
$^3He + p \rightarrow {}^4He + e^+ + \nu_e$ Weak capture

Source of Highest energy ν_e from sun

$E_{max} = 19$ MeV

S-Factor $\equiv \alpha\, 10^{-20}$ keV b.

Calculation by Marcucci et. al with
Argonne v_{18} + Urbana IX interactions
& "exact" Hyperspherical harmonic wave fun.
give $\alpha = 10.1$



Global Structure of Light Nuclei

Intrinsic Density of ^{8}Be

^{8}Be w.f.: ^{4}He core + 4 p-shell nucleons + pair corr.

M. C. [redacted]: random walk in $|\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_8)|^2$ [redacted]

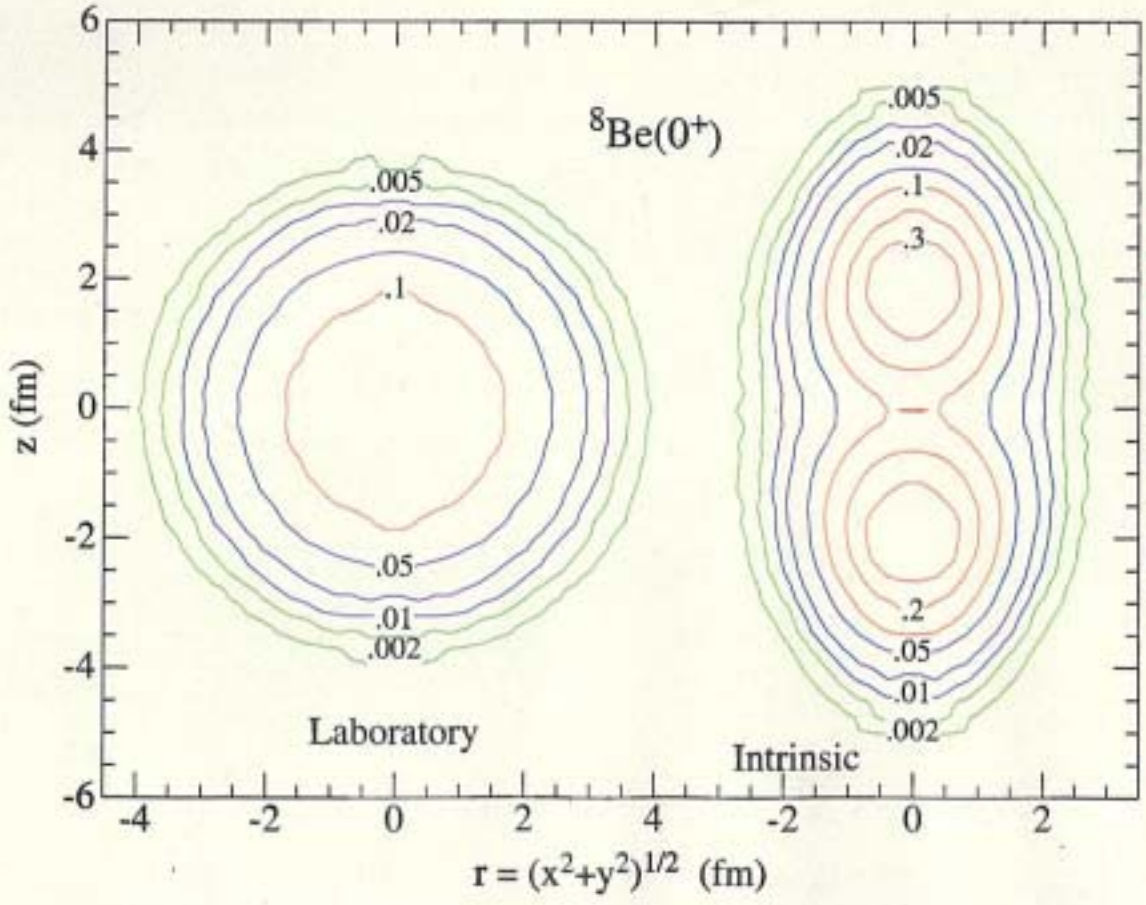
[redacted] each set $(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_8)$ is a picture of nucleons in the nucleus.

Lab $\rho(\mathbf{r})$: bin $\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_8$

Intrinsic $\rho(\mathbf{r})$: find eigenvectors of moment of inertia matrix:

$$\mathcal{M} = \sum_i \begin{pmatrix} x_i^2 & x_i y_i & x_i z_i \\ y_i x_i & y_i^2 & y_i z_i \\ z_i x_i & z_i y_i & z_i^2 \end{pmatrix} ,$$

rotate to them, and bin $\mathbf{r}'_1, \mathbf{r}'_2, \cdots, \mathbf{r}'_8$.



$\rho_0 = .16$ fm^{-3}

$\rho_{max} \sim 2\rho_0$

^{8}Be has $0^+, 2^+, 4^+$ rotational band.

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Many-Body Theory of Nuclei and Nuclear Matter

Vijay Pandharipande

(September 2003)

Lecture III Green's function Monte Carlo Calculations

This is what we want to do

I. EVOLUTION IN IMAGINARY TIME

Let Ψ_i be eigenstates of H belonging to eigenvalue E_i

All of these have the same chosen spin, parity, isospin, ...

Ψ_0 has the lowest energy E_0.

Suppose we have an approximation Ψ_V for the Ψ_0,

$$\Psi_V = \sum_{i \geq 0} a_i \Psi_i$$

We can project Ψ_0 from Ψ_V by evolution in imaginary time

The evolution operator e^{-iHt} becomes $e^{-H\tau}$ for imaginary time $\tau = it$

We use the evolution operator $e^{-(H-E_T)\tau}$ to control the normalization

$$\begin{aligned}\Psi(\tau) &= e^{-(H-E_T)\tau}\Psi_V \\ &= \sum_{i \geq 0} a_i e^{(E_T-E_i)\tau}\Psi_i \\ &= a_0 e^{(E_T-E_0)\tau}\Psi_0 \quad lim\ \tau \to \infty\end{aligned}$$

Because $(E_T - E_0) > (E_T - E_{i \geq 1})$

When $E_T = E_0$ then the norm of $\Psi(\tau \to \infty)$ is a_0^2 independent of τ.

The estimate of E_0 obtained by tuning the "trial energy" E_T to keep the norm of $\Psi(\tau \to \infty)$ fixed is called the **Growth Estimate**

We can also calculate E_0 from:

$$\frac{\langle \Psi_V | H | \Psi(\tau \to \infty) \rangle}{\langle \Psi_V | \Psi(\tau \to \infty) \rangle} = E_0 \frac{\langle \Psi_V | \Psi(\tau \to \infty) \rangle}{\langle \Psi_V | \Psi(\tau \to \infty) \rangle} = E_0$$

This is called the **Mixed Estimate**

 How can we do it?

II. THE SHORT TIME GREEN'S FUNCTION

In general the imaginary time evolution operator, or propagator, is very difficult to calculate. However, the propagator, or Green's function for a small time $\Delta\tau$ is relatively simple. We use:

$$e^{-(H-E_T)\tau} = \left(e^{-(H-E_T)\Delta\tau}\right)^n \; ; \quad n = \frac{\tau}{\Delta\tau}$$

This gives: (We omit spin-isospin labels now for brevity)

$$\begin{aligned}\Psi(\tau) &= e^{-(H-E_T)\tau}\Psi_V \\ &= \left(e^{-(H-E_T)\Delta\tau}\right)\ldots\left(e^{-(H-E_T)\Delta\tau}\right)\left(e^{-(H-E_T)\Delta\tau}\right)\Psi_V\end{aligned}$$

Now insert complete sets $\int d\mathbf{R}|\mathbf{R}\rangle\langle\mathbf{R}|$ after each). This gives

$$\Psi(\mathbf{R}_n,\tau) = \int d\mathbf{R}_{n-1}\ldots d\mathbf{R}_1\; d\mathbf{R}_0\;\; G(\mathbf{R}_n,\mathbf{R}_{n-1})\ldots G(\mathbf{R}_1,\mathbf{R}_0)\;\Psi_V(\mathbf{R}_0)$$

$$Where \quad G(\mathbf{R},\mathbf{R}') = \langle\mathbf{R}|e^{-(H-E_T)\Delta\tau}|\mathbf{R}'\rangle$$

is the Green's Function of Green's Function Monte Carlo (GFMC)

The set of configuration points $\mathbf{R}_n,\ldots\mathbf{R}_1,\ \mathbf{R}_0$ make a path, denoted by $\mathbf{P}_n$ in the $3A$ dimensional configuration space. We use

$$\mathbf{P}_n = \mathbf{R}_n,\ldots\mathbf{R}_1,\mathbf{R}_0$$

$$d\mathbf{P}_n = d\mathbf{R}_n,\ldots d\mathbf{R}_1,d\mathbf{R}_0$$

III. FEYNMAN'S APPROXIMATION FOR SHORT TIME GREEN'S FUNCTION

$$H = T + V(\mathbf{R})$$

$$T = \sum_{i=1,A} \left(-\frac{1}{2m} \nabla_i^2 \right) \quad \textit{The kinetic energy}$$

$$V(\mathbf{R}) = \left(\sum_{i<j} v(ij) + \sum_{i<j<k} V(ijk) + ... \right) \quad \textit{The total potential energy}$$

For now we assume that $v(ij)$, $V(ijk)$ are spin-isospin independent functions of the interparticle distances which depend only on $\mathbf{R}$

$$e^{-(H-E_T)\Delta\tau} = e^{E_T \Delta\tau} e^{-H\Delta\tau} \textbf{ since } E_T \textbf{ commutes with } H$$

But T and V do not commute with each other

$$\begin{aligned} e^{-H\Delta\tau} &= e^{-(T+V)\Delta\tau} \\ &= 1 - (T+V)\Delta\tau + \frac{1}{2}(T+V)^2\Delta\tau^2 - \frac{1}{6}(T+V)^3\Delta\tau^3 + ... \\ &= 1 - (T+V)\Delta\tau + \frac{1}{2}\left(T^2 + TV + VT + V^2\right)\Delta\tau^2 \\ &\quad - \frac{1}{6}\left(T^3 + TV^2 + V^2T + VTV + T^2V + VT^2 + TVT + V^3\right)\Delta\tau^3 \end{aligned}$$

Now consider the expansion of $e^{-V\Delta\tau/2} e^{-T\Delta\tau} e^{-V\Delta\tau/2}$ in powers of $\Delta\tau$

$$e^{-V\Delta\tau/2} e^{-T\Delta\tau} e^{-V\Delta\tau/2} = 1 - (T+V)\Delta\tau + \frac{1}{2}\left(T^2 + TV + VT + V^2\right)\Delta\tau^2$$
$$-\frac{1}{6}\left(T^3 + \frac{3}{4}TV^2 + \frac{3}{4}V^2T + \frac{3}{2}VTV + \frac{3}{2}T^2V + \frac{3}{2}VT^2 + (0)TVT + V^3\right)\Delta\tau^3$$

Obviously the two are not the same, **BUT**

$$e^{-H\Delta\tau} = e^{-(T+V)\Delta\tau} = e^{-V\Delta\tau/2} e^{-T\Delta\tau} e^{-V\Delta\tau/2}$$
$$+ \textit{ terms of order } \Delta\tau^3 \textit{ and higher}$$

We calculate $\Psi(\tau)$ taking n time steps using the approximate Green's function.

$$\langle \mathbf{R}|e^{-(H-E_T)\Delta\tau}|\mathbf{R}'\rangle \sim \langle \mathbf{R}|e^{E_T\Delta\tau}e^{-V\Delta\tau/2}e^{-T\Delta\tau}e^{-V\Delta\tau/2}|\mathbf{R}'\rangle$$

In each time step we make an error of order $\Delta\tau^3$.

$$Total\ error = n\Delta\tau^3 = \frac{\tau^3}{n^2} \to 0 \quad lim\ n \to \infty$$

verify that the error is negligible by doubling n

In fact we can use the more approximate Green's function:

$$\langle \mathbf{R}|e^{-(H-E_T)\Delta\tau}|\mathbf{R}'\rangle \sim \langle \mathbf{R}|e^{E_T\Delta\tau}\left(1-\frac{1}{2}V\Delta\tau\right)e^{-T\Delta\tau}\left(1-\frac{1}{2}V\Delta\tau\right)\mathbf{R}'\rangle$$

which has an error of order $\Delta\tau^2$. We then have an error of order n^{-1}, and need much larger values of n to obtain a desired accuracy.

For spin-isospin independent interactions $V(\mathbf{R})\Delta\tau$ is a real number, and

$$\begin{aligned}\langle \mathbf{R}|e^{E_T\Delta\tau}e^{-V\Delta\tau/2}e^{-T\Delta\tau}e^{-V\Delta\tau/2}\mathbf{R}'\rangle &= e^{E_T\Delta\tau}e^{-V(\mathbf{R})\Delta\tau/2}\langle \mathbf{R}|e^{-T\Delta\tau}|\mathbf{R}'\rangle e^{-V(\mathbf{R}')\Delta\tau/2} \\ &= e^{E_T\Delta\tau}e^{-V(\mathbf{R})\Delta\tau/2}G_0(\mathbf{R},\mathbf{R}')e^{-V(\mathbf{R}')\Delta\tau/2}\end{aligned}$$

The Green's function of noninteracting particles is a simple gaussian:

$$G_0(\mathbf{R},\mathbf{R}') = \langle \mathbf{R}|e^{-T\Delta\tau}|\mathbf{R}'\rangle = \left[\sqrt{\frac{m}{2\pi\Delta\tau}}\right]^{3A} exp\left[\frac{-(\mathbf{R}-\mathbf{R}')^2}{2\Delta\tau/m}\right]$$

When the interactions are spin-isospin independent functions of interparticle distances the short time Green's function is a simple, real, positive function of R and R′

IV. IMPROVED FORM FOR THE SHORT TIME GREEN'S FUNCTION

It is possible to improve the accuracy of the Feynman Green's function. It has errors of order $\Delta\tau^3$; for example it misses the TVT term.

Consider a configuration in which particles $1, 2$ are close to each other, so that v_{12} and ∇_{12}^2 are large. In this case most of the error in the Feynman's approximation will come from terms having many powers of v_{12} and ∇_{12}^2 such as:

$$(v_{12})^2\nabla_{12}^2, \quad \nabla_{12}^2 v_{12}\nabla_{12}^2, \quad \ldots.$$

We can calculate the two-particle Green's function:

$$g_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij}) = \langle \mathbf{r}_{ij}|e^{-H_{ij}\Delta\tau}|\mathbf{r}'_{ij}\rangle$$
$$H_{ij} = -\frac{1}{m}\nabla_{ij}^2 + v_{ij}$$

very accurately. The Green's function:

$$G_2(\mathbf{R}, \mathbf{R}') = G_0(\mathbf{R}, \mathbf{R}')\left[\prod_{i<j}\frac{g_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij})}{g_{0,ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij})}\right]$$

is more accurate. It has errors from terms like $v_{ij}Tv_{jk}$ which are large only when three particles are close. **Bottomline : we can take bigger $\Delta\tau$, smaller n with this G_2.**

Since $V(ijk)$ is smaller than $v(ij)$ we can use

$$G(\mathbf{R}, \mathbf{R}') = e^{E_T\Delta\tau}e^{-V_3(\mathbf{R})\Delta\tau/2}G_2(\mathbf{R}, \mathbf{R}')e^{-V_3(\mathbf{R}')\Delta\tau/2}$$

$$V_3(\mathbf{R}) = \sum_{i<j<k} V(ijk) \;\; in\; configuration\; \mathbf{R}$$

V. MIXED ESTIMATES

$$\langle \mathbf{O} \rangle_{Mixed} = \frac{\langle \Psi_V | \mathbf{O} | \Psi(\tau) \rangle}{\langle \Psi_V | \Psi(\tau) \rangle}$$
$$= \frac{\int d\mathbf{P}_n \Psi_V(\mathbf{R}_n)^\dagger \mathbf{O} G(\mathbf{R}_n, \mathbf{R}_{n-1}) ... G(\mathbf{R}_1, \mathbf{R}_0) \Psi_V(\mathbf{R}_0)}{\int d\mathbf{P}_n \Psi_V(\mathbf{R}_n)^\dagger G(\mathbf{R}_n, \mathbf{R}_{n-1}) ... G(\mathbf{R}_1, \mathbf{R}_0) \Psi_V(\mathbf{R}_0)}$$

$$\langle \mathbf{O} \rangle_{Exact} = \frac{\langle \Psi(\tau) | \mathbf{O} | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle}$$
$$= 2\langle \mathbf{O} \rangle_{Mixed} - \langle \mathbf{O} \rangle_V + terms\ of\ order\ (\Psi_0 - \Psi_V)^2$$
$$\langle \mathbf{O} \rangle_V = \frac{\langle \Psi_V | \mathbf{O} | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle}$$

Fortunately

$$\langle H \rangle_{Mixed} = \frac{\langle \Psi(\tau/2) | H | \Psi(\tau/2) \rangle}{\langle \Psi(\tau/2) | \Psi(\tau/2) \rangle} = E(\tau)$$
$$E(\tau) > E_0 \quad and \quad = E_0 \quad lim\ \tau \to \infty$$

Use Monte Carlo For $\int d\mathbf{P}_n$

Sample Paths from a probability function : $\mathrm{P}(\mathbf{P})$

$$let \quad : \quad N_{\mathbf{P}} = \Psi_V(\mathbf{R}_n)^\dagger \mathbf{O} G(\mathbf{R}_n, \mathbf{R}_{n-1}) ... G(\mathbf{R}_1, \mathbf{R}_0) \Psi_V(\mathbf{R}_0) / P(\mathbf{P})$$
$$D_{\mathbf{P}} = \Psi_V(\mathbf{R}_n)^\dagger G(\mathbf{R}_n, \mathbf{R}_{n-1}) ... G(\mathbf{R}_1, \mathbf{R}_0) \Psi_V(\mathbf{R}_0) / P(\mathbf{P})$$

For path $\vec{P}$

$$\langle \mathbf{O} \rangle_{Mixed} = \frac{\Sigma_{\{\mathbf{P}\}} N_{\mathbf{P}}}{\Sigma_{\{\mathbf{P}\}} D_{\mathbf{P}}}$$

$\{\mathbf{P}\}$ is the ensemble of sampled paths

We must choose $P(\vec{P})$ correctly.

Sampling Paths in Simple Systems with $v(\mathrm{r}_{ij})$: Kalos's Method

$\Psi(\mathbf{R})$ *and* $G(\mathbf{R}, \mathbf{R}')$ *are real scalar functions*

$$P(\mathbf{P}) = \left[\prod_{i=1,n} I(\mathbf{R}_i) G(\mathbf{R}_i, \mathbf{R}_{i-1}) \frac{1}{I(\mathbf{R}_{i-1})}\right] I(\mathbf{R}_0) |\Psi_V(\mathbf{R}_0)|$$

$$I(\mathbf{R}) = |\Psi_V(\mathbf{R})| \quad \textit{Importance function}$$

All the $I(\mathbf{R}_i)$ except the last $I(\mathbf{R}_n)$ cancel

$$P(\mathbf{P}) = |\Psi_V(\mathbf{R}_n)| G(\mathbf{R}_n, \mathbf{R}_{n-1}) ... G(\mathbf{R}_1, \mathbf{R}_0) |\Psi_V(\mathbf{R}_0)|$$

$$D_{\mathbf{P}} = \frac{\Psi_V(\mathbf{R}_n)\Psi_V(\mathbf{R}_0)}{|\Psi_V(\mathbf{R}_n)||\Psi_V(\mathbf{R}_0)|}$$

$$= \quad 1 \quad When\ \Psi_V(\mathbf{R}_n)\ and\ \Psi_V(\mathbf{R}_0)\ have\ same\ sign$$

$$= -1 \quad When\ \Psi_V(\mathbf{R}_n)\ and\ \Psi_V(\mathbf{R}_0)\ have\ opposite\ signs$$

In a similar way

$$N_{\mathbf{P}} = \frac{\Psi_V(\mathbf{R}_n)\mathbf{O}(\mathbf{R}_n)\Psi_V(\mathbf{R}_0)}{|\Psi_V(\mathbf{R}_n)||\Psi_V(\mathbf{R}_0)|}$$

In the special case $\mathbf{O} = H$ and $\Psi_V(\mathbf{R}_n)H(\mathbf{R}_n) \sim E_0\Psi_V(\mathbf{R}_n)$

$$N_{\mathbf{P}} \sim \quad E_0 \quad When\ \Psi_V(\mathbf{R}_n)\ and\ \Psi_V(\mathbf{R}_0)\ have\ same\ sign$$

$$\sim -E_0 \quad When\ \Psi_V(\mathbf{R}_n)\ and\ \Psi_V(\mathbf{R}_0)\ have\ opposite\ signs$$

THE FERMION SIGN PROBLEM

Both $\Sigma_{\{\mathbf{P}\}} N_{\mathbf{P}}$ and $\Sigma_{\{\mathbf{P}\}} D_{\mathbf{P}} \to 0$ as $\tau \to \infty$

we will deal with it later

WEIGHTS

$$I(\mathbf{R}_i)G(\mathbf{R}_i,\mathbf{R}_{i-1})\frac{1}{I(\mathbf{R}_{i-1})} = Importance\ sampled\ Green's\ function$$
$$= G_0(\mathbf{R}_i,\mathbf{R}_{i-1})\ w(\mathbf{R}_i,\mathbf{R}_{i-1})$$
$$w(\mathbf{R}_i,\mathbf{R}_{i-1}) = \frac{I(\mathbf{R}_i)}{I(\mathbf{R}_{i-1})}\prod_{m<n}\frac{g_{mn}}{g_{0,mn}}...$$

Where ... represent contributions of three-body interactions to $G(\mathbf{R}_i,\mathbf{R}_{i-1})$.

The simplest way to sample the paths uses the probability

only for learning

$$P'(\mathbf{P}) = G_0(\mathbf{R}_n,\mathbf{R}_{n-1})...G_0(\mathbf{R}_1,\mathbf{R}_0)|\Psi_V(\mathbf{R}_0)|^2$$

For this probability function we have:

$$D'_{\mathbf{P}} = \Psi_V(\mathbf{R}_n)G(\mathbf{R}_n,\mathbf{R}_{n-1})...G(\mathbf{R}_1,\mathbf{R}_0)\Psi_V(\mathbf{R}_0)/P'(\mathbf{P})$$
$$= w(\mathbf{R}_n,\mathbf{R}_{n-1})...w(\mathbf{R}_1,\mathbf{R}_0)\ \times\ sign[\Psi_V(\mathbf{R}_n)\Psi_V(\mathbf{R}_0)]$$

and similarly

$$N'_{\mathbf{P}} = \left(\frac{\Psi_V(\mathbf{R}_n)\mathcal{O}}{\Psi_V(\mathbf{R})}\right) w(\mathbf{R}_n,\mathbf{R}_{n-1})...w(\mathbf{R}_1,\mathbf{R}_0)\ \times\ sign[\Psi_V(\mathbf{R}_n)\Psi_V(\mathbf{R}_0)]$$
$$= \mathcal{O}(\mathbf{R}_n)w(\mathbf{R}_n,\mathbf{R}_{n-1})...w(\mathbf{R}_1,\mathbf{R}_0)\ \times\ sign[\Psi_V(\mathbf{R}_n)\Psi(\mathbf{R}_0)]$$

$$\langle\mathbf{O}\rangle_{Mixed} = \frac{\Sigma_{\{\mathbf{P}\}}N'_{\mathbf{P}}}{\Sigma_{\{\mathbf{P}\}}D'_{\mathbf{P}}}$$

In Quantum Monte Carlo $\mathbf{R}_i$ are called walkers on step i

The number of walkers = number of paths in the ensemble = $\mathcal{N}_P$

$w(\mathbf{R}_i,\mathbf{R}_{i-1})...w(\mathbf{R}_1,\mathbf{R}_0)$ = Weight of walker at step i

Implementation of the "simple" method

Principle : Sample $\mathbf{R}_0,\ \mathbf{R}_1, ...\mathbf{R}_n$ sequentially

1. Get $\mathcal{N}_P$ configurations (walkers) $\mathbf{R}_0(I = 1, \mathcal{N}_P)$ by sampling $|\Psi_V(\mathbf{R})|^2$ by Metropolis method.

2. Assign weight $W_0(I) = 1$ to each walker

3. For each I, sample $G_0(\mathbf{R}, \mathbf{R}_0(I))$ to get the $\mathbf{R}_1(I)$. **The 1st step.**

The $G_0(\mathbf{R}, \mathbf{R}')$ is a gaussian, and there are many analytic methods to sample gaussians.

4. Set weights : $W_1(I) = w(\mathbf{R}_1(I), \mathbf{R}_0(I))W_0(I)$

5. For each I, sample $G_0(\mathbf{R}, \mathbf{R}_1(I))$ to get the $\mathbf{R}_2(I)$. **The 2ed step.**

6. Set weights : $W_2(I) = w(\mathbf{R}_2(I), \mathbf{R}_1(I))W_1(I)$

7. Repeat steps 5-6 to take n steps

$$\langle \mathbf{O} \rangle_{Mixed} = \frac{\Sigma_I \mathcal{O}(\mathbf{R}_n(I))W_n(I) \times sign(I)}{\Sigma_I W_n(I) \times sign(I)}$$

"Simple", BUT it does not work

All $W_n(I) \to 0$ as $n \to \infty$

This happens even in Bose systems

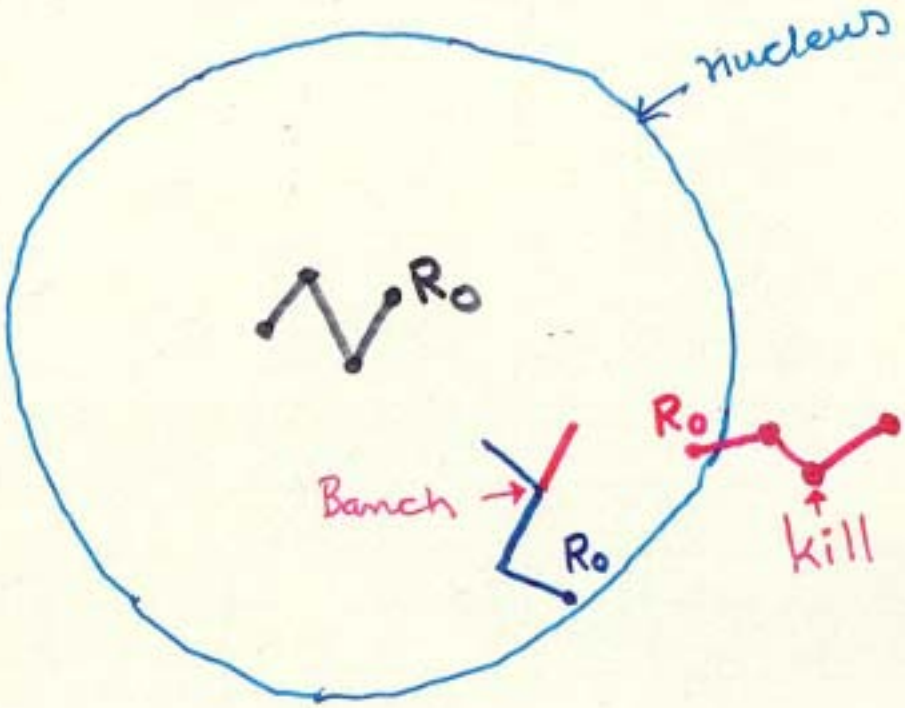
Independent of the Fermion $sign(I) = sign[\Psi_V(\mathbf{R}_n(I))\Psi_V(\mathbf{R}_0(I))]$

What is wrong?

WHY ? The paths leave the nucleus and go in space where

$$\Psi_V(\mathbf{R}_n(I)) \sim 0$$

The $G_0(\mathbf{R}, \mathbf{R}')$ does not know where the nucleus is !!!



At each step

$$I(\mathbf{R}_i)G(\mathbf{R}_i, \mathbf{R}_{i-1})\frac{1}{I(\mathbf{R}_{i-1})} = |\Psi_V(\mathbf{R}_i)|G(\mathbf{R}_i, \mathbf{R}_{i-1})\frac{1}{|\Psi_V(\mathbf{R}_{i-1})|}$$

The Kalos $P(\mathbf{P})$

$$P(\mathbf{P}) = |\Psi_V(\mathbf{R}_n)|G(\mathbf{R}_n, \mathbf{R}_{n-1})...G(\mathbf{R}_1, \mathbf{R}_0)|\Psi_V(\mathbf{R}_0)|$$

Knows where the nucleus is

We want walkers distributed with $P(\mathbf{P})$ NOT with $P'(\mathbf{P})$

BRANCHING AND GROWTH

At each step i we have walkers $\mathbf{R}_i(I)$ distributed with $P'(\mathbf{P})$ and the weighted walkers are distributed with the desired $P(\mathbf{P})$.

Branching is used to produce walkers distributed with $P(\mathbf{P})$ by redefining the ensemble $\{\mathbf{R}_i(I)\}$ of the walkers

In the new ensemble the number of walkers with $\mathbf{R} = \mathbf{R}_i(I)$ is

$$= \textit{Integer part of } W_i(I)$$

$$+ 1 \textit{ with probability } [W_i(I) - \textit{Integer part of } W_i(I)]$$

Example 1. $W_i(I) = 1.3$ Number of walkers $= 1+1$ *with probability* 0.3

Example 2. $W_i(I) = 0.8$ Number of walkers $= 1$ *with probability* 0.8

The new walkers have unit weight, and are distributed with $P(\mathbf{P})$

Walkers do not leave the nucleus and calculation becomes possible

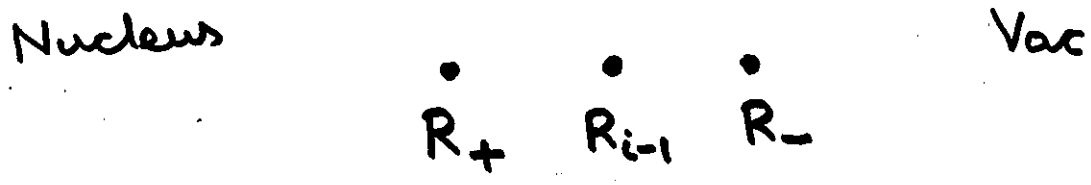
The number of walkers is NOT constant

The $G(\mathbf{R}, \mathbf{R}')$ has a factor $e^{E_T \Delta\tau}$. It controls the magnitude of $G(\mathbf{R}, \mathbf{R}')$, and is also a factor in $w(\mathbf{R}, \mathbf{R}')$.

When $E_T > E_0$ the weights are large and the walker population grows. An $E_T < E_0$ will reduce the population.

The Growth Estimate of E_0 is obtained by tuning E_T such that the population stays stable.

Gradient Correction : One more trick for efficient sampling



The $G_0(\mathbf{R}, \mathbf{R}_{i-1})$ is spherically symmetric gaussian in $3A$ dimensions centered at $\mathbf{R}_{i-1}$. We can go to

$$\mathbf{R}_+ = \mathbf{R}_{i-1} + \Delta\mathbf{R} \quad or \quad \mathbf{R}_- = \mathbf{R}_{i-1} - \Delta\mathbf{R}$$

with equal probability when sampling $G_0(\mathbf{R}, \mathbf{R}_{i-1})$.

Suppose we have a large number, $2\mathcal{M}$ walkers with unit weight at $\mathbf{R}_{i-1}$ and we let them go to $\mathbf{R}_\pm$. We will have $\mathcal{M}$ walkers at $\mathbf{R}_\pm$

Their weights are:

$$W_+ = w(\mathbf{R}_+, \mathbf{R}_{i-1}) \quad and \quad W_- = w(\mathbf{R}_-, \mathbf{R}_{i-1})$$

After branching we will have $\mathcal{M}W_+$ walkers at $\mathbf{R}_+$ and $\mathcal{M}W_-$ at $\mathbf{R}_-$

We can reproduce this result by moving each walker to

$$\mathbf{R}_+ with\ probability = \frac{W_+}{W_+ + W_-}\ , weight = \frac{W_+ + W_-}{2}$$
$$\mathbf{R}_- with\ probability = \frac{W_-}{W_+ + W_-}\ , weight = \frac{W_+ + W_-}{2}$$

This is better because we have walkers with similar weights.

Less load on branching

VI. ISSUES IN GFMC CALCULATIONS OF NUCLEI

The Short Time Propagator

The Green's Function : $G_{\alpha,\beta}(\mathbf{R},\mathbf{R}') = \langle \mathbf{R},\alpha | e^{-(H-E_0)\Delta\tau} | \mathbf{R}',\beta \rangle$

is a $Max \times Max$ Matrix function of $\mathbf{R}$ and $\mathbf{R}'$. $|\alpha\rangle$, $|\beta\rangle$ are spin-isospin states.

we will suppress α, β subscripts for brevity

$$G(\mathbf{R},\mathbf{R}') = e^{E_0\Delta\tau} G_0(\mathbf{R},\mathbf{R}') I_3(\mathbf{R}) \left[\mathcal{S} \prod_{i<j} \frac{g_{ij}(\mathbf{r}_{ij},\mathbf{r}'_{ij})}{g_{0,ij}(\mathbf{r}_{ij},\mathbf{r}'_{ij})} \right] I_3(\mathbf{R}')$$

$$I_3(\mathbf{R}) = \left[1 - \frac{\Delta\tau}{2} \sum_{i<j<k} V_{ijk}(\mathbf{R}) \right]$$

$g_{ij}(\mathbf{r}_{ij},\mathbf{r}'_{ij}) = The \;\; exact \;\; 2-body \;\; Green's \;\; function$

$g_{0,ij}(\mathbf{r}_{ij},\mathbf{r}'_{ij}) = The \;\; noninteracting \;\; 2-body \;\; Green's \;\; function$

$G_0(\mathbf{R},\mathbf{R}') = The \;\; noninteracting \;\; many-body \;\; Green's \;\; function$

The two particle Green's functions $g_{ij}(\mathbf{r}_{ij},\mathbf{r}'_{ij})$ are noncommuting matrix operators. We have to symmetrize their product. As in VMC we write:

$$\mathcal{S} \prod_{i<j} \frac{g_{ij}(\mathbf{r}_{ij},\mathbf{r}'_{ij})}{g_{0,ij}(\mathbf{r}_{ij},\mathbf{r}'_{ij})} = \sum_{\xi} \prod_{i<j}(\xi) \frac{g_{ij}(\mathbf{r}_{ij},\mathbf{r}'_{ij})}{g_{0,ij}(\mathbf{r}_{ij},\mathbf{r}'_{ij})}$$

$\Pi(\xi)$ denotes the product of g_{ij} in the order denoted by ξ

The sum over the order labels ξ is done together with the path integrals by Monte Carlo sampling.

$P(\mathbf{P})$ For Sampling Paths

In Simple Systems $\Psi(\mathbf{R})$ and $G(\mathbf{R}, \mathbf{R}')$ are real scalar functions and we use the *Kalos*

$$P(\mathbf{P}) = \left[\prod_{i=1,n} |\Psi_V(\mathbf{R}_i)| G(\mathbf{R}_i, \mathbf{R}_{i-1}) \frac{1}{|\Psi_V(\mathbf{R}_{i-1})|}\right] \Psi_V^2(\mathbf{R}_0)$$

In nuclei $\Psi(\mathbf{R})$ is a complex vector, $G(\mathbf{R}, \mathbf{R}')$ is a complex matrix

Carlson's $P(\mathbf{P})$

Vector : $\Psi_i(\mathbf{R}_i) = G(\mathbf{R}_i, \mathbf{R}_{i-1}) \Psi_{i-1}(\mathbf{R}_{i-1})$

$$I[\Psi_V(\mathbf{R}_i), \Psi_i(\mathbf{R}_i)] = |\Psi_V^\dagger(\mathbf{R}_i) \Psi_i(\mathbf{R}_i)| + \epsilon \sum_\alpha |\Psi_{\alpha,V}^*(\mathbf{R}_i) \Psi_{\alpha,i}(\mathbf{R}_i)|$$

In the following we set $\epsilon = 0$ for simplicity

$$P(\mathbf{P}) = \left[\prod_{i=1,n} \frac{I[\Psi_V(\mathbf{R}_i), \Psi_i(\mathbf{R}_i)]}{I[\Psi_V(\mathbf{R}_{i-1}), \Psi_{i-1}(\mathbf{R}_{i-1})]}\right] I[\Psi_V(\mathbf{R}_0), \Psi_V(\mathbf{R}_0)]$$

$$= I[\Psi_V(\mathbf{R}_n), \Psi_n(\mathbf{R}_n)]$$

NOTE : In the simple case:

$$\frac{I[\Psi_V(\mathbf{R}_i), \Psi_i(\mathbf{R}_i)]}{I[\Psi_V(\mathbf{R}_{i-1}), \Psi_{i-1}(\mathbf{R}_{i-1})]} = \frac{|\Psi_V(\mathbf{R}_i) G(\mathbf{R}_i, \mathbf{R}_{i-1}) \Psi_{i-1}(\mathbf{R}_{i-1})|}{|\Psi_V(\mathbf{R}_{i-1}) \Psi_{i-1}(\mathbf{R}_{i-1})|}$$

$$= |\Psi_V(\mathbf{R}_i)| G(\mathbf{R}_i, \mathbf{R}_{i-1}) \frac{1}{|\Psi_V(\mathbf{R}_{i-1})|}$$

Carlson's $P(\mathbf{P})$ = Kalos $P(\mathbf{P})$.

Carlson's $P(\mathbf{P}) = |\Psi_V^\dagger(\mathbf{R}_n)[\Pi_{i=1,n}\, G(\mathbf{R}_i, \mathbf{R}_{i-1})]\Psi_V(\mathbf{R}_0)|$

It gives:

$$D_{\mathbf{P}} = \frac{\Psi_V^\dagger(\mathbf{R}_n)[\Pi_{i=1,n}\, G(\mathbf{R}_i, \mathbf{R}_{i-1})]\Psi_V(\mathbf{R}_0)}{I[\Psi_V(\mathbf{R}_n), \Psi_n(\mathbf{R}_n)]}$$

$$= \frac{\Psi_V^\dagger(\mathbf{R}_n)\Psi_n(\mathbf{R}_n)}{|\Psi_V^\dagger(\mathbf{R}_n)\Psi_n(\mathbf{R}_n)|} \quad lim \;\; \epsilon = 0$$

$$= \pm 1$$

Has Fermion Sign Problem

In simple systems we have regions in which $\Psi_V(\mathbf{R})$ is > 0 and < 0. These are seperated by nodal surfaces on which $\Psi_V(\mathbf{R}) = 0$. The requirement that $\Psi_V(\mathbf{R}') = -\Psi_V(\mathbf{R})$ when $\mathbf{R}'$ is obtained from $\mathbf{R}$ by interchanging the positions of two identical (two $\uparrow p$ for example) particles implies the existance of such regions and nodal surfaces.

The $D_{\mathbf{P}} = 1$ when $\Psi_V(\mathbf{R}_n)$ and $\Psi_V(\mathbf{R}_0)$ have the same sign, and -1 when they have opposite signs.

After many steps approximately half of the paths have $D_{\mathbf{P}} = 1$ and the other half have -1. The average value of the $\Sigma_{\{\mathbf{P}\}}\, D_{\mathbf{P}} \to 0$. The statistical sampling error however continues to decrease as $1/\sqrt{N_C}$ and the relative error increases.

$$E_0 = \frac{\overline{\Psi_V^\dagger(\vec{R}_n) H \Psi(\vec{P}_n)}}{\overline{|\Psi_V^\dagger(\vec{R}_n)\Psi(\vec{P}_n)|}} \Big/ \frac{\overline{\Psi_V^\dagger(\vec{R}_n)\Psi(\vec{P}_n)}}{\overline{|\Psi_V^\dagger(\vec{R}_n)\Psi(\vec{P}_n)|}}$$

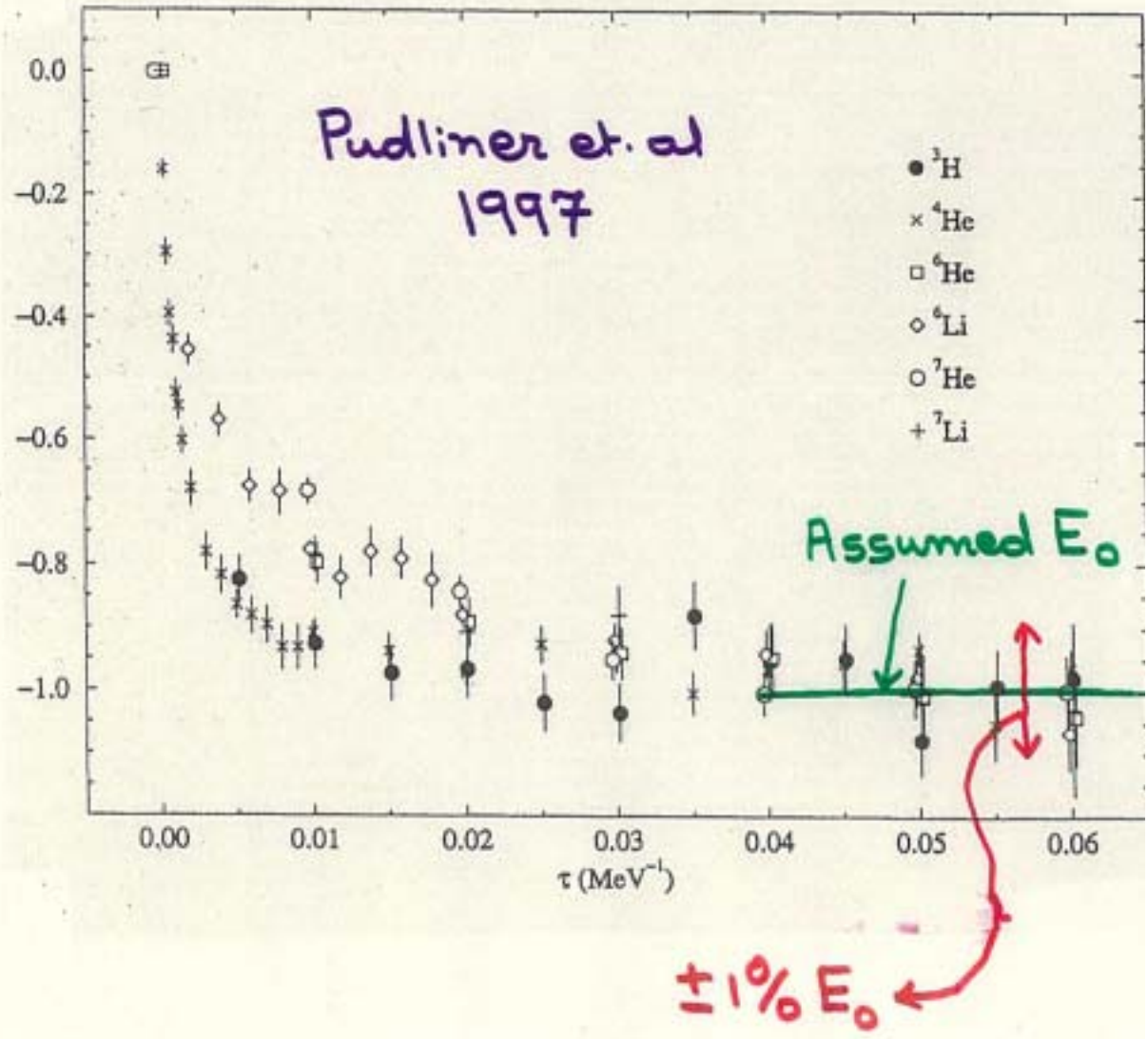
Has Fermion sign problem.

But we can ignore it for $A \leq 7$

if we want only a 1% accuracy

$\tau)-E_V$

$_0-E_V|$



For $A \leq 7$ Fermion Sign is No Problem

The growth of Statistical Error is Tolerable

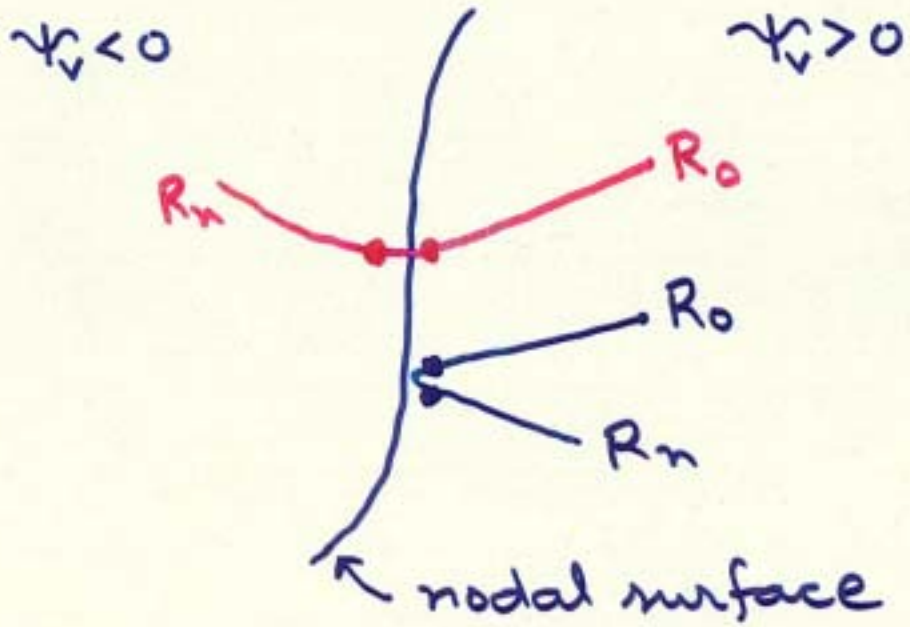
Constrained Path Calculations For $A \geq 8$

Principle : We can discard configurations for which $\Psi_0(\mathbf{R}_i)^\dagger \Psi_i(\mathbf{R}_i) = 0$

$\Psi_0(\mathbf{R})$ is the exact ground state : we do not know it.

We approximate it with $\Psi_V(\mathbf{R})$.

Fixed Node Calculations in Simple Systems



Discard configuration $\mathbf{R}_i$ when $\Psi_V(\mathbf{R}_i) = 0$ or changes sign between two moves

The calculated energy is $> E_0$ in this case. It is the energy of the lowest energy state with nodes of Ψ_V.

In nuclei $\Psi_V(\mathbf{R})$ is a vector and we do not calculate it

We sample the order of $\prod \mathcal{F}_{ij}$

The Chosen Algorithm

Discard configurations with probability function $\xi(Re[\Psi_V^\dagger(\mathbf{R}_n)\Psi_n(\mathbf{R}_n)]/I)$

$\xi(x<0)=1$ and $\xi(x)\to 1$ rapidly as x becomes larger than 0

Constrain : $\sum_{discarded} Re[\Psi_V^\dagger(\mathbf{R}_n)\Psi_n(\mathbf{R}_n)]/I = 0$

One obtains stable statistical errors,

BUT calculated energy can be above/below the E_0

A very useful trick

Release constraint and propagate.

If the constraint provided by Ψ_V is "good"

The $E(\tau)$ remains the same or goes down a bit.

If not improve Ψ_V

$A \geq 8$ Constrained Path Calculations

Problem: Nuclear $\Psi = \sum_{\alpha=1,M} \psi_\alpha(\vec{R}) |\alpha\rangle$

Each ψ_α has different nodal surfaces

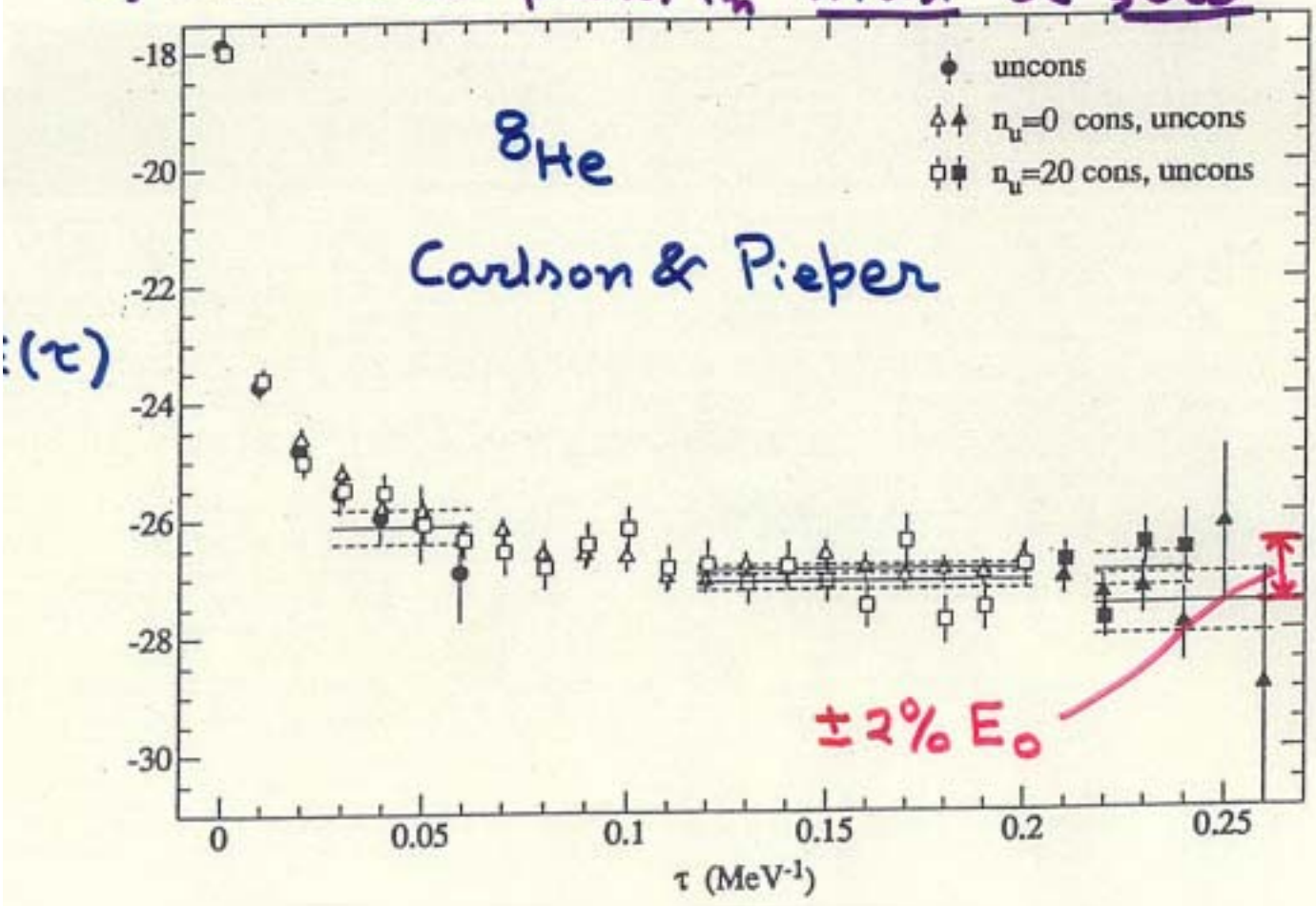
Simple fixed node propogation not possible

Solution: Discard configurations with a probab

dependent on $\Psi^\dagger_{V,A}(\vec{R}_n)\Psi(\vec{P}_n)$

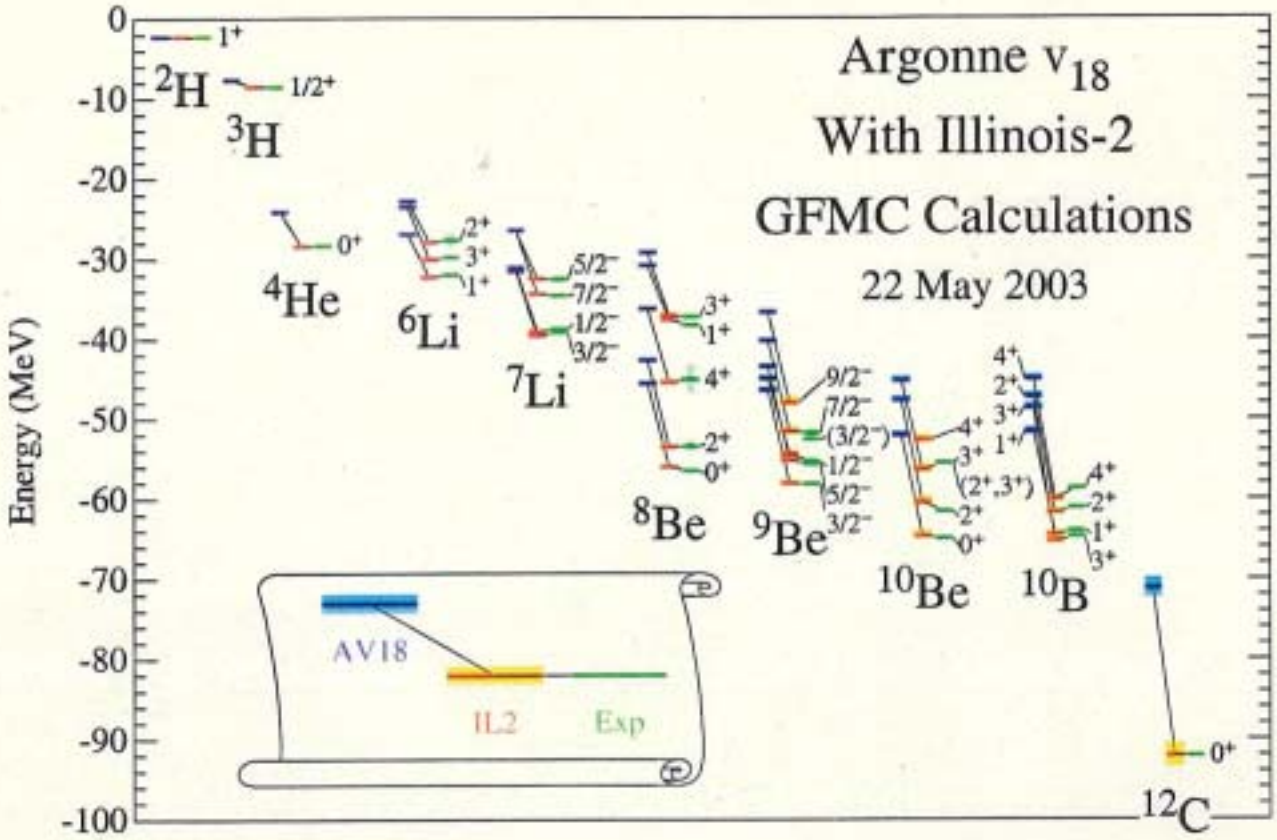
Weighted average: $\dfrac{\mathrm{Re}\ \Psi^\dagger_{V,A}(\vec{R}'_n)\Psi(\vec{P}'_n)}{|\Psi^\dagger_{V,A}(\vec{R}'_n)\Psi(\vec{P}'_n)|}$

of discarded paths $\vec{P}'_n$ must be zero



$\Sigma(\tau)$

Spectra of Light Nuclei



- AV18: Argonne v_{18} with no *NNN* potential
  - significantly underpredicts experimental values
  - error increases with increasing size of nucleus
- IL2: Argonne v_{18} and Illinois-2 *NNN* potential
  - generally very good agreement with experiment
  - note correct ground-state spin for ^{10}B obtained only with *NNN* potential
- Many other nuclei and levels have been computed
- ^{12}C results are preliminary

IV. REALISTIC MODELS OF THREE-NUCLEON INTERACTION

Based on terms with theoretical spin - isospin and spatial dependence and with strengths obtained from experiment

$$\begin{aligned} Illinois\ V_{ijk} &= V_{ijk}^{2\pi,PW} : Fujita - Miyazawa \\ &+ V_{ijk}^{2\pi,SW} : 2 - pion\ \ S - wave \\ &+ V^{3\pi,\Delta R} : 3 - pions\ \ and\ \ 1\ \ or\ \ 2\ \ delta \\ &+ V_{ijk}^{R} \quad : Phenomenological\ \ repulsion \end{aligned}$$

This V_{ijk} has FIVE parameters

strengths of the 4 terms + short range cut off

We fit energies of all the 17 bound / narrow states of $A \leq 8$ nuclei, calculated accurately with the Green's function Monte Carlo method, and the density of nuclear matter, calculated with approximate variational-chain summation calculations.

PROBLEM : We can determine at most three parameters from this data

Need to calculate more observables

Table of parameters in Urbana-Argonne V_{ijk} Models

Parameters with * are not varied. They have "theoretically plausible values"

Short range cutoff = $(1 - e^{-cr^2})$; A's are the strengths

Model	c	$A_{2\pi}^{PW}$	$A_{2\pi}^{SW}$	$A_{3\pi}^{\Delta R}$	A_R	
	fm^{-2}	MeV	MeV	MeV	MeV	
UIX	2.1*	−0.0293	–	–	0.00480	← Not ok
IL1	2.1*	−0.0385	0.0*	0.0026*	0.00705*	ok
IL2	2.1*	−0.037	−1.0*	0.0026	0.00705	← "best"
IL3	1.5	−0.07*	−1.0*	0.0065	0.032	ok
IL4	2.1*	−0.028*	−1.0*	0.0021	0.0039	ok

The strengths are reasonable within a factor of ~ 2

$V_{SW}^{2\pi}$ contribution is typically few % of $V_{PW}^{2\pi}$. Its strength $A_{2\pi}^{SW}$ can not be determined from nuclear binding energies . Compare IL1 and IL2

Nuclear matter calculations (in progress) will eliminate IL2 or IL4

IL3 uses χPT strengths $A_{2\pi}^{PW}$ and $A_{2\pi}^{SW}$

Illinois V_{ijk} models do not explain the A_y in d-n scattering

Kievsky : $V_{ijk}^{LS} = [w(r_{ij}, r_{jk}, r_{ki}) \ , \ \mathbf{L}_{ij} \cdot \mathbf{S}_{ij}]$

can be added to Illinois V_{ijk} to fit both the energies and the n-d scattering.

Problem : Origin of Kievsky V_{ijk}^{LS} is unclear

Pion Exchange Interactions Give Large Contributions

Contributions of two- and three-nucleon pion and reminder ($v_{ij}^R = v_{ij} - v_{ij}^\pi$) potentials in MeV for Av18+IL2 Hamiltonian.

	v^π	v^R	$V^{2\pi}$	$V^{3\pi}$	V^R
^{3}H	−45.0(2)	−13.5(2)	−2.98(2)	0.182(3)	1.34(1)
^{4}He	−105.4(4)	−30.9(5)	−16.3(1)	0.63(1)	7.26(7)
^{6}He	−127.(1)	−44.(2)	−20.3(4)	−0.91(6)	9.6(3)
^{6}Li	−150.(1)	−38.(2)	−19.8(4)	−0.44(5)	9.1(2)
^{7}Li	−178.(2)	−54.(3)	−25.6(6)	−1.1(1)	12.3(4)
^{8}He	−153.(1)	−66.(3)	−25.6(6)	−4.0(2)	13.3(4)
^{8}Li	−211.(1)	−67.(2)	−34.2(5)	−3.8(1)	17.4(3)
^{8}Be	−234.(2)	−69.(3)	−38.5(9)	−0.9(2)	18.3(6)
^{7}n	−10.11(9)	−49.(1)	−0.07(5)	−5.4(3)	1.9(1)
^{8}n	−12.0(1)	−61.(1)	0.31(9)	−5.9(4)	2.6(2)

$V^{3\pi}$ is essential to reproduce the energy of ^{8}He and ^{8}Li

The dominant term of $V^{3\pi}$ is attractive in isospin $T = 3/2$ triplets and zero in isospin $T = 1/2$ triplets (*i. e.* in ^{3}H and ^{4}He)

$V^{2\pi}$ is strong and attractive in isospin $T = 1/2$ triplets

In stable nuclei $V^{2\pi}$ is the largest of all V_{ijk} terms

BUT in neutron drops in external wells and in pure neutron matter the $V^{3\pi}$ dominates over $V^{2\pi}$ and v^R over v^π

Euclidean Response

(Carlson & Schiavilla)

Response to $\mathcal{O}(\vec{k}) = \sum_i \theta_i e^{i\vec{k}\cdot\vec{r}_i}$

$$R(\vec{k},\omega) = \sum_I |\langle I|\mathcal{O}(\vec{k})|0\rangle|^2 \delta(\omega + E_0 - E_I)$$

It is difficult to calculate

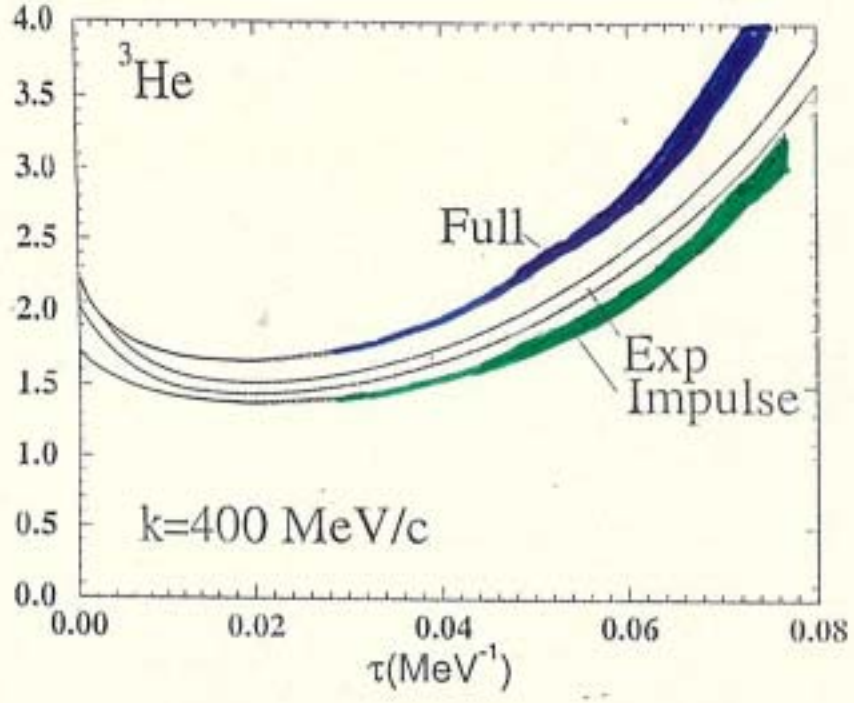
$$E(\vec{k},\tau) = \int d\omega\, e^{-\omega\tau} R(\vec{k},\omega)$$

$$= \langle 0|\mathcal{O}^+(\vec{k}) e^{-(H-E_0)\tau} \mathcal{O}(\vec{k})|0\rangle$$

Calculate with GFMC technique

$$\mathcal{O}_T(\vec{k}) = \sum_i \mathcal{O}_T^{(1)}(i) + \sum_{i<j} \mathcal{O}_T^{(2)}(ij)$$

Scaled $E_T(\vec{k},\tau)$



Scaled $E_T(\vec{k},\tau)$

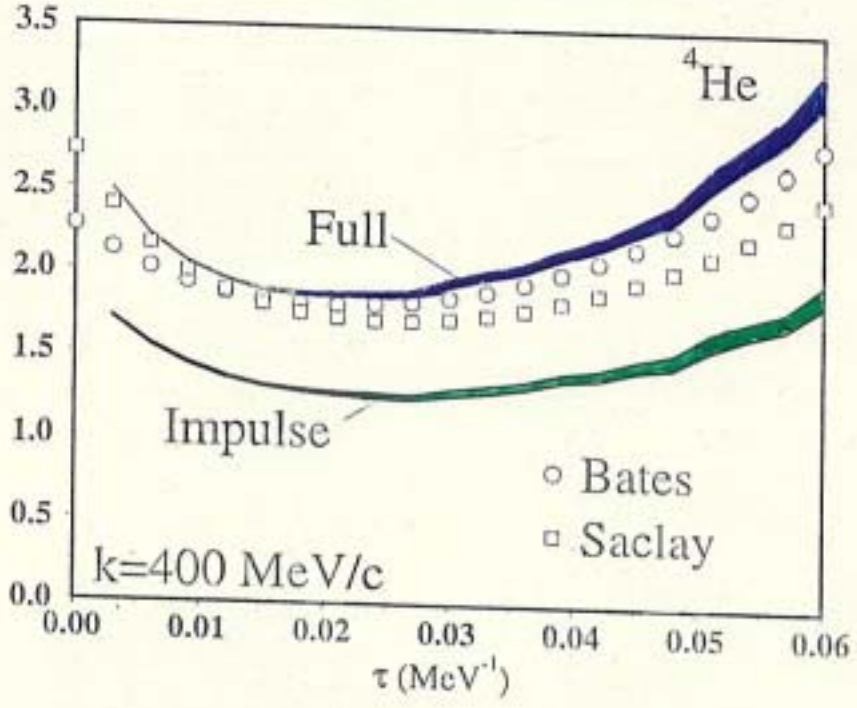


FIG. 72. Transverse Euclidean responses as in Fig. 71, but for ^{4}He. Experimental data are from Bates (Dytman, 1988) and Saclay (Zghiche *et al.* 1993 and erratum 1995). Impulse (one-body current) and full calculations are taken from Carlson and Schiavilla, 1994b.

→ There are pair current effects → π

→ Present model overestimates them.

References for additional reading

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(First applications of GFMC to nuclei with realistic interactions)

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3. R. B. Wiringa *et al.* Phys. Rev. C 62, 014001 (2000)

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4. S. C. Pieper *et al.* Phys. Rev. C 64, 014001 (2001)

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5. S. C. Pieper, K. Varga and R. B. Wiringa, Phys. Rev. C 66, 044310 (2002)

(GFMC for nuclei with $A = 9$ and 10)

6. J. Carlson *et al.*, Phys. Rev. Lett. (in press, 2003)

(GFMC for dilute superfluid gases)

7. J. Carlson and R. Schiavilla, Phys. Rev. Lett. 68, 3682 (1992), Phys. Rev. C 49, R2880 (1994) and Rev. Mod. Phys. 70, 743 (1998)

(Euclidean response. The Rev. Mod. Phys. article has a review of all recent work with VMC, GFMC and other methods)

Many-Body Theory of Nuclei and Nuclear Matter

Vijay Pandharipande

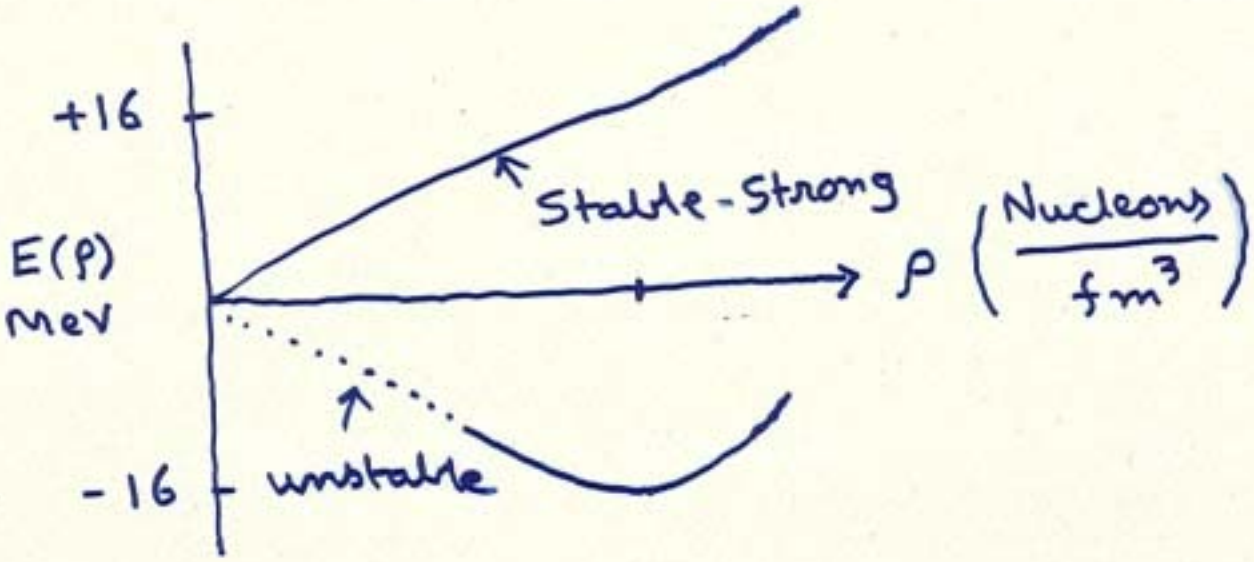
(September 2003)

Lecture IV Variational Theory of Nuclear Matter

SNM : Symmetric nuclear matter with $N = Z = A/2$ without Coulomb

PNM : Pure neutron matter with $N = A$

Ground State Energy Per Nucleon, E(ρ)



Basic Equations

$$Degeneracy \;:\; d = 4\ (SNM) \quad and \quad 2\ (PNM)$$

$$Fermi\ momentum \;:\; k_F = \left(\frac{6\pi^2\rho}{d}\right)^{1/3}$$

$$Pressure \;:\; P(\rho) = \rho^2 \frac{\partial E(\rho)}{\partial \rho}$$

$$(In)compressibility \;:\; K(\rho_o) = 9\rho^2 \frac{\partial^2 E(\rho)}{\partial \rho^2}\Big|_{\rho=\rho_o}$$

Equilibrium ($P = 0$) Values of SNM

$$\rho_0 \sim 0.16\ \ fm^{-3} \qquad E(\rho_0) \sim -16\ \ MeV$$

$$K(\rho_0) \sim 240\ \ MeV$$

Variational Wave Functions for Nuclear Matter

Fermi Gas Product Wave Function : Φ_P

$$\Phi_P(\mathbf{x}_1, \mathbf{x}_2 ... \mathbf{x}_A) = \phi_1(\mathbf{x}_1)\phi_2(\mathbf{x}_2)...\phi_A(\mathbf{x}_A)$$

$$\mathbf{x}_i = \mathbf{r}_i, \sigma_i, \tau_i \quad of\ nucleon\ i$$

$$\phi_i(\mathbf{x}) = e^{i\mathbf{k}_i \cdot \mathbf{r}} \chi_i^\sigma \chi_i^\tau \quad with \quad |\mathbf{k}_i| < k_F$$

The $\phi_i(\mathbf{x})$ are occupied single particle states. The number of ϕ_i equals the number of nucleons A.

In the product wave function Φ_P nucleon i occupies state ϕ_i

Sums over particles $i = 1, A$ and states $i = 1, A$ are equivalent

Antisymmetric Fermi Gas Wave Function : $\Phi_A = \Phi$

$$\Phi(\mathbf{X}) = \Phi_A(\mathbf{X}) = \mathcal{A}\Phi_P(\mathbf{X})$$

$$\mathbf{X} = \mathbf{x}_1, \mathbf{x}_2, ...\mathbf{x}_A$$

For any symmetric operator $\mathcal{O}$ such as H

$$\frac{\langle \Phi_A | \mathcal{O} | \Phi_A \rangle}{\langle \Phi_A | \Phi_A \rangle} = \frac{\langle \Phi_A | \mathcal{O} | \Phi_P \rangle}{\langle \Phi_A | \Phi_P \rangle}$$

We need to antisymmetrize only one side of the expectation value

$$\text{Correlated} \quad \Psi_V = \mathcal{S} \prod_{i<j} \mathcal{F}_{ij} \Phi_A(\mathbf{X})$$

The Energy Expectation Value

To begin with omit $V(ijk)$ and use the simpler

$$H = \sum_{i=1,A} \frac{1}{2m}\nabla_i^2 + \sum_{i<j\leq A} v(ij) = T_i + v_{ij}$$

The variational energy is given by:

$$\begin{aligned} AE_V &= \frac{\langle \Phi_A | \mathcal{S}\prod\mathcal{F}(T_i + v_{ij})\mathcal{S}\prod\mathcal{F}|\Phi_P\rangle}{\langle \Phi_A | \mathcal{S}\prod\mathcal{F}\ \ \mathcal{S}\prod\mathcal{F}|\Phi_P\rangle} \\ &= \frac{\int d\mathbf{R}\Phi_A^\dagger(\mathbf{X})\mathcal{S}\prod\mathcal{F}(T_i + v_{ij})\mathcal{S}\prod\mathcal{F}\Phi_P(\mathbf{X})}{\int d\mathbf{R}\Phi_A^\dagger(\mathbf{X})\mathcal{S}\prod\mathcal{F}\ \ \mathcal{S}\prod\mathcal{F}\Phi_P(\mathbf{X})} \end{aligned}$$

Now both Φ_P and Φ_A are eigenstates of T_i with eigenvalue:

$$E_{FG} = \frac{3}{10m}k_F^2 \ \ per\ nucleon$$

It is then convenient to write:

$$E_V = E_{FG} + \frac{1}{A}\frac{\int d\mathbf{R}\Phi_A^\dagger(\mathbf{X})\mathcal{S}\prod\mathcal{F}(T_i' + v_{ij})\mathcal{S}\prod\mathcal{F}\Phi_P(\mathbf{X})}{\int d\mathbf{R}\Phi_A^\dagger(\mathbf{X})\mathcal{S}\prod\mathcal{F}\ \ \mathcal{S}\prod\mathcal{F}\Phi_P(\mathbf{X})}$$

Where T_i' does not act on Φ_P. E_V is energy per particle.

The Cluster Expansion

The pair correlation operator $\mathcal{F}_{ij}$ has a finite range beyond which it is 1.

Most of the pairs in uniform nuclear matter are outside the range of correlations and have $\mathcal{F}_{ij} = 1$.

Cluster Expansions are obtained by replacing $\mathcal{F}_{ij} = 1 + (\mathcal{F}_{ij} - 1)$ in the expectation values.

Expand in powers of $(\mathcal{F}_{ij}-1)$

$$E_V = E_{FG} + \frac{1}{A}\frac{\int d\mathbf{R}\Phi_A^\dagger(\mathbf{X})\mathcal{S}\prod[1+(\mathcal{F}_{ij}-1)](T_i'+v_{ij})\mathcal{S}\prod[1+(\mathcal{F}_{ij}-1)]\Phi_P(\mathbf{X})}{\int d\mathbf{R}\Phi_A^\dagger(\mathbf{X})\mathcal{S}\prod[1+(\mathcal{F}_{ij}-1)]\ \ \mathcal{S}\prod[1+(\mathcal{F}_{ij}-1)]\Phi_P(\mathbf{X})}$$

Rules of the expansion

1. Do not approximate the $\mathcal{F}_{mn}$ by 1 in the expectation value of v_{mn}. The range of v_{mn} is often shorter than that of $\mathcal{F}_{mn}$.

2. For the same reason do not replace $\mathcal{F}_{mn}$ in $\Psi_V^\dagger$ by 1 in the terms containing $\nabla_m^2\mathcal{F}_{mn}$ and $\nabla_m\mathcal{F}_{mn}\cdot\nabla_m$ in the expectation value of T_m'

3. For the same reason do not approximate $\mathcal{F}_{ij}$ by 1 only on one side of H, (Ψ_V or $\Psi_V^\dagger$). Either in both or none.

4. The antisymmetric Φ_A has $A!$ terms. Of these the one in which nucleons $1,2,...A$ are in single particle states $\phi_1,\phi_2,...\phi_A$, as in Φ_P, gives the **direct** contributions. The rest give **exchange** contributions.

5. Terms in which uncorrelated nucleons are exchanged give zero contribution since the single particle states ϕ_i are orthogonal.

6. Normalization of the ϕ_i, (Ω is the normalization volume)

$$\phi_i(\mathbf{x}) = \frac{1}{\sqrt{\Omega}}e^{i\mathbf{r}\cdot\mathbf{k}_i}\chi_i^\sigma\chi_i^\tau$$

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}$$

$$A = \rho\Omega$$

7. The sum over nucleons or single particle states is given by

$$\sum_{i=1,A} = \sum_{\mathbf{k}_i<k_F}\ \sum_{\chi_i^\sigma=\uparrow,\downarrow}\ \sum_{\chi_i^\tau=p,n}$$

Division of Cluster Contributions

$$The \;\; v_{ij} = \sum_{p=1,14} v^p(\mathbf{r}_{ij}) O^p_{ij} \quad \mathcal{F}_{ij} = \sum_{p=1,8} f^p(\mathbf{r}_{ij}) O^p_{ij}$$

1. **Static contributions** contain only the static parts ($O^{p=1,6}_{ij}$) of v_{ij} and $\mathcal{F}_{ij}$. These are large and calculated most accurately.

2. **Spin-Orbit contributions** contain one or more spin-orbit operators from either v_{ij} or $\mathcal{F}_{ij}$. Most difficult to calculate due to gradient operators in spin-orbit correlations.

3. **Quadratic contributions** contain quadratic $v^{p>8}_{ij}$ and static $f^{p<7}_{ij}$.

Note: contributions from quadratic v and spin-orbit f are included in the spin-orbit contributions.

Note: No quadratic correlations
$v^q = (v_{14} - v_8)$ is "small perturbation"

$[v^s - 2b - dir]$: Two-body direct cluster contribution to the static potential energy

The denominator is approximated by 1, and in the numerator we keep only the $\mathcal{F}^s_{ij}$; all other $\mathcal{F}$ are approximated by 1. This gives:

$$[v^s - 2b - dir] = \frac{1}{A}\frac{1}{\Omega^2} \sum_{i<j} \int d\mathbf{r}_i d\mathbf{r}_j e^{-i(\mathbf{k}_i\cdot\mathbf{r}_i + \mathbf{k}_j\cdot\mathbf{r}_j)} \chi^{\sigma\dagger}_i \chi^{\tau\dagger}_i \chi^{\sigma\dagger}_j \chi^{\tau\dagger}_j$$
$$\times \left(\sum_{p,q,r=1,6} f^p(r_{ij}) v^q(r_{ij}) f^r(r_{ij}) O^p_{ij} O^q_{ij} O^r_{ij} \right) e^{i(\mathbf{k}_i\cdot\mathbf{r}_i + \mathbf{k}_j\cdot\mathbf{r}_j)} \chi^{\sigma}_i \chi^{\tau}_i \chi^{\sigma}_j \chi^{\tau}_j$$

$$= \frac{A}{32}\frac{1}{\Omega} \sum_{\chi^\sigma_i, \chi^\tau_i, \chi^\sigma_j, \chi^\tau_j} \int d\mathbf{r}_{ij} \;\; \chi^{\sigma\dagger}_i \chi^{\tau\dagger}_i \chi^{\sigma\dagger}_j \chi^{\tau\dagger}_j$$
$$\times \left(\sum_{p,q,r=1,6} f^p(r_{ij}) v^q(r_{ij}) f^r(r_{ij}) O^p_{ij} O^q_{ij} O^r_{ij} \right) \chi^{\sigma}_i \chi^{\tau}_i \chi^{\sigma}_j \chi^{\tau}_j$$

Operator Algebra

The static operators $O_{ij}^{p=1,6}$ have a closed algebra for multiplication:

$$O_{ij}^{p} O_{ij}^{q} = \sum_{r=1,6} K^{pqr} O_{ij}^{r}$$

where K^{pqr} are real numbers. For example:

$$S_{ij}\sigma_i \cdot \sigma_j = S_{ij}$$

$$\sigma_i \cdot \sigma_j \; \sigma_i \cdot \sigma_j = 3 - 2\sigma_i \cdot \sigma_j$$

$$S_{ij}S_{ij} = 6 + 2\sigma_i \cdot \sigma_j - 2S_{ij}$$

Using this algebra we can express any product of $O_{ij}^{p\leq 6}$ operators as a sum of these operators:

$$O_{ij}^{p} O_{ij}^{q} \ldots = \sum_{r} \gamma_r O_{ij}^{r}$$

The γ_1 associated with the unit operator has special significance. It is called the C-part of the product of operators. For example:

$$C[S_{ij}\sigma_i \cdot \sigma_j] = 0$$

$$C[\sigma_i \cdot \sigma_j \; \sigma_i \cdot \sigma_j] = 3$$

$$C[S_{ij}S_{ij}] = 6$$

The sum

$$\sum_{\chi_i^\sigma, \chi_i^\tau, \chi_j^\sigma, \chi_j^\tau} \chi_i^{\sigma\dagger} \; \chi_i^{\tau\dagger} \; \chi_j^{\sigma\dagger} \; \chi_j^{\tau\dagger} \;\; O_{ij}^{p} \;\; \chi_i^{\sigma} \; \chi_i^{\tau} \; \chi_j^{\sigma} \; \chi_j^{\tau} = 16 \;\; \delta_{p1}$$

Note that there are 16 two-nucleon spin-isospin states $\chi_i^\sigma, \chi_i^\tau, \chi_j^\sigma, \chi_j^\tau$, and we can consider the above sum as the trace of the 16×16 matrix representing the operator O_{ij}^{p} in the basis of these 16 states.

Only the $C[O_{ij}^p O_{ij}^q O_{ij}^r]$ contributes to the $[v^s - 2b - dir]$. We obtain:

$$[v^s - 2b - dir] = \frac{\rho}{2} \sum_{p,q,r=1,6} C[O_{ij}^p O_{ij}^q O_{ij}^r] \int d\mathbf{r}_{ij} \;\; f^p(r_{ij}) v^q(r_{ij}) f^r(r_{ij})$$

$[v^s - 2b - ex]$: Two-body exchange cluster contribution to the static potential energy

$$[v^s - 2b - ex] = -\frac{1}{A}\frac{1}{\Omega^2} \sum_{i<j} \int d\mathbf{r}_i d\mathbf{r}_j e^{-i(\mathbf{k}_i \cdot \mathbf{r}_j + \mathbf{k}_j \cdot \mathbf{r}_i)} \chi_i^{\sigma\dagger}(j) \chi_i^{\tau\dagger}(j) \chi_j^{\sigma\dagger}(i) \chi_j^{\tau\dagger}(i)$$
$$\times \left(\sum_{p,q,r=1,6} f^p(r_{ij}) v^q(r_{ij}) f^r(r_{ij}) O_{ij}^p O_{ij}^q O_{ij}^r \right) e^{i(\mathbf{k}_i \cdot \mathbf{r}_i + \mathbf{k}_j \cdot \mathbf{r}_j)} \chi_i^\sigma \chi_i^\tau \chi_j^\sigma \chi_j^\tau$$

Here $\chi_i^\sigma(j)$ means that nucleon j is in the spin state χ_i^σ.

The spin-isospin exchange operator e_{ij}

It is more convenient to have $\chi_i^{\sigma\dagger}\chi_i^{\tau\dagger}\chi_j^{\sigma\dagger}\chi_j^{\tau\dagger} = \chi_i^{\sigma\dagger}(i)\chi_i^{\tau\dagger}(i)\chi_j^{\sigma\dagger}(j)\chi_j^{\tau\dagger}(j)$ than $\chi_i^{\sigma\dagger}(j)\chi_i^{\tau\dagger}(j)\chi_j^{\sigma\dagger}(i)\chi_j^{\tau\dagger}(i)$ in 2-body cluster contrbutions. We can then take the trace of the product of operators, which is just 16 $\times$ their C-part. The operators for spin and isospin exchange are respectively:

$$P_{ij}^\sigma = \frac{1}{2}(1 + \sigma_i \cdot \sigma_j) \quad and \quad P_{ij}^\tau = \frac{1}{2}(1 + \tau_i \cdot \tau_j)$$

The spin-isospin exchange operator:

$$e_{ij} = P_{ij}^\sigma P_{ij}^\tau = \frac{1}{4}(1 + \sigma_i \cdot \sigma_j)(1 + \tau_i \cdot \tau_j)$$

We can varify that:

$$\chi_i^{\sigma\dagger}(j)\chi_i^{\tau\dagger}(j)\chi_j^{\sigma\dagger}(i)\chi_j^{\tau\dagger}(i) = \chi_i^{\sigma\dagger}\chi_i^{\tau\dagger}\chi_j^{\sigma\dagger}\chi_j^{\tau\dagger}\; e_{ij}$$

The Slater Function $\ell(k_F r)$

The exchange contributions contain:

$$\sum_{\mathbf{k}_i<k_F} e^{i\mathbf{k}_i\cdot(\mathbf{r}_i-\mathbf{r}_j)} = \frac{A}{d}\ell(k_F r)$$

$$\ell(x) = 3[sin(x) - x\ cos(x)]/x^3 \qquad x = k_F r$$

The Slater function is normalized such that $\ell(x=0)=1$

Using the exchange operator and the Slater function, we obtain

$$[v^s - 2b - ex] = -\frac{\rho}{2}\sum_{p,q,r=1,6} C[e_{ij}O^p_{ij}O^q_{ij}O^r_{ij}]\int d\mathbf{r}\ell^2(k_F r)f^p(r_{ij})v^q(r_{ij})f^r(r_{ij})$$

$$= -\frac{\rho}{2}\int d\mathbf{r}\ell^2(k_F r)C[e_{ij}\mathcal{F}^s_{ij}v^s_{ij}\mathcal{F}^s_{ij}]$$

Two-body Kinetic Energy Contribution

These are divided in to two parts. The first denoted by T^s_1 contains $(\nabla^2_i + \nabla^2_j)\mathcal{F}^s_{ij}$, and the second denoted by T^s_2 has terms with $(\nabla_i\mathcal{F}_{ij})\cdot(\nabla_i\Phi)$. The $\nabla^2_i\Phi$ terms give the Fermi-gas kinetic energy E_{FG}, and are not included in the cluster expansion. We obtain:

$$[T^s_1 - 2b - dir] = \frac{\rho}{2m}\int d\mathbf{r}C[\mathcal{F}^s_{ij}(-\nabla^2_{ij}\mathcal{F}^s_{ij})]$$

$$[T^s_1 - 2b - ex] = -\frac{\rho}{2m}\int d\mathbf{r}\ell^2(k_F r)C[e_{ij}\mathcal{F}^s_{ij}(-\nabla^2_{ij}\mathcal{F}^s_{ij})]$$

In most cases it is convenient to combine the T^s_1 and v^s because the Schrödinger like equations for $\mathcal{F}$ imply a cancellation between them.

The $[T_2^s - 2b - ex]$

$$[T_2^s - 2b - ex] = \frac{16}{A}\frac{1}{\Omega^2}\frac{1}{m}\sum_{\mathbf{k}_i,\mathbf{k}_j<k_F}\int d\mathbf{r}_i d\mathbf{r}_j e^{-i(\mathbf{k}_i\cdot\mathbf{r}_j+\mathbf{k}_j\cdot\mathbf{r}_i)} \times C[e_{ij}\mathcal{F}_{ij}\nabla_i\mathcal{F}_{ij}]\cdot(i\mathbf{k}_i)e^{i(\mathbf{k}_i\cdot\mathbf{r}_i+\mathbf{k}_j\cdot\mathbf{r}_j)}$$

$$= \frac{\rho}{m}\int d\mathbf{r}_{ij}\ell(r_{ij})\ell'(r_{ij}) \times C[e_{ij}\mathcal{F}_{ij}\nabla_i\mathcal{F}_{ij}]\cdot\hat{\mathbf{r}}_{ij}$$

Here $\ell'(r) = \partial\ell(r)/\partial r$ and $\hat{\mathbf{r}}$ is a unit vector. Note :

$$\sum_{\mathbf{k}_i<k_F} e^{-i\mathbf{k}_i\cdot\mathbf{r}_j}(i\mathbf{k}_i)e^{i\mathbf{k}_i\cdot\mathbf{r}_i} = \frac{A}{d}\ell'(r_{ij})\hat{\mathbf{r}}_{ij}$$

The $[T_2^s - 2b - dir] = 0$

The total 2-body static contribution is given by:

$$[2b-s] = [v^s - 2b - dir] + [v^s - 2b - ex] + [T_1^s - 2b - dir] + [T_1^s - 2b - ex] + [T_2^s - 2b - ex]$$

In a similar way we calculate the $[2b-q]$ contribution containing interactions dependent on $\mathbf{p}^2$ or $\mathbf{L}^2$ and static correlations. The $[2b-q]$ does not have any kinetic energy terms.

The last 2-body contribution is $[2b-ls]$. It containes potential and kinetic energy terms with either v_{ij}^{ls} or f_{ij}^{ls} or both.

All the 2-body contributions have been calculated exactly. The $[2b-total]$ containing all the 2-body contributions is the largest term (by magnitude) in the cluster expension of the energy of SNM.

The Three-body Cluster Contribution: $[v^s - 3b - dir]$

We consider $[v^s - 3b - dir]$ as an example of three-body cluster contributions.

The 3-body correlation operator is denoted by:

$$\mathcal{M}_{ijk} = \mathcal{S}[\mathcal{F}_{ij}\mathcal{F}_{jk}\mathcal{F}_{ki}]$$

$$= \mathcal{F}_{ijk}\,\mathcal{S}[\mathcal{F}_{ij}\mathcal{F}_{jk}\mathcal{F}_{ki}]$$ Most general

By expanding the numerator of the $\langle H \rangle$ we get the 3-body term:

$$[v^s - 3b - \mathcal{N}] = \mathcal{M}_{ijk} v^s_{ij} \mathcal{M}_{ijk} - \mathcal{F}_{ij} v^s_{ij} \mathcal{F}_{ij}$$

The above result is obtained by replacing:

$$\mathcal{F}_{jk}\mathcal{F}_{ki} \to [1 + (\mathcal{F}_{jk} - 1)][1 + (\mathcal{F}_{ki} - 1)]$$

in both $\Psi^\dagger$ and Ψ, and expanding $\Psi^\dagger v^s_{ij} \Psi$ in powers of $(\mathcal{F} - 1)$. The 0 th order term: $\mathcal{F}_{ij} v^s_{ij} \mathcal{F}_{ij}$ gives the $[v^s - 2b]$, and all the three body terms are contained in $[v^s - 3b - \mathcal{N}]$

In addition we have 3-body terms from the expansion of the denominator:

$$\mathcal{D} = \int d\mathbf{R} \Phi^\dagger_A(\mathbf{X}) \mathcal{S} \prod [1 + (\mathcal{F}_{ij} - 1)] \;\; \mathcal{S} \prod [1 + (\mathcal{F}_{ij} - 1)] \Phi_P(\mathbf{X})$$

$$= \int d\mathbf{R} \Phi^\dagger_A(\mathbf{X}) \left(1 + \sum_{i<j} (\mathcal{F}^2_{ij} - 1) + \ldots \right) \Phi_P(\mathbf{X})$$

They contain

$$[v^s - 3b - \mathcal{D}] = \mathcal{F}_{ij} v^s_{ij} \mathcal{F}_{ij} (\mathcal{F}^2_{jk} - \mathcal{F}^2_{ki} - 2)$$

where $\mathcal{F}_{ij} v^s_{ij} \mathcal{F}_{ij}$ comes from the numerator.

The: $[v^s - 3b - dir]$

Including $[v^s - 3b - \mathcal{N}]$ and $[v^s - 3b - \mathcal{D}]$ we obtain:

$$[\ v^s - 3b - dir] = \frac{1}{A} \sum_{k,(i<j)} \int d\mathbf{r}_i d\mathbf{r}_j d\mathbf{r}_k$$
$$\times\ \chi_i^{\sigma\dagger}\chi_i^{\tau\dagger}\chi_j^{\sigma\dagger}\chi_j^{\tau\dagger}\chi_k^{\sigma\dagger}\chi_k^{\tau\dagger}\left(\mathcal{M}v_{ij}^s\mathcal{M} - \mathcal{F}_{ij}v_{ij}^s\mathcal{F}_{ij}(\mathcal{F}_{jk}^2 + \mathcal{F}_{ki}^2 - 1)\right)\chi_i^\sigma\chi_i^\tau\chi_j^\sigma\chi_j^\tau\chi_k^\sigma\chi_k^\tau$$
$$= \frac{\rho^2}{2}\frac{1}{d^3}\int d\mathbf{r}_{ij}d\mathbf{r}_{ik}\ Tr\ \left(\mathcal{M}v_{ij}^s\mathcal{M} - \mathcal{F}_{ij}v_{ij}^s\mathcal{F}_{ij}(\mathcal{F}_{jk}^2 + \mathcal{F}_{ki}^2 - 1)\right)$$

In the exact calculation of $[v^s - 3b - dir]$ in SNM (PNM) there are $d^3 = 64$ (8) 3-body spin-isospin states. We consider the v_{ij}^s and the $\mathcal{F}$ as $d^3 \times d^3$ matrix functions of $\mathbf{R}$ and calculate the trace as in quantum Monte Carlo method.

The other 3-body contributions can be calculated in a similar way. For example:

$$[v^s - 3b - e_{ij}] = \frac{\rho^2}{2}\frac{1}{d^3}\int d\mathbf{r}_{ij}d\mathbf{r}_{ik}\ \ell_{ij}^2$$
$$\times\ Tr\ \left(e_{ij}\mathcal{M}v_{ij}^s\mathcal{M} - e_{ij}\mathcal{F}_{ij}v_{ij}^s\mathcal{F}_{ij}(\mathcal{F}_{jk}^2 + \mathcal{F}_{ki}^2 - 1)\right)$$

The static, potential and kinetic and quadratic potential contributions have been calculated in this way by Morales, Pandharipande and Ravenhall (Phys. Rev. C 66, 054308 (2002)). The $\geq$3-body spin-orbit contributions are more difficult to calculate. They contain new terms in which the gradients in $(\mathbf{L}\cdot\mathbf{S})_{jk}$ operate on $\mathcal{F}_{ij}$ and $\mathcal{F}_{ik}$. Only selected terms are sumed to estimate the $[3b - ls]$ contribution.

FHNC-SOC Chain Summation Method

Fermi Hypernetted Chain and Single Operator Chain

Sum all FHNC diagrams with central links: only irreducible exist

Sum all diagrams with rings of single operator links: irreducible and those that can be seperated in to two or more rings.

Single operator chains with open ends give zero contribution

Sum multiple operator diagrams to the extent that they can be treated as single operator rings.

The FHNC-SOC sum gives

1. Two-body contribution exactly
2. Exact 3-body for central links
3. **Approximate** 3-body with operator links
4. **Approximate** contributions of all $\geq$ 4-body clusters.
5. The approximations can be good in many cases.
6. It is always better to use FHNC-SOC than to neglect many-body cluster contributions.

Argonne v_{18} + Urbana IX V_{ijk}

TABLE II. Cluster contributions calculated with CSM: SNM at $\rho=\rho_0$, $\alpha=0.80$, $d_c=1.80$ fm, and $d_t=4.80$ fm, $T_F=22.1$ MeV, and $E_v^{CSM}=-8.9$ MeV.

n	2	3	4	5	>5	Total
v_{ij}^s	−66.7	11.1	−6.9	3.4	−1.1	−60.2
T_s	20.3	−2.0	2.4	−1.1	0.4	20.0
v_{ij}^q	4.5	3.5	0.2	0.0	0.0	8.1
V_{ijk}		1.9	1.0	0.3	−0.1	3.1
$v_{ij}^b+T_b$	−1.8	−0.1	−0.1	0	0	−2.0
$E_v^{CSM}-T_F$	−43.7	14.4	−3.4	2.6	−0.8	−31.0

$\rho=\rho_0$

"interaction energy"

−43.7

Exact: 10.8

TABLE III. Cluster contributions calculated with CSM: SNM at $\rho=1.5\rho_0$, $\alpha=0.89$, $d_c=1.50$ fm, and $d_t=3.99$ fm; $T_F=29.0$ and $E_v^{CSM}=-3.3$ MeV.

n	2	3	4	5	>5	Total
v_{ij}^s	−92.1	10.9	−6.2	2.8	−0.9	−85.5
T_s	28.7	−0.5	2.5	−0.8	0.2	30.1
v_{ij}^q	9.9	8.0	0.6	−0.1	−0.1	18.4
V_{ijk}		4.7	2.7	0.8	−0.3	7.9
$v_{ij}^b+T_b$	−2.7	−0.3	−0.1	0	0	−3.1
$E_v^{CSM}-T_F$	−56.2	22.8	−0.5	2.7	−1.1	−32.3

$\rho=\frac{3}{2}\rho_0$

−56.2

Exact: 18.7

TABLE I. Cluster contributions calculated with CSM: SNM at $\rho=0.5\rho_0$, $\alpha=0.60$, $d_c=2.23$ fm and $d_t=8.93$ fm; $T_F=13.9$ MeV and $E_v^{CSM}=-7.1$ MeV.

n	2	3	4	5	>5	Total
v_{ij}^s	−36.5	7.4	−4.9	2.6	−0.9	−32.3
T_s	10.0	−1.6	1.4	−0.7	0.1	9.2
v_{ij}^q	1.2	0.8	0.0	0.0	0.0	1.9
V_{ijk}		0.6	0.1	0.1	0.0	0.7
$v_{ij}^b+T_b$	−0.6	0	0	0	0	−0.6
$E_v^{CSM}-T_F$	−25.9	7.2	−3.4	2.0	−0.8	−21.0

$\rho=\frac{\rho_0}{2}$

−25.9

5.0

TABLE X. The 3-body cluster contribution from F^s correlations calculated exactly and with CSM for SNM in MeV.

	$0.5\rho_0$		ρ_0		$1.5\rho_0$	
	Exact	CSM	Exact	CSM	Exact	CSM
T_s	−1.8	−1.6	−2.5	−2.0	−1.1	−0.5
v^s_{ij}	5.7	7.4	9.3	11.1	10.4	10.9
v^q_{ij}	0.9	0.8	3.2	3.5	6.3	8.0
V^R_{ijk}	1.7	1.6	6.3	6.0	13.7	13.3
$V^{2\pi}_{ijk}$	−1.6	−1.0	−5.4	−4.1	−10.2	−8.6
Total 3b	5.0	7.2	10.9	14.5	19.0	23.1

Morales, Pandharipande, Ravenhall

Phys. Rev. C 66, 054308 (2002)

Test of AV_{18} + U-IX + δv ; FHNC-SOC-5

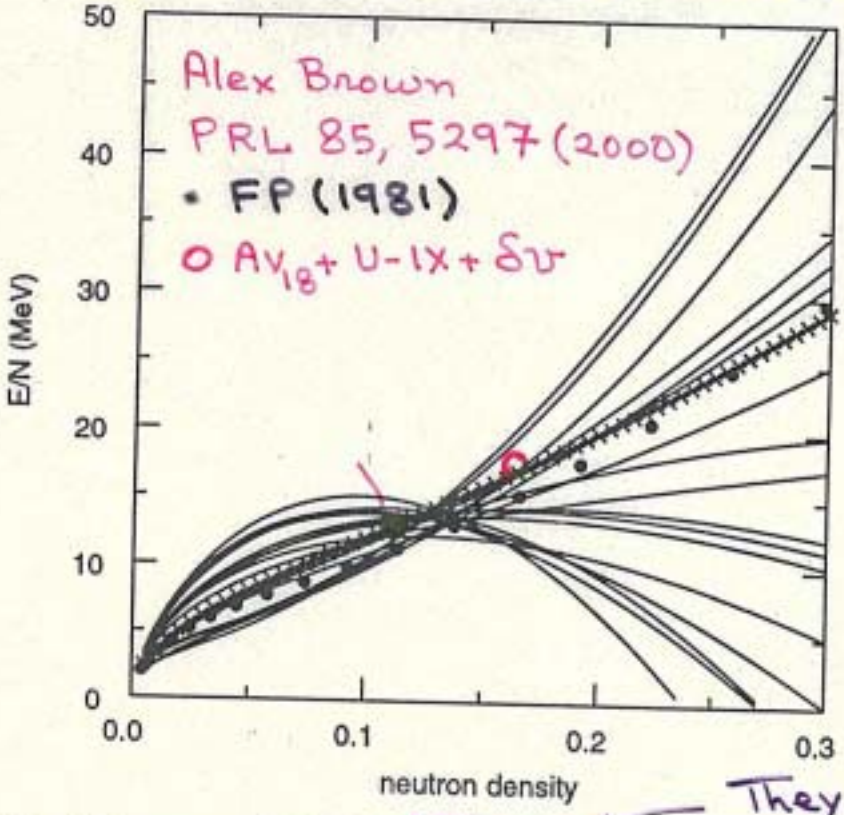
Symmetric nuclear matter $\rho \sim \rho_0$

2002 Urbana Calculations (Variational) of Symmetric Nuclear Matter with Argonne v_{ij} and Urbana V_{ijk}, $E(\rho)$ in MeV/A.

Density [$\mathbf{fm}^{-3}$]	0.08	0.16	0.24	
1-b T_{FG}	13.9	22.1	29.1	Exact
2-b all	−25.9	−43.7	−56.2	"
3-b static	4.9	10.9	19.1	"
3-b $(\mathbf{L}\cdot\mathbf{S})$ + ≥ 4-b all	−2.2	−1.7	+0.8	Approx.
$(E_0 - E_V)$ Pert.	−0.6	−1.8	−3.3	"
Calculated $E_0(\rho)$	−9.9	−14.2	−10.6	Total
Empirical $E_0(\rho)$	−12.1	−16.0	−12.9	"

We have a 15% underbinding

$E(\rho \sim \rho_0)$ of Pure neutron matter



They all fit a set of nuclear data including $E(^{132}Sn) - E(^{100}Sn)$

FIG. 2. The neutron EOS for 18 Skyrme parameter sets. The filled circles are the Friedman-Pandharipande (FP) variational calculations and the crosses are SkX. The neutron density is in units of neutron/fm^3.

Quantum Monte Carlo Calculations of Uniform Matter

Use "Periodic Box" : Box with periodic boundary conditions.

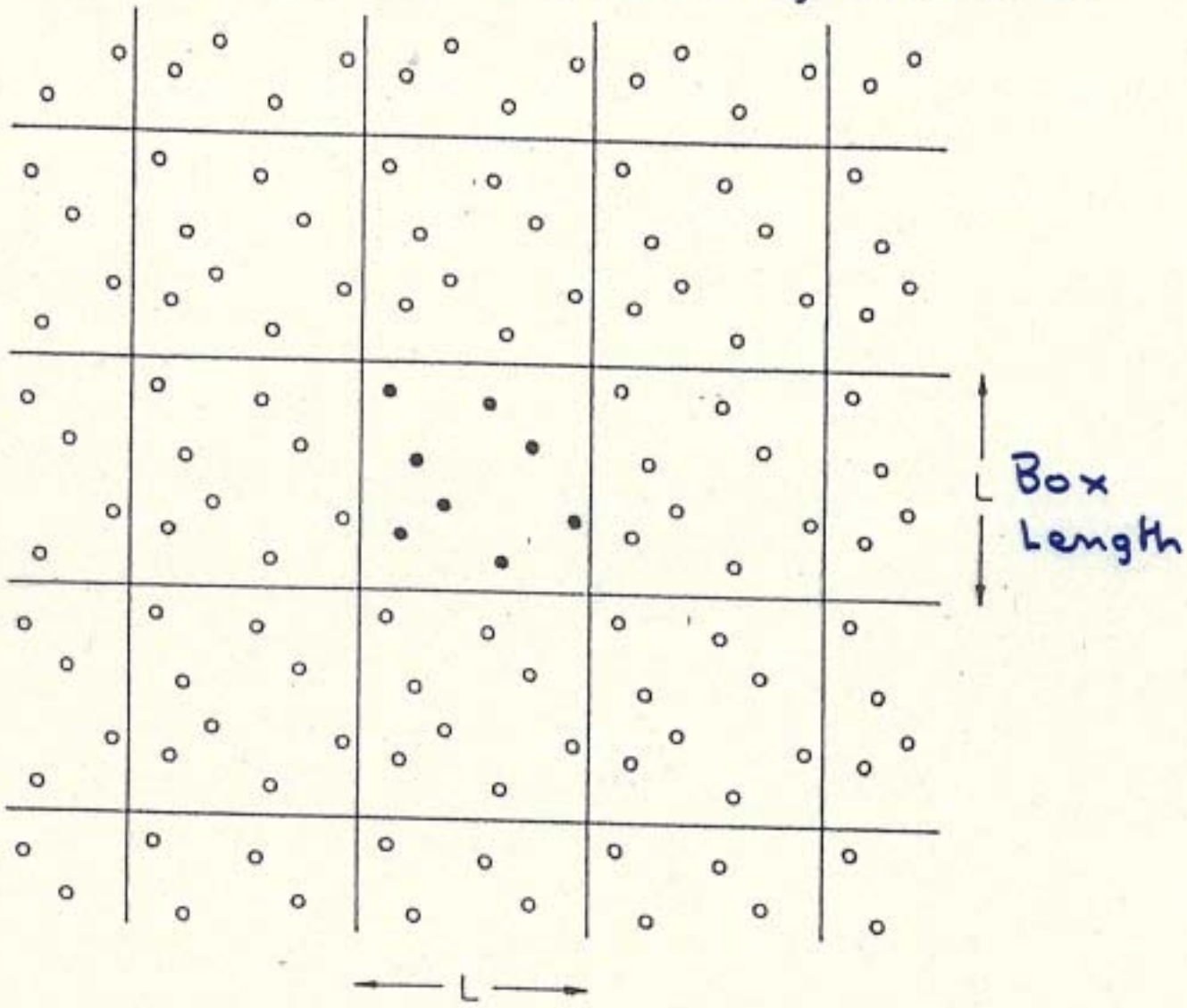


Illustration of the periodic box in two dimensions. The solid dots give positions of particles in the simulation square, while the circles show positions of assumed image particles filling the entire plane.

Single Particle states in Periodic Box

General condition: $k_i = n_i k_B \quad i = x, y, z$

$$k_B = \frac{2\pi}{L}$$

$$n_i = 0, \pm 1, \pm 2 \ldots .$$

Energy $E = \frac{\hbar^2}{2m} k_B^2 \left(n_x^2 + n_y^2 + n_z^2 \right)$

Spectrum

			N
———	$E = \hbar^2 k_B^2 / m$	$d = 12$	19
———	$E = \hbar^2 k_B^2 / 2m$	$d = 6$	7
———	$E = 0$	$d = 1$	1

We get a good approximation to uniform matter with $N = 7$ for <u>each</u> <u>spin-isospin</u>

Neutron matter $N = 14$ (possible)

Nuclear matter $N = 28$ (<u>not</u> possible)

Simplest PB calculations use:

truncated $v_{ij}^{tr} = v_{ij}$ for $r < L/2$

$= 0$ for $r > L/2$

For fixed N $(=14)$

$\rho L^3 = N$ gives $L = (N/\rho)^{1/3}$

Truncation effects limit ρ_{max} possible

$N=14$, $\rho = \rho_0 = 0.16\ fm^{-3}$: $L = 4.44\ fm$

Method

- Calculate PNM using $N=14$ PB & v_{ij}^{tr}
- Calculate the Box corrections:

$$\left[E_{UM}(v^{tr}) - E_{PB}(v^{tr})\right]$$

$$\& \quad \left[E_{UM}(v) - E_{UM}(v^{tr})\right]$$

using chain-summation methods

Box corrections are small for $\rho \leq \rho_0$

Results of PB (N=14) : v_6^{tr} (No L.S) MeV

Density (fm^{-3})	0.04	0.08	0.16	0.24	
GFMC - Const.	6.72	10.64	19.80	31.90	<1% Difference
GFMC - Unconst.	6.75	10.64	19.91	32.15	
VCS	7.6	11.9	21.2	33.6	

Results of PB (N=14): $v_8'^{tr}$ (Av_8')

GFMC - const	6.43	10.02	18.54	30.04	
GFMC - Uncon.	6.32	9.50	17.00	28.35	?
VCS	7.0	10.3	17.4	26.3	

Problem: l.s contributions do ≥ 3b clusters

OR in constrains ?

Best Estimates of E(ρ) with AV8'

GFMC - Uncon	6.3	9.5	17.0	28.4
ΔE (Box)	−0.2	−0.4	−0.6	−0.8
$v(r > L/2)$	−0.1	−0.8	−4.5	−10.7
E(ρ)	6.0	8.4	12.1	16.9
$\frac{E(\rho)}{E_{FG}(\rho)}$	0.43	0.38	0.34	0.37

Does not → 1 as ρ → 0

Properties of Neutron Stars

Energy of Low Density Neutron Matter

The nn scattering length $a \sim -18$ fm

Low density means $|k_F a| < 1$ or $\rho < 4 \times 10^{-5} \rho_0$

At densities of interest $|k_F a| >> 1$

Dilute (range of interaction $< r_0$) superfluid Fermi Gases with $|k_F a| >> 1$ have (see Phys. Rev. Lett. 91, 05041 (2003))

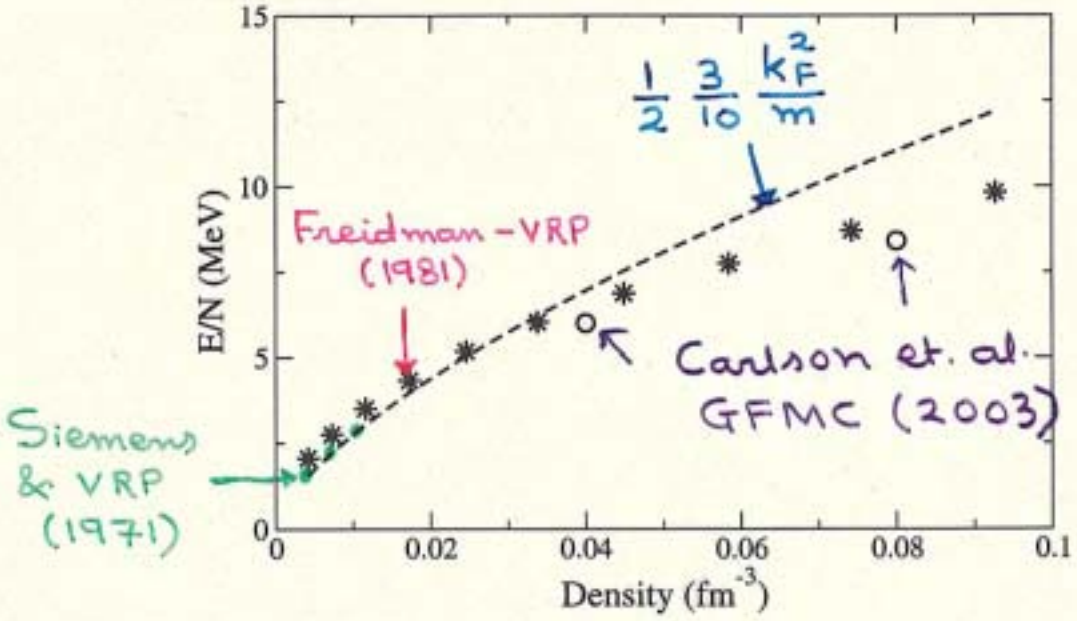
$$E(\rho = \frac{k_F^3}{3\pi^2}) = 0.44 \frac{3}{10} \frac{k_F^2}{m} + \text{terms of order } \frac{1}{k_F a}$$

Nonrelativistic (Skyrme) and relativistic mean field EOS have

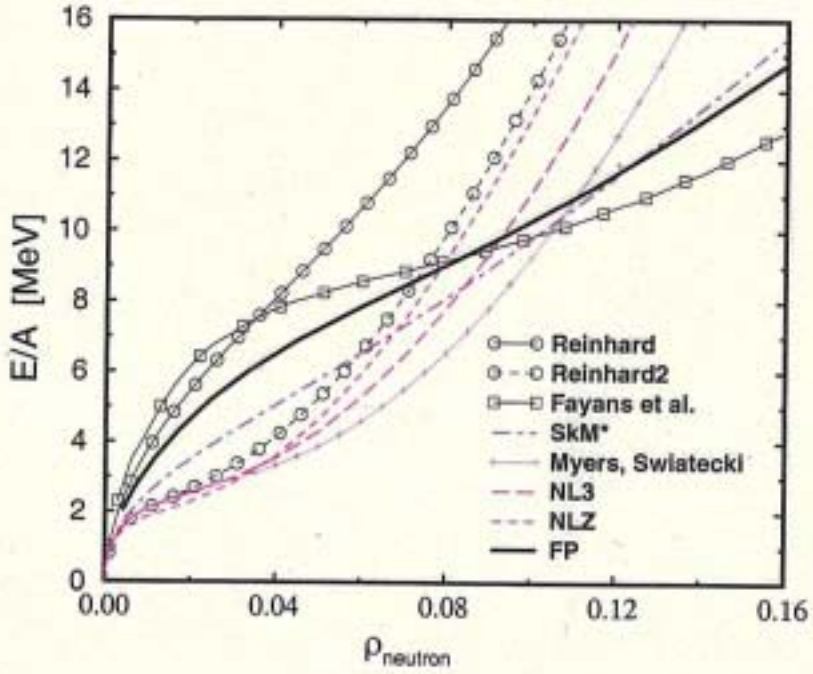
$$E(\rho = \frac{k_F^3}{3\pi^2}) = \frac{3}{10} \frac{k_F^2}{m} + \text{terms of order } k_F^3 \text{ or } \rho.$$

↑ Leading term to big by a factor $\gtrsim 2$

Results of Neutron Matter Calculation

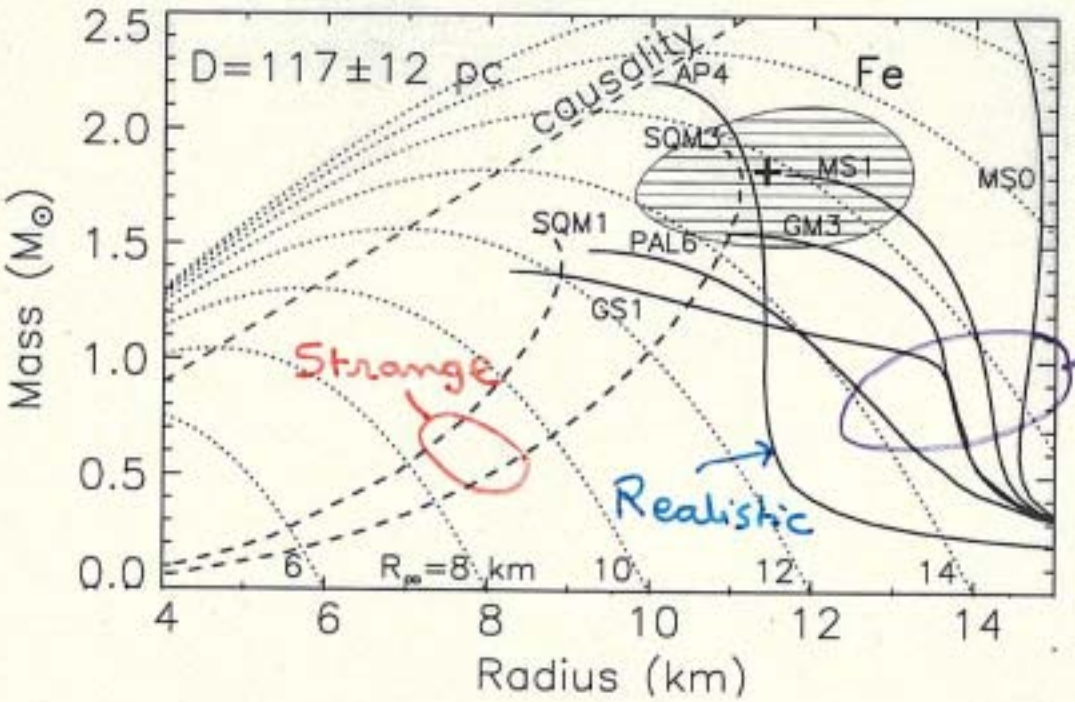


Realistic E(ρ) and Mean-field Models



Can not overcome a factor of 2 difference in leading term

Walter and Lattimer (2002)



Radii of Mean Field model stars are larger than "realistic"

Asymmetric Nuclear Matter

Asymmetry $\beta \equiv \frac{N-Z}{A} = \frac{\rho_n - \rho_p}{\rho}$

Energy per nucleon:

$$E(\rho,\beta) = E(\rho,0) + \beta^2 E_2(\rho) + \beta^4 E_4(\rho) + \cdots$$

Present theory indicates

$E_{n\geq 4}(\rho)$ are very small

$$E(\rho,\beta) = E(\rho,0) + \beta^2 E_2(\rho)$$

$$= E_{SNM}(\rho) + \beta^2 \left(E_{PNM}(\rho) - E_{SNM}(\rho) \right)$$

$E_{SNM}(\rho)$: Experiment

$E_{PNM}(\rho)$: theory

$E_{PNM}(\rho)$ constrains the density dependance of symmetry energy.

Correlated Basis Theory: Feenberg, et.al.(1969)

Many approaches.

Present approach: Fantoni and Pandharipande (1988)

The correlated state: $|X) = (S \prod_{i<j} F_{ij})|\Phi_X\rangle$,
where $|\Phi_X\rangle$ are uncorrelated Fermi gas (or Shell model) states and F_{ij} are pair correlation operators.

The $|X)$ are *not* orthonormal.

The FP orthonormalization: ($|X\rangle$ are orthonormal)

$|X) \longrightarrow |X\rangle$ such that (diagonal matrix elements are preserved)

$$\begin{aligned}\langle X|H|X\rangle &= \tfrac{(X|H|X)}{(X|X)} \\ &= \langle\Phi_X|\sum_i -\tfrac{1}{2m}\nabla_i^2 + \sum_{i<j} v_{eff}^{CB}(ij) + \sum_{i<j<k} V_{eff}^{CB}(ijk) + \cdots|\Phi_X\rangle\end{aligned}$$

and

$$\langle Y|\sum_i O_{bare}(i)|X\rangle = \langle\Phi_Y|\sum_i O_{eff}^{(1)}(i) + \sum_{i<j} O_{eff}^{(2)}(ij) + \cdots|\Phi_X\rangle \ .$$

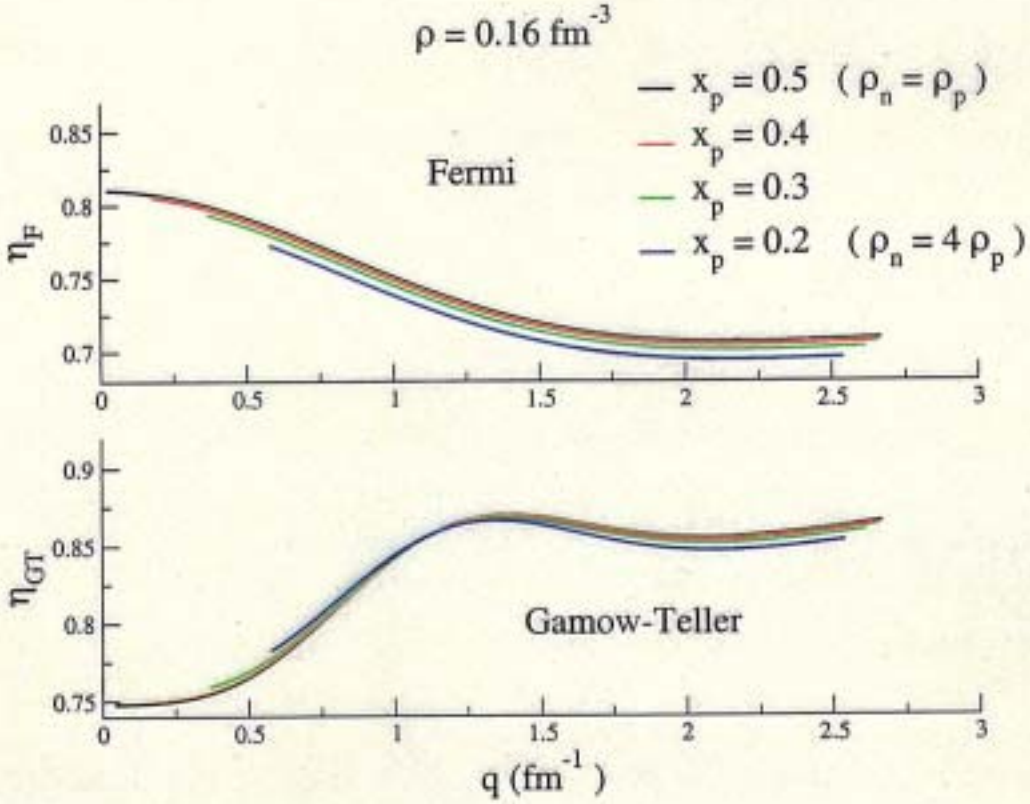
Past Applications: including 2nd order v_{eff}^{CB} (neglect V_{ijk}^{CB})

- Real and imaginary parts of optical potential (Fantoni, et.al. (1983))
- Response of nucleon matter to electromagnetic probes (Fabrocini, et.al. (1989))
- Weak interactions in nuclear matter (2002)

Results Quenching of Weak Interactions

Including All 2-body Direct+Exchange Terms

$$\eta = \frac{|\langle \Phi_F | O_{eff} | \Phi_I \rangle|^2}{|\langle \Phi_F | O_{bare} | \Phi_I \rangle|^2}: \text{ Charge Current}$$



General Properties:

- Relatively independent of proton fraction: x_p.
- q-dependence introduced through 1+2nd order : j terms.
- η depends upon the initial and final nucleon momenta by $< 3\%$ through the exchange contributions.
- η also depends slightly upon total density of system: ρ.

Correlated Basis Effective Interaction

$$\langle X|H|X\rangle = \langle \Phi_X| - \frac{1}{2m}\sum_i \nabla_i^2 + \sum_{i<j} v_{eff}^{CB}(ij) + \cdots |\Phi_X\rangle$$

In two-body cluster approximation:

$$v_{eff}^{CB}(ij) = v_{eff}^{CBS}(ij) + v_{eff}^{MD}(ij) \ .$$

$$v_{eff}^{CBS}(ij) = F_{ij}(v_{ij} - \frac{1}{m}\nabla^2)F_{ij}$$

$$v_{eff}^{MD}(ij) = -\frac{1}{m}[\overleftarrow{\nabla}\cdot(F_{ij}\overleftarrow{\nabla})F_{ij} + F_{ij}(\overrightarrow{\nabla}F_{ij})\cdot\overrightarrow{\nabla}]$$

Several studies of weak interactions in nuclei and nucleon matter use Landau-Migdal effective interactions derived from spin and isospin susceptibilities of nucleon matter.

We therefore study the susceptibilities of symmetric nuclear matter which are proportional to $E^{-1}_{\tau,\sigma,\sigma\tau}$ defined as:

$$\begin{aligned} E(\rho,x,y,z) &= E_0(\rho) + E_\tau(\rho)x^2 + E_\sigma(\rho)y^2 + E_{\sigma\tau}(\rho)z^2 \ , \\ x &= (\rho_{n\uparrow} + \rho_{n\downarrow} - \rho_{p\uparrow} - \rho_{p\downarrow})/\rho \ : \tau \text{ polarization} \\ y &= (\rho_{n\uparrow} - \rho_{n\downarrow} + \rho_{p\uparrow} - \rho_{p\downarrow})/\rho \ : \sigma \text{ polarization} \\ z &= (\rho_{n\uparrow} - \rho_{n\downarrow} - \rho_{p\uparrow} + \rho_{p\downarrow})/\rho \ : \sigma\tau \text{ polarization} \end{aligned}$$

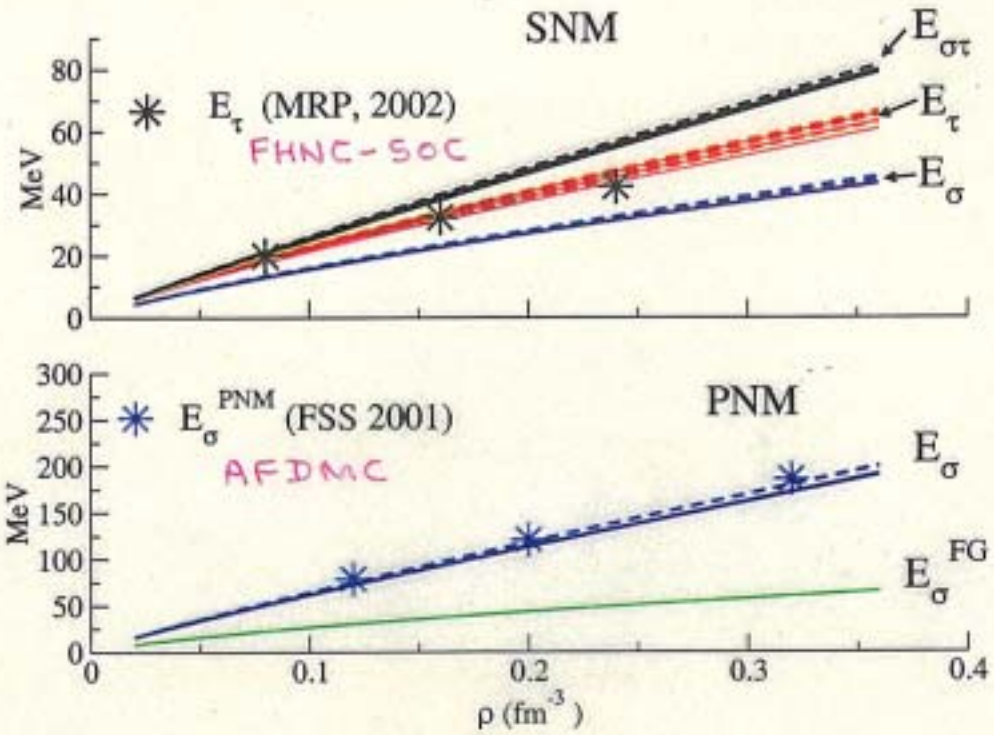
and that of pure neutron matter proportional to E_σ^{-1} defined as:

$$E(\rho, x=1, y, z=y) = E_0^{PNM}(\rho) + E_\sigma^{PNM}(\rho)y^2 \ .$$

Susceptibilities

Dashed lines : v_{eff}^{CB} Solid lines: v_{eff}^{CBS}

Results using SNM F_{ij} for $\rho = 0.08, 0.16$, and 0.24 fm^{-3}.

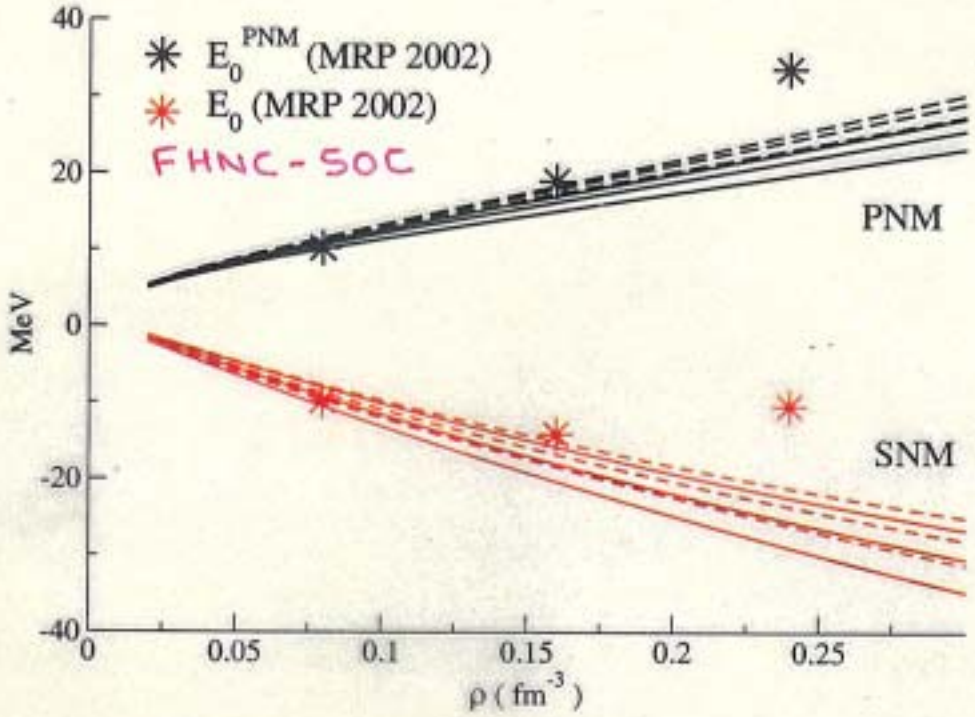


- Contribution of momentum dependent terms is small.
- E_σ, $E_{\sigma\tau}$ and E_σ^{PNM} are insensitive to the density dependence of the effective interaction via F_{ij}.
- Two-body v_{eff}^{CB} gives a fair approximation to symmetry energy, E_τ.
- F_{ij} for SNM ($\rho_n = \rho_p$) reproduce E_σ^{PNM} of pure neutron matter.
- The above four simplifications are possible because Fermi-gas and v_{eff}^{CB} contributions to E_σ, E_τ and $E_{\sigma\tau}$ **ADD**.

$E_0(\rho)$: Total Energy

Dashed lines : v_{eff}^{CB} Solid lines: v_{eff}^{CBS}

Results using SNM F_{ij} for $\rho = 0.08, 0.16$, and 0.24 fm^{-3}.



- At low densities, the two-body v_{eff}^{CB} gives a fair approximation to the $E_0(\rho)$ of PNM and SNM.
- Minimum of SNM $E_0(\rho)$ at $\rho_0 = 0.16$ fm^{-3} is not obtained at the two-body level. Three-body interactions and cluster contributions are repulsive and essential to obtain this minimum.
- These complications are because Fermi-gas and v_{eff}^{CB} contributions to $E_0(\rho)$ **CANCEL**.

Need V_{ijk}^{CB} & more

Single-particle energies in SNM

Fermi gas: $|0\rangle$, $|p\rangle = a_p^\dagger |0\rangle$, $|h\rangle = a_h |0\rangle$ ...

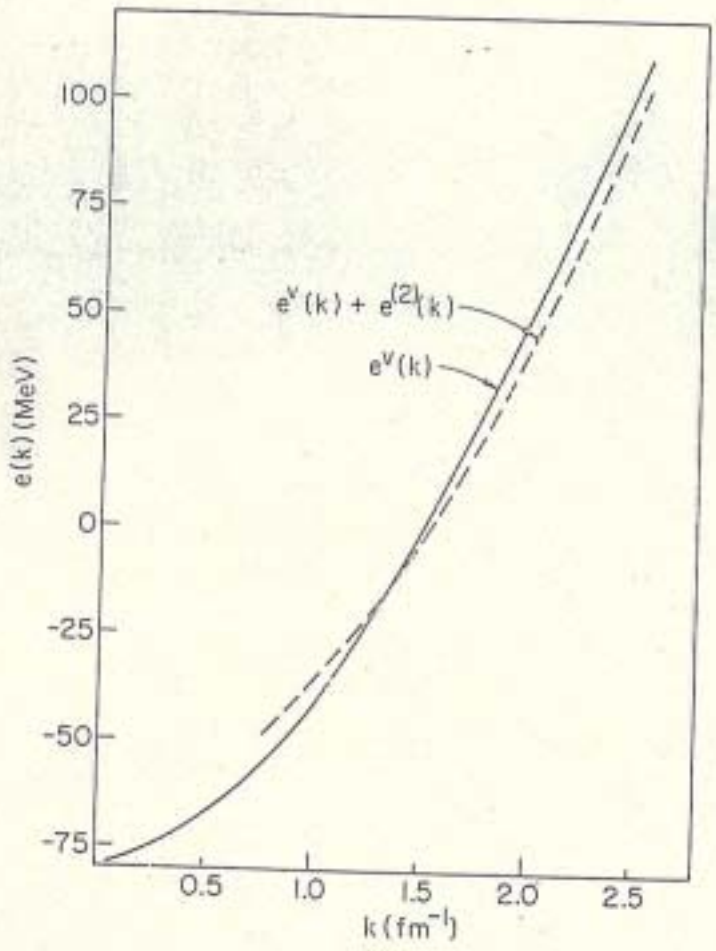
Corrosponding correlated states $|0\rangle_c$, $|p\rangle_c$, $|h\rangle_c$ ...

Orthogonalized

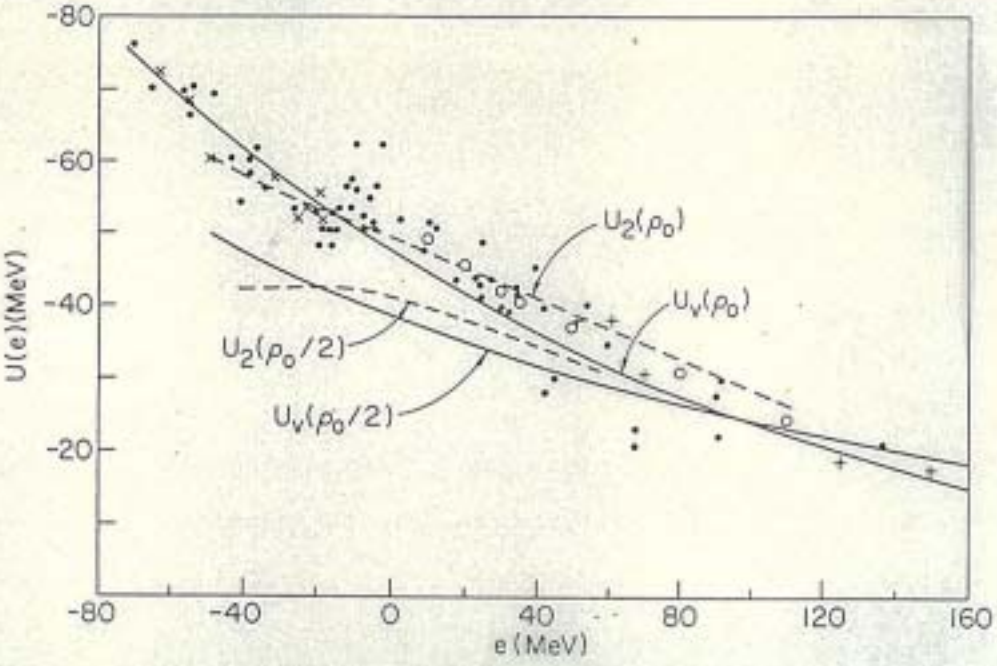
First order $E^{(1)}(p) = \dfrac{{}_c\langle p|H|p\rangle_c}{{}_c\langle p|p\rangle_c} - \dfrac{{}_c\langle 0|H|0\rangle_c}{{}_c\langle 0|0\rangle_c}$ Real

Second order via coupling of $|p\rangle_c$ to $|p_1 p_2 h_1\rangle_c$ by v_{eff}^{CB}

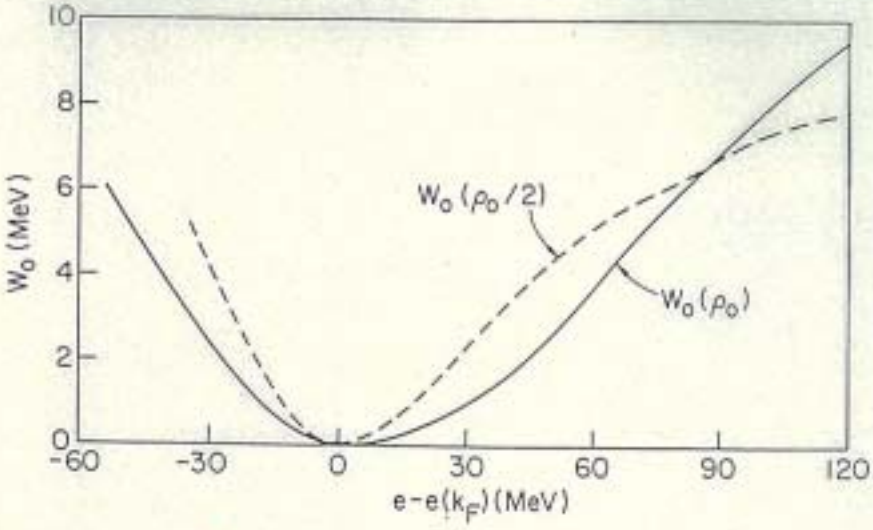
Gives Real $\delta E^{(2)}(p)$ and imaginary $W(p)$



Extract Real & Imaginary parts of optical potential in SNM



Real part



Imaginary part
(agrees well with expt.)

Fantoni et.al. Nucl. Phys. A399, 51 (1983).

TDA Calculations : RPA ?? (in progress)

Calculate the response of an infinite system utilizing the effective weak operators, O_{eff} :

$$R(\omega, \vec{q}) = \sum_F |\langle \Phi_F | O_{eff} | \Phi_I \rangle|^2 \quad \delta(\omega_F - \omega_I - \omega)$$

Note: $|\Psi_I\rangle = (\mathcal{S}\Pi F)|\Phi_I\rangle$
$|\Psi_F\rangle = (\mathcal{S}\Pi F)|\Phi_F\rangle$.
Effects of correlations are in v_{eff} and O_{eff}.

Obtain final state wave functions, Φ_F, using Tamm-Dancoff Approximation (TDA) using Hartree-Fock $|\Phi_I\rangle$.

Current TDA Calculation

Φ_F obtained by diagonalization of the effective Hamiltonian matrix calculated between (> 1000) particle-hole states of total momentum $\vec{q}$.

Infinite system is approximated as a Fermi Gas contained in a periodic box.

Single particle states, $\phi_i = e^{i\vec{k}_i \cdot \vec{r}_i}\, \chi_{\sigma\tau}(i)$ where $\vec{k}_i = \frac{2\pi}{L}\, \vec{n}_i$. Increase box size, L, to increase the size of p-h Hamiltonian matrix.

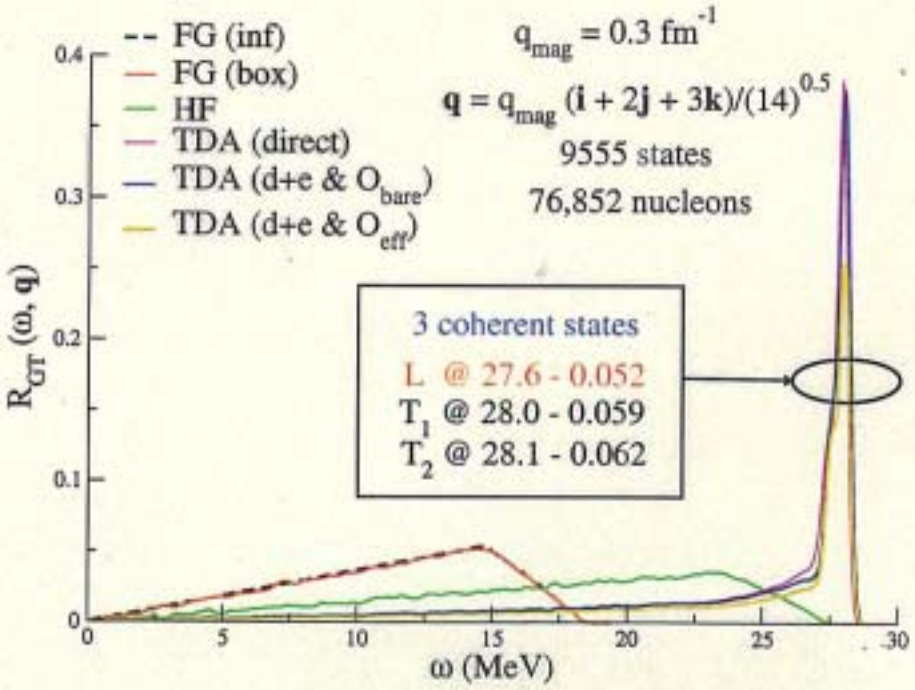
$|\Phi_F\rangle = \sum_{\vec{h}} \alpha^F_{\vec{h}} |\vec{p} = \vec{h} + \vec{q}\rangle$ $(h < k_F, p > k_F)$

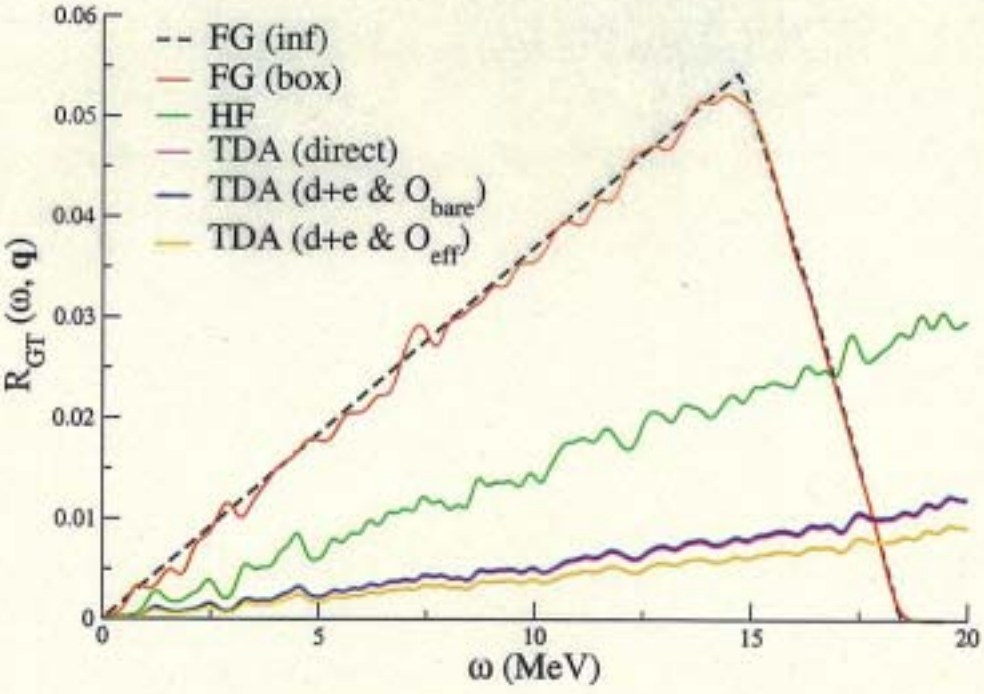
Diagonalize $H^{eff}_{HF} + v^{cB}_{eff}$ to get $\alpha^F_{\vec{h}}$

$\Uparrow$

Hartree-Fock H^{eff}_{HF} is also calculated from v^{cB}_{eff}

TDA Response Functions - Gamow-Teller



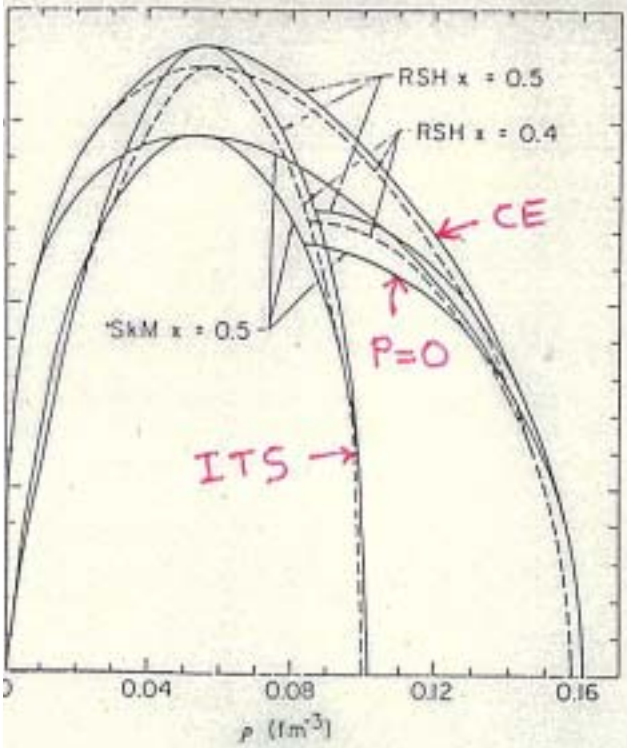


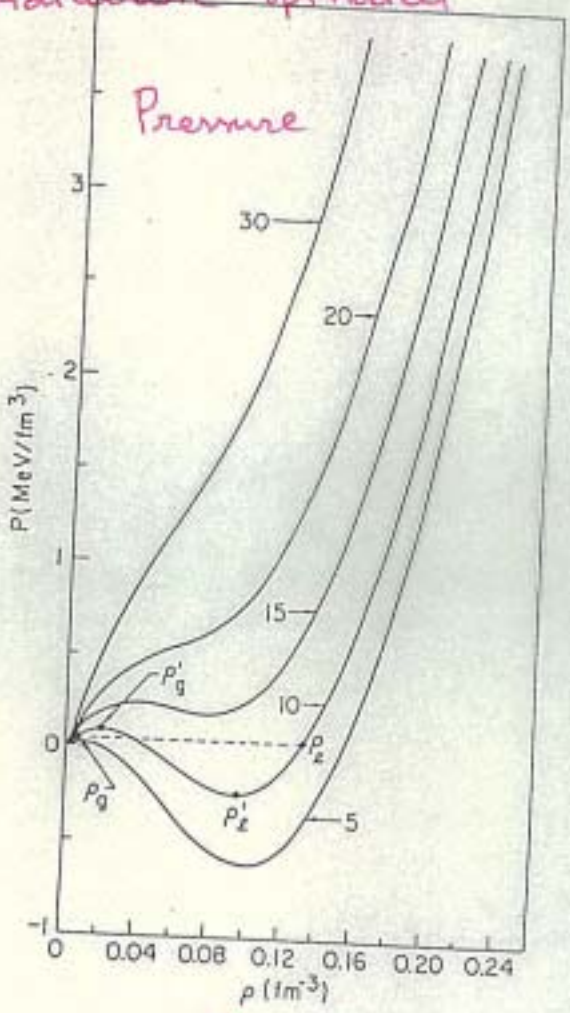
v_{eff} exchange matrix elements have small effect

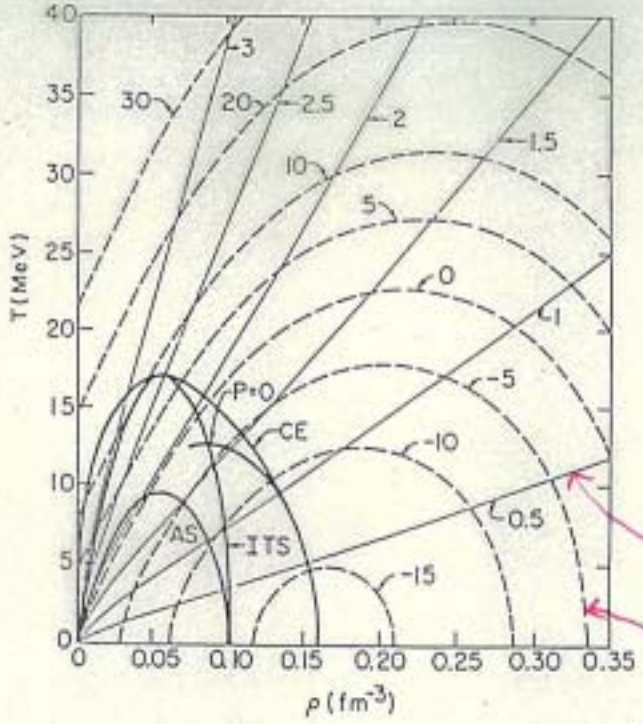
Minimize Free Energy = $\langle H \rangle - TS$ to study matter at Finite Temp.

SNM

CE: Liquid-gas coexistance
ITS: Isothermal spinodal
AS: Adiabatic spinodal







Constant entropy

Constant $\langle H \rangle$

GFMC Studies of Fermi Superfluids

Normal $\Phi_{FG} = \mathcal{A} \prod_i e^{i k_i \cdot r_i} |\uparrow\rangle \prod_{i'} e^{i k_{i'} \cdot r_{i'}} |\downarrow\rangle$

$$\Psi_V = \left(S \prod_{i<j} F_{ij}\right) \Phi_{FG}$$

Constrained Path **OR** Fixed Node GFMC

$$\Psi_0^{FN} = e^{-(H-E_0)\tau} \Psi_V \Big\|_{FN}$$

Gives lowest energy Ψ_0^{FN} with nodes of Ψ_V

Superfluid : Particle number conserved

$$\Phi_{BCS}(\text{N-particle}) = \mathcal{A}\, \phi(r_{11'}) \phi(r_{22'}) \cdots \phi(r_{\frac{N}{2},\frac{N}{2}'})$$

$$\phi(r) = \sum_k \frac{v_k}{u_k} e^{i \vec{k} \cdot \vec{r}}$$

$$|BCS\rangle = \prod_k \left(u_k + v_k a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}\right)|0\rangle$$ N not conserved

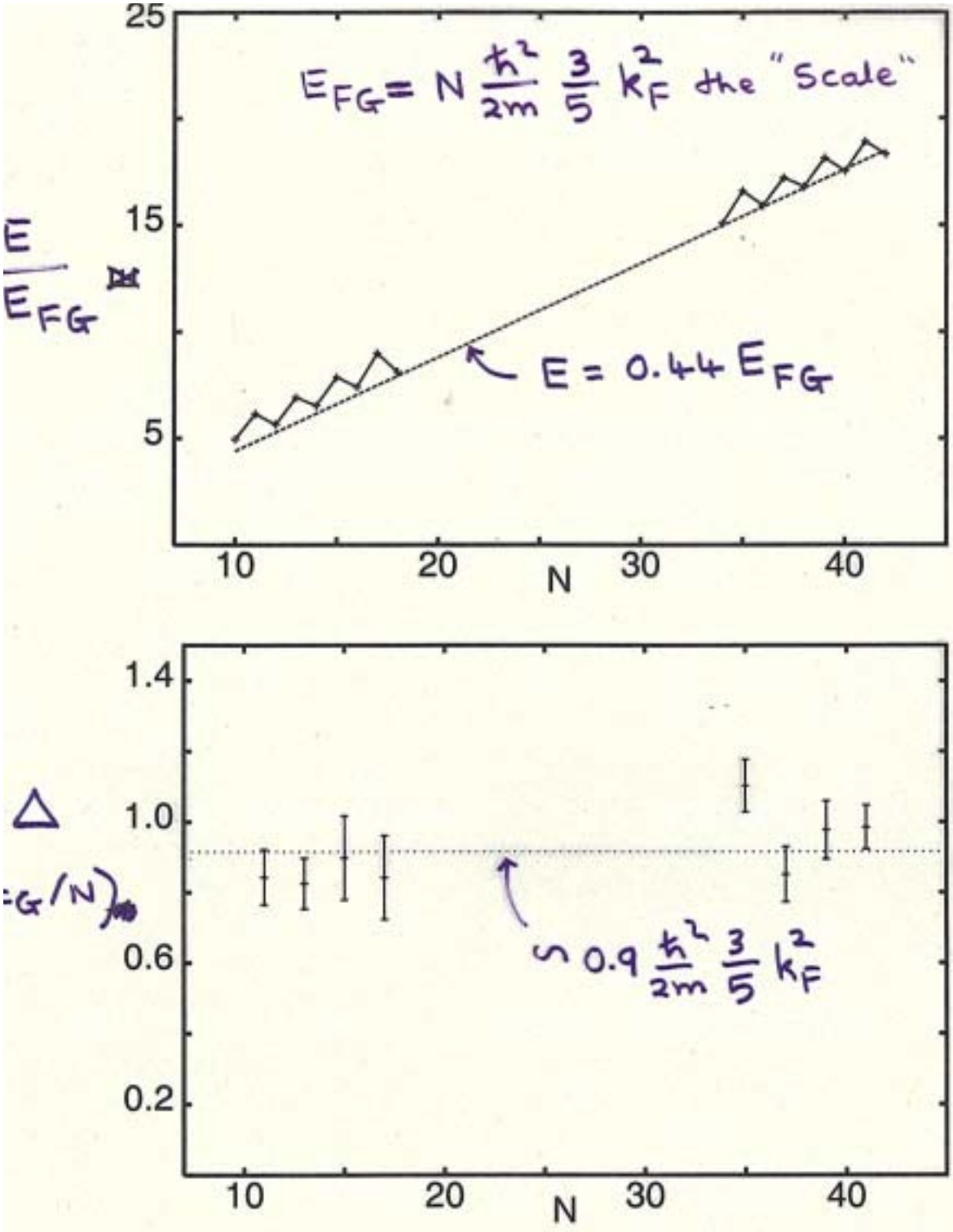
$$\Psi_{V,BCS} = \left(S \prod_{i<j} F_{ij}\right) \Phi_{BCS}$$

$$\Psi^{FN}_{BCS} = e^{-(H-E_0)\tau} \Psi_{V,BCS} \Big\|_{FN}$$

Depend upon the pair $\phi(r)$

Minimize ground state energy E_0

to find optimum $\phi(r)$ & Ψ_{BCS}.



Dilute Fermi superfluid gas

with $ak_F \to -\infty$: "Bertsch problem"

Carlson et. al. PRL 91, 050401 (2003).

References for additional reading

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