Quantum Monte Carlo
J. Carlson - LANL

- Simple Explanation
- History
- Some Applications
- Ground-States
-     Weak Binding
-     Efimov Regime
- Low-Energy Scattering
- Static Response
- Dynamic Response
- Challenges

GFMC/DMC

exp [- H t]
Evolve Particle Coordinates

MC for kinetic term

$$\exp[-T\delta\tau] = \exp[-\frac{(R-R')^2}{4\frac{\hbar^2}{2m}\delta\tau}]$$

exp [- V t] explicitly

Some Applications:
Electron Gas
Liquid He
Light Nuclei
Cold Atoms

AFMC/SMMC

exp [- H t]
Evolve Single-Particle Orbitals

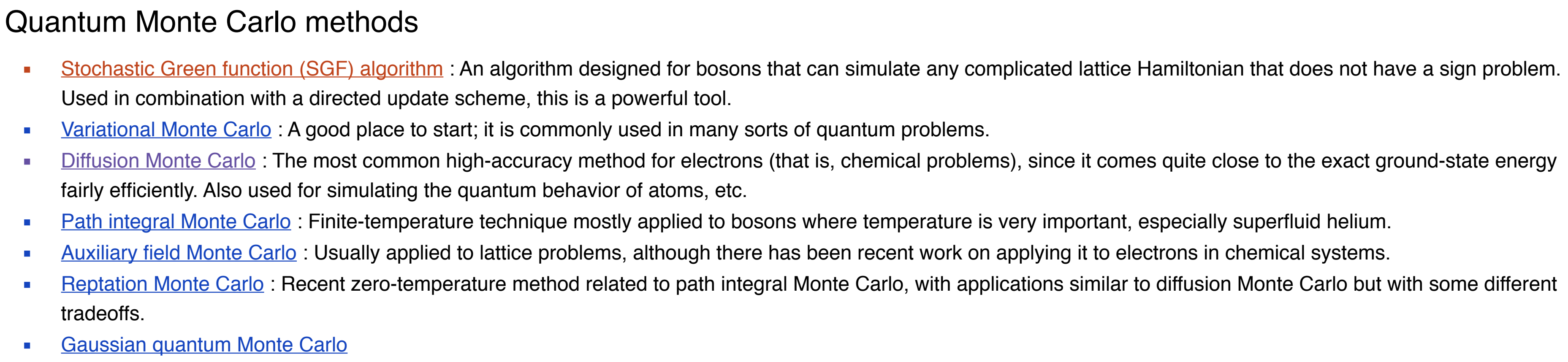
MC for interaction

$$\exp\left\{-\frac{a}{2}x^2\right\} = \sqrt{\frac{1}{2\pi a}} \int_{-\infty}^{\infty} \exp\left[-\frac{y^2}{2a} - ixy\right] dy,$$

exp [- T t] explicitly

Some Applications:
Hubbard Model, ...
Shell Model of Nuclei
Cold Atoms

http://en.wikipedia.org/wiki/Quantum_Monte_Carlo



Quantum Monte Carlo methods

- Stochastic Green function (SGF) algorithm : An algorithm designed for bosons that can simulate any complicated lattice Hamiltonian that does not have a sign problem. Used in combination with a directed update scheme, this is a powerful tool.
- Variational Monte Carlo : A good place to start; it is commonly used in many sorts of quantum problems.
- Diffusion Monte Carlo : The most common high-accuracy method for electrons (that is, chemical problems), since it comes quite close to the exact ground-state energy fairly efficiently. Also used for simulating the quantum behavior of atoms, etc.
- Path integral Monte Carlo : Finite-temperature technique mostly applied to bosons where temperature is very important, especially superfluid helium.
- Auxiliary field Monte Carlo : Usually applied to lattice problems, although there has been recent work on applying it to electrons in chemical systems.
- Reptation Monte Carlo : Recent zero-temperature method related to path integral Monte Carlo, with applications similar to diffusion Monte Carlo but with some different tradeoffs.
- Gaussian quantum Monte Carlo

Implementations

- ALPS
- CASINO
- CHAMP
- Monte Python
- PIMC++
- pi-qmc
- QMcBeaver
- QmcMol
- QMCPACK
- Qumax
- Qwalk
- TurboRVB
- Zori

(some) History:

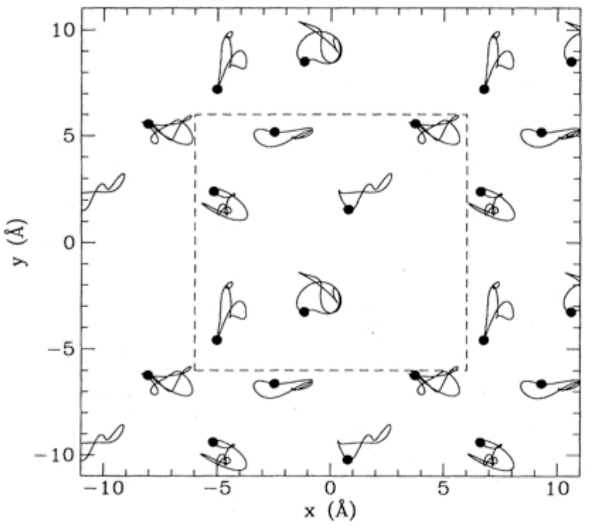
MC calculation of the ground state
of 3- and 4-body nuclei, M. H. Kalos, PR 128, 1797(1962).

Helium at Zero Temperature with Hard-Sphere and Other Forces,
M. H. Kalos, D. Levesque, L. Verlet, PRA, 2178 (1974).

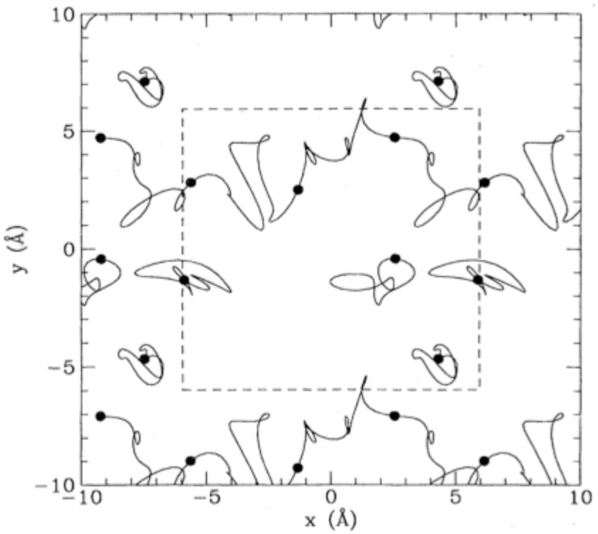
Ground State of the Electron Gas by a Stochastic Method,
D. M. Ceperley, B. J. Alder, PRL 45, 565 (1980).

Path Integrals in the Theory of Condensed Helium
D. M. Ceperley, RMP 67, 279 (1995).

Superfluid/Normal
Transition



High T



Low T

DMC Algorithm (shortest version)

- Start with a set of 'configurations'
  each configuration with coordinates R
  (spin-isospin amplitudes α_i),
  initially from VMC with probability $|\sum_i \beta_i^\star \alpha_i|$
  where $\beta_i = \alpha_i$ determined from trial state

- For each sample new R' from $\exp[-(R_i' - R_i)^2/(\frac{4\hbar^2}{2m_i}\Delta\tau)]$

- Calculate new amplitudes $\alpha_j' = \exp[-V\delta\tau]_{ji}\alpha_i$
  and β_j from trial state at R'

- Form new weight $|\sum_i \beta_i^\star \alpha_i|$ sample
  configurations proportional to weights

- Measure observables & repeat

Real work (insight) in:

Good trial state or source:

$$|\Psi_T^i\rangle = \mathcal{S} \prod_{i<j} F_{ij} |\Phi_T^i\rangle$$

Nuclear Physics: Fij spin/isospin dependent; $|\Phi_T^i\rangle$ shell-model `like'

Improved propagator exp [- H t]

$$\exp[-H\Delta\tau] \approx \mathcal{S} \prod \frac{\exp[-H_{ij}\Delta\tau]}{\exp[-H_{ij}^0\Delta\tau]} \exp[-T\delta\tau]$$

Fixed Node

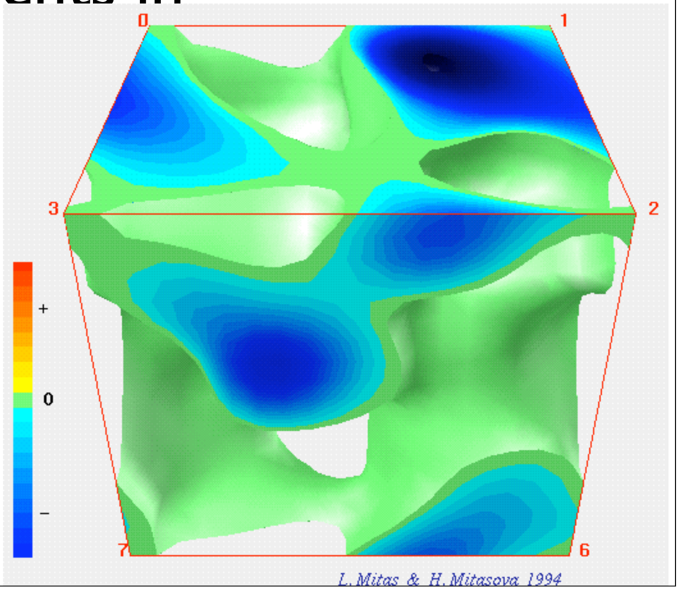
For fermions in a spin-independent potential, do not allow diffusion across surfaces where the trial function is zero.

Variational upper bound, can optimize the fixed-node surface.

Optimize at variational level, or try to optimize by including parameters as diffusing elements in random walk.

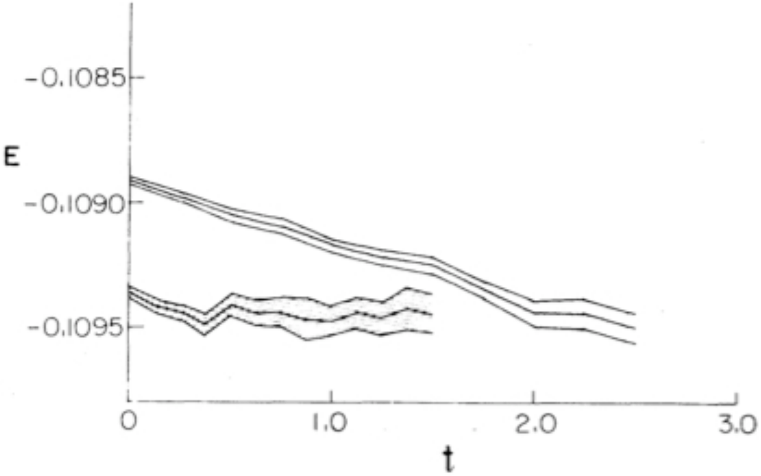
Test results by relaxing nodal constraint.

Nitrogen Solid



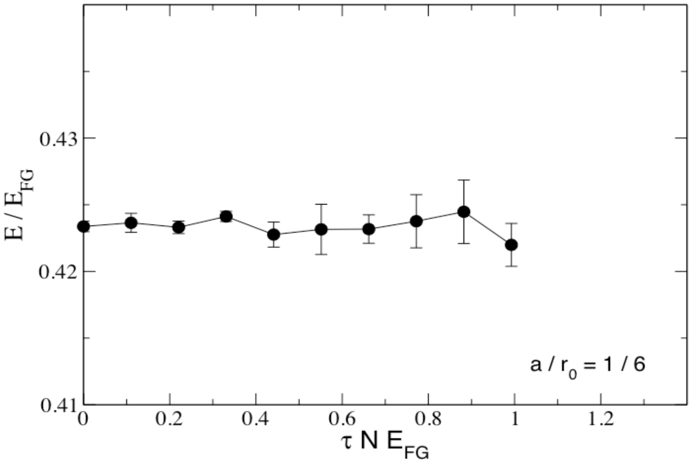
Transient Estimation

Electron Gas

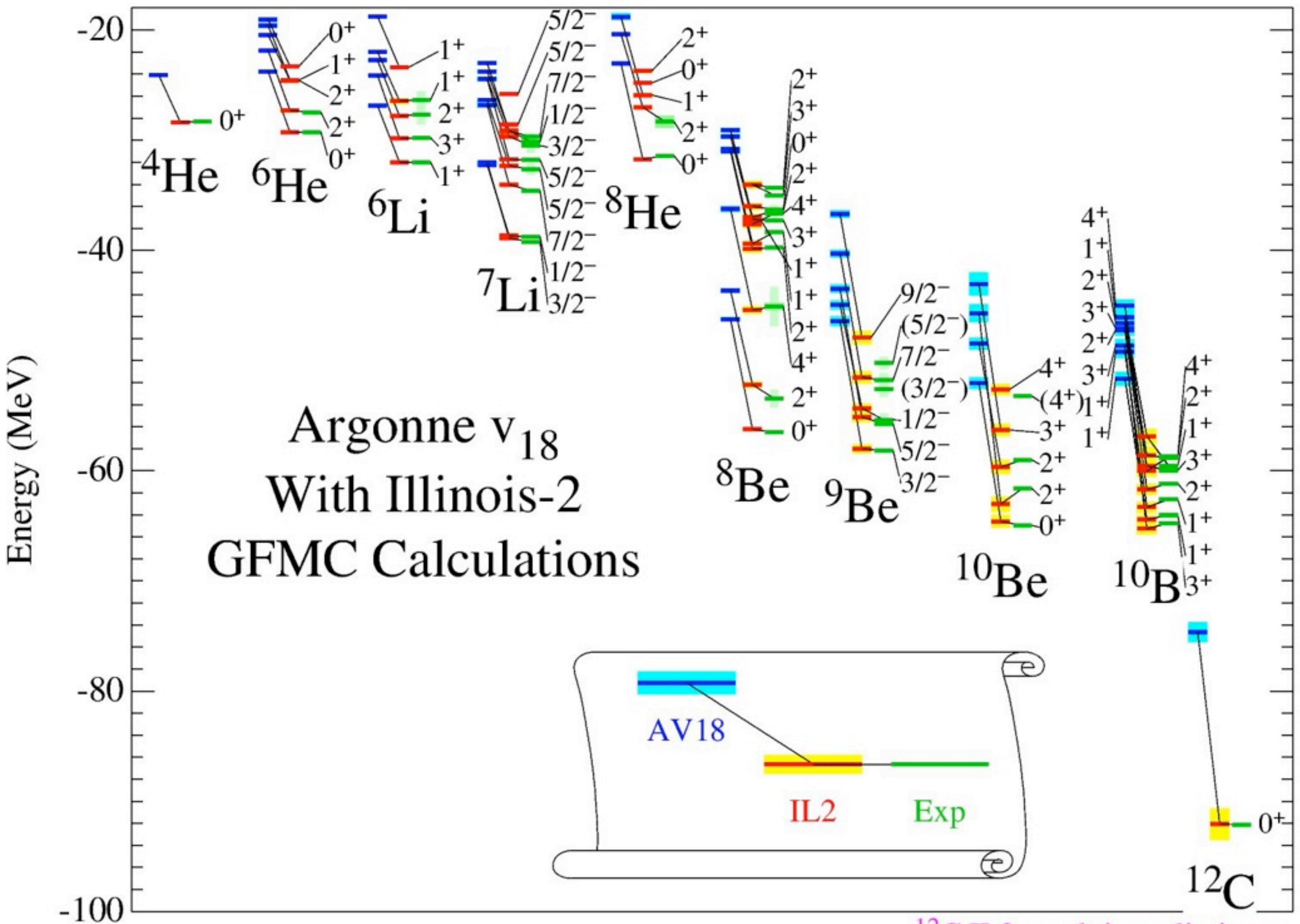


Ceperley and Alder, PRL 1980

Cold Atoms



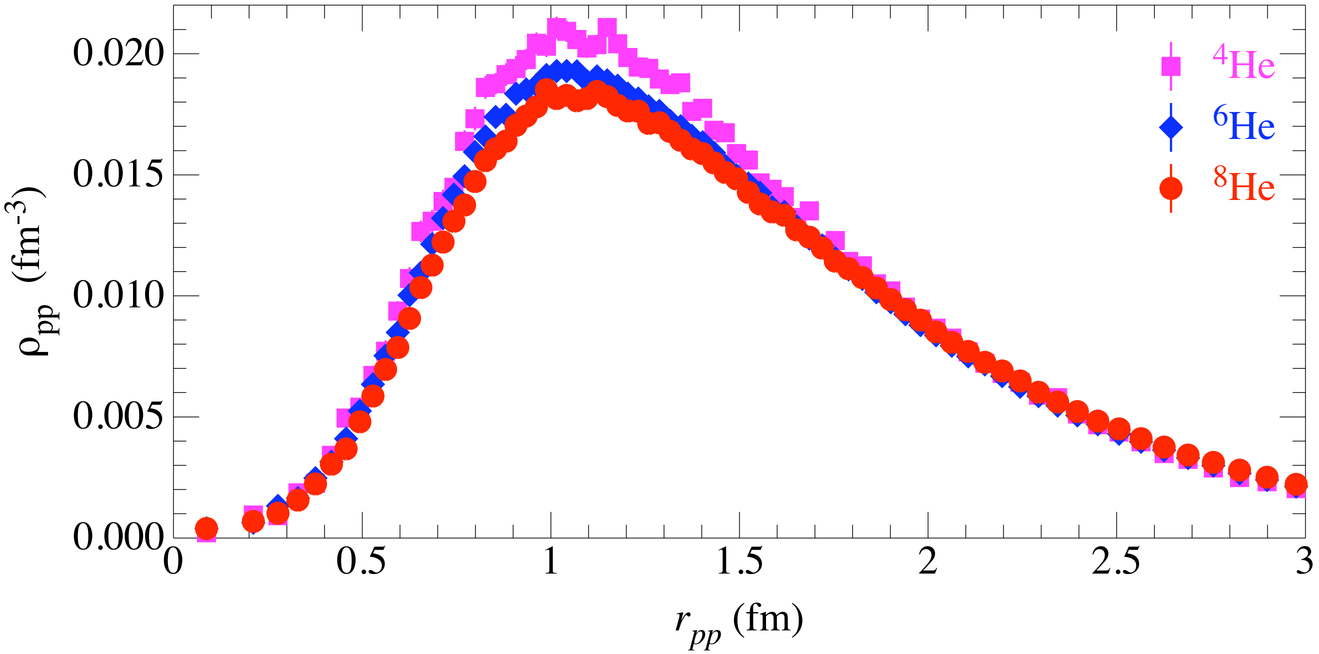
Light Nuclear Spectra



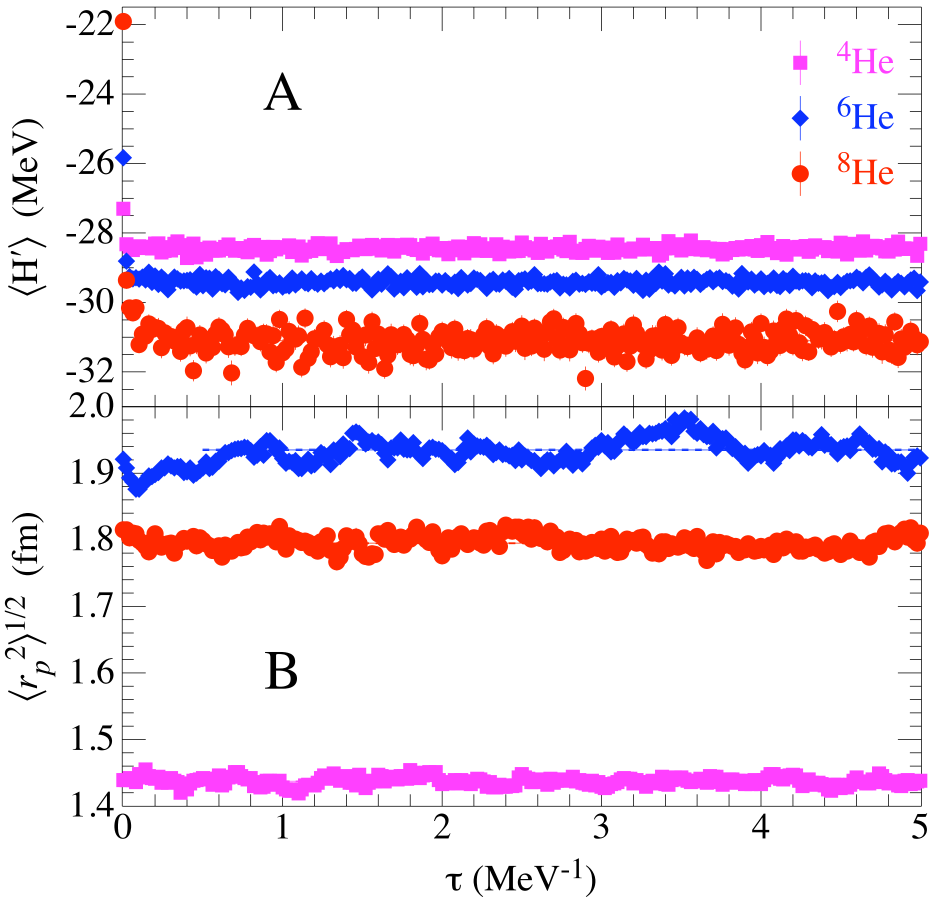
^{12}C IL2 result is preliminary.

Weakly Bound Helium Isotopes

To what extent is the alpha core changed in He isotopes?



Convergence vs. Imaginary Time

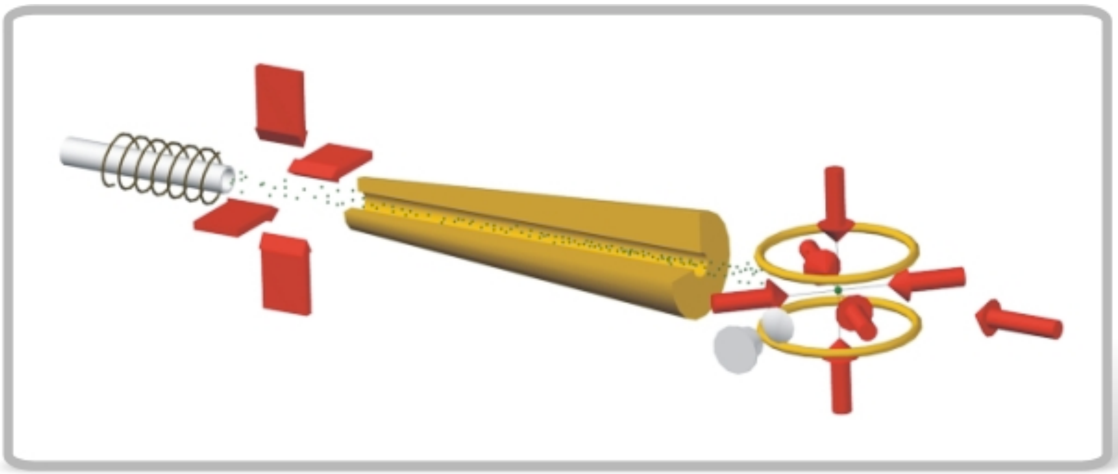


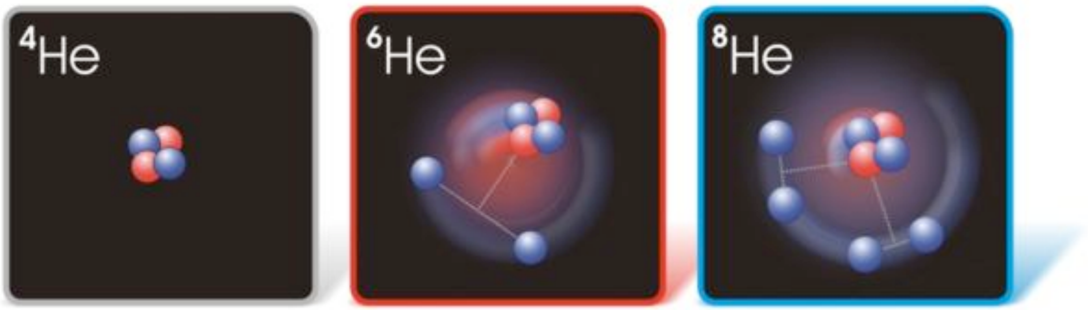
Energy

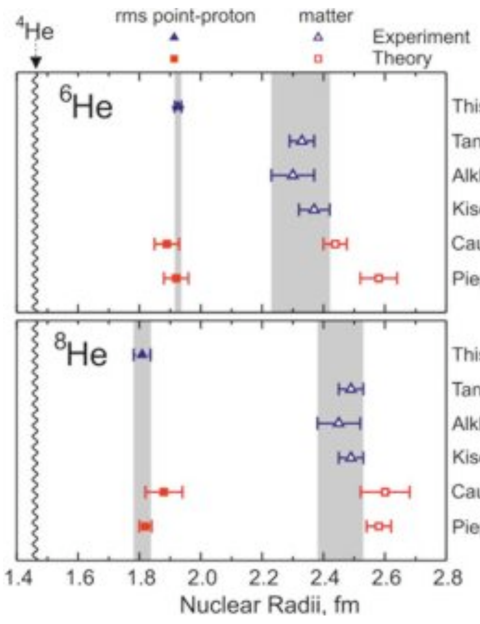
Charge Radius

Note: long correlations in imaginary time (low-E modes)

Helium Charge Radii







Mueller, et al, PRL 2007
Norterhauser, et al, PRL 2009

Hamiltonian for Cold Atoms

$$H = \sum_{i=1,n_l} \frac{-\hbar^2}{2m_l}\nabla_i^2 + \sum_{j=1,n_h} \frac{-\hbar^2}{2m_h}\nabla_j^2 + \sum_{i,j} V(r_{ij})$$

$$v(r) = -\frac{2}{m}\frac{\mu^2}{\cosh^2(\mu r)}$$

strength, μ ⇔ scattering length & effective range

for cold atoms want μ ⇒ ∞, range ⇒ 0

for heavy-light compare at same reduced mass

Gap and Effective Mass

$$|\psi_{BCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow}) |0\rangle \ ,$$

$$\Psi_0 \ = \ \Psi_{BCS} = \prod_{k} \ [v_k/u_k] \ a^{\dagger}_{\uparrow}(k) a^{\dagger}_{\downarrow}(-k) \ |0\rangle$$

particle projected BCS state

Add a particle of momentum k

$$\Psi_1(k') \ = \ a^{\dagger}_{\uparrow}(k') \Psi_{BCS} = a^{\dagger}_{\uparrow}(k') \prod_{k} \ [v_k/u_k] \ a^{\dagger}_{\uparrow}(k) a^{\dagger}_{\downarrow}(-k) \ |0\rangle$$

`Easy' to add excitation with different quantum numbers

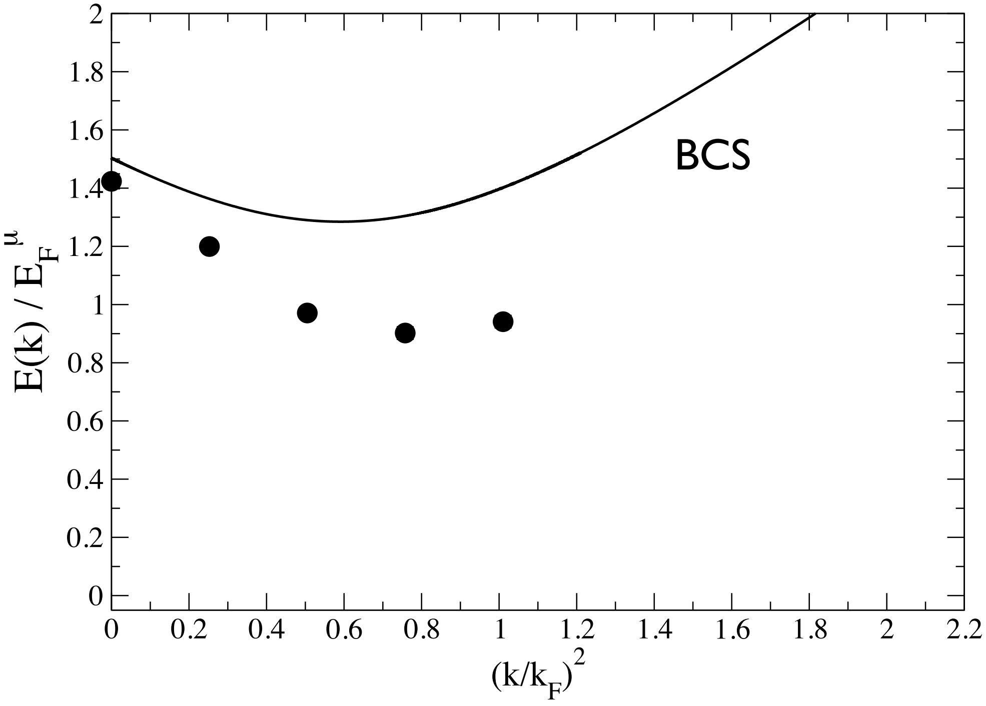
Superfluid at Equal Mass, T=0

BCS (Mean-Field) Theory: Strongly-paired Superfluid gap of same order as Fermi Energy

$\xi \sim 0.40(0.01) = E / E_{FG}$

$\Delta = 0.5\ (0.05)\ E_F$

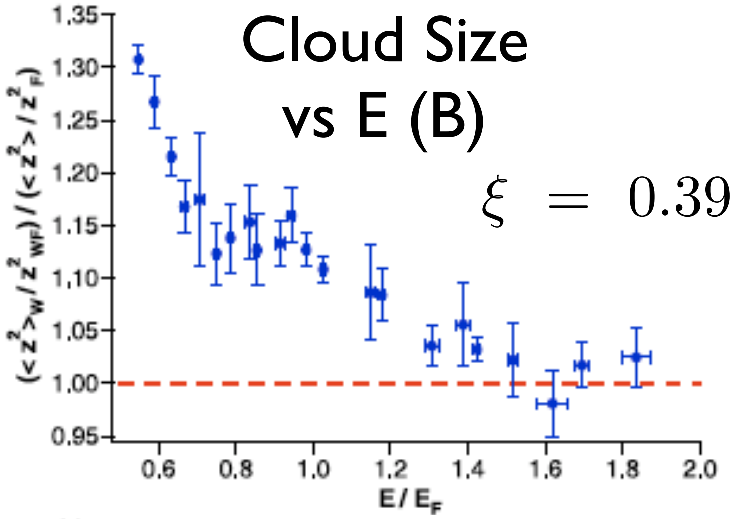
Quasiparticle Dispersion



Experiments at Unitarity: # ↑ = # ↓
Cloud Size and Sound Velocity

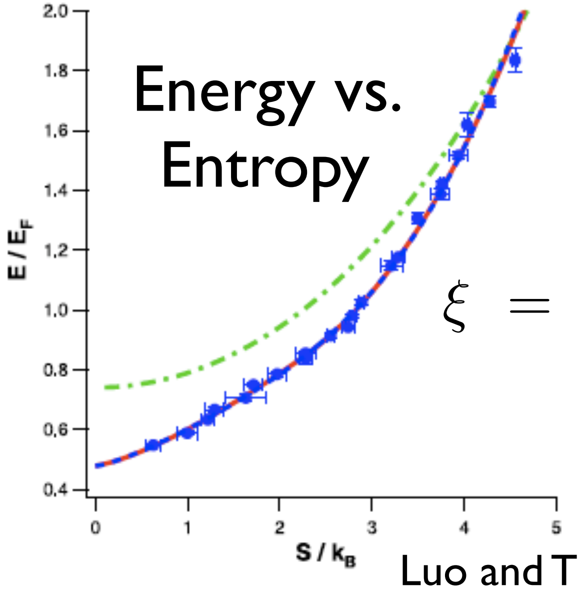
Cloud Size vs E (B)

$$\xi = 0.39(02)$$



Energy vs. Entropy

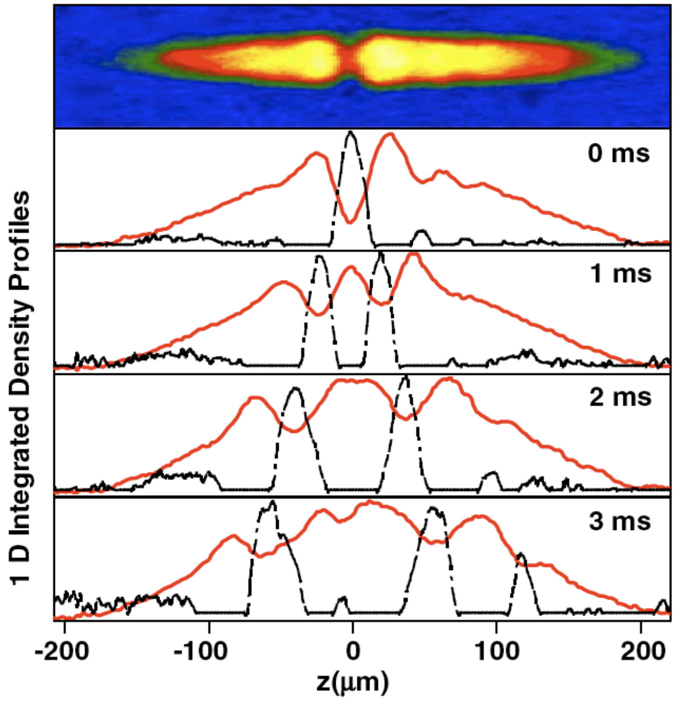
$$\xi = 0.41(02)$$



Luo and Thomas, JLTP, 2009

Sound Propagation

Joseph, et al., PRL 2007



$$\frac{c_0}{v_f} = \frac{\xi^{1/4}}{\sqrt{(5)}}$$

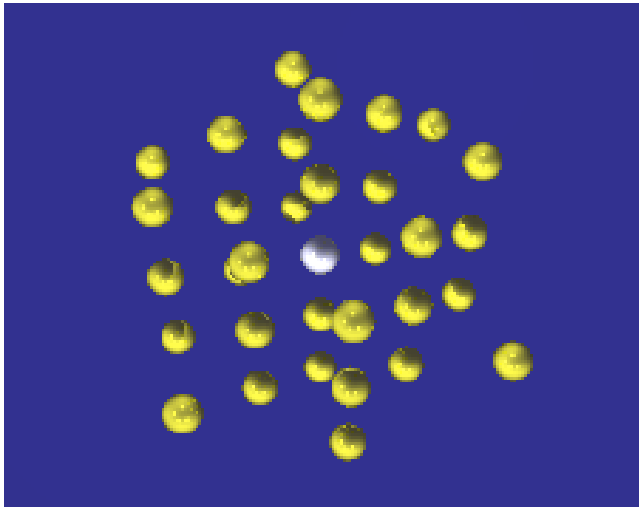
scaling verified as ρ varied by 30!

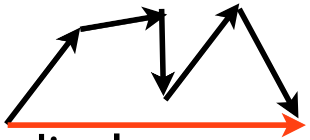
$$\xi = 0.435(15)$$

Normal State at Large P

One particle in a sea of non-interacting fermions

Binding ~ 0.6 Ef
Effective mass ~ 1





rms displacement of the impurity
measures effective mass

Calculate systems w/ total momentum k, extract E(k)
k=0 gives Binding, curvature gives effective mass

Unequal Masses

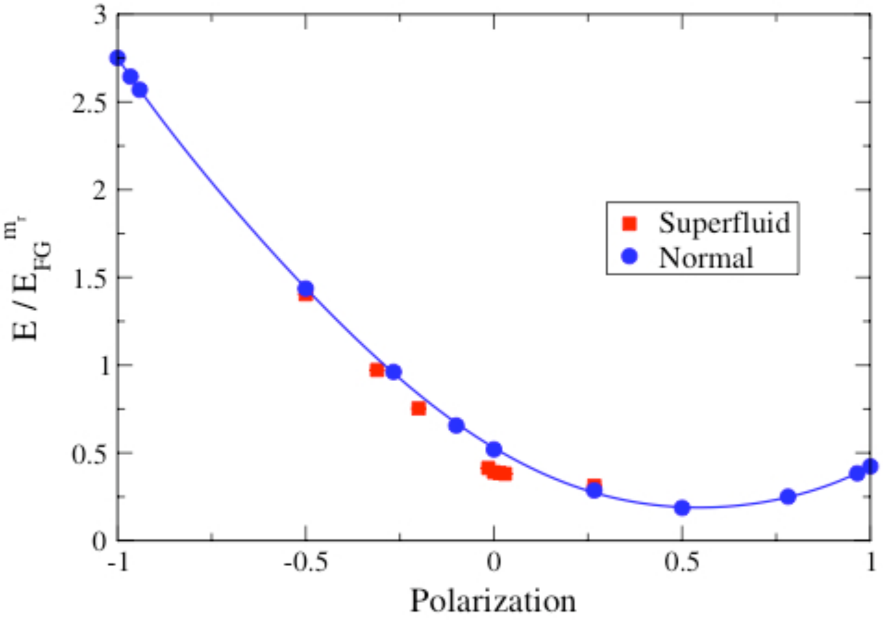
We concentrate on Mh/Ml = 6.5
approximate K/Li ratio

BCS Equations unchanged for constant reduced mass
Individual Quasiparticle Excitation Energies:

$$E_{h(l)}(k) = \frac{\xi_{h(l)}(k) - \xi_{l(h)}(k)}{2} + \sqrt{\left(\frac{\xi_h(k) + \xi_l(k)}{2}\right)^2 + \Delta^2(k)},$$

ξ Unchanged
Average Quasiparticle Energy Unchanged

Heavy-Light Fermions at Unitarity



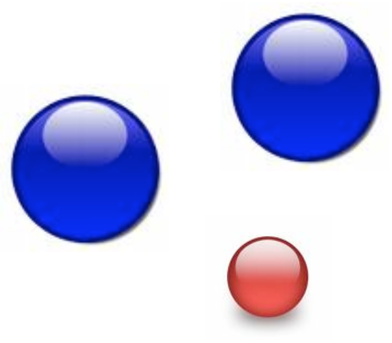
M/m = 6.5

Understand structure
for Nh >> Nl

Gezerlis, Gandolfi, Schmidt, JC, PRL 2009

Larger Mass Ratios

For 2H, 1L get collapse and Efimov States at M/m > 13.6



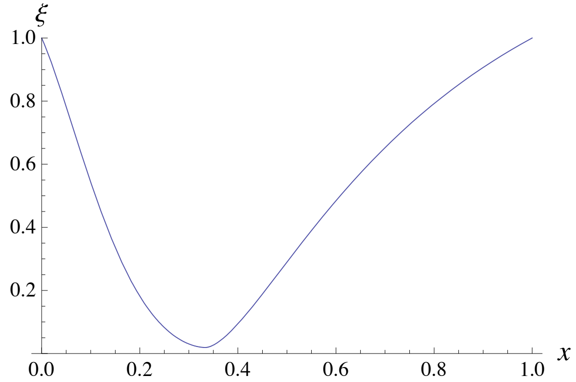
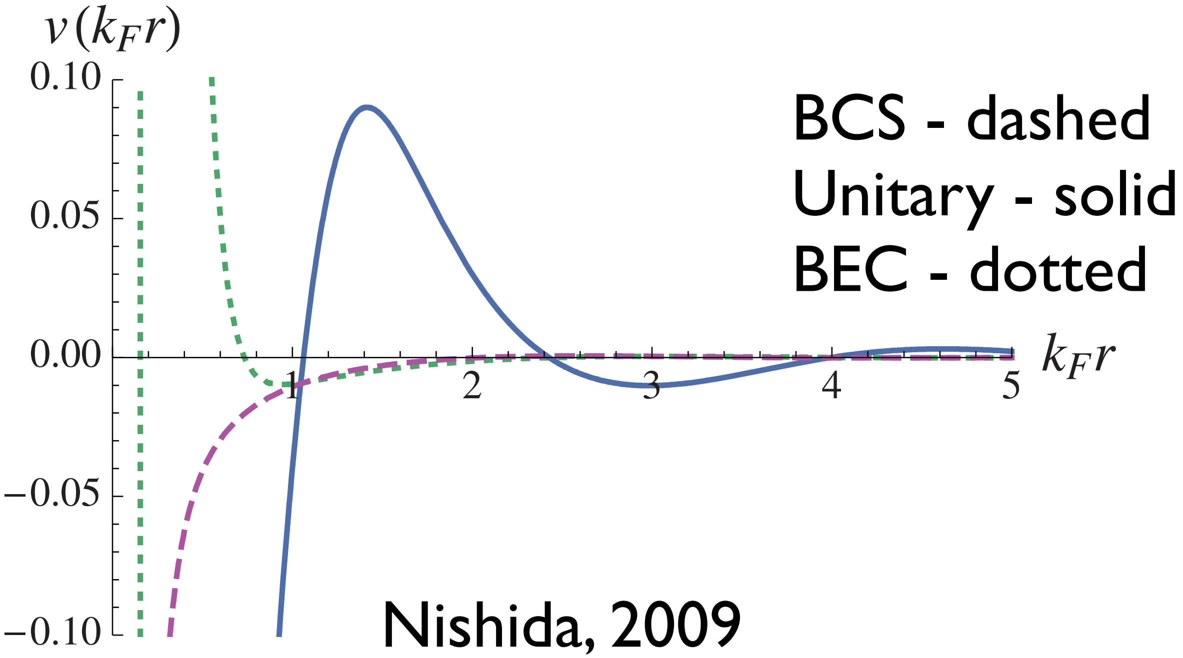


FIG. 1: The variational bound on ξ as a function of the abundance of light fermions x at $M/m = 8.62 + \epsilon$.

Nishida, Son, Tan 2008

For M/m = 8.62-13.6 can get weakly interacting gas of dimers and trimers

Born Oppenheimer Treatment

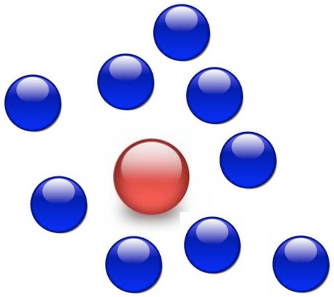


Nishida, 2009

In a gas of light particles, heavy particles are attractive
at moderate distances

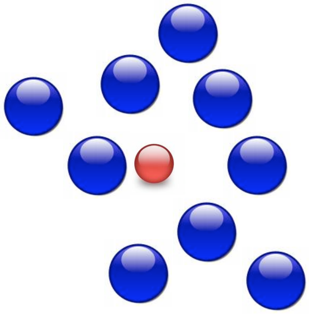
Three and four heavy centers at fixed pair distances
approximately equal to sum of pair interactions

Binding of One Heavy or One Light



$B(H) = 0.36\ E_F(L)$

effective mass ~1.0



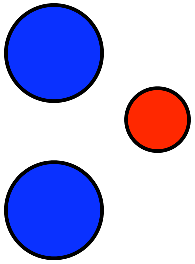
$B(L) = 2.3\ E_F(H)$

effective mass ~ 1.3

Agreement w/ previous calculations

R. Combescot et al., Phys. Rev. Lett. 98, 180402 (2007)

Efimov Physics in Few-Body Heavy Light Systems

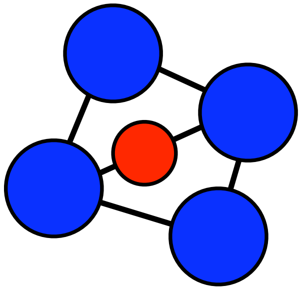


2 Heavy Fermions - 1 Light

Collapse at M/m = 13.6

Efimov, NPA 210, 157

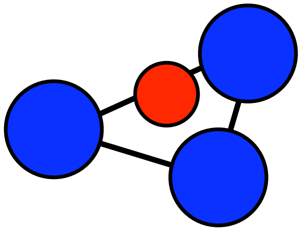
Assume nodes independent of light particle



Nh = 2 $\mathbf{r}_{12} \cdot \hat{z}$

Nh = 3 $\mathbf{r}_{12} \times \mathbf{r}_{13} \cdot \hat{z}$

Nh = 4 $\mathbf{r}_{12} \times \mathbf{r}_{13} \cdot \mathbf{r}_{1;234}$



Nodes when ‘volume’ goes to zero

Collapse: 2H 1L M/m = 13.6

3H 1L M/m ~ 10.5

4H 1L M/m ~ 9.5

Gandolfi & JC , 2010

Low Energy Scattering: Explicit States

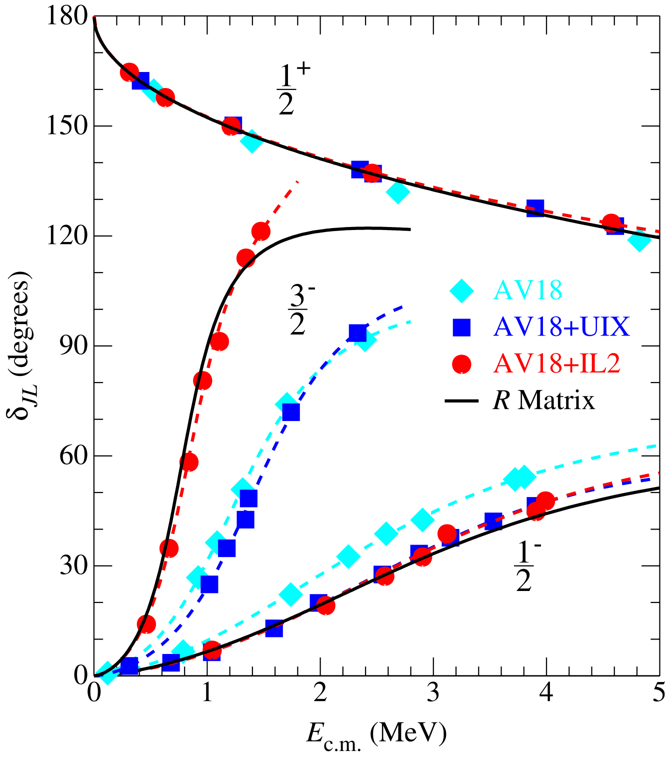
Enforce Logarithmic Derivative at R

$$\Psi_{n+1}(\mathbf{R}') = \int_{|\mathbf{r}|<R_0} d\mathbf{R}_{c1}\, d\mathbf{R}_{c2}\, d\mathbf{r}\, G(\mathbf{R}', \mathbf{R}; \Delta\tau) \times \left[\Psi_n(\mathbf{R}) + \frac{G(\mathbf{R}', \mathbf{R}_e; \Delta\tau)}{G(\mathbf{R}', \mathbf{R}; \Delta\tau)} \left(\frac{r_e}{r}\right)^3 \Psi_n(\mathbf{R}_e) \right].$$

Multiple Solutions at same E for multi-channel scattering.

Also useful for Asymptotic constants

Viviani talk, Nollett, ...



Nollett, et al, PRL 2007

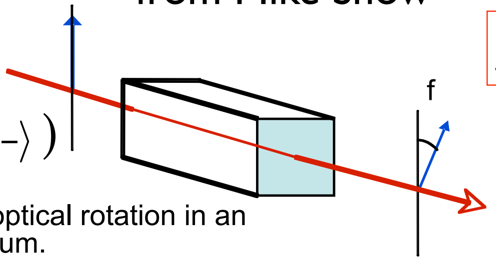
Shorter-Range Correlations required for Parity Violation
PV Interaction: Pion exchange plus short-range

A Parity-Violating Observable: Neutron Spin Rotation

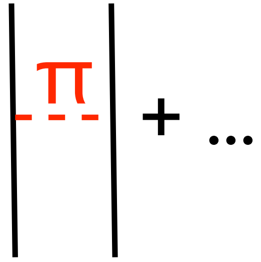
from Mike Snow

Also: np→dγ, ...

$$f(0) = f_{PC} + f_{PV}(\vec{\sigma}\cdot\vec{k})$$



$$|\uparrow\rangle_i = \frac{1}{\sqrt{2}}\left(|+\rangle + |-\rangle\right)$$



- Analogous to optical rotation in an “handed” medium.
- Transversely-polarized neutrons corkscrew due to the NN weak interaction
- ***PV Spin Angle*** is independent of incident neutron energy in cold neutron regime, $d\phi_{PV}/dx \sim 10^{-6}$ rad/m based on dimensional analysis
- $d\phi_{PC}/dx$ (due to B field) can be much larger than $d\phi_{PV}/dx$, and is v_n dependent

Refractive index dependent on neutron helicity

$$\frac{1}{\sqrt{2}}\left(e^{-i(\phi_{PC}+\phi_{PV})}|z\rangle + e^{-i(\phi_{PC}-\phi_{PV})}|-z\rangle\right)$$

$$\phi_{PV} = \varphi_+ - \varphi_- = 2\pi l \rho f_{PV}$$

Dmitriev *et al.* Phys Lett **125** 1 (1983)

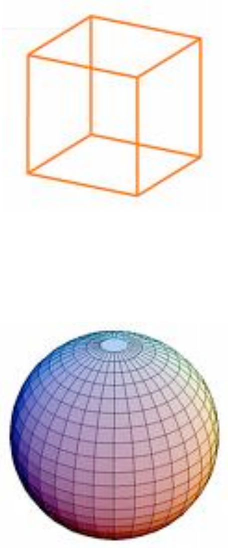
$$\phi_{PV}(\vec{n},{}^4\mathrm{He}) = -\left(0.97 f_\pi + 0.22 h^0_\omega - 0.22 h^1_\omega + 0.32 h^0_\rho - 0.11 h^1_\rho - 0.02 h'^1_\rho\right)\ \mathrm{rad/m}$$

$$\phi_{\mathrm{PV}}(n\,{}^4\mathrm{He}) = (1.2\lambda_s^{nn} + 0.6\lambda_s^{np} + 1.3\lambda_t - 2.7\rho_t)\ m_n$$

Zhu *et al.* Nucl. Phys. A **748** 435-498 (2005)

For complicated case (multi-particle breakup), we can enforce simple (unphysical) boundary conditions. (for example 11Li).

What information does this contain about the S-matrix?

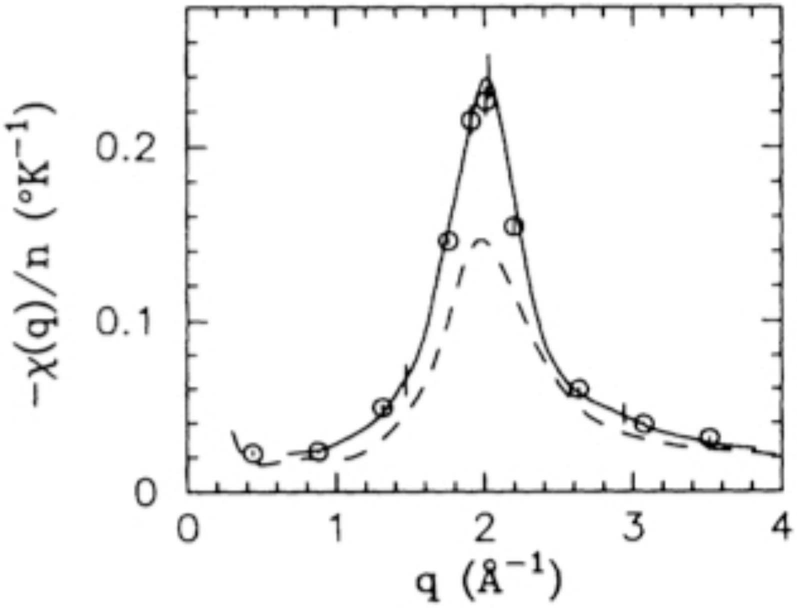


Static Response

$V_{ext}(r) = 2v_q cos(\mathbf{q} \cdot \mathbf{r})$

$n_{\mathbf{q}} = \chi(\mathbf{q})v_{\mathbf{q}} + C_3 v\mathbf{q}^3$

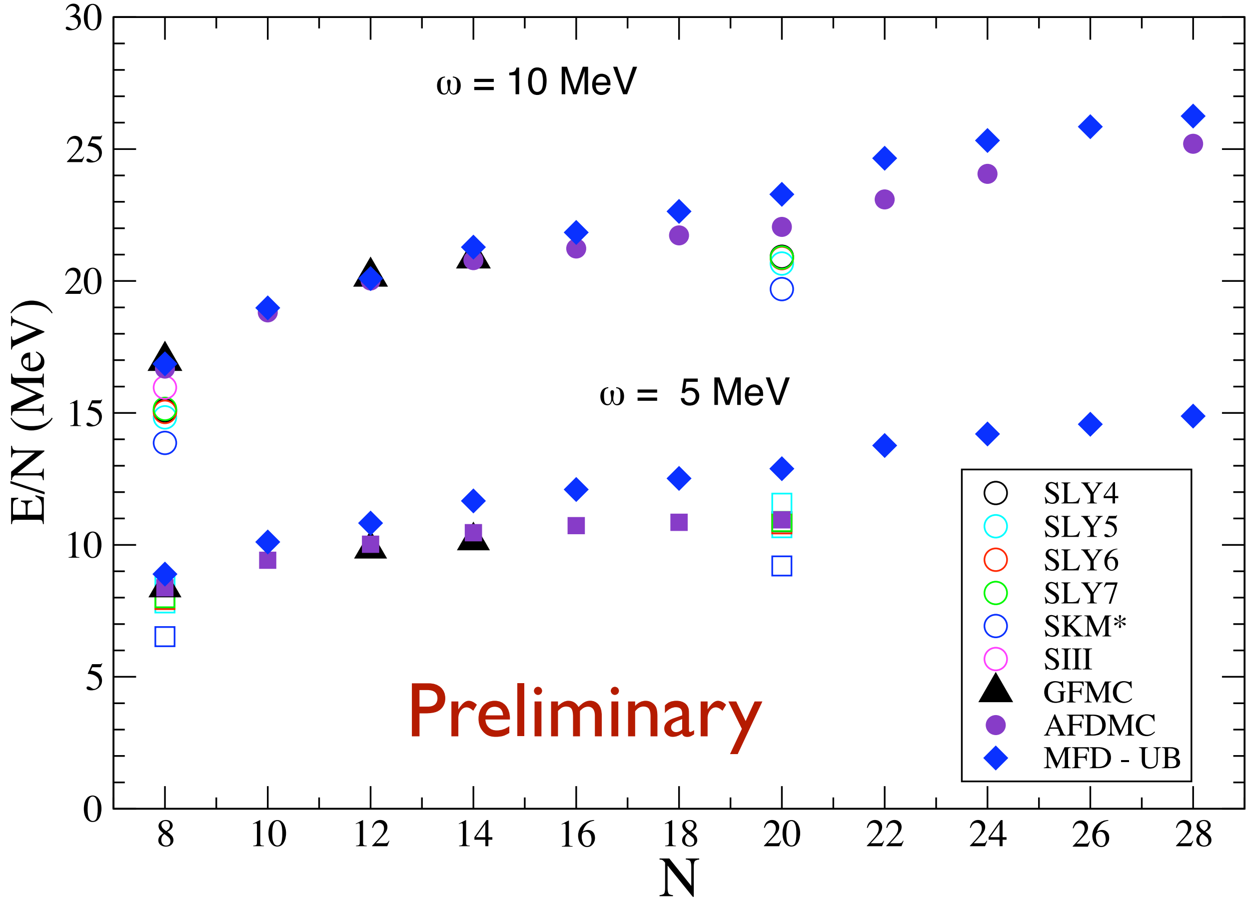
$E_v = E_0 + \chi(q)v_{\mathbf{q}}^2 + C_4 v_{\mathbf{q}}^4$



Liquid He-4

Moroni, et al PRL 1992

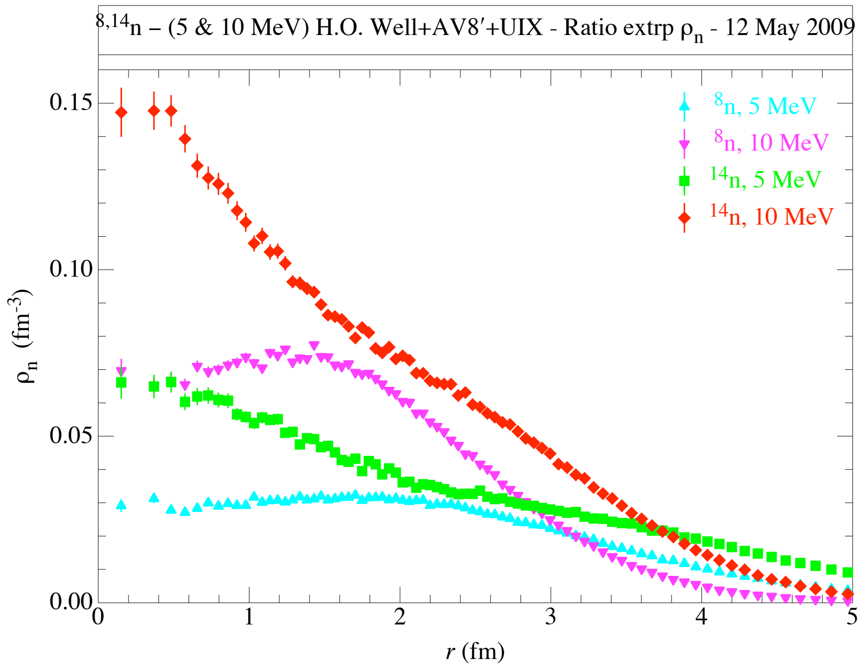
Neutron Drops in an External Well (HO)

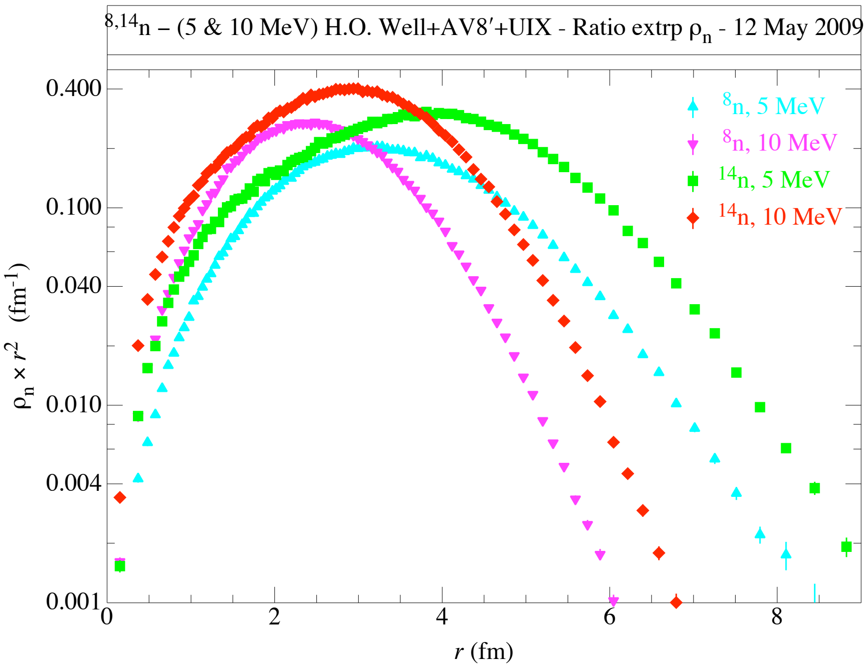


Implies significantly more repulsive isovector gradient terms

Carlson, Pieper, Gandolfi, preliminary

Neutron Drop Densities





Dynamic Response

Inclusive Scattering at Higher Energy
- Imaginary Time Response

Linear Response

$$S(k,\omega) = \sum_f \langle 0|\rho^\dagger(\mathbf{k})|f >< f|\rho(\mathbf{k})|0\rangle \delta(E_f - E_0 - \omega)$$

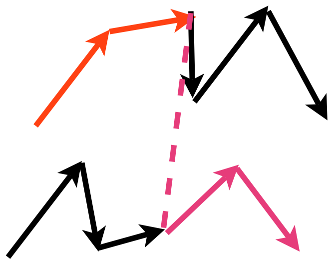
for example for electron scattering longitudinal response

$$\rho(\mathbf{k}) = \sum_i \exp(i\mathbf{k}\cdot r)\ [1+\tau_z(i)]/2$$

Can really only calculate imaginary time response

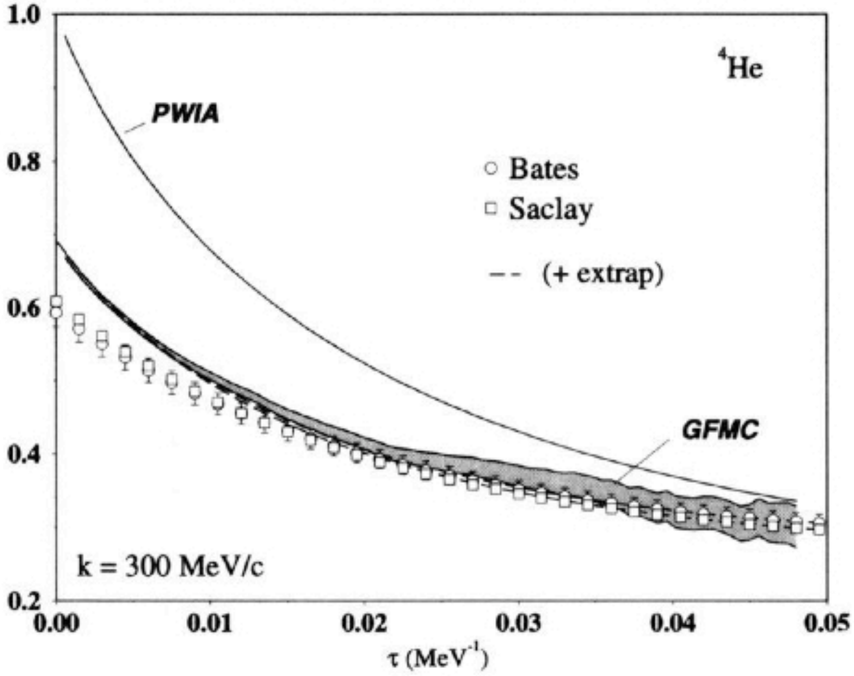
$$E(k,\tau) = \int d\omega\ S(k,\tau)\exp[-\omega\tau]$$

$$E(k,\tau) = \langle 0|\ \rho^\dagger(\mathbf{k})\ \ \exp[-H\tau]\ \rho(\mathbf{k})\ |0\rangle$$



Longitudinal Respone

300 MeV/c



400 MeV/c

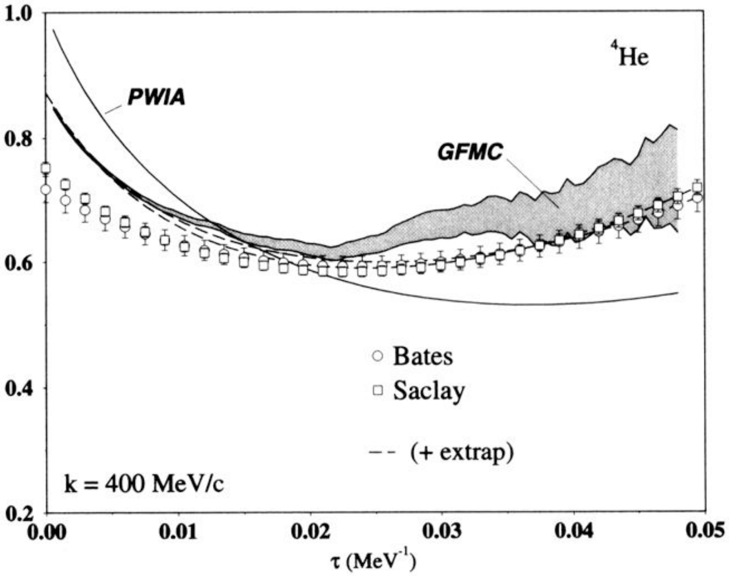


FIG. 3. Same as Fig. 2, but at $k = 400$ MeV/c.

Transverse response shows
importance of 2-body currents

Maximum Entropy Techniques used to reconstruct S(k,w)

Would be very interesting to do neutrino scattering on 12C

Major Challenges

More complete scattering (more channels), breakup
Bigger Nuclei / Nuclear - Neutron Matter
More General Interactions
Improved/ More Response Calculations