CISS07 8/30/2007

Comprehensive treatment of correlations at different energy scales in nuclei using Green's functions

Lecture 1: 8/28/07	Propagator description of single-particle motion and the link with experimental data
Lecture 2: 8/29/07	From Hartree-Fock to spectroscopic factors < 1: inclusion of long-range correlations
Lecture 3: 8/29/07	Role of short-range and tensor correlations associated with realistic interactions
Lecture 4: 8/30/07	Dispersive optical model and predictions for nuclei towards the dripline
Adv. Lecture 1: 8/30/07	Saturation problem of nuclear matter & pairing in nuclear and neutron matter
Adv. Lecture 2: 8/31/07	Quasi-particle density functional theory

Wim Dickhoff
Washington University in St. Louis

The two "most elusive" numbers in nuclear physics

- What are these numbers?
- In what sense are they elusive?
- What is the history?
- Three-body forces? Relativity? Give up?
- What has been learned from (e,e´p)?
- What really decides the saturation density?
- Nuclear Matter with SRC? No LRC?
- Conclusions
- Pairing …

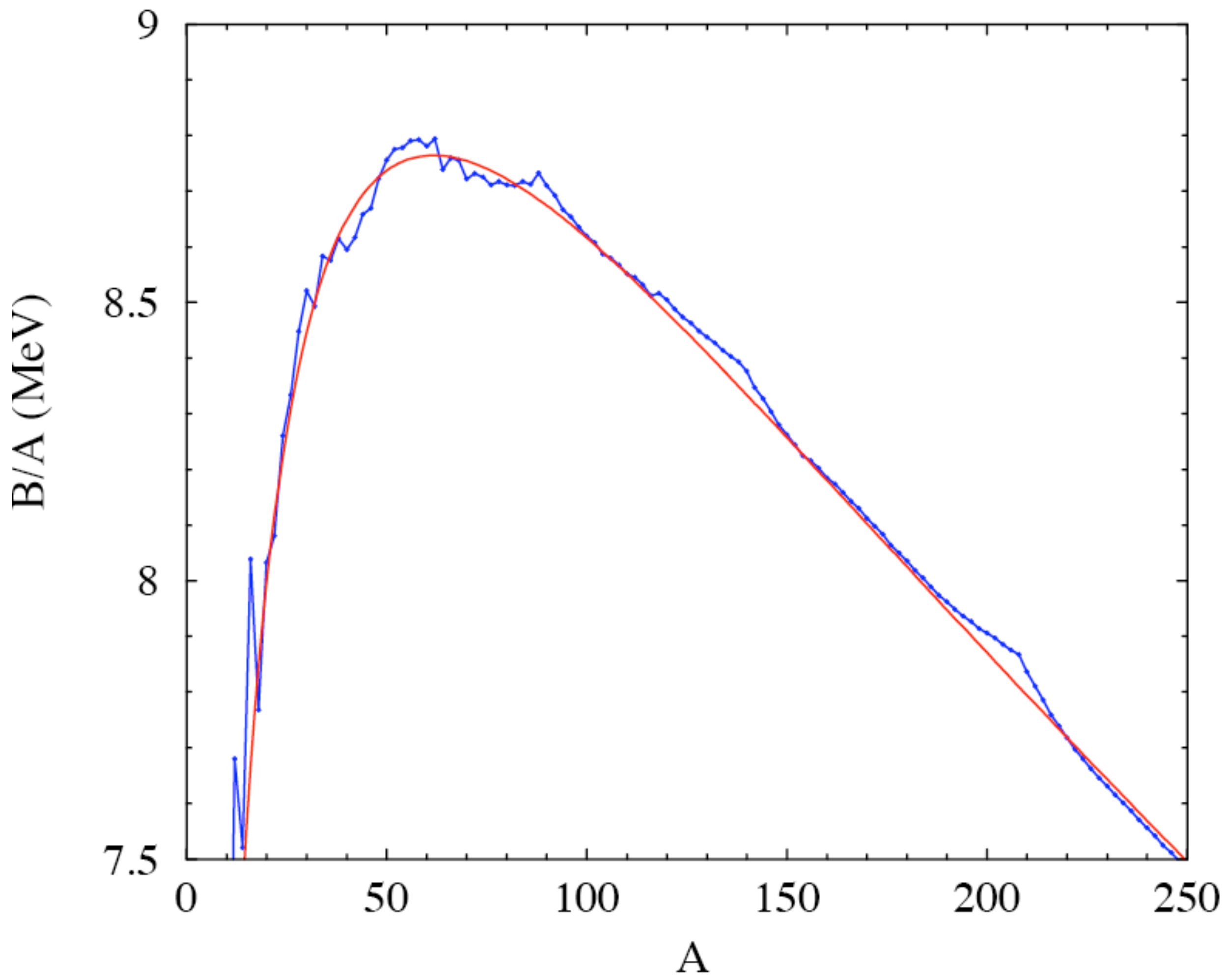
Empirical Mass Formula

Global representation of nuclear masses (Bohr & Mottelson)

$$B = b_{vol}A - b_{surf}A^{2/3} - \tfrac{1}{2}b_{sym}\frac{(N-Z)^2}{A} - \tfrac{3}{5}\frac{Z^2e^2}{R_c}$$

- Volume term $b_{vol} = 15.56$ MeV
- Surface term $b_{surf} = 17.23$ MeV
- Symmetry energy $b_{sym} = 46.57$ MeV
- Coulomb energy $R_c = 1.24\, A^{1/3}$ fm
- Pairing term must also be considered

Empirical Mass Formula



Plotted: most stable nucleus for a given A

Central density of nuclei

Multiply charge density at the origin by A/Z

$\Rightarrow$ Empirical density = 0.16 nucleons / fm^3

$\Rightarrow$ Equivalent to $k_F = 1.33$ fm^{-1}

Nuclear Matter

N = Z

No Coulomb

$A \Rightarrow \infty$, $V \Rightarrow \infty$ but $A/V = \rho$ fixed

"Two most important numbers"

b_{vol} = 15.56 MeV and $k_F = 1.33$ fm^{-1}

Historical Perspective

- First attempt using scattering in the medium — *Brueckner* 1954
- Formal development (linked cluster expansion) — *Goldstone* 1956
- Low-density expansion — *Galitskii* 1958
- Reorganized perturbation expansion (60s) involving ordering in the number of hole lines — *Bethe & students*, *BBG*-expansion
- Variational Theory vs. Lowest Order *BBG* (70s) — *Clark, Pandharipande*
- Variational results & next hole-line terms (80s) — *Day, Wiringa*
- Three-body forces? Relativity? (80s) — *Urbana, CUNY*
- Confirmation of three hole-line results (90s) — *Baldo et al.*
- New insights from experiment about what nucleons are up to in the nucleus (90s & 00s) — ***NIKHEF* Amsterdam**, *JLab*

Old pain and suffering!

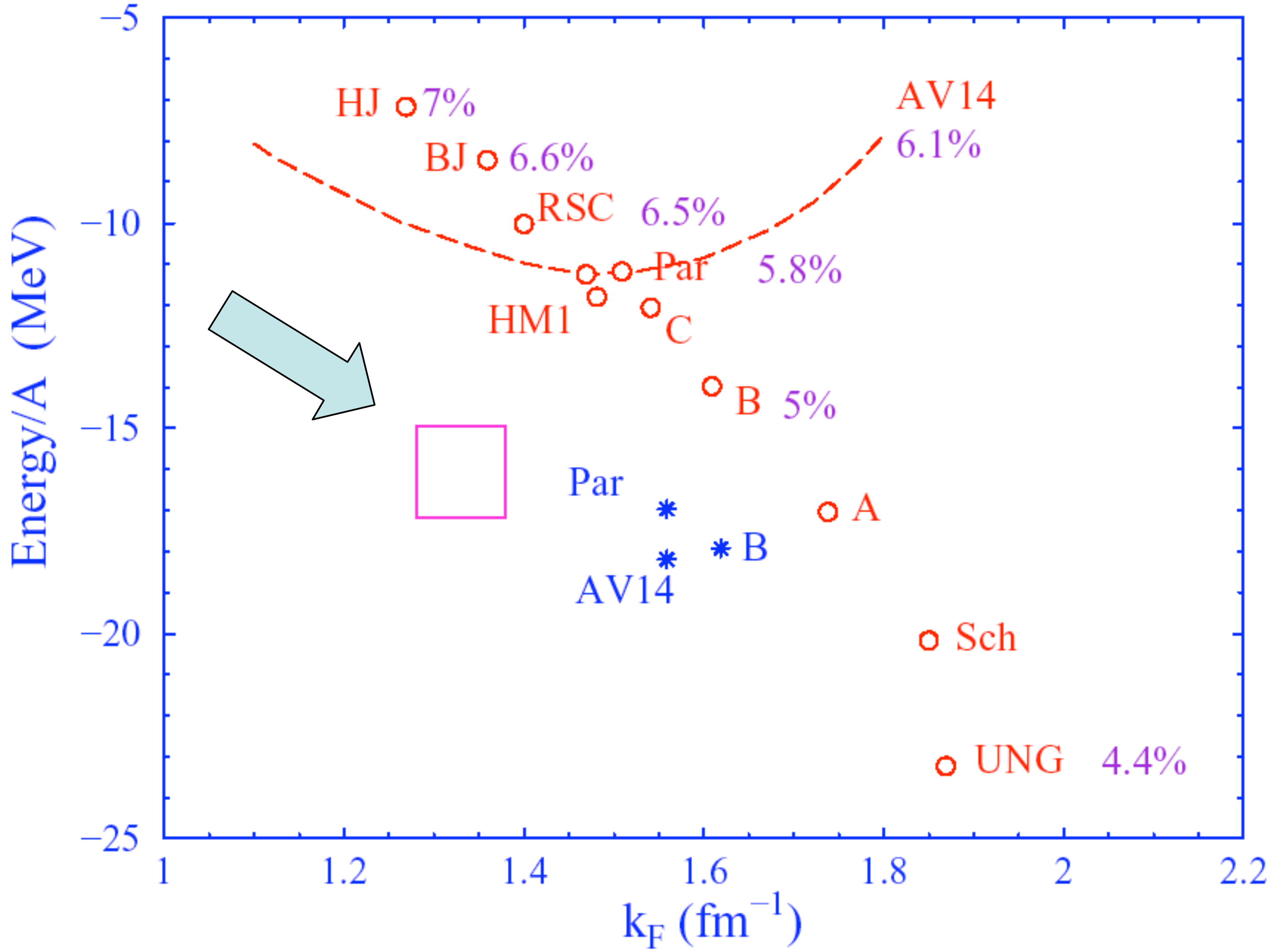
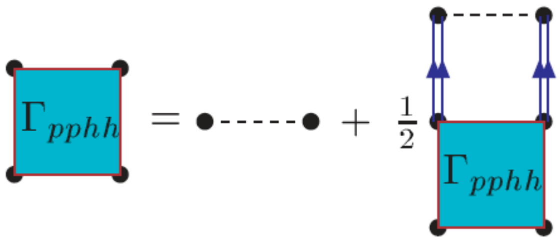


Figure adapted from Marcello Baldo (Catania)

Lowest-order Brueckner theory (two hole lines)



G^f_{BG} angle-average of

$$G^f_{BG}(k_1,k_2;E)=\frac{\theta(k_1-k_F)\theta(k_2-k_F)}{E-\varepsilon(k_1)-\varepsilon(k_2)+i\eta}$$

$$\langle k\ell|G^{JST}(K,E)|k'\ell'\rangle=\langle k\ell|V^{JST}|k'\ell'\rangle+\frac{1}{2}\sum_{\ell''}\int_0^\infty\frac{dq}{(2\pi)^3}q^2\langle k\ell|V^{JST}|q\ell''\rangle G^f_{BG}(q;K,E)\langle q\ell''|G^{JST}(K,E)|k'\ell'\rangle$$

Spectrum
$$\varepsilon_{BHF}(k)=\frac{\hbar^2k^2}{2m}+\Sigma_{BHF}(k;\varepsilon_{BHF}(k))$$

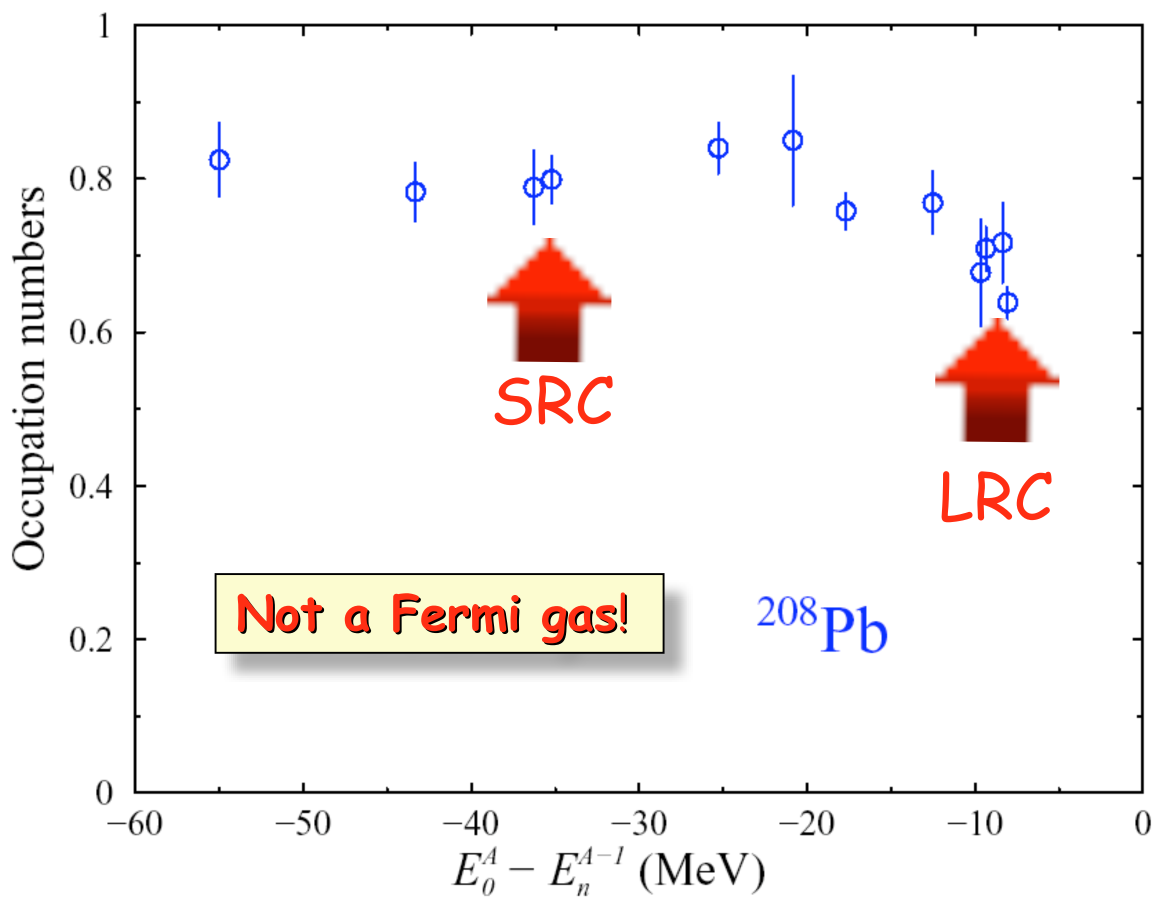
$k < k_F \Rightarrow$ standard choice
all $k \Rightarrow$ continuous choice

Self-energy
$$\Sigma_{BHF}(k;E)=\frac{1}{\nu}\sum_{m,m'}\int\frac{d^3k'}{(2\pi)^3}\theta(k_F-k')\left\langle\vec{k}\vec{k}'mm'\right|G\left(\vec{k}+\vec{k}';E+\varepsilon_{BHF}(k')\right)\left|\vec{k}\vec{k}'mm'\right\rangle$$

Energy
$$\frac{E}{A}=\frac{4}{\rho}\int\frac{d^3k}{(2\pi)^3}\theta(k_F-k)\frac{\hbar^2k^2}{2m}$$
$$+\frac{1}{2\rho}\sum_{m,m'}\int\frac{d^3k}{(2\pi)^3}\theta(k_F-k)\int\frac{d^3k'}{(2\pi)^3}\theta(k_F-k')\left\langle\vec{k}\vec{k}'mm'\right|G\left(\vec{k}+\vec{k}';\varepsilon_{BHF}(k)+\varepsilon_{BHF}(k')\right)\left|\vec{k}\vec{k}'mm'\right\rangle$$

M. van Batenburg (thesis, 2001) & L. Lapikás from ^{208}Pb (e,e´p) ^{207}Tl

Occupation of deeply-bound proton levels from **EXPERIMENT**



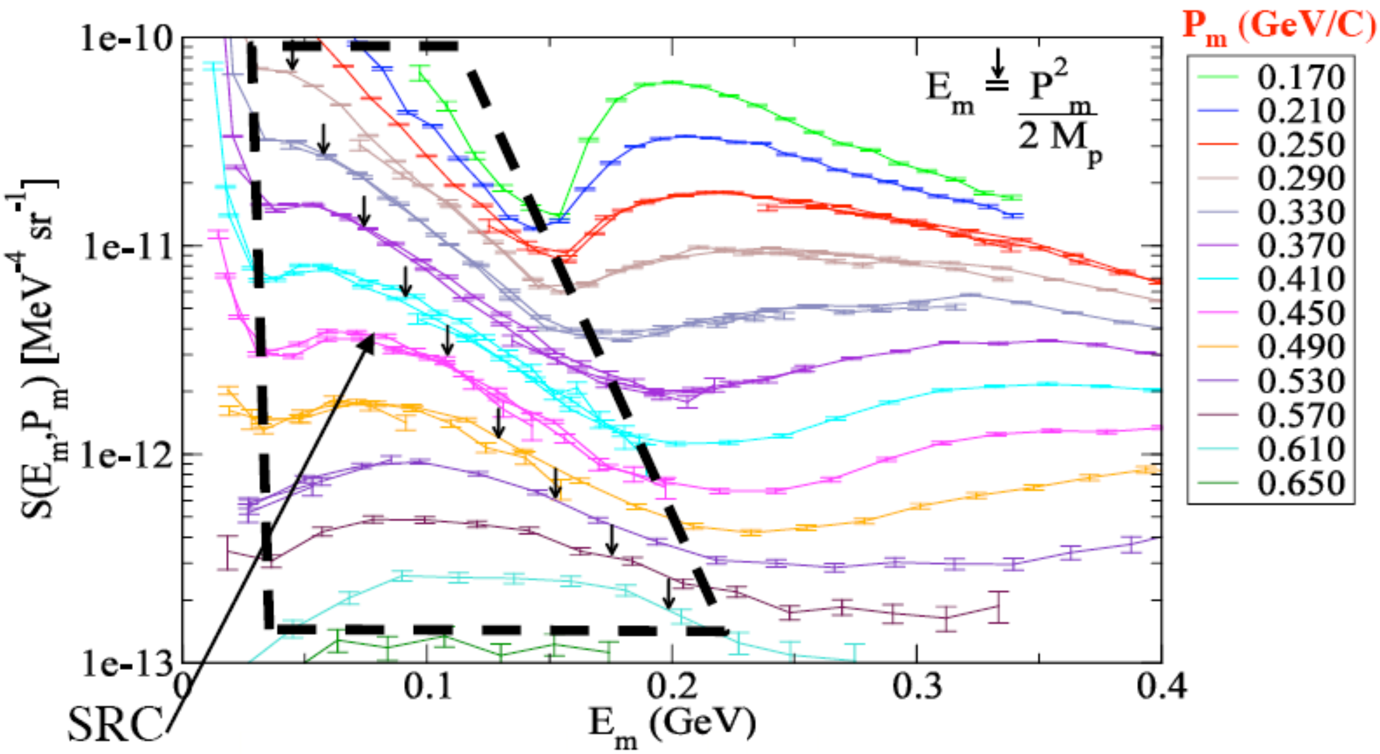
Up to 100 MeV missing energy and 270 MeV/c missing momentum

Covers the whole mean-field domain for the FIRST time!!

Confirmation of theory

What are the rest of the protons doing?

Jlab E97-006 Phys. Rev. Lett. 93, 182501 (2004) D. Rohe et al.



^{12}C

- Location of high-momentum components
- Integrated strength agrees with theoretical prediction Phys. Rev. C49, R17 (1994)

  $\Rightarrow$ 0.6 protons for ^{12}C

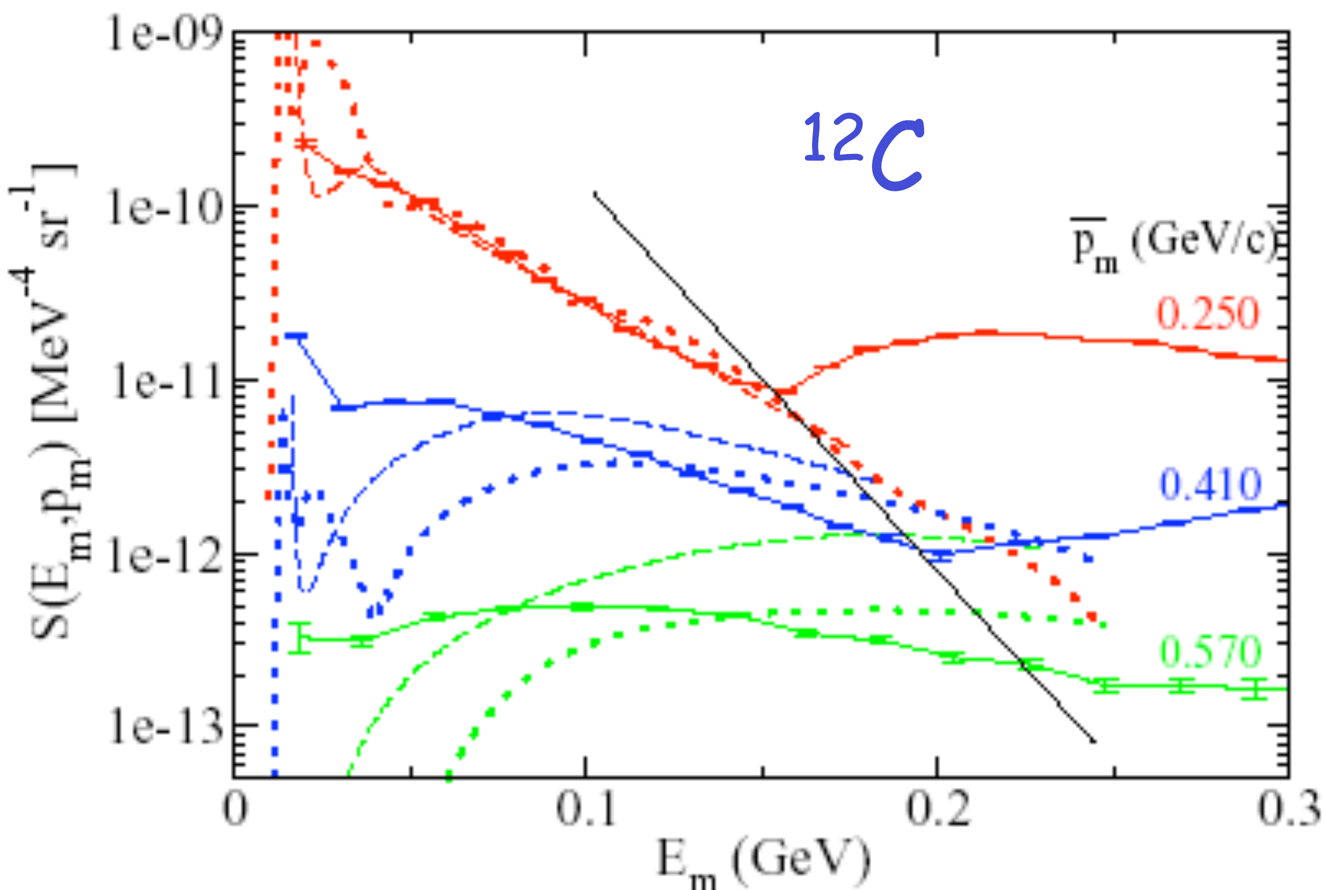
Green's function V 10

Where are the last protons? Answer is coming!

Jlab data
PRL**93**,182501 (2004)
Rohe et al.

Location of high-momentum component

integrated strength OK!



There are high-momentum components
in the nuclear ground state!

Energy Sum Rule (Migdal, Galitskii, Koltun ...)

Finite nuclei

$$E_0^A = \langle \Psi_0^A | \hat{H} | \Psi_0^A \rangle = \frac{1}{2} \sum_{\alpha\beta} \langle \alpha | T | \beta \rangle n_{\alpha\beta} + \frac{1}{2} \sum_{\alpha} \int_{-\infty}^{\varepsilon_F^-} dE \; E \, S_h(\alpha; E)$$

$$n_{\alpha\beta} = \langle \Psi_0^A | a_\alpha^+ a_\beta | \Psi_0^A \rangle = \frac{1}{\pi} \int_{-\infty}^{\varepsilon_F^-} dE \; \mathrm{Im}\, G(\beta, \alpha; E)$$

$$S_h(\alpha; E) = \sum_n \left| \langle \Psi_n^{A-1} | a_\alpha | \Psi_0^A \rangle \right|^2 \delta\left(E - \left(E_0^A - E_n^{A-1} \right) \right) = \frac{1}{\pi} \mathrm{Im}\, G(\alpha, \alpha; E)$$

Nuclear matter

$$\frac{E}{A} = \frac{1}{2} \left\{ \frac{4}{\rho} \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\varepsilon_F} dE \left(\frac{\hbar^2 k^2}{2m} + E \right) S_h(k; E) \right\}$$

- Presumes only two-body interactions!
- Correct description of experimental spectral function should yield good *E/A*!!

Where does binding come from (really)?

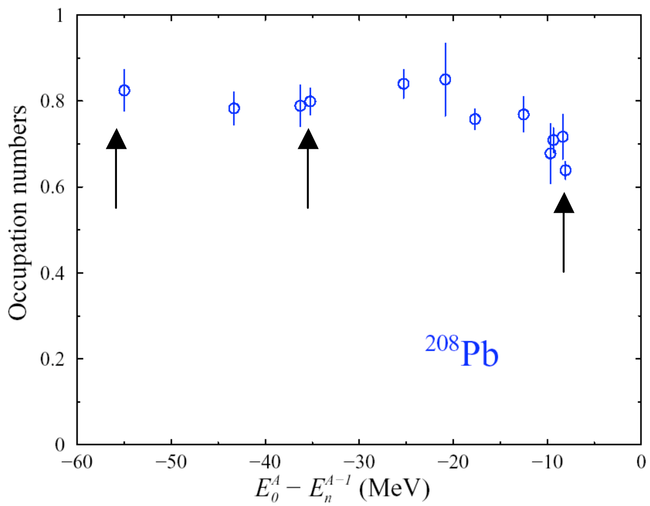
^{16}O PRC51,3040(1995)

lj	"BHF" ϵ	t	ΔE	Total ϵ	t	ΔE
$s\frac{1}{2}$ qh	-36.9	11.8	-50.3	-34.3	11.2	-36.0
$s\frac{1}{2}$ c				-90.4	17.1	-22.9
$p\frac{3}{2}$ qh	-15.4	17.6	9.1	-17.9	18.1	0.4
$p\frac{3}{2}$ c				-95.2	35.2	-10.0
$p\frac{1}{2}$ qh	-11.5	16.6	10.3	-14.1	17.2	5.5
$p\frac{1}{2}$ c				-103.6	35.9	-5.8
$\ell > 1$ c				-98.9	63.2	-12.3
E/A(MeV)		-1.9			-5.1	
$\langle r \rangle$(fm)		2.59			2.55	

Quasiholes contribute 37% to the total energy
High-momentum nucleons (continuum) contribute 63%
but represent **only** about 10% of the particles!!

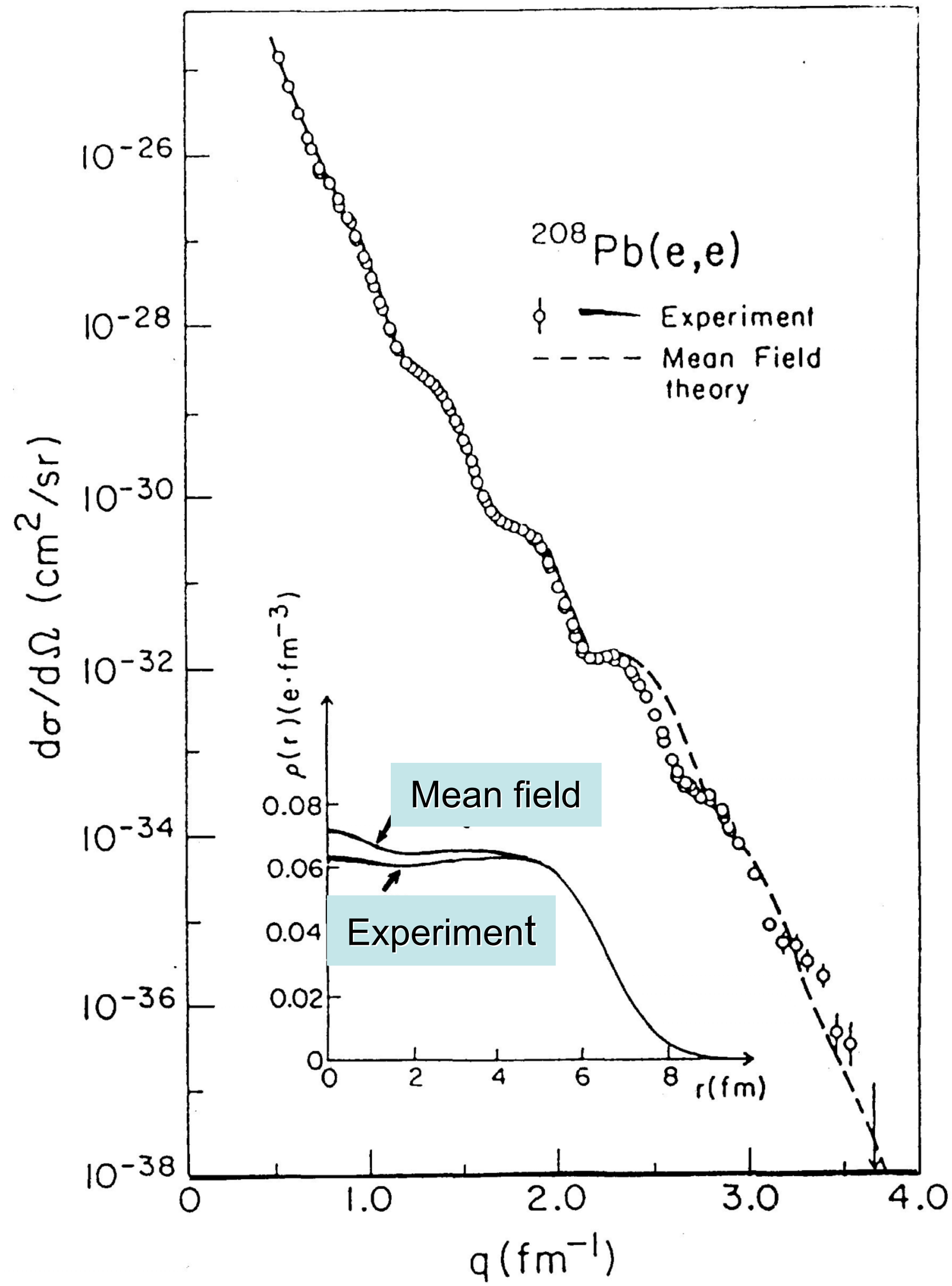
Saturation density and SRC

- Saturation density related to nuclear charge density at the origin. Data for ^{208}Pb $\Rightarrow$ $A/Z * \rho_{ch}(0) = 0.16\ fm^{-3}$
- Charge at the origin determined by protons in *s* states
- Occupation of 0*s* and 1*s* totally dominated by SRC as can be concluded from recent analysis of ^{208}Pb(e,e´p) data and theoretical calculations of occupation numbers in nuclei and nuclear matter.
- Depletion of 2*s* proton also dominated by SRC:
  15% of the total depletion of 25% (n_{2s} = 0.75)



- Conclusion: **Nuclear saturation dominated by SRC and therefore high-momentum components**

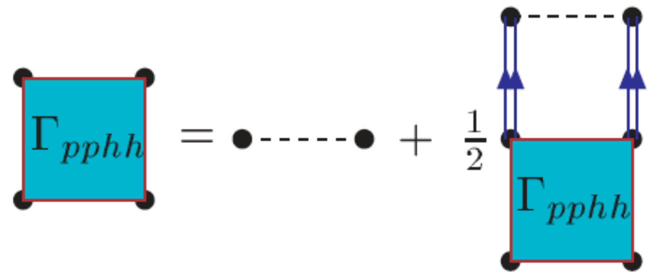
Elastic electron scattering from ^{208}Pb



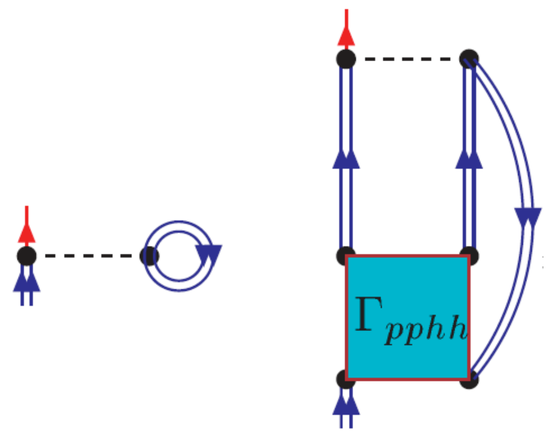
B. Frois *et al.*

Phys. Rev. Lett. **38**, 152 (1977)

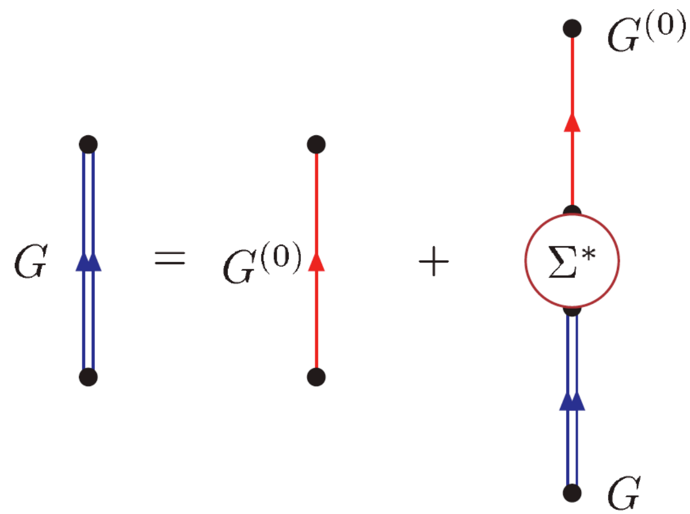
Self-consistent treatment of SRC in nuclear matter



Interaction



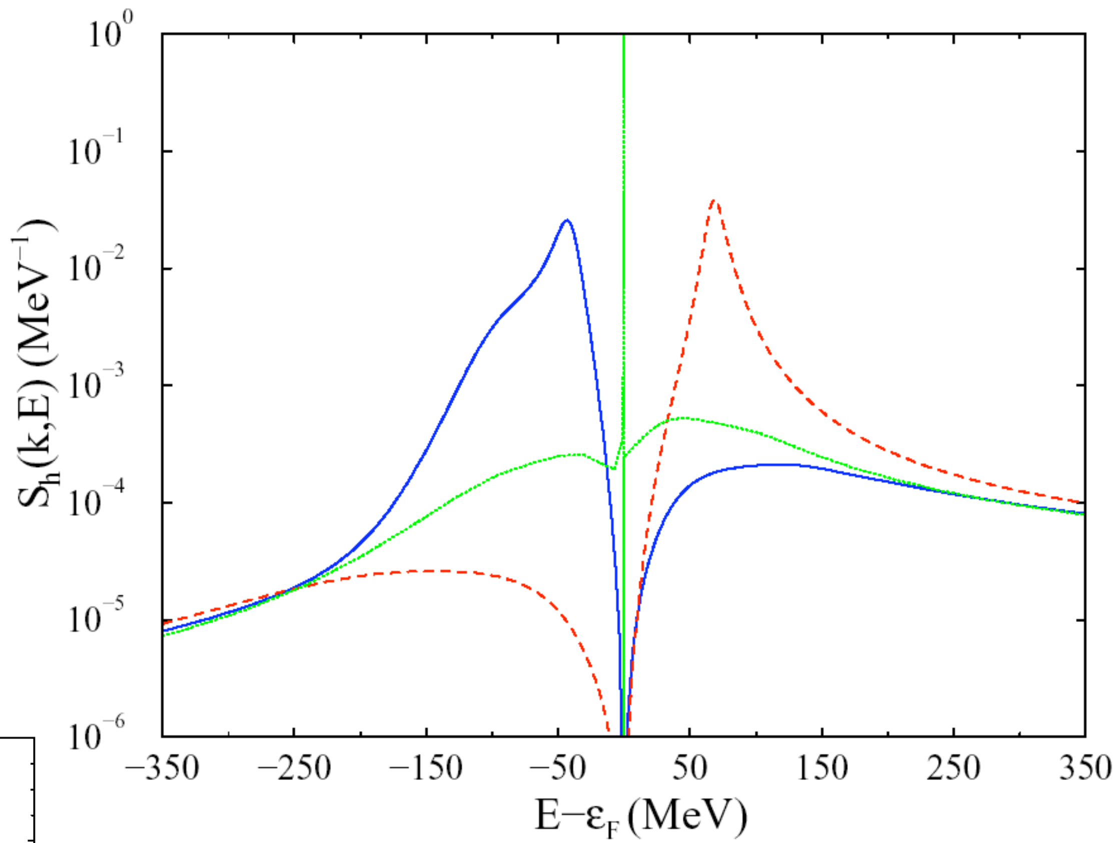
Self-energy

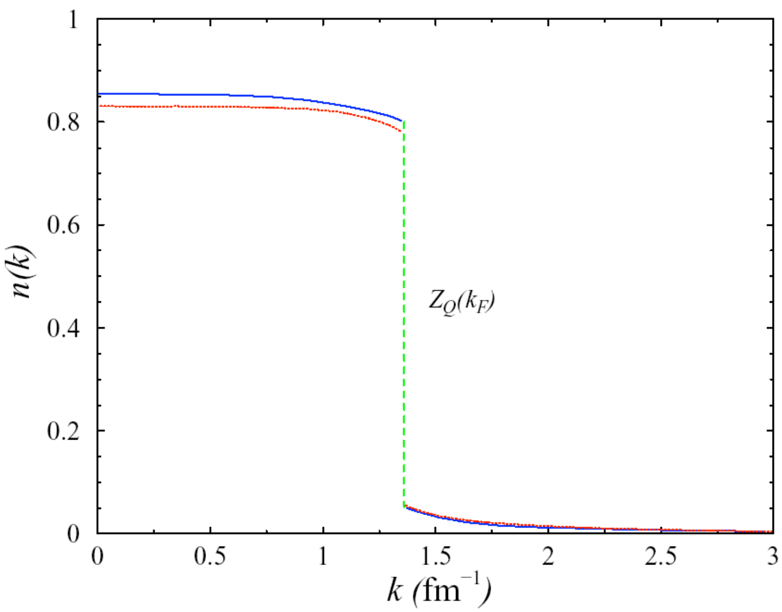


Dyson equation

Results from Nuclear Matter
2nd generation (2000)

- Spectral functions for k = 0, 1.36, & 2.1 fm^{-1}
- Common tails on both sides of ε_F





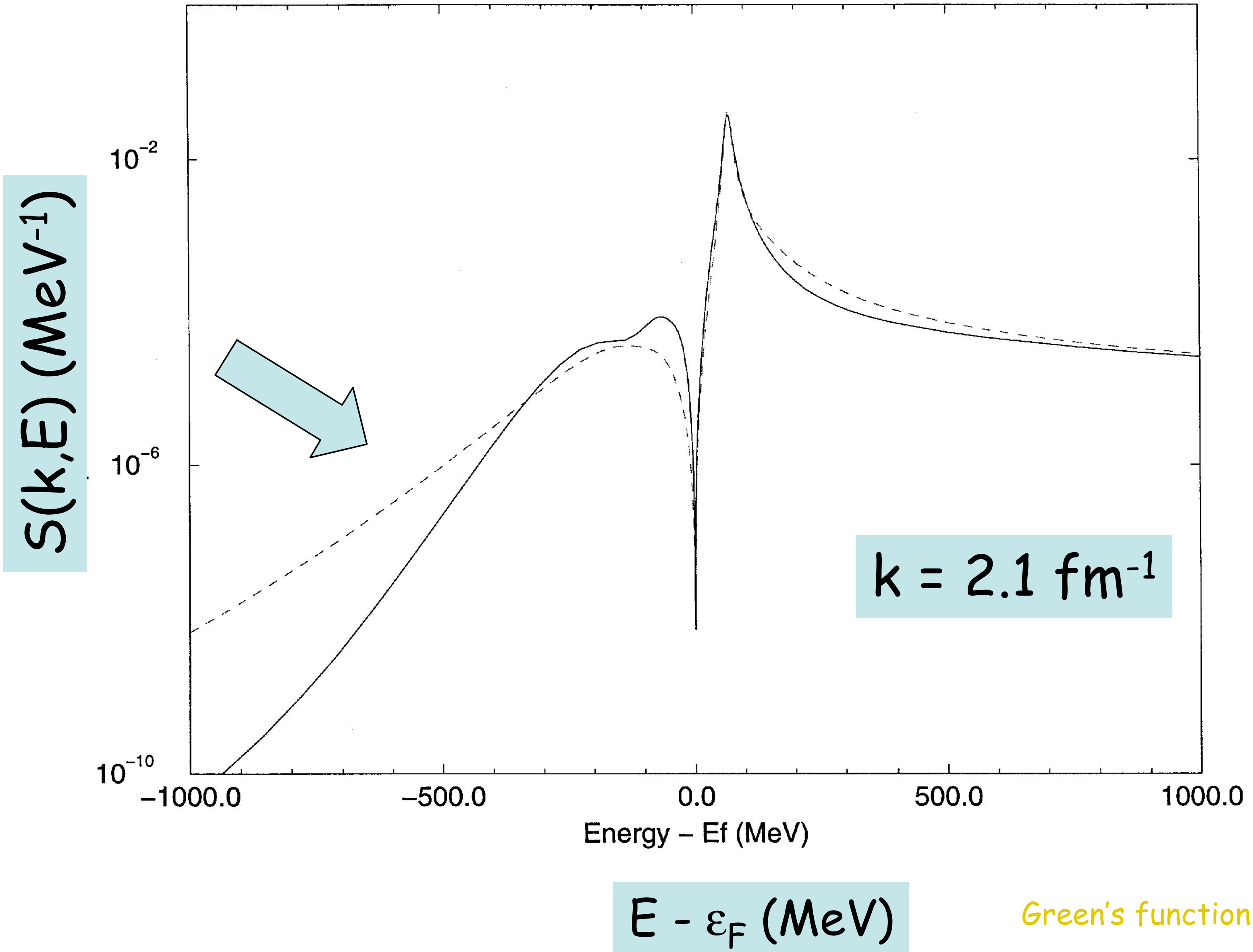
Momentum distribution :

only minor changes

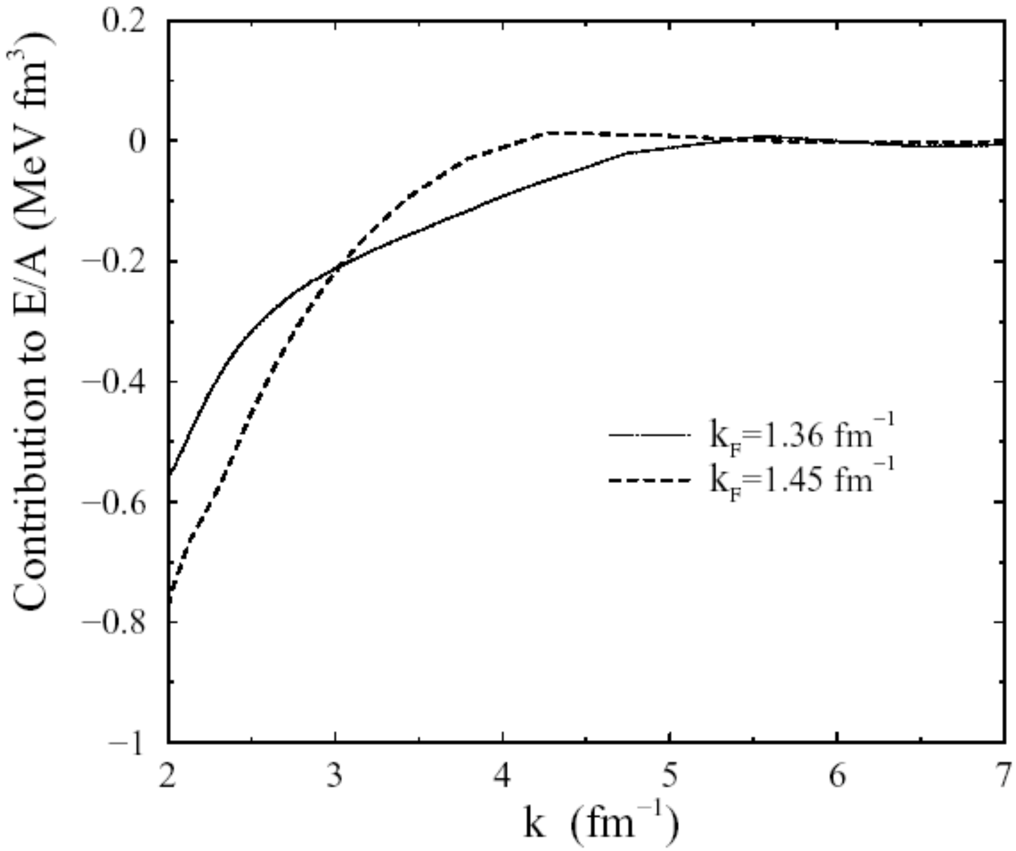
occupation in nuclei

depleted similarly!?!

Self-consistent spectral functions



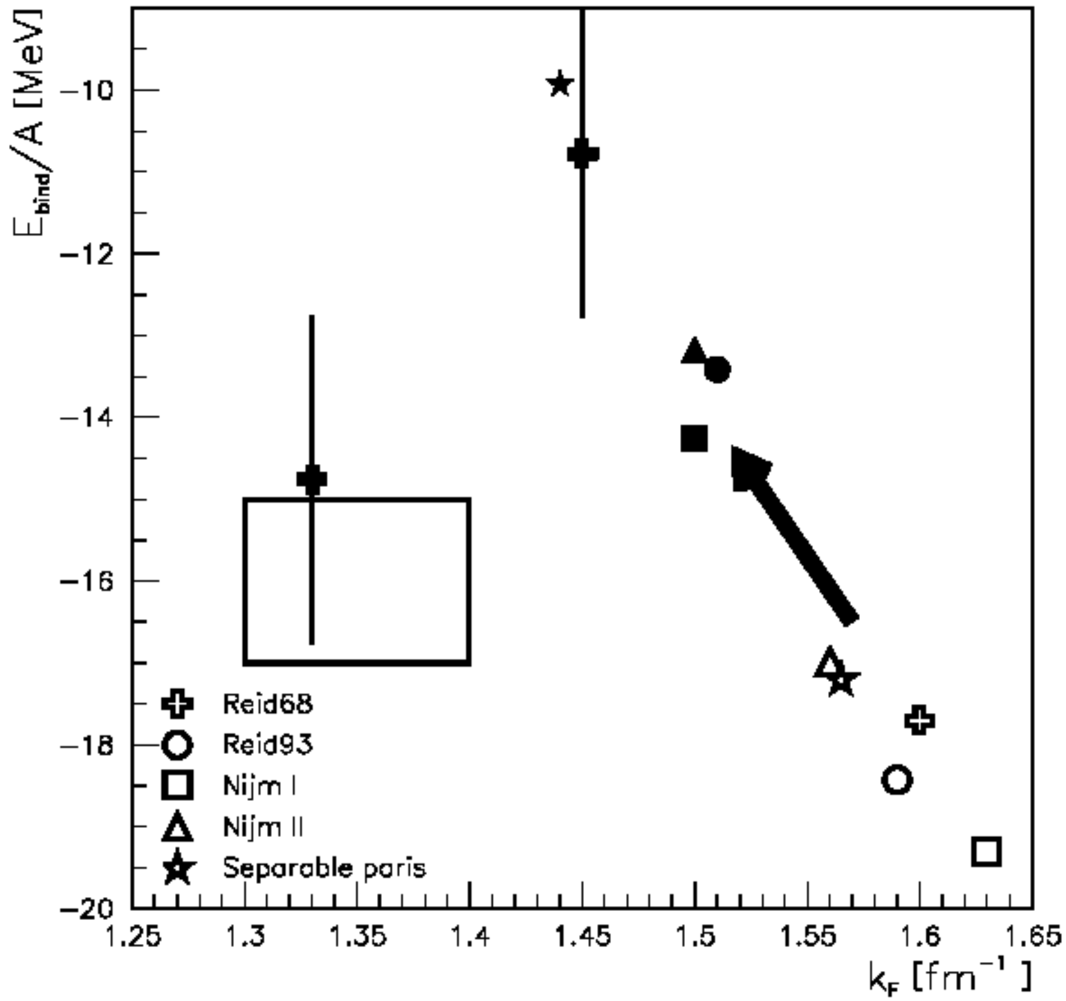
Saturation with self-consistent spectral functions in nuclear matter ⇒ reasonable saturation properties



Contribution to the energy per particle before integration over the single-particle momentum at high momentum for two densities

Saturation of Nuclear Matter
Ladders and self-consistency for Nuclear Matter

- Ghent group
  Dewulf, Van Neck & Waroquier
- St. Louis
  Stoddard, WD



Phys. Rev. Lett. **90**, 152501 (2003)

Self-consistent spectral functions

- Distribution below ε_F broadens for high momenta and develops a common tail at high missing energy
- Slight increase in occupation $k < k_F$ to 85% at $k_F = 1.36\ \mathrm{fm}^{-1}$ compared to Phys. Rev. *C***44**, R1265 (1991) & Nucl. Phys. **A555**, 1 (1993)
- Self-consistent treatment of Pauli principle
- Interaction between dressed particles weaker (reduced cross sections for both pn and nn)
- Pairing instabilities disappear in all channels
- Saturation with lower density than before and reasonable binding
- **Contribution of long-range correlations excluded**

Self-consistent Green's functions and the energy of the ground state of the electron gas

GW approximation
G — self-consistent sp propagator
W — screened Coulomb interaction
$\Rightarrow$ RPA with dressed sp propagators

Electron gas : -XC energies (Hartrees)

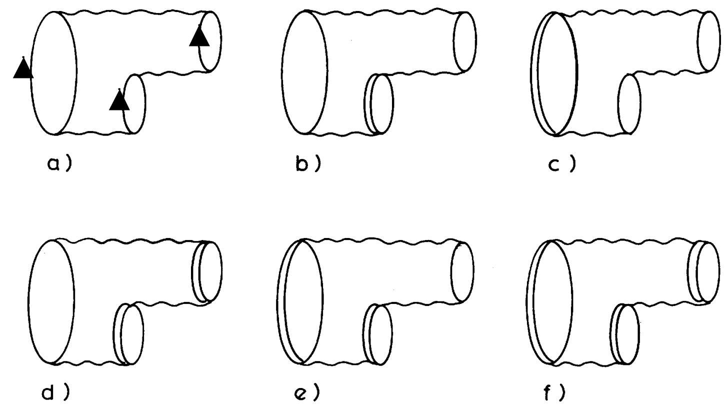
Method	$r_s = 1$	$r_s=2$	$r_s=4$	$r_s=5$	$r_s=10$	$r_s=20$	Reference
QMC	0.5180	0.2742	0.1464	0.1197	0.0644	0.0344	CA80
	0.5144	0.2729	0.1474	0.1199	0.0641	0.0344	OB94;OHB99
GW	0.5160	0.2727	0.1450	0.1185	0.0620	0.032	GG01
		0.2741	0.1465				HB98
RPA	0.5370	0.2909	0.1613	0.1340	0.0764	0.0543	

What about long-range correlations in nuclear matter?

- Collective excitations in nuclei very different from those in nuclear matter
- Long-range correlations normally associated with small q
- Contribution to the energy like $dq\, q^2 \Rightarrow$ very small (except for e-gas)
- Contributions of collective excitations to the binding energy of nuclear matter dominated by pion-exchange induced excitations?!?

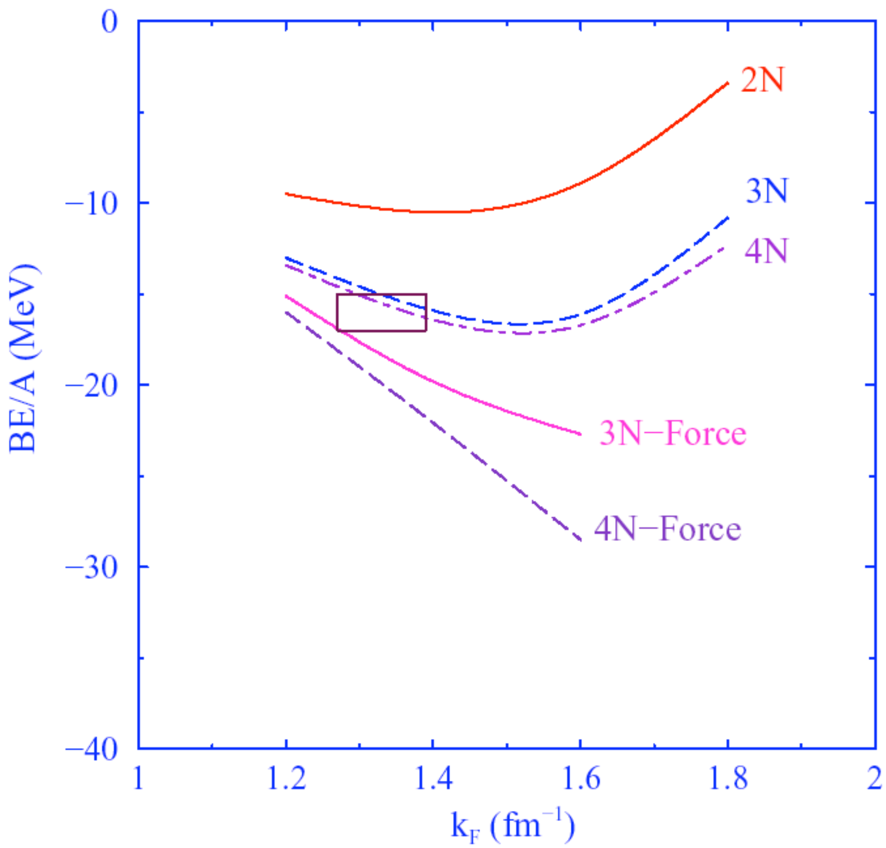
Inclusion of Δ-isobars as "3N-" and "4N-force"

Nucl. Phys. **A389**, 492 (1982)



k_F [fm^{-1}]	1.0	1.2	1.4	1.6
third order				
a)	-0.303	-1.269	-3.019	-5.384
b)	-0.654	-1.506	-2.932	-5.038
c)	-0.047	-0.164	-0.484	-1.175
d)	0.033	0.095	0.220	0.447
e)	-0.104	-0.264	-0.589	-1.187
f)	0.041	0.137	0.385	0.962
Sum	-1.034	-2.971	-6.419	-11.375

Inclusion of Δ-isobars as 3N- and 4N-force



2N,3N, and 4N from
B.D.Day, PRC24,1203(81)

Rings with Δ-isobars :

Nucl. Phys. **A389**, 492 (1982)

PPNPhys **12**, 529 (1983)

⇒ No sensible convergence with Δ-isobars

Nuclear Saturation without π-collectivity

- Variational calculations treat LRC (on average) and SRC simultaneously (Parquet equivalence) so **difficult** to separate LRC and SRC
- Remove 3-body ring diagram from Catania hole-line expansion calculation $\Rightarrow$ about the correct saturation density
- Hole-line expansion doesn't treat Pauli principle very well
- Present results improve treatment of Pauli principle by self-consistency of spectral functions => more reasonable saturation density and binding energy acceptable

- Neutron matter: pionic contributions must be included (Δ)

Pion collectivity: nuclei vs. nuclear matter

- Pion collectivity leads to pion condensation at higher density in nuclear matter (including Δ-isobars) => Migdal ...
- No such collectivity observed in nuclei $\Rightarrow$ LAMPF / Osaka data

Sakai/Wakasa group may disagree

- Momentum conservation in nuclear matter dramatically favors amplification of π-exhange interaction at fixed q
- In nuclei the same interaction is sampled over all momenta Phys. Lett. **B146**, 1(1984)

$$V_\pi(q) = -\frac{f_\pi^2}{m_\pi^2}\frac{q^2}{m_\pi^2 + q^2}$$

Needs further study

$\Rightarrow$ Exclude collective pionic contributions to nuclear matter binding energy

Two Nuclear Matter Problems

The usual one

- With π-collectivity and only nucleons
- Variational + CBF and
  three hole-line results presumed OK (for *E/A*) but not directly relevant for comparison with nuclei!
- **NOT OK** if Δ-isobars are included
- Relevant for neutron matter

The relevant one?!

- Without π-collectivity
- Treat only SRC
- But at a sophisticated level by using self-consistency
- Confirmation from Ghent results $\Rightarrow$ Phys. Rev. Lett. **90**, 152501 (2003)
- 3N-forces difficult $\Rightarrow$ π ...
- Relativity?

Comments

Relativity

- Saturation depends on NNσ-coupling in medium but underlying correlated two-pion exchange behaves differently in medium
- $m^* \rightarrow 0$ with increasing ρ opposite in liquid ^{3}He
  appears unphysical
- Dirac sea under control?
- sp strength overestimated too many nucleons for $k<k_F$

Three-body forces

- Microscopic models yield only attraction in matter and more so with increasing ρ
- Microscopic background of phenomenological repulsion in 3N-force (if it exists)?
- 4N-, etc. forces yield increasing attraction with ρ
- Needed in light nuclei and attractive!
- Mediated by π-exchange
- Argonne group can't get nuclear matter right with new 3N-force

Conclusions

- Good understanding of role of short-range correlations
  - Depletion of Fermi sea: nuclear matter OK for nuclei
    - Confirmed by experiment
  - High-momentum components
    - # of protons experimentally confirmed
      (Long-range correlations crucial
      for distribution of sp strength)

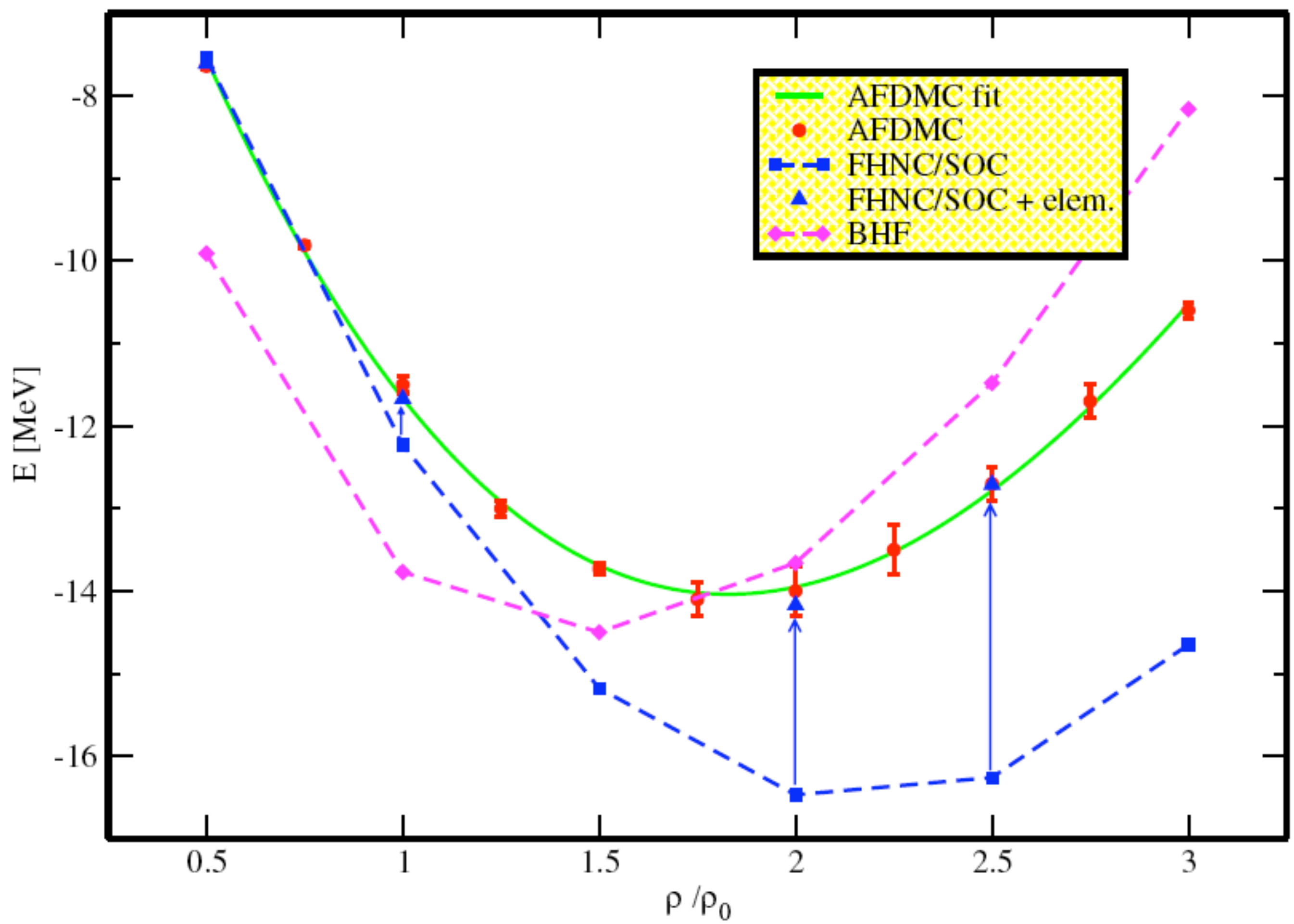
- Energy per particle from self-consistent Green's functions

- Better understanding of nuclear matter saturation
  $\Rightarrow$ SRC dominate (don't treat LRC from pions)

- We know what protons are up to in stable closed-shell nuclei!!

New stochastic results for ArV8'

Gandolfi et al., Phys. Rev. Lett. 98, 102593 (2007)

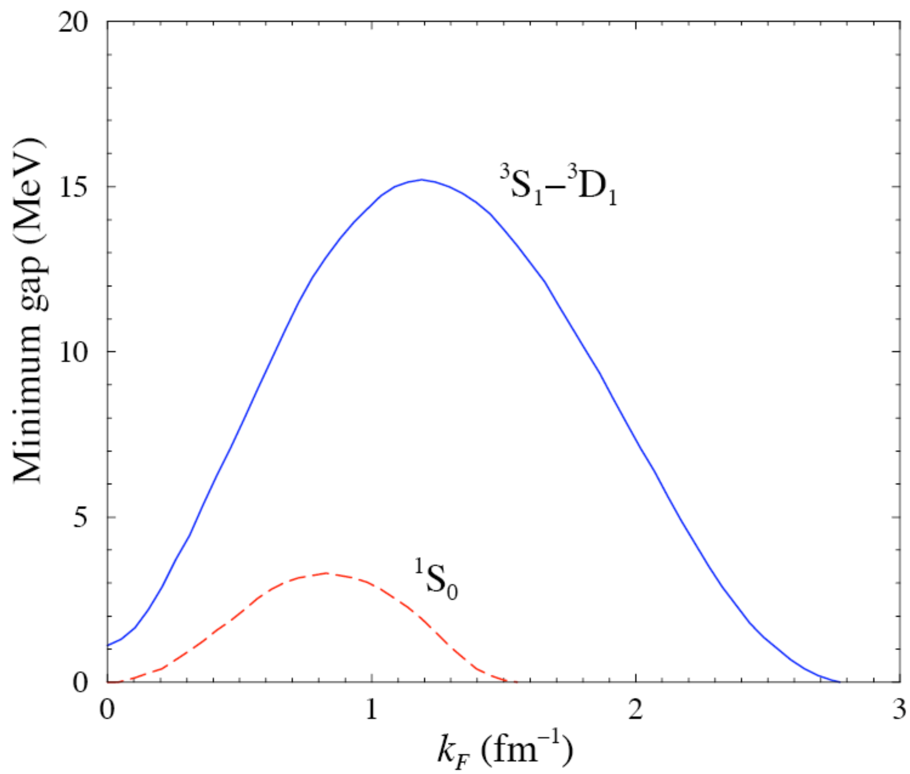


Some pairing issues in infinite matter

- Gap size in nuclear matter & neutron matter
- Density & temperature range of superfluidity
- Resolution of $^3S_1$-$^3D_1$ puzzle (size of pn pairing gap)
- Influence of short-range correlations (SRC)
- Influence of polarization contributions
- Relation of infinite matter results & finite nuclei

Review: e.g. Dean & Hjorth-Jensen, RMP75, 607 (2003)

Puzzle related to gap size in $^3S_1$-$^3D_1$ channel



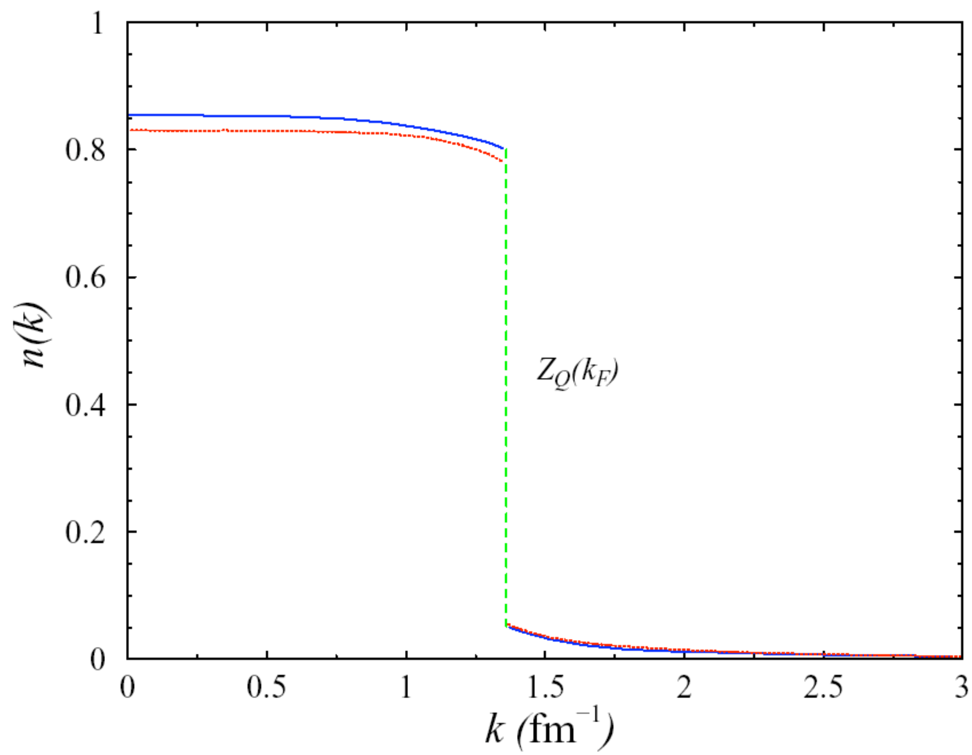
Mean-field particles

Early nineties: BCS gaps ~ 10 MeV

Alm et al. Z.Phys.A337,355 (1990)
Vonderfecht et al. PLB253,1 (1991)
Baldo et al. PLB283, 8 (1992)

Dressing nucleons is expected to reduce pairing strength as suggested by in-medium scattering

Results from Nuclear Matter (N=Z)
2nd generation (2000)



Momentum distribution: only minor changes
when self-consistency is included

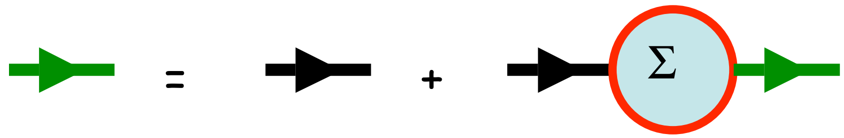
Occupation in nuclei: Depleted similarly!

Thesis Libby Roth Stoddard (2000)

Green´s function and Γ-matrix approach (ladders)

Single-particle Green´s function $G(k,t_1,t_2) = -i\langle T\, c_k(t_1) c_k^+(t_2)\rangle$

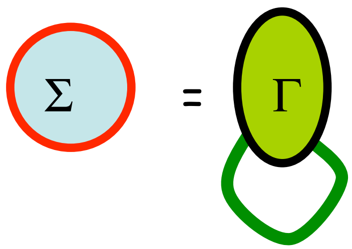
Dyson equation:



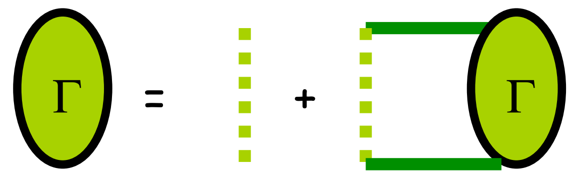
$$G(k,\omega) = G^{(0)}(k,\omega) + G^{(0)}(k,\omega)\Sigma(k,\omega)G(k,\omega)$$

$$G(k,\omega) \quad = \quad \frac{1}{\omega - k^2/2m - \Sigma(k,\omega)} \qquad \Rightarrow \qquad S(k,\omega) = -2\,\mathrm{Im}\,G(k,\omega)$$

Self-energy



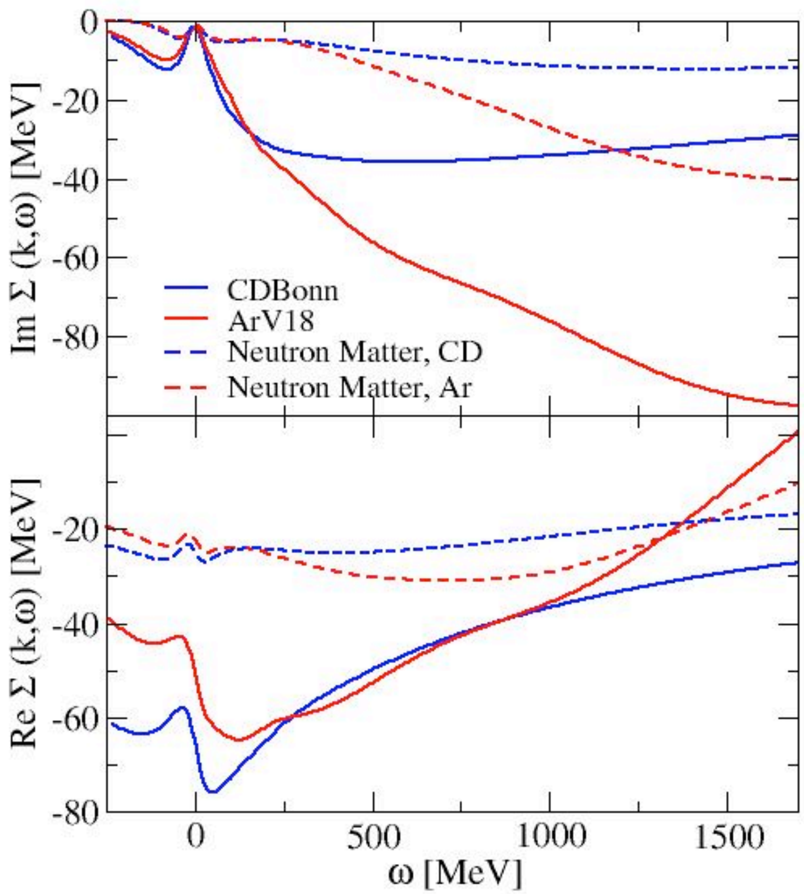
, Γ-matrix



- Pairing instability possible
- Finite temperature calculation can avoid this

Self-energy

$$G(k,\omega) = \frac{1}{\omega - k^2/2m - \Sigma(k,\omega)} \quad \Rightarrow \quad S(k,\omega) = -2\,\mathrm{Im}\,G(k,\omega)$$



Real and imaginary part of the retarded self-energy

- $k_F = 1.35\ \mathrm{fm}^{-1}$
- $T = 5$ MeV
- $k = 1.14\ \mathrm{fm}^{-1}$

Note differences due to NN interaction

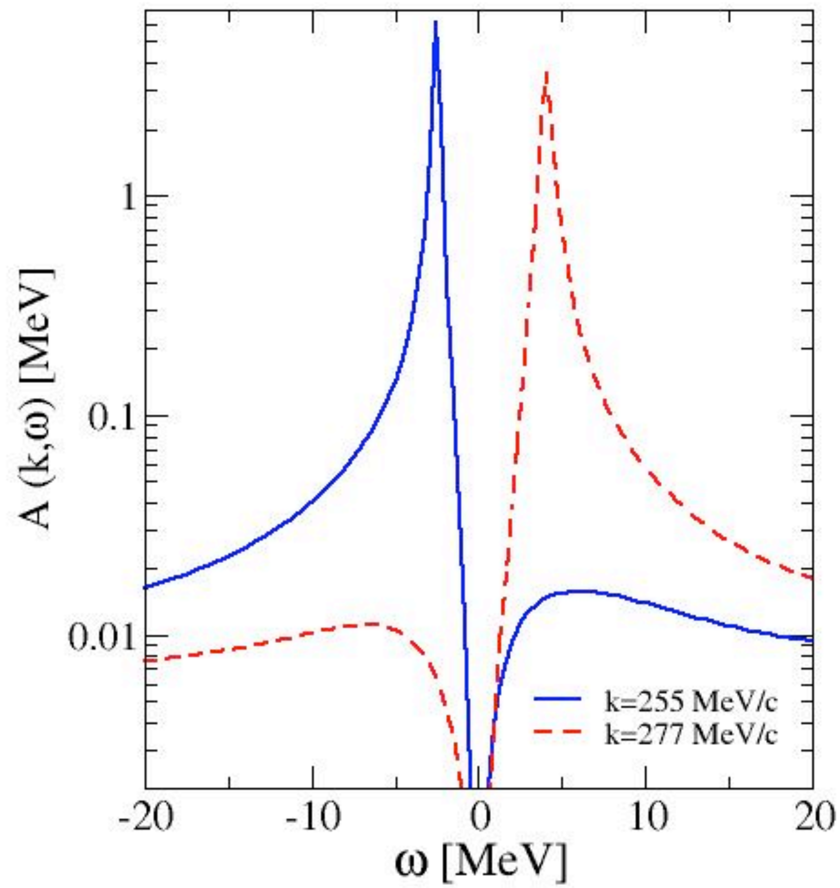
Spectral functions

•Strength above and below the Fermi energy as in BCS

• But broad distribution in energy

• BCS not just a cartoon of SCGF but both features must be considered in a consistent way

• CDBonn interaction at "T=0"



BCS: a reminder

NN correlations on top of Hartree-Fock: $\varepsilon_k\,, \quad c_k^+$

Bogoliubov transformation $\quad a_k^+ \;=\; u_k c_k^+ + v_k c_{\bar{k}}$

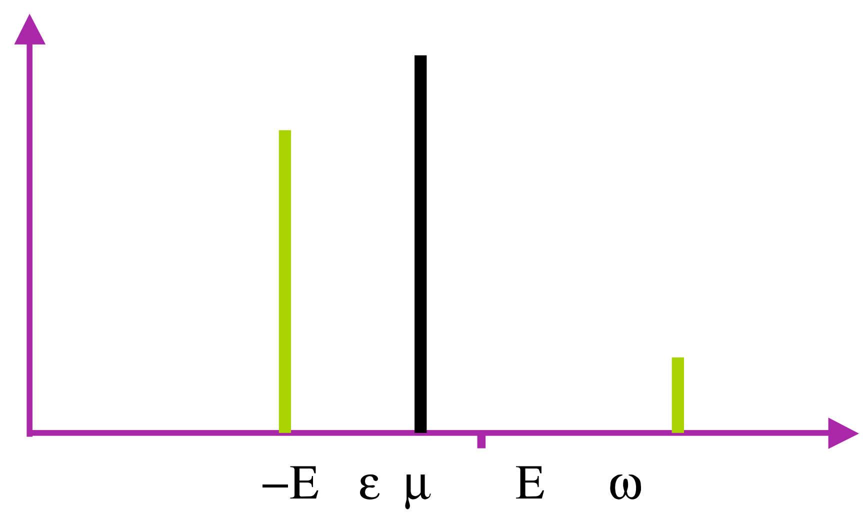
with

$$\begin{matrix} u_k^2 \\ v_k^2 \end{matrix} \;=\; \frac{1}{2}\left[1 \pm \frac{\varepsilon_k - \mu}{\sqrt{(\varepsilon_k - \mu)^2 + \Delta(k)^2}}\right] \quad , \quad E(k) = \sqrt{(\varepsilon_k - \mu)^2 + \Delta(k)^2}$$

Gap equation

$$\Delta(k) = \int k'^2 dk' < k, \bar{k} \,|\, V \,|\, k', \bar{k}' > \frac{\Delta(k')}{-2E(k)}$$

Spectral function S(k,ω)



Solution of the gap equation

$$\Delta(k) = \sum_{k'} \langle k,\bar{k} | V | k',\bar{k}' \rangle \frac{\Delta(k')}{\omega - 2E(k)}$$ with $$E(k) = \sqrt{(\varepsilon_k - \mu)^2 + \Delta(k)^2}$$ and $\omega=0$

Define: $$\delta(k) = \frac{\Delta(k)}{\omega - 2E(k)}$$

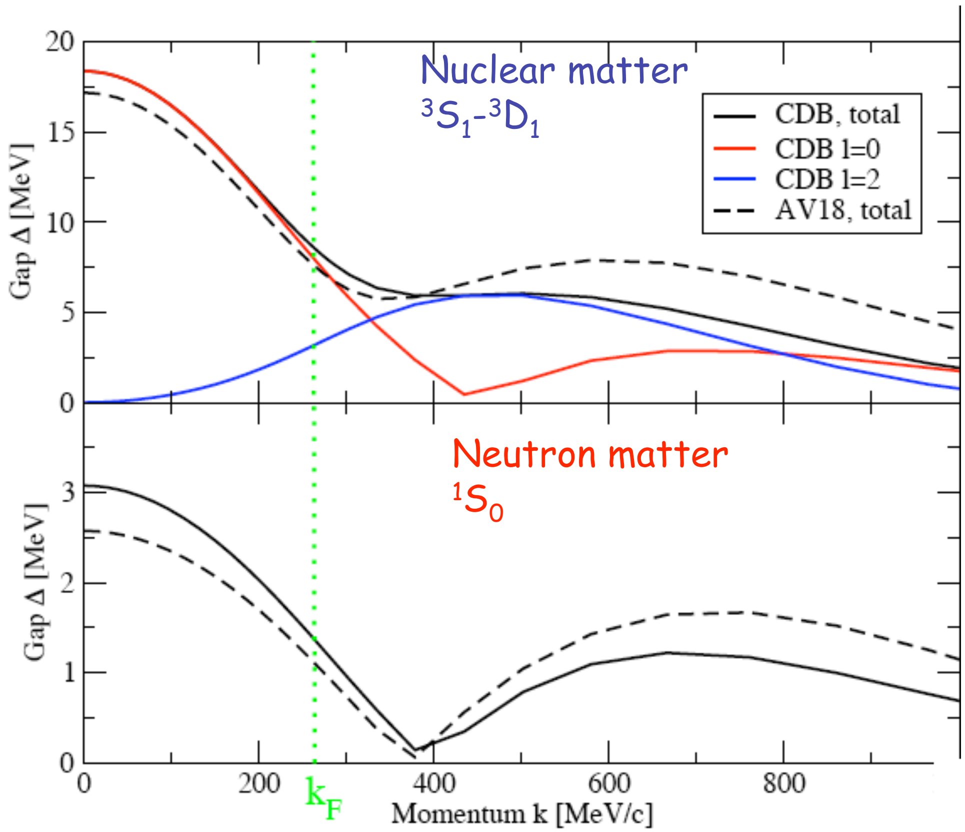
$$\begin{pmatrix} 2E(k) + \langle k|V|k\rangle, & \ldots, & \langle k|V|k'\rangle \\ \vdots & \ddots & \vdots \\ \langle k'|V|k\rangle, & \cdots, & 2E(k') + \langle k'|V|k'\rangle \end{pmatrix} \begin{pmatrix} \delta(k) \\ \vdots \\ \delta(k') \end{pmatrix} = \omega \begin{pmatrix} \delta(k) \\ \vdots \\ \delta(k') \end{pmatrix}$$

Eigenvalue problem for a pair of nucleons at $\omega=0$

Steps of the calculation:

- Assume $\Delta(k)$ and determine E(k)
- Solve eigenvalue equation and evaluate new $\Delta(k)$
  - If lowest eigenvalue $\omega<0$ enhance $\Delta(k)$ (resp. $\delta(k)$)
  - If lowest eigenvalue $\omega>0$ reduce $\Delta(k)$
- Repeat until convergence

Gaps from BCS for realistic interactions



T = 0
Mean-field particles

- momentum dependence Δ(k)
- different NN interactions
- very similar to pairing gaps in finite nuclei for like particles...!?
- for np pairing no strong empirical evidence...?!

Early nineties: BCS gaps ~ 10 MeV

Alm et al. Z.Phys.A337,355 (1990)
Vonderfecht et al. PLB253,1 (1991)
Baldo et al. PLB283, 8 (1992)

Beyond BCS in the framework of SCGF

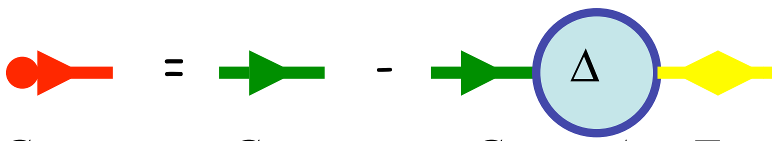
Generalized Green's functions: Extend $G(k,t_1,t_2) = -i\langle T\, c_k(t_1) c_k^+(t_2)\rangle$

Anomalous propagators

$$G(k,t_1,t_2) = \begin{pmatrix} -i\langle T cc^+\rangle & -i\langle Tcc\rangle \\ i\langle Tc^+c^+\rangle & i\langle Tc^+c\rangle \end{pmatrix} = \begin{pmatrix} G & F \\ F^+ & \overline{G} \end{pmatrix}$$

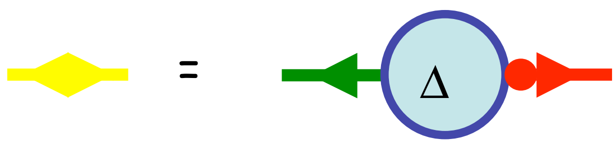
Generalized Dyson equation: Gorkov equations

Leads to e.g.

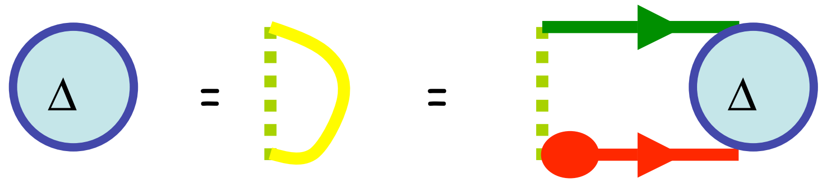


$$G_{pair} = G - G \quad \Delta \quad F$$

G includes all normal self-energy terms



Anomalous self-energy: Δ & generalized Gap equation



$$\Delta(k) \quad = \quad \int k'^2 dk' \langle k|V|k'\rangle \int d\omega \int d\omega' \frac{1-f(\omega)-f(\omega')}{-\omega-\omega'} S(k',\omega)\, S_{pair}(k',\omega') \quad \Delta(k')$$

$$f(\omega) = \frac{1}{e^{\beta\omega}+1}$$

Fermi function

If we replace $S(k,\omega)$ by "HF" approx. and $S_{pair}(k,\omega)$ by BCS:

⇨ Usual Gap equation

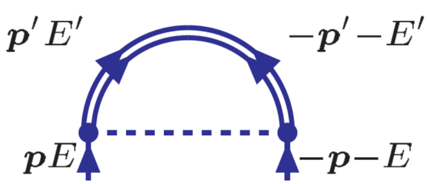
If we take $S_{pair}(k,\omega) = S(k,\omega)$:

⇨ Corresponds to the homogeneous solution of Γ-matrix eq.

With $S_{pair}(k,\omega)$:

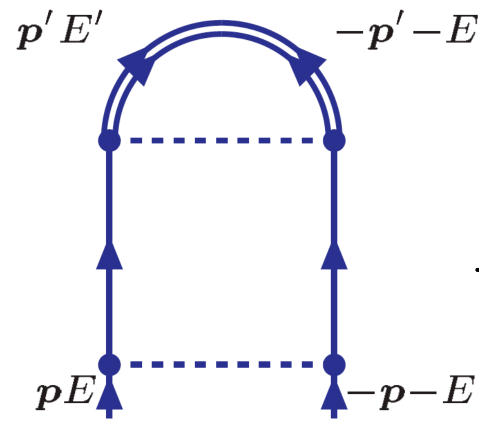
⇨ The above and self-consistency

Consistency of Gap equation (anomalous self-energy) and Ladder diagrams



Iteration of Gorkov equations for anomalous

propagator generates $\Rightarrow$



+ ...

... and all other ladder diagrams at
total momentum and energy zero (w.r.t. 2μ)
plus anomalous self-energy terms in normal part of propagator

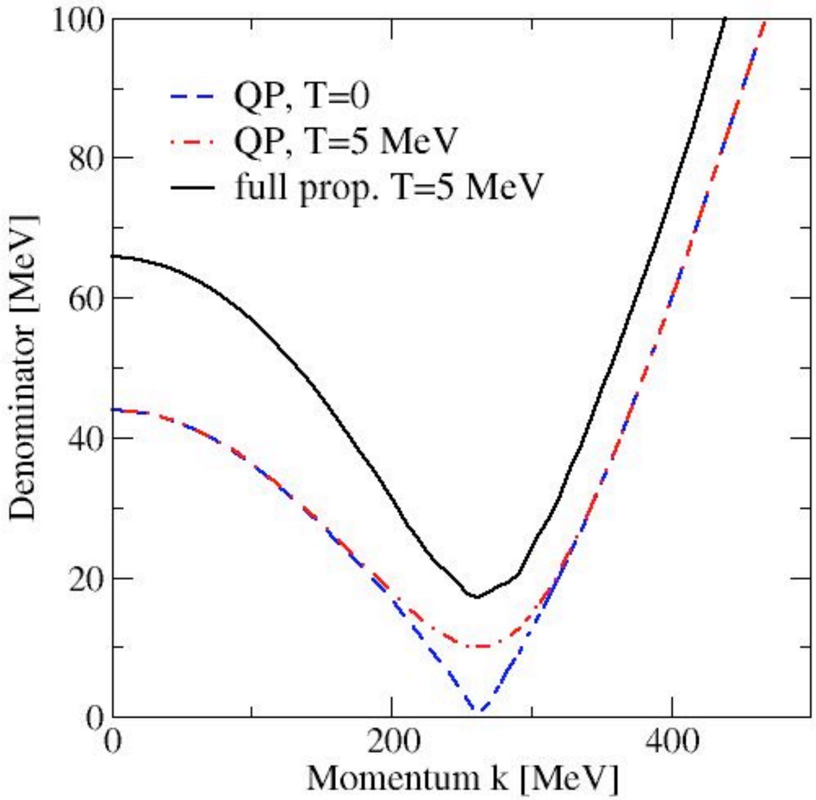
So truly consistent with inclusion of ladder diagrams at other total momenta and energies

Features of generalized gap equation

$$\Delta(k) \quad = \quad \int k'^2 dk' \langle k|V|k'\rangle \int d\omega \int d\omega' \frac{1-f(\omega)-f(\omega')}{-\omega-\omega'} S(k',\omega)\, S_{\cancel{pair}}(k',\omega') \quad \Delta(k')$$

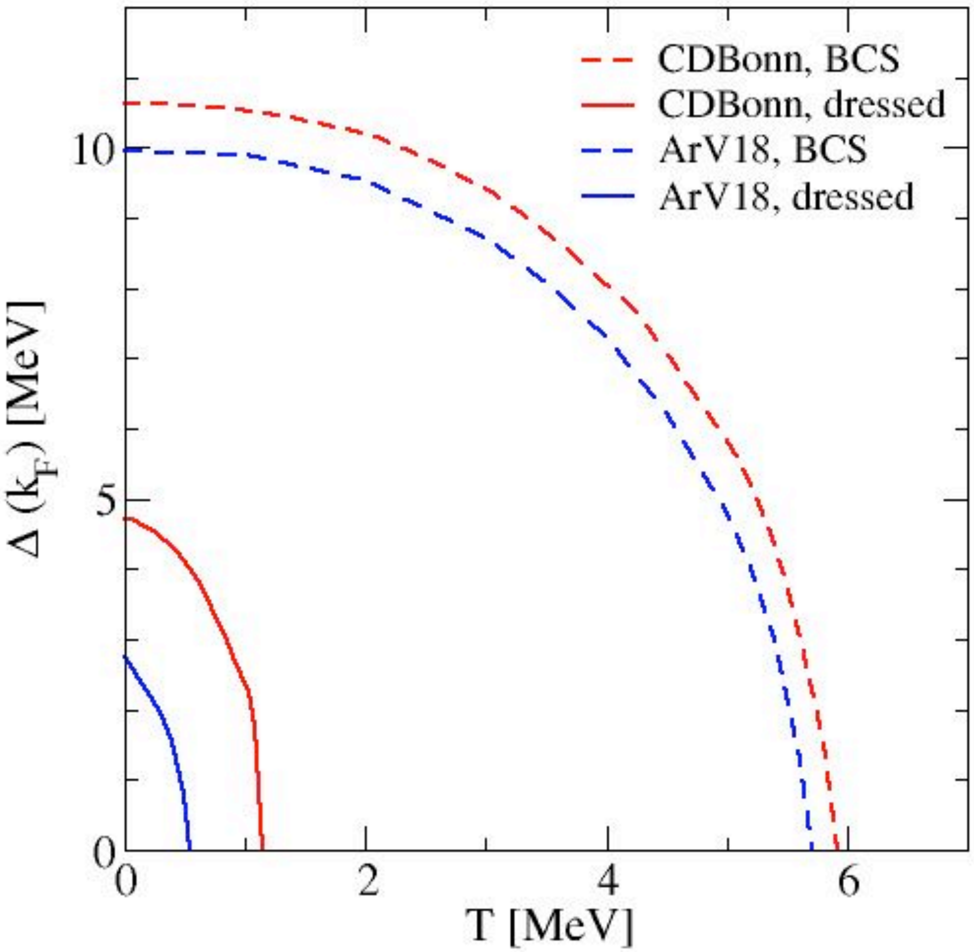
$$-\frac{1}{2\tilde{\chi}_{k'}}$$

$\tilde{\chi}_k$



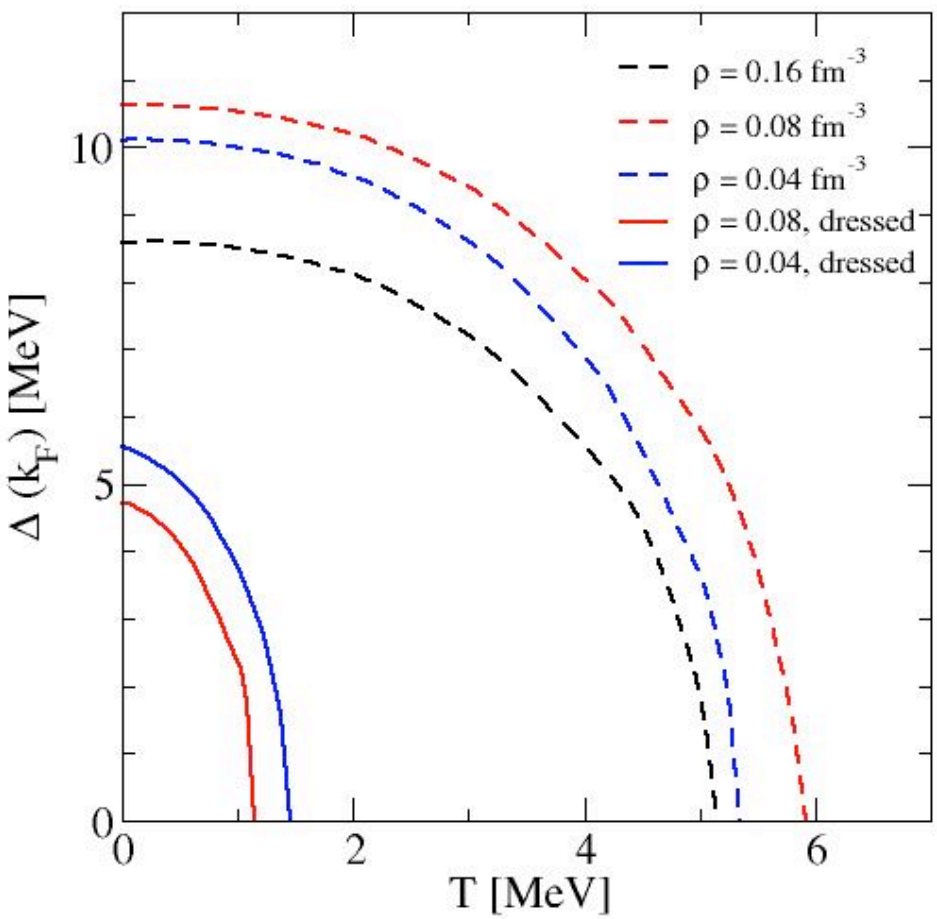
Dashed:
Spectral strength only at 1 energy
Dashed-dot:
Effect of temperature (5 MeV)
Solid:
Includes complete strength distribution due to SRC

Related studies by
Baldo, Lombardo, Schuck et al.
use BHF self-energy



CDBonn yields stronger pairing than ArV18

Proton-neutron pairing in symmetric nuclear matter



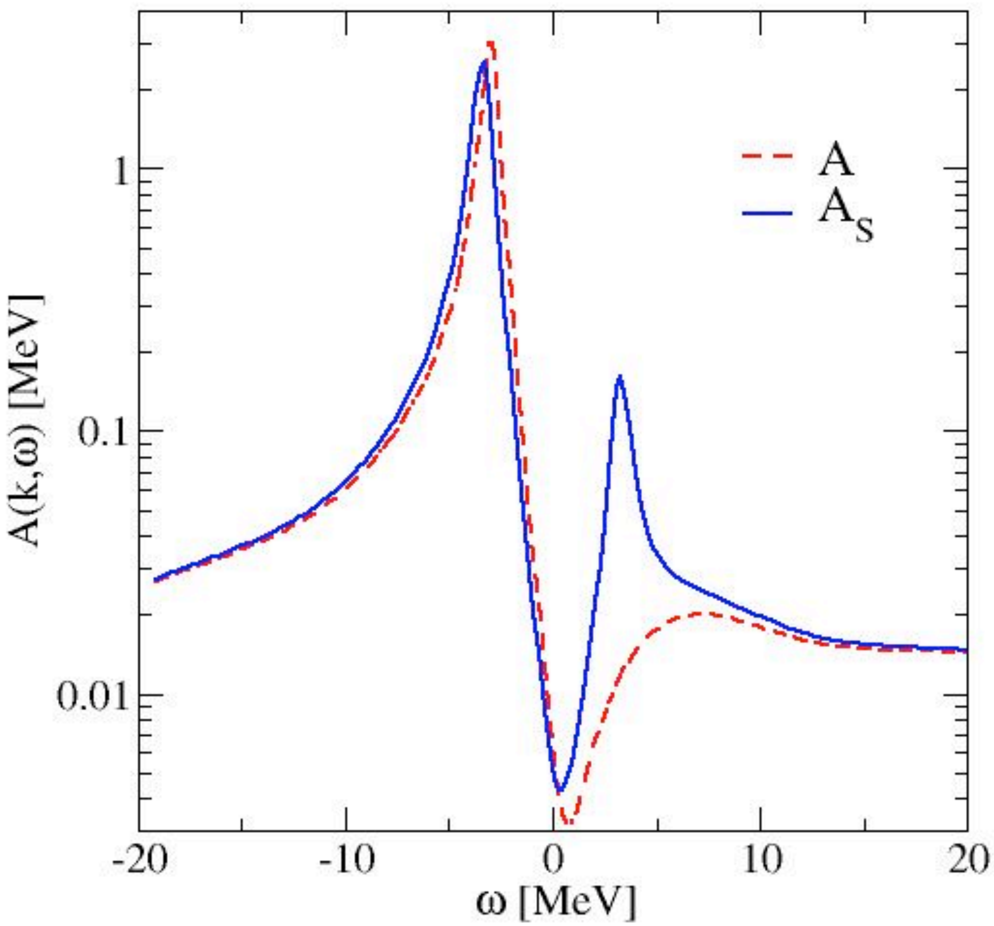
Using CDBonn

Dashed lines:
quasiparticle poles

Solid lines:
dressed nucleons

No pairing at saturation density!

Pairing and spectral functions



Spectral functions

$S(k,\omega)$ dashed = $A(k,\omega)$

$S_{pair}(k,\omega)$ solid = $A_S(k, \omega)$

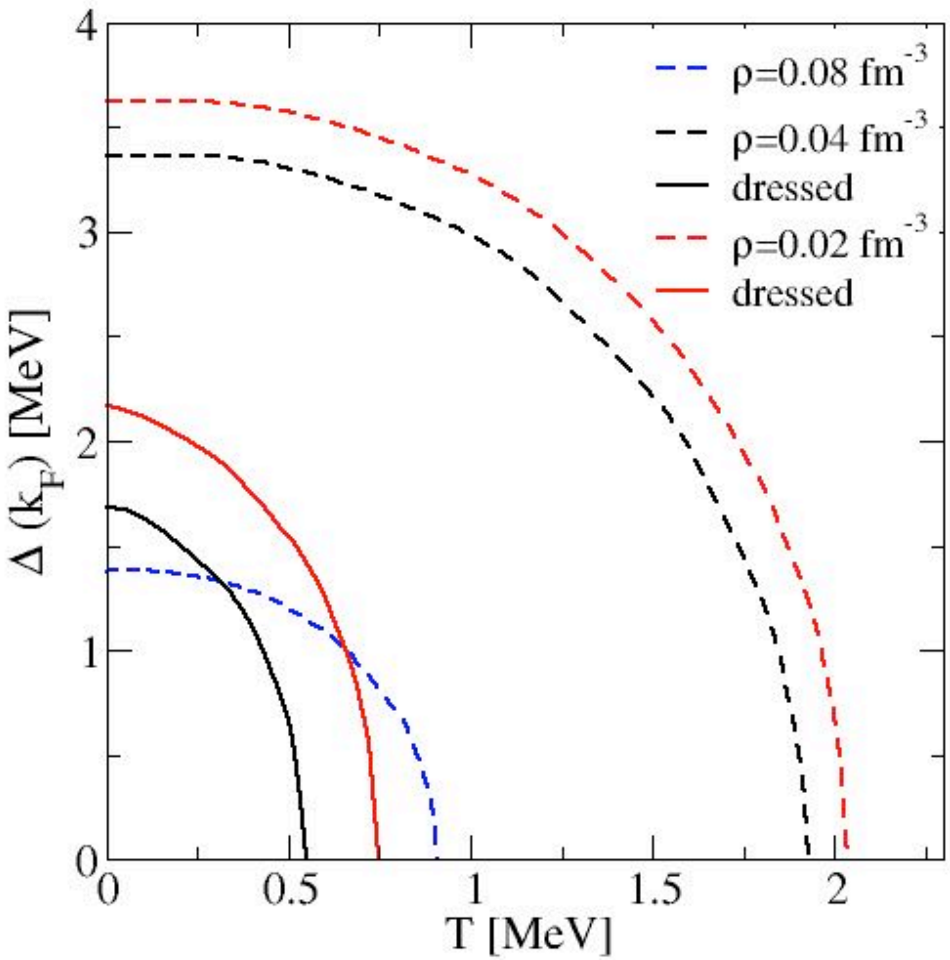
ρ = 0.08 fm^{-3}

T = 0.5 MeV

k = 193 MeV/c 0.9 k_F

Expected effect

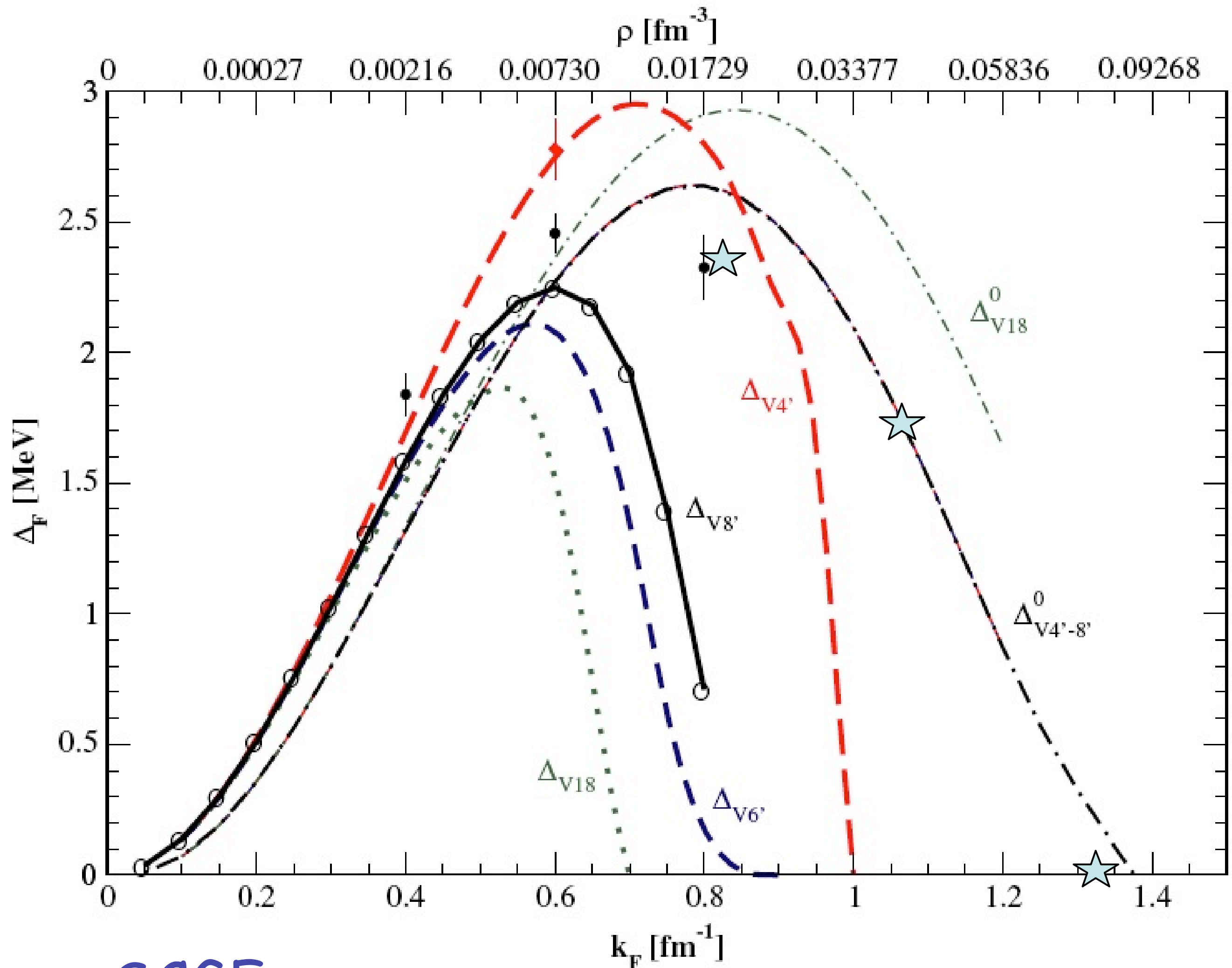
Pairing in neutron matter



Dressing effects weaker, but non-negligible

CDBonn

Comparison for neutron matter with CBF & Monte Carlo PRL95,192501(2005)



☆ ⇒ SCGF