CISS07 8/29/2007

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

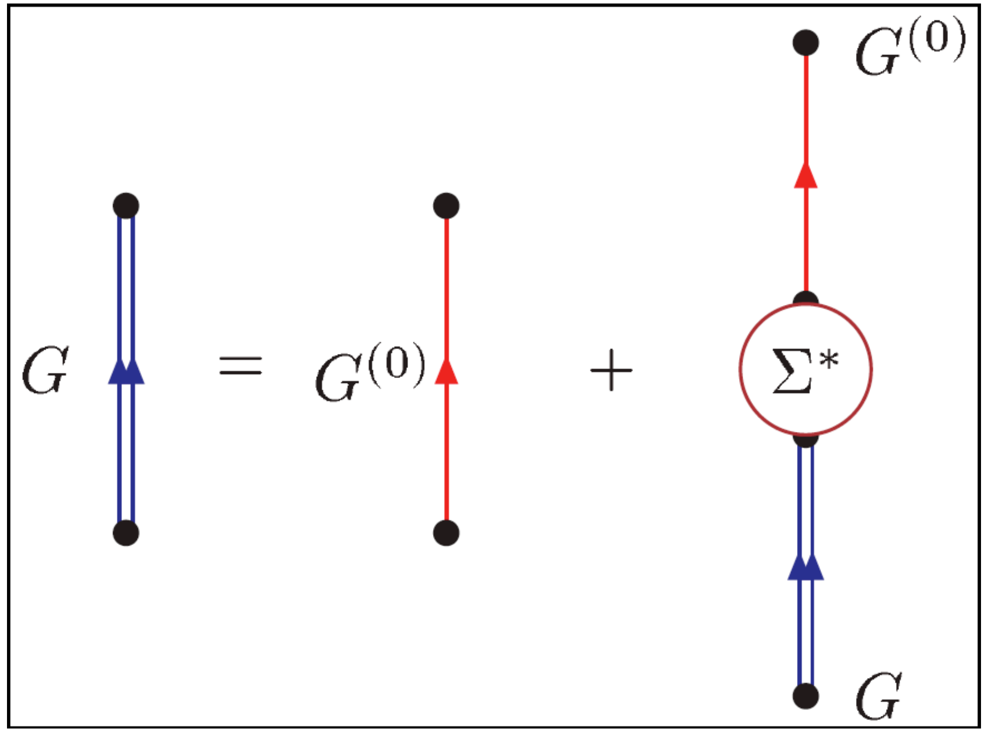
Lecture 1: 8/28/07	Propagator description of single-particle motion and the link with experimental data
Lecture 2: 8/29/07	From Hartree-Fock to spectroscopic factors < 1: inclusion of long-range correlations
Lecture 3: 8/29/07	Role of short-range and tensor correlations associated with realistic interactions
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

Outline

- Link between sp and two-particle propagator
- Self-consistent Green's functions
- Hartree-Fock
- Dynamical self-energy and spectroscopic factors < 1
- Self-energy using "*G*-matrix" in second order
- Qualitative features; missing ingredients!
- Excited states and $G \Leftrightarrow G$ and excited states
- Conserving approximations; HF ⇔ RPA *e.g.*
- E(xtended) RPA & results (Giant Resonances)
- Collective excitations in the self-energy
- Influence of "long-range"correlations
- Recent developments (Faddeev summation)
- Why does (e,e´p) yield "absolute" spectroscopic factors

Dyson equation



Looks like the propagator equation for a single particle

$$G(\alpha,\beta;E) = G^{(0)}(\alpha,\beta;E) + \sum_{\gamma,\delta} G^{(0)}(\alpha,\gamma;E)\Sigma^*(\gamma,\delta;E)G(\delta,\beta;E)$$

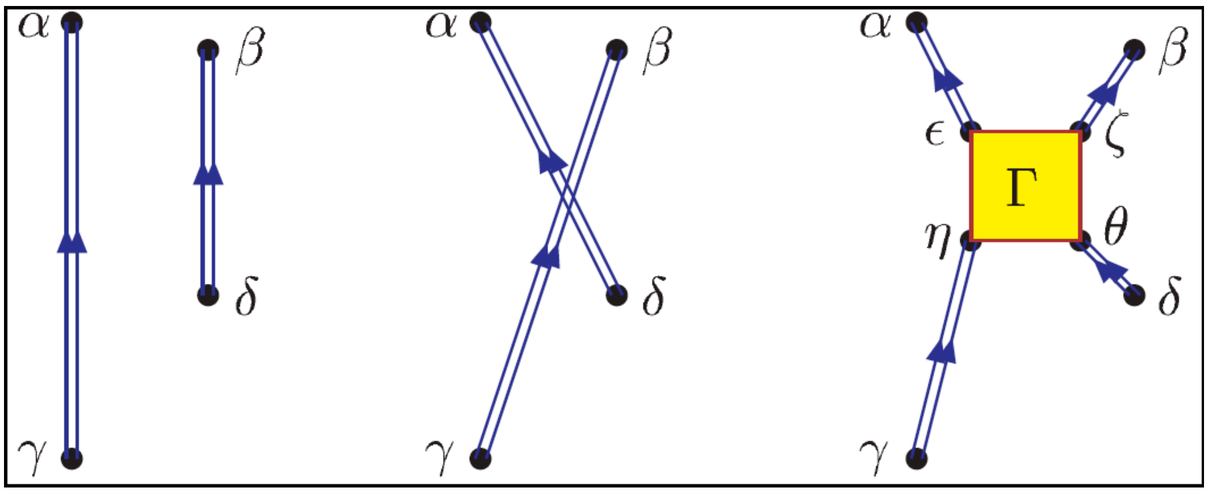
with the irreducible self-energy acting as the in-medium (complex) potential.

Link with two-particle propagator

Equation of motion for G

$$i\hbar\frac{\partial}{\partial t}G(\alpha,\beta;t-t') = \delta(t-t')\delta_{\alpha,\beta} + \varepsilon_\alpha G(\alpha,\beta;t-t') - \sum_\delta \langle\alpha|U|\delta\rangle G(\delta,\beta;t-t')$$
$$+\frac{1}{2}\sum_{\delta\xi\vartheta}\langle\alpha\delta|V|\vartheta\zeta\rangle\left\{-\frac{i}{\hbar}\left\langle\Psi_0^N\right|T\left[a^+_{\delta_H}(t)a_{\zeta_H}(t)a_{\vartheta_H}(t)a^+_{\beta_H}(t')\right]\left|\Psi_0^N\right\rangle\right\}$$

Diagrammatic analysis of G^{II} yields



Γ is the effective interaction (vertex function) between correlated particles in the medium.

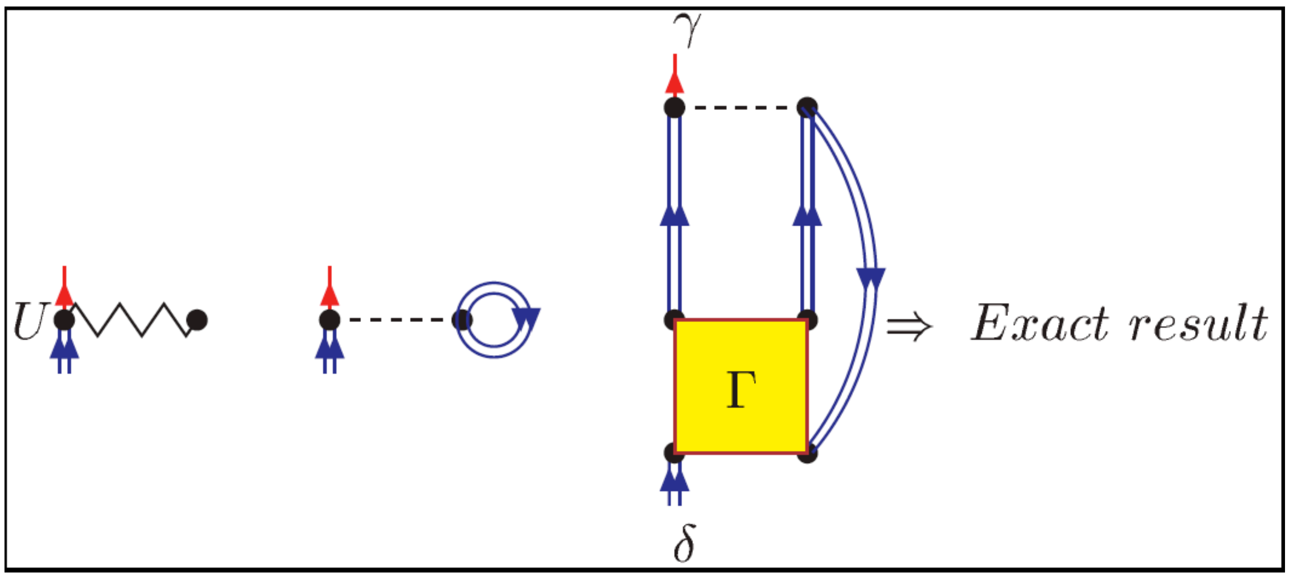
Dyson equation and vertex function

Fourier transform of equation of motion for *G* yields again the Dyson equation with the self-energy

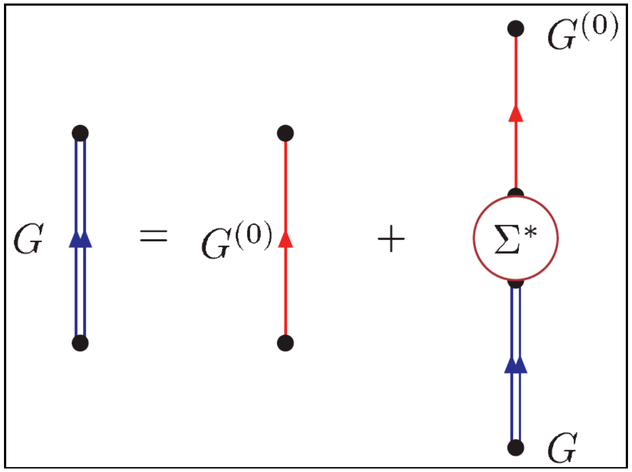
$$\Sigma^*(\gamma,\delta;E) = -\langle\gamma|U|\delta\rangle - i\int_{C\uparrow}\frac{dE'}{2\pi}\sum_{\mu\nu}\langle\gamma\mu|V|\delta\nu\rangle G(\nu,\mu;E')$$

$$+\frac{1}{2}\int\frac{dE_1}{2\pi}\int\frac{dE_2}{2\pi}\sum_{\varepsilon\mu\nu\zeta\rho\sigma}\langle\gamma\mu|V|\varepsilon\nu\rangle G(\varepsilon,\zeta;E_1)G(\nu,\rho;E_2)G(\sigma,\mu;E_1+E_2-E)\langle\zeta\rho|\Gamma(E_1,E_2;E)|\delta\sigma\rangle$$

In diagram form



Dyson Equation and "experiment"



Equivalent to ….!!

Schrödinger-like equation with: $E_n^- = E_0^N - E_n^{N-1}$

$$-\frac{\hbar^2\nabla^2}{2m}\left\langle \Psi_n^{N-1}\middle| a_{\vec{r}m} \middle| \Psi_0^N \right\rangle + \sum_{m'} \int d\vec{r}\,'\, \Sigma'^*(\vec{r}m, \vec{r}\,'m'; E_n^-) \left\langle \Psi_n^{N-1}\middle| a_{\vec{r}\,'m'} \middle| \Psi_0^N \right\rangle = E_n^- \left\langle \Psi_n^{N-1}\middle| a_{\vec{r}m} \middle| \Psi_0^N \right\rangle$$

Self-energy: non-local, energy-dependent potential (no *U*)

With energy dependence: spectroscopic factors < 1

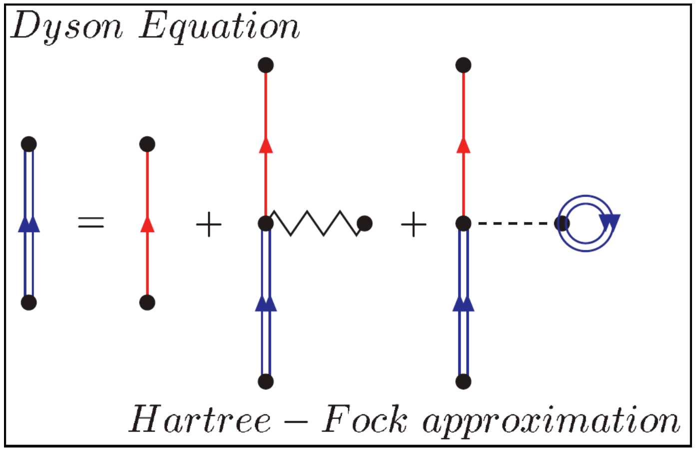
$$S = \left| \left\langle \Psi_n^{N-1} \middle| a_{\alpha_{qh}} \middle| \Psi_0^N \right\rangle \right|^2 = \frac{1}{1 - \left.\dfrac{\partial \Sigma'^*\left(\alpha_{qh}, \alpha_{qh}; E\right)}{\partial E}\right|_{E_n^-}}$$

α_{qh} solution of DE at E_n^-

Physics is in the choice of the approximation to the self-energy

Hartree-Fock

For weakly interacting particles: independent propagation dominates
$\Rightarrow$ neglect vertex function in self-energy



Democracy in action
$\Leftrightarrow$ self-consistency

$$\Sigma^{HF}(\gamma,\delta) = -\langle\gamma|U|\delta\rangle - i\int_{C\uparrow}\frac{dE'}{2\pi}\sum\langle\gamma\mu|V|\delta\nu\rangle G^{HF}(\nu,\mu;E')$$

No energy dependence $\Rightarrow$ static mean field
Not a valid strategy for realistic *NN* interactions
With "effective" interactions can yield good quasihole wave functions
HF levels full or empty; spectroscopic factors 1 or 0 accordingly

HF for “closed”-shell atoms

		Removal energies		Total energy	
		HF	Exp.	HF	Exp.
He	$1s$	-0.918	-0.9040	-2.862	-2.904
Be	$1s$	-4.733	-4.100	-14.573	-14.667
	$2s$	-0.309	-0.343		
Ne	$1s$	-32.77	-31.70	-128.547	-128.928
	$2s$	-1.930	-1.782		
	$2p$	-0.850	-0.793		
Mg	$1s$	-49.03	-47.91	-199.615	-200.043
	$2s$	-3.768	-3.26		
	$2p$	-2.283	-1.81		
	$3s$	-0.253	-0.2811		
Ar	$1s$	-118.6	-117.87	-526.818	-527.549
	$2s$	-12.32	-12.00		
	$2p$	-9.571	-9.160		
	$3s$	-1.277	-1.075		
	$3p$	-0.591	-0.579		

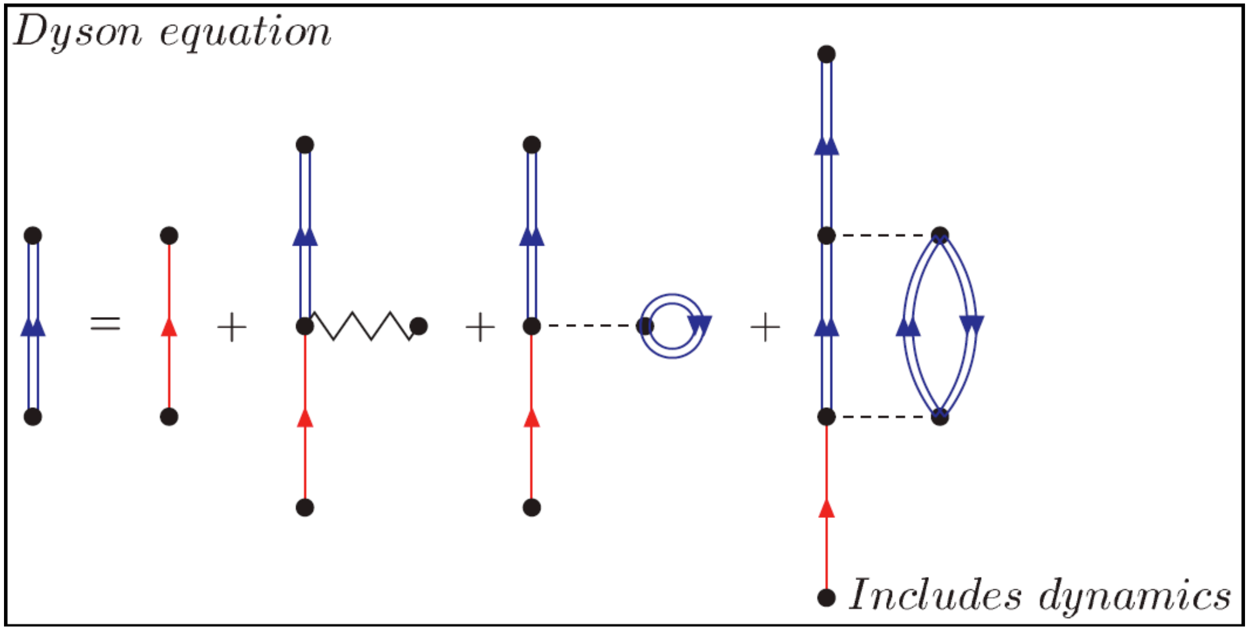
HF good starting point for atoms but total energy dominated by core electrons.

Description of valence electrons not good enough to do chemistry.

Spectroscopic factors not OK.
Wave functions ✓

Energies in atomic units (Hartree)

Beyond HF $\Rightarrow$ dynamical self-energy



Approximate vertex function by $\Gamma = V$

Use HF propagator to initiate self-consistent solution

$$\Sigma^{(2)}(\gamma,\delta;E) = \frac{1}{2}\left\{ \sum_{p_1 p_2 h_3} \frac{\langle \gamma h_3 | V | p_1 p_2 \rangle \langle p_1 p_2 | V | \delta h_3 \rangle}{E - (\varepsilon_{p_1} + \varepsilon_{p_2} - \varepsilon_{h_3}) + i\eta} + \sum_{h_1 h_2 p_3} \frac{\langle \gamma p_3 | V | h_1 h_2 \rangle \langle h_1 h_2 | V | \delta p_3 \rangle}{E - (\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_3}) - i\eta} \right\}$$

Poles at 2*p*1*h* and 2*h*1*p* energies

Interesting consequences for solution of Dyson equation

Diagonal approximation

Further simplification: assume no mixing between major shells

$$\Sigma^{(2)}(\alpha;E) = \frac{1}{2}\left\{ \sum_{p_1p_2h_3} \frac{\left|\langle \alpha h_3 | V | p_1 p_2 \rangle\right|^2}{E - \left(\varepsilon_{p_1} + \varepsilon_{p_2} - \varepsilon_{h_3}\right) + i\eta} + \sum_{h_1h_2p_3} \frac{\left|\langle \alpha p_3 | V | h_1 h_2 \rangle\right|^2}{E - \left(\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_3}\right) - i\eta} \right\}$$

Corresponding Dyson equation

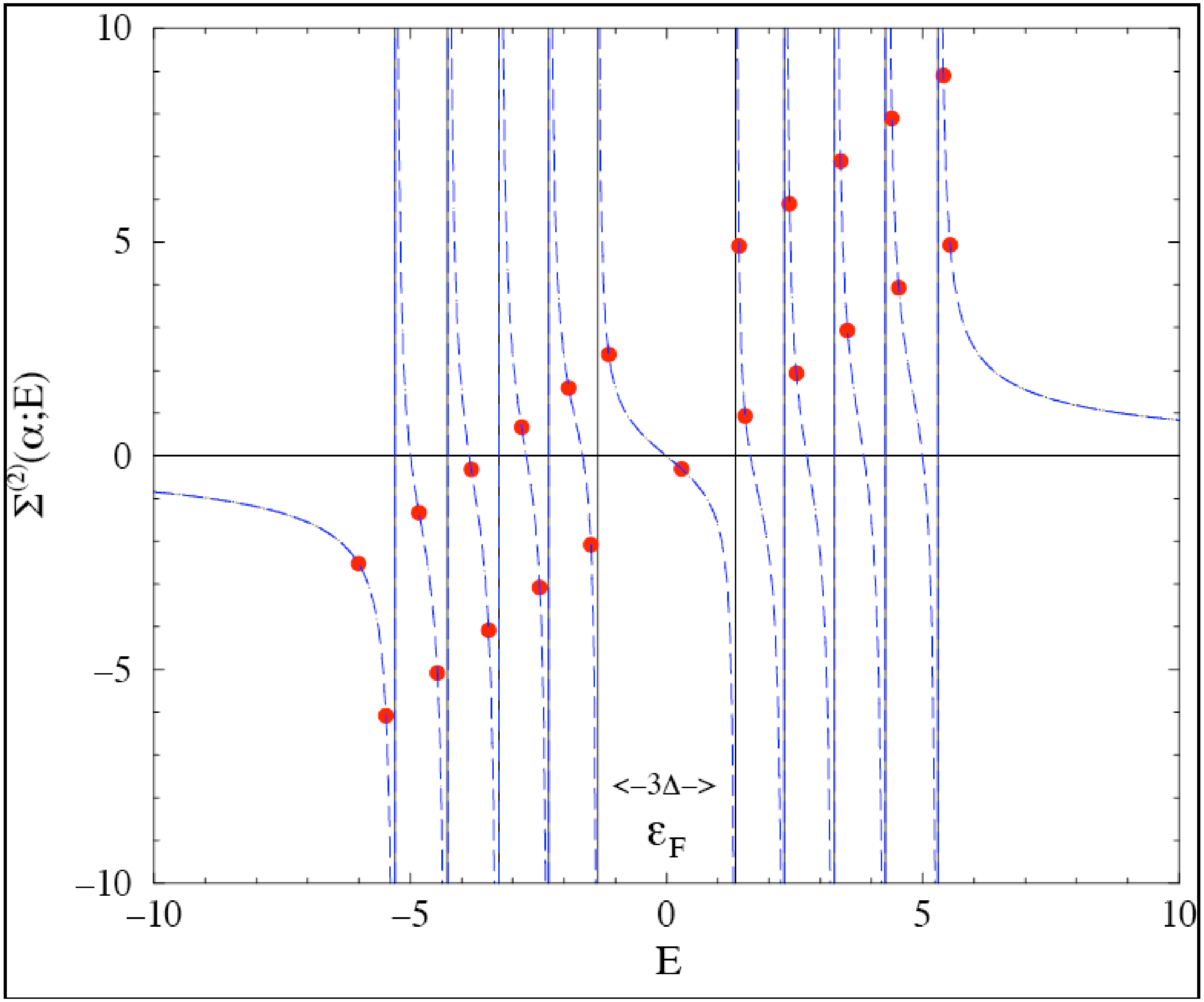
$$G(\alpha;E) = G^{HF}(\alpha;E) + G(\alpha;E)\Sigma^{(2)}(\alpha;E)G^{HF}(\alpha;E) = \frac{1}{E - \varepsilon_\alpha - \Sigma^{(2)}(\alpha;E)}$$

Assume discrete poles in Σ, then discrete solution (poles of G) for

$$E_{n\alpha} = \varepsilon_\alpha + \Sigma^{(2)}(\alpha;E_{n\alpha})$$

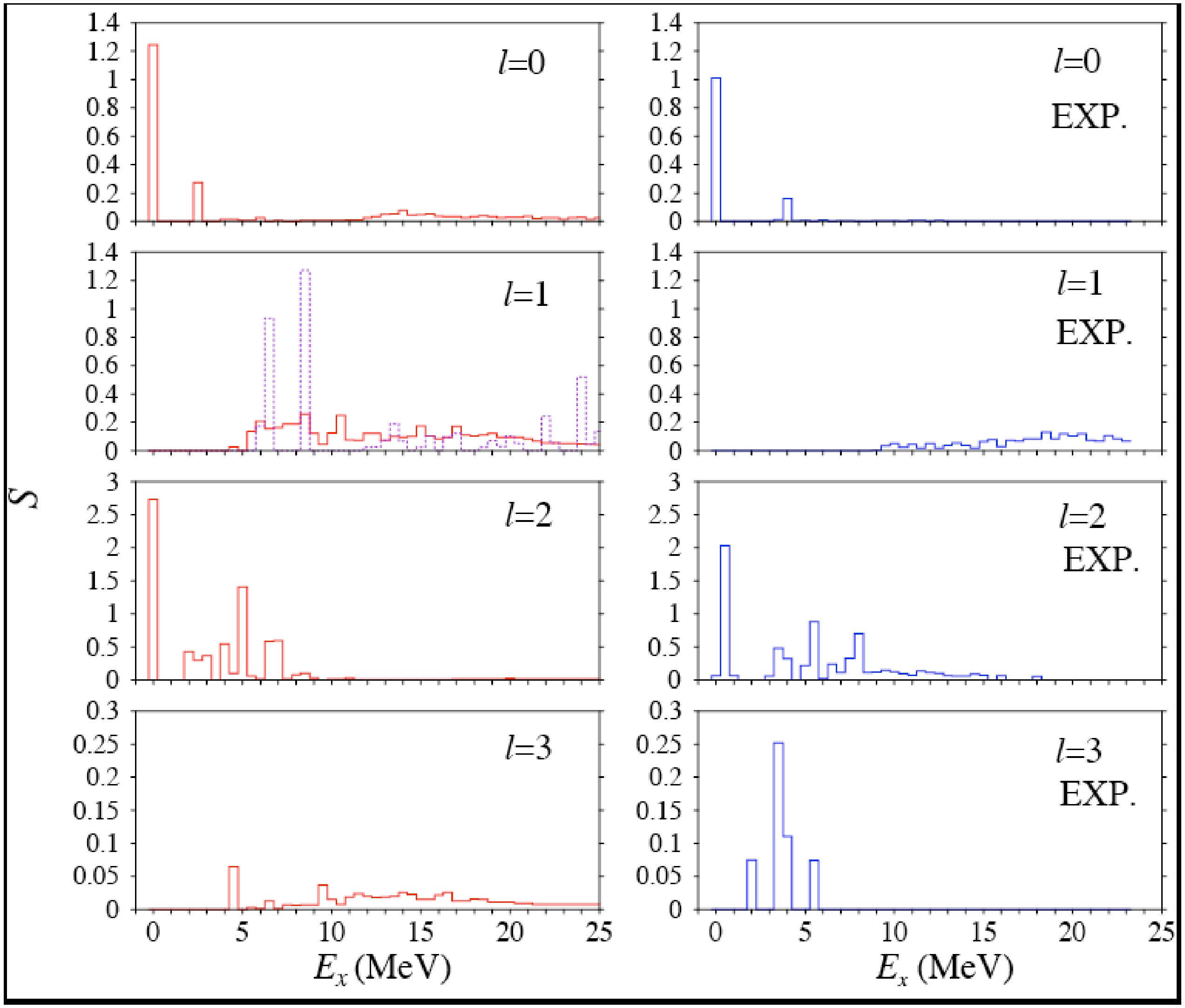
With residue (spectroscopic factor) $$R_{n\alpha} = \frac{1}{1 - \left.\frac{\partial \Sigma^{(2)}(\alpha;E)}{\partial E}\right|_{E_{n\alpha}}}$$

Solutions



Explains all qualitative features of sp strength distribution in nuclei!

Self-consistent calculation with Skyrme force

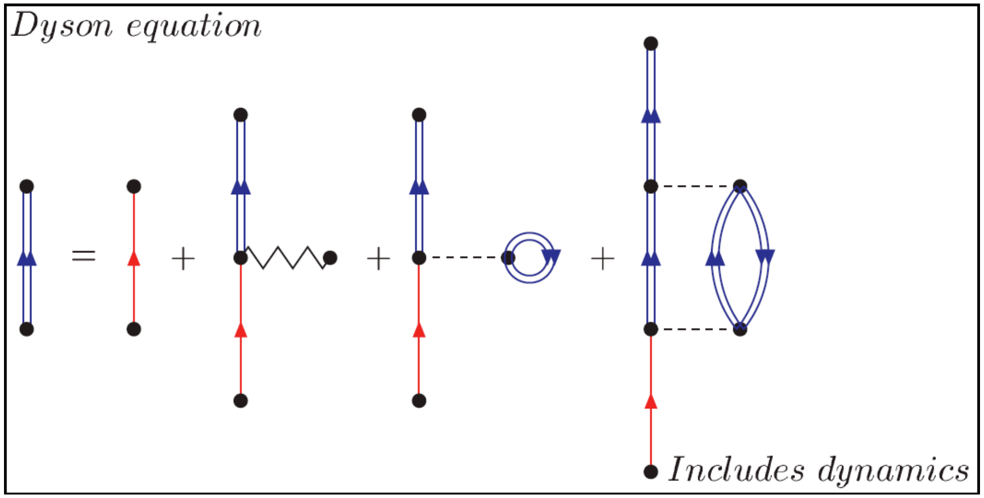


Data: ^{48}Ca(e,e´p)
Kramer NIKHEF
(1990)

Qualitatively OK
No relation with
realistic *V* yet!

Van Neck *et al.* NPA**530**,347(1991)

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



Dyson(2)

Van Neck, Peirs, Waroquier
J. Chem. Phys. **115**, 15 (2001)
Dahlen & von Barth
J. Chem. Phys. **120**, 6826 (2004)

Atoms : total ground state energies (a.u.)

Method	He	Be	Ne	Mg	Ar
DFT	-2.913	-14.671	-128.951	-200.093	-527.553
HF	-2.862	-14.573	-128.549	-199.617	-526.826
CI	-2.891	-14.617	-128.733	-199.63	-526.807
Dyson(2)	-2.899	-14.647	-128.939	-200.027	-527.511
Exp.	-2.904	-14.667	-128.928	-200.043	-527.549

How to proceed from a realistic *V*?

Must take effects of short-range and tensor correlations into account. Well known procedure: from *V* to "*G*"-matrix.

$$\langle\alpha\beta|G(E)|\gamma\delta\rangle = \langle\alpha\beta|V|\gamma\delta\rangle + \frac{1}{2}\sum_{\sigma\tau}\langle\alpha\beta|V|\sigma\tau\rangle\frac{\theta(\sigma-M)\theta(\tau-M)}{E-\varepsilon_\sigma-\varepsilon_\tau}\langle\sigma\tau|G(E)|\gamma\delta\rangle$$

Well-behaved; takes excitations outside configuration space *M* into account. Used inside *M* $\Rightarrow$ therefore this procedure doesn't **yet** completely include the effect of short-range and tensor correlations on sp motion.

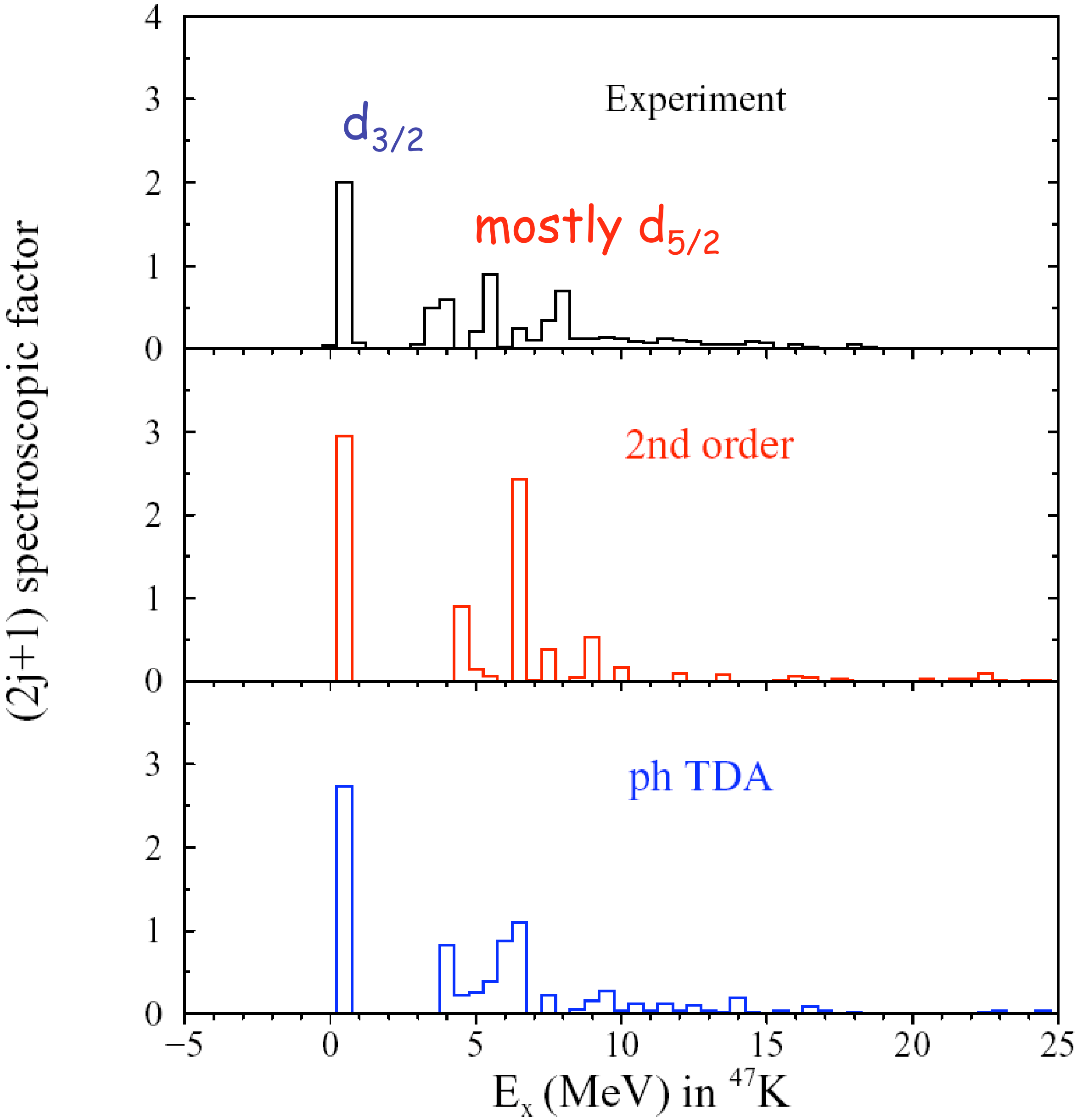
Neglect energy dependence of *G* then

$$\Sigma^{(2)}(\gamma,\delta;E) = \frac{1}{2}\left\{\sum_{p_1p_2h_3}\frac{\langle\gamma h_3|G|p_1p_2\rangle\langle p_1p_2|G|\delta h_3\rangle}{E-\left(\varepsilon_{p_1}+\varepsilon_{p_2}-\varepsilon_{h_3}\right)+i\eta} + \sum_{h_1h_2p_3}\frac{\langle\gamma p_3|G|h_1h_2\rangle\langle h_1h_2|G|\delta p_3\rangle}{E-\left(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_3}\right)-i\eta}\right\}$$

Summations only inside *M*!

Spectral function $^{48}Ca\ (e,e'p)\ ^{47}K\ (\ell=2)$

NIKHEF data
G. Kramer, Thesis



Brand *et al.*
Nucl. Phys. **A531**, 253 (1991).
Rijsdijk *et al.*
Nucl.Phys. **A550**, 159 (1992)

Configuration space: includes three major shells above ε_F

Distribution of fragments ± 100 MeV around ε_F

G-matrix strong enough to distribute strength in this interval

Excited states and G …
G and excited states …

Before improving self-energy with a better description of the intermediate $2p1h$ and $2h1p$ states, it is instructive to clarify the deep relation between excited states and the sp propagator G.

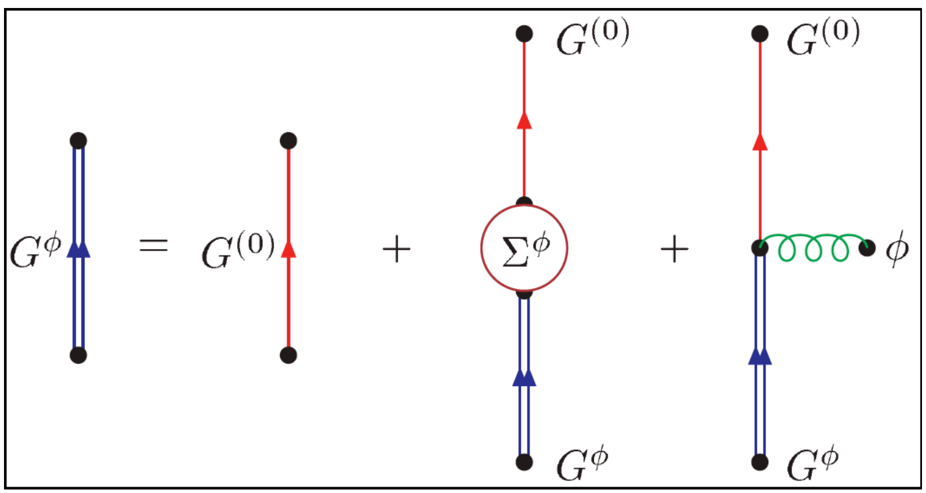
$\Rightarrow$ Study time-dependent external fields that can probe excited states

$$\hat{\phi}(t) = \sum_{\gamma\delta} \langle \gamma | \phi(\vec{x},t) | \delta \rangle a_\gamma^{+} a_\delta$$

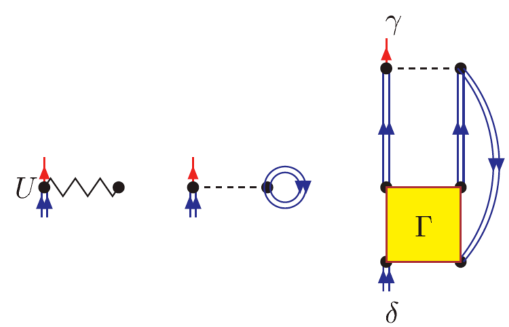
So Hamiltonian reads

$$\hat{H}^{\phi}(t) = \hat{H} + \hat{\phi}(t)$$

Equations of motion as before



Σ^{ϕ} as before with $G \Rightarrow G^{\phi}$



Conserving approximations (Baym, Kadanoff, Pitaevskii, Luttinger, Ward)

Conservation laws implied by the Hamiltonian are fulfilled by imposing certain conditions on the approximate self-energy and, consequently, the vertex function Γ: in particular the issue of self-consistency is critical!

$\Rightarrow$ particle number, momentum, energy, …conservation

$\Rightarrow$ study consequences for the description of excited states

Write $G^{\phi}\left(\alpha,\overline{\beta},t-t'\right) = -\frac{i}{\hbar}\frac{\left\langle \Psi_0 \middle| T\left[\hat{S} a_{\alpha_F}(t) a^{+}_{\overline{\beta}_F}(t')\right] \middle| \Psi_0 \right\rangle}{\left\langle \Psi_0 \middle| T\left[\hat{S}\right] \middle| \Psi_0 \right\rangle}$ as an expansion in ϕ

In linear response (lowest order in ϕ):

Functional derivative of G^{ϕ} yields

$$\frac{\delta G^{\phi}\left(\alpha,\overline{\beta},t-t'\right)}{\delta\phi_{\gamma\overline{\delta}}\left(t''\right)} = \frac{i}{\hbar}\Pi\left(\alpha t,\beta^{-1}t';\gamma t'',\delta^{-1}t''\right)$$

corresponding to the *ph* limit of the two-particle propagator.

Conserving description of excited states

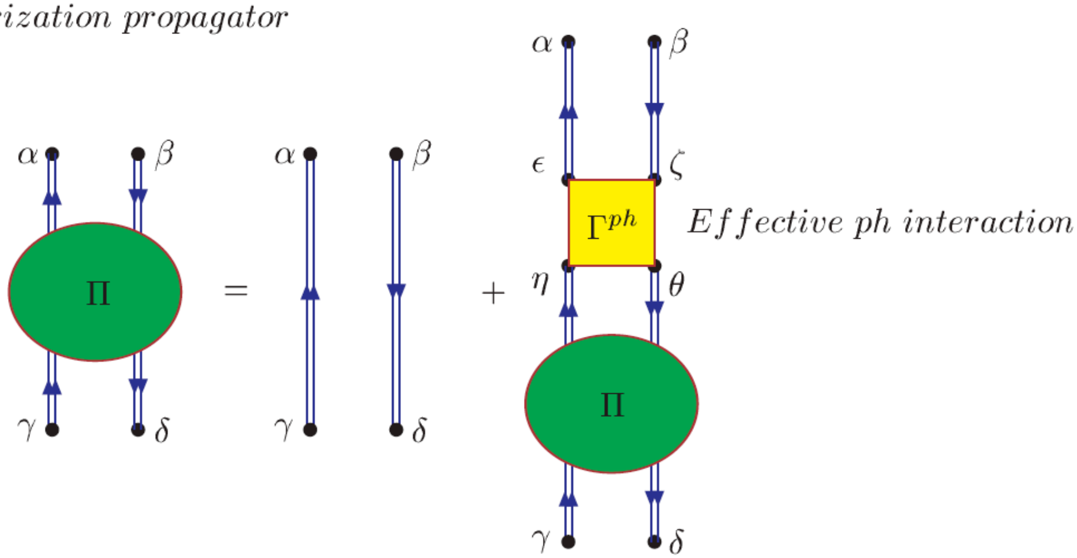
Fourier transform of two-time "polarization" propagator

$$\Pi\left(\alpha,\beta^{-1};\gamma,\delta^{-1};E\right)=\sum_{n\neq 0}\frac{\langle\Psi_0|a_{\bar\beta}^{+}a_{\alpha}|\Psi_n\rangle\langle\Psi_n|a_{\gamma}^{+}a_{\bar\delta}|\Psi_0\rangle}{E-\left(E_n-E_0\right)+i\eta}-\sum_{n\neq 0}\frac{\langle\Psi_0|a_{\gamma}^{+}a_{\bar\delta}|\Psi_n\rangle\langle\Psi_n|a_{\bar\beta}^{+}a_{\alpha}|\Psi_0\rangle}{E+\left(E_n-E_0\right)-i\eta}$$

contains all relevant information about excited states (location and one-body transition strength).

Integral equation for three-time polarization propagator from Dyson equation!

Polarization propagator



Propagators are dressed according to approximation (must be self-consistent)

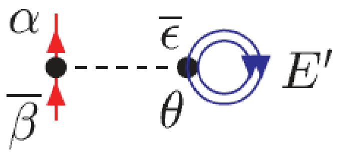
Particle-hole interaction

$$\Gamma^{ph}\left(\alpha t_1, \beta^{-1} t_2, \gamma t_3, \delta t_4\right) = \frac{\delta\Sigma\left(\alpha, \overline{\beta}; t_1 - t_2\right)}{\delta G\left(\gamma, \overline{\delta}; t_3 - t_4\right)}$$

If G is conserving, so is Π with this Γ^{ph}

Looks complicated … but …

Hartree-Fock and RPA



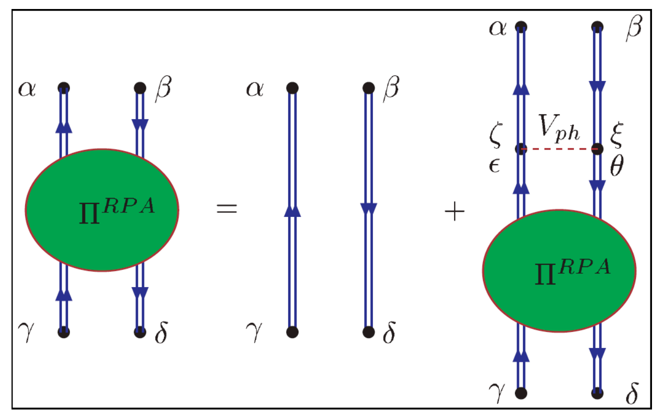
$$\Rightarrow \quad -i\hbar\delta(t-t') \sum_{\theta\overline{\epsilon}} \langle \alpha\overline{\epsilon}| V |\overline{\beta}\theta\rangle G^{HF}(\theta, \overline{\epsilon}; t - t^+)$$

Functional derivative equivalent to breaking internal propagator line so

$$\Gamma^{ph}_{HF}\left(\alpha t_1, \beta^{-1} t_2, \gamma t_3, \delta^{-1} t_4\right) = -i\hbar\delta\left(t_1 - t_2\right)\delta\left(t_1 - t_3\right)\delta\left(t_1 - t_4\right)\left\langle \alpha\overline{\delta}\middle| V \middle|\overline{\beta}\gamma\right\rangle$$

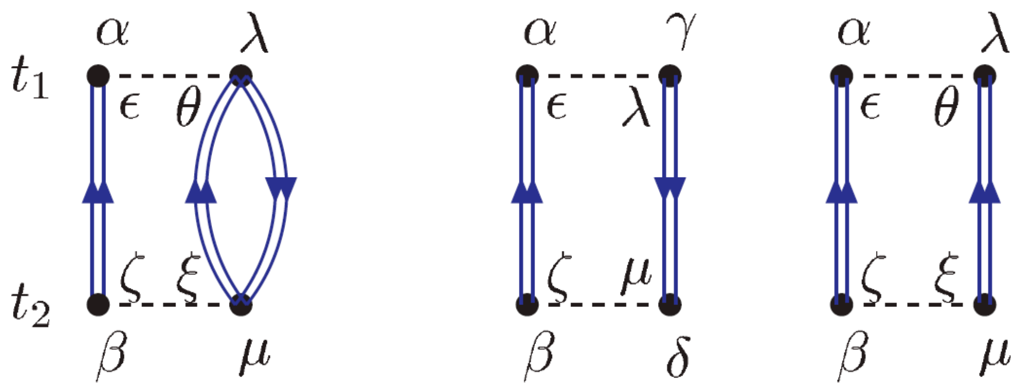
resulting in the RPA approximation to Π!!

sp propagators $\Rightarrow$ HF

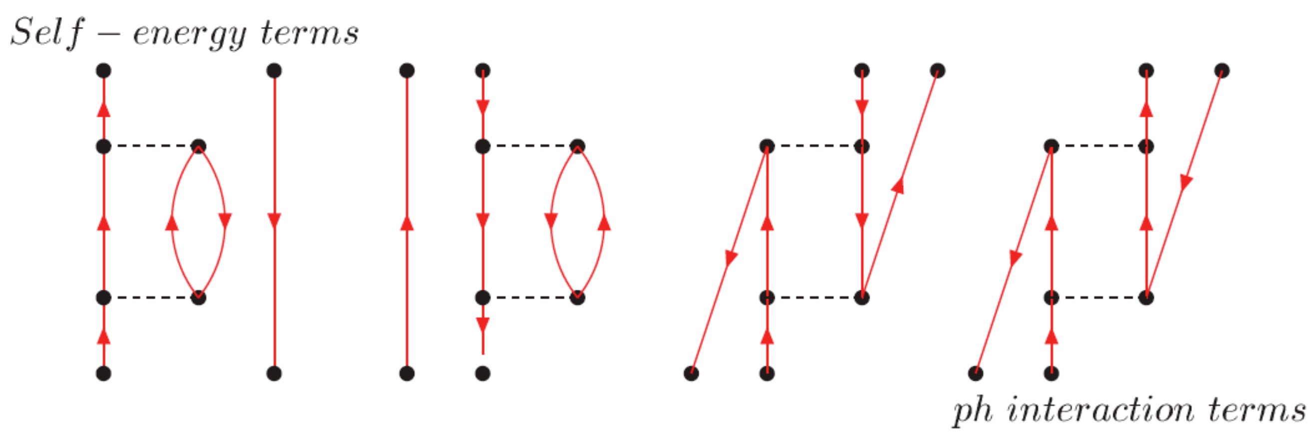


Beyond RPA = beyond mean-field for *G*

Second-order self-energy

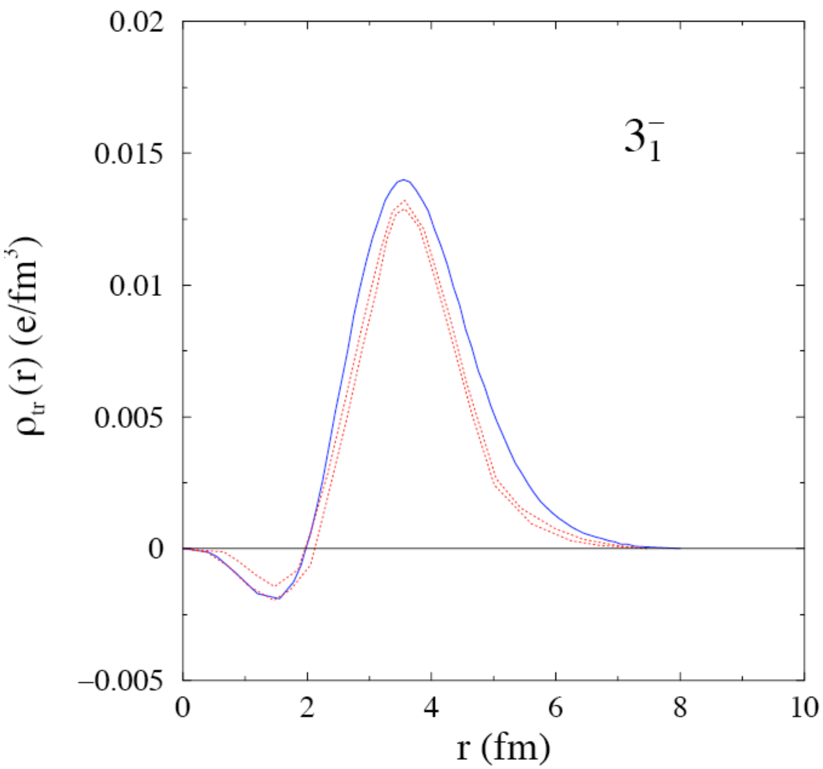


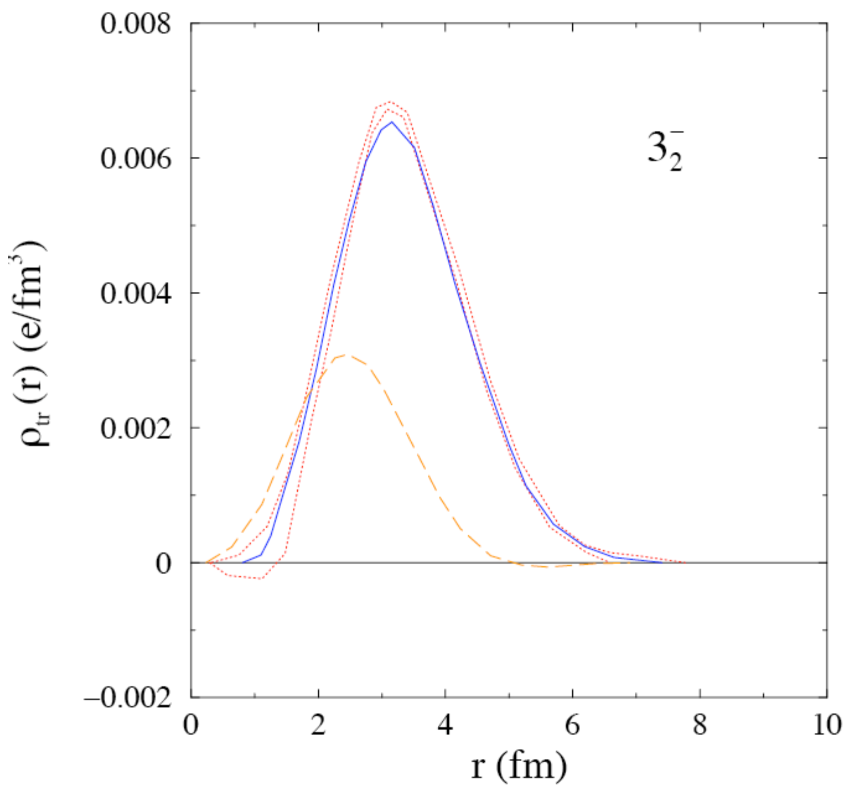
Leads to a consistent coupling of 1*p*1*h* to 2*p*2*h* configurations!



E(xtended)RPA results

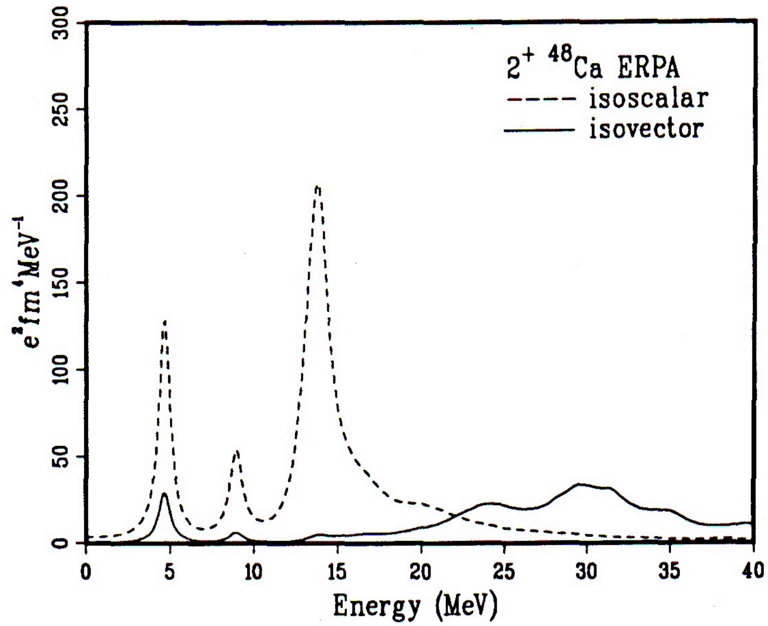
Transition densities in ^{48}Ca





Brand *et al.* Nucl.Phys.A509, 1 (1990)

Giant Quadrupole



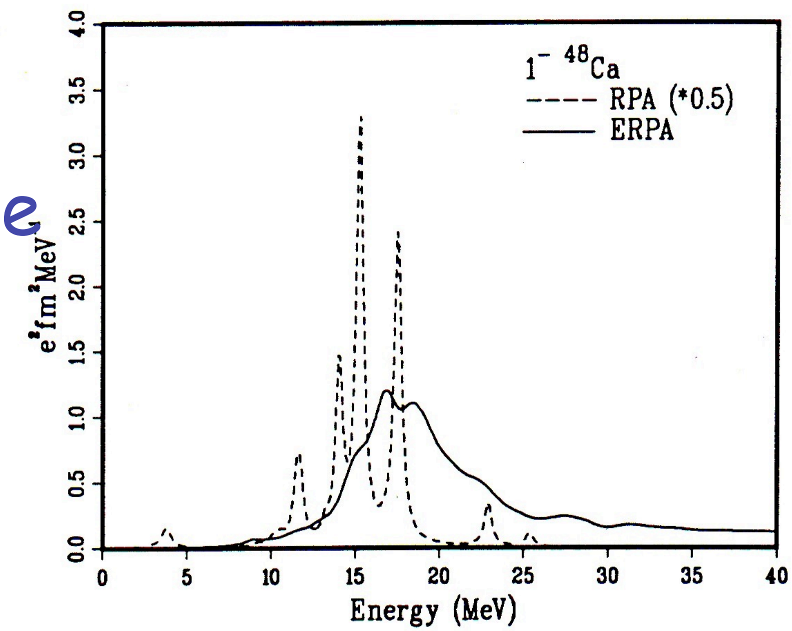
Giant Resonances only correct when sp fragmentation is included!

In turn:

Excited states

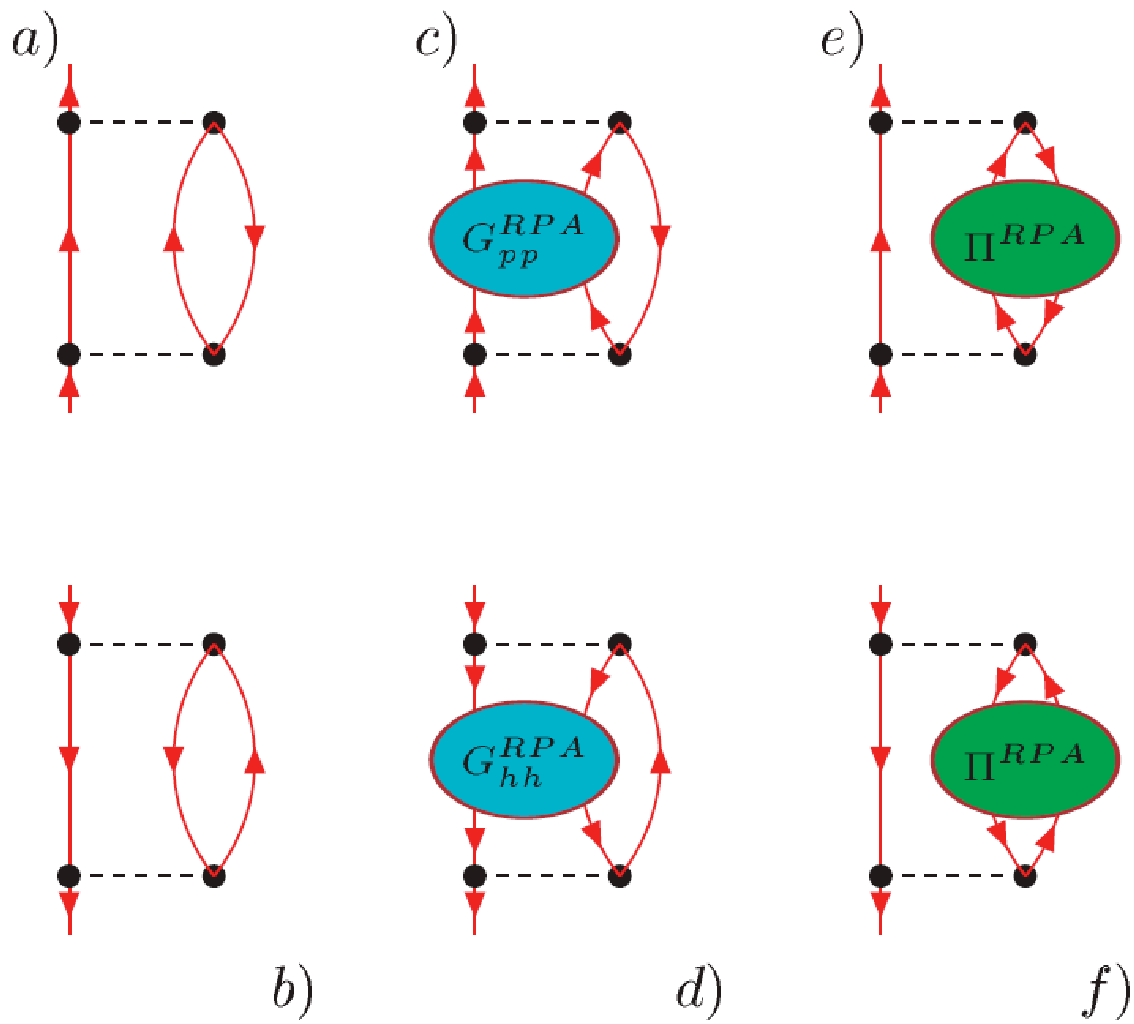
determine sp fragmentation

Giant Dipole



M. G. E. Brand, K. Allaart, and W. D.
Phys. Lett. **214B**, 483 (1988);
Nucl. Phys. **A509**, 1 (1990).

Long-range correlations ⇒ typical self-energy contributions



TDA or RPA

Link with excited states at low energy and their collective features

Results for TDA & RPA self-energies

Need:

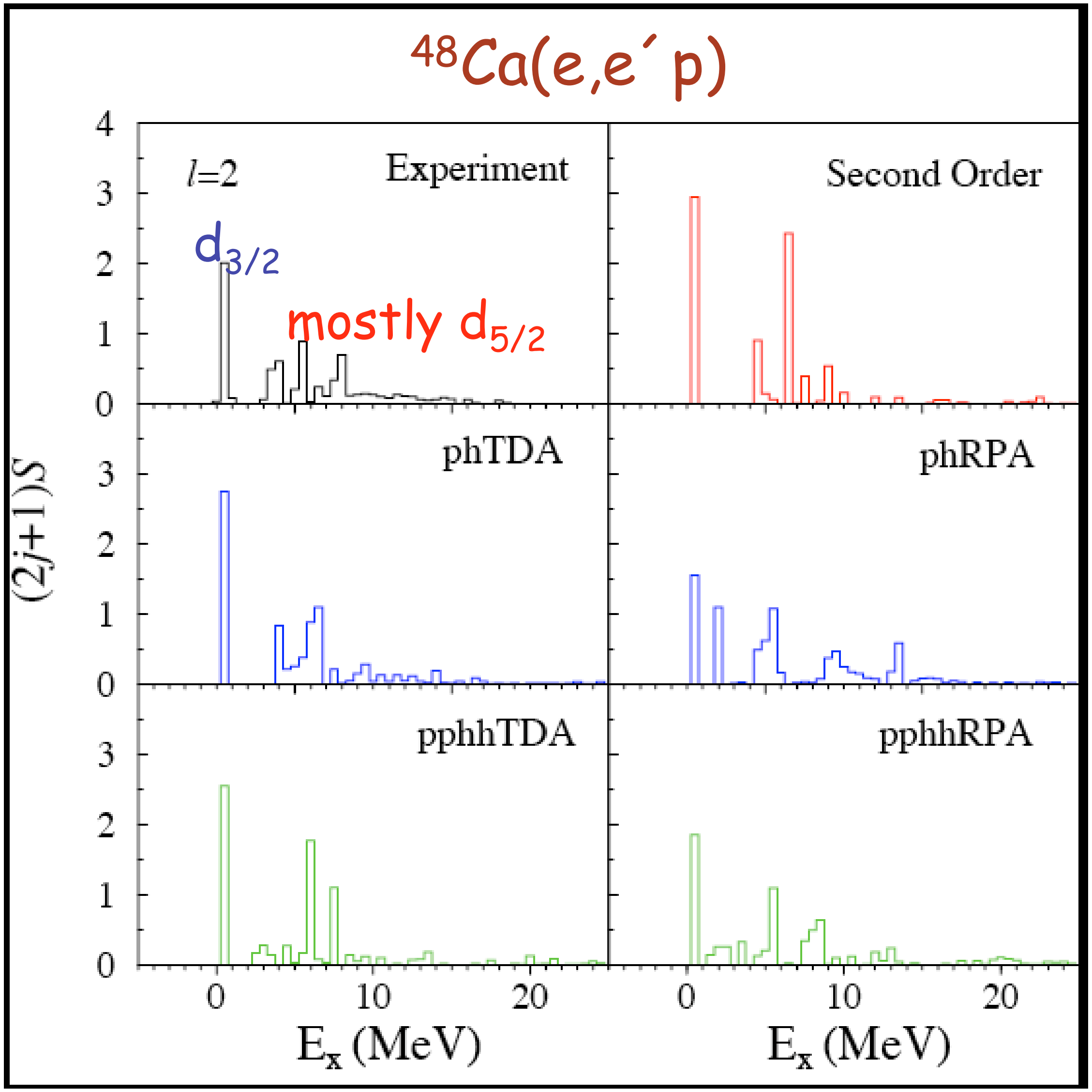
Better fragmentation at low energy
⇒ Excited states beyond RPA (unstable)

Less strength at low energy
⇒ Effect of SRC

Calculations yield:

10% strength at more bound energies!

10% depletion for states near the Fermi energy



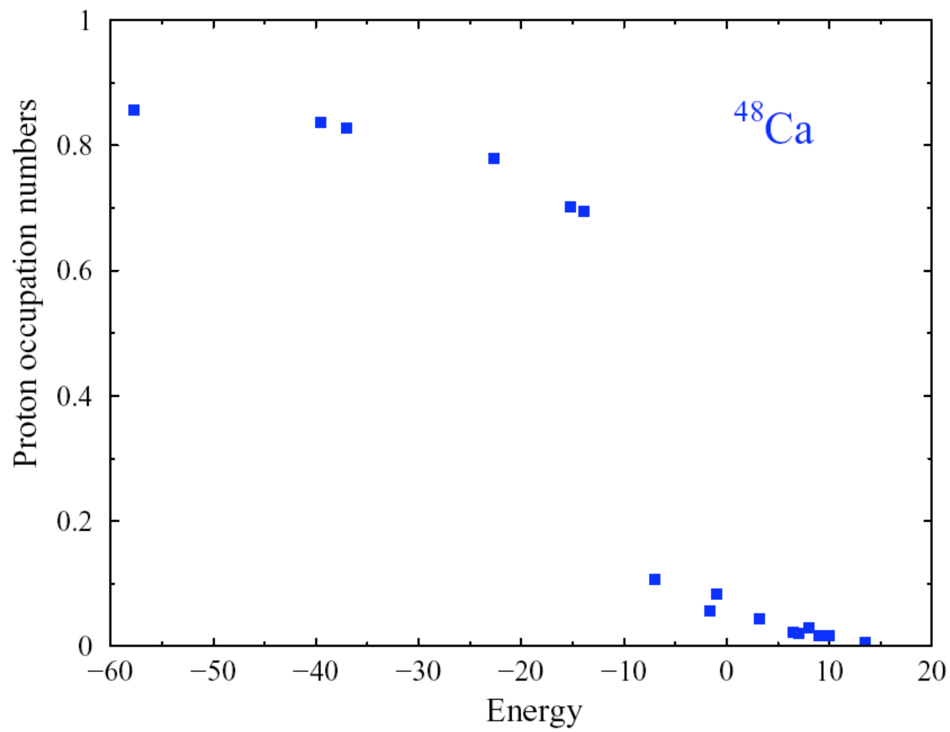
Occupation numbers ^{48}Ca

Shell	$\Sigma^{(2)}$	Σ^{TDA}_{ph}	Σ^{RPA}_{ph}	Σ^{TDA}_{pphh}	Σ^{RPA}_{pphh}
$0s\frac{1}{2}$	.967	.968	.963	.965	.952
$0p\frac{3}{2}$	.955	.956	.944	.950	.930
$0p\frac{1}{2}$	.951	.951	.939	.944	.920
$0d\frac{5}{2}$	.920	.925	.915	.898	.867
$0d\frac{3}{2}$	.877	.885	.891	.842	.780
$1s\frac{1}{2}$	.869	.860	.907	.818	.773
$0f\frac{7}{2}$	.060	.063	.048	.082	.120
$0f\frac{5}{2}$	.048	.044	.043	.064	.092
$1p\frac{3}{2}$	.033	.031	.036	.049	.063
$1p\frac{1}{2}$	.030	.028	.035	.042	.050
$0g\ 1d\ 2s$	.014	.014	.019	.018	.026
$0h\ 1f\ 2p$	.006	.006	.006	.007	.009
Total	20.053	20.093	20.125	20.165	20.370

Occupation numbers from low-energy correlations

Shell	$n(\alpha)$
$0s_{1/2}$	0.968
$0p_{3/2}$	0.956
$0p_{1/2}$	0.951
$0d_{5/2}$	0.925
$0d_{3/2}$	0.885
$1s_{1/2}$	0.860
$0f_{7/2}$	0.063
$0f_{5/2}$	0.044
$0p_{3/2}$	0.031
$0p_{1/2}$	0.028
….	

Including SRC depletion effect by treating energy dependence of *G*-matrix



Spectroscopic Strength in ^{16}O

Data: PRC49, 955 (94)

- Influence of SRC ✓✓
- Translational Invariance ✖
- Influence of LRC "✓"

  TDA for 2p1h and 2h1p

  Geurts et al.

  PRC**53**, 2207 (1996)

- Influence of LRC ✓✓

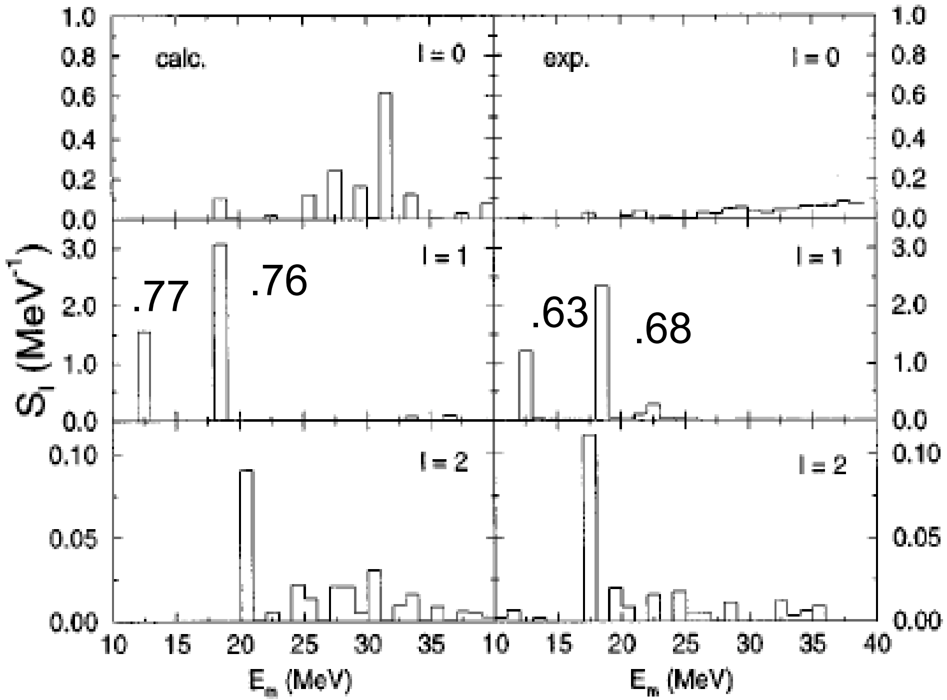
  RPA + Faddeev

  C. Barbieri and WHD,

  PRC**65**, 064313 (2002)

Still not solved because RPA is not good enough for ^{16}O!!

TDA



Shell	TDA	RPA
$d_{3/2}$	0.866	0.838
$s_{1/2}$	0.882	0.842
$d_{5/2}$	0.894	0.875
$p_{1/2}$	0.775	0.745
$p_{3/2}$	0.766	0.725

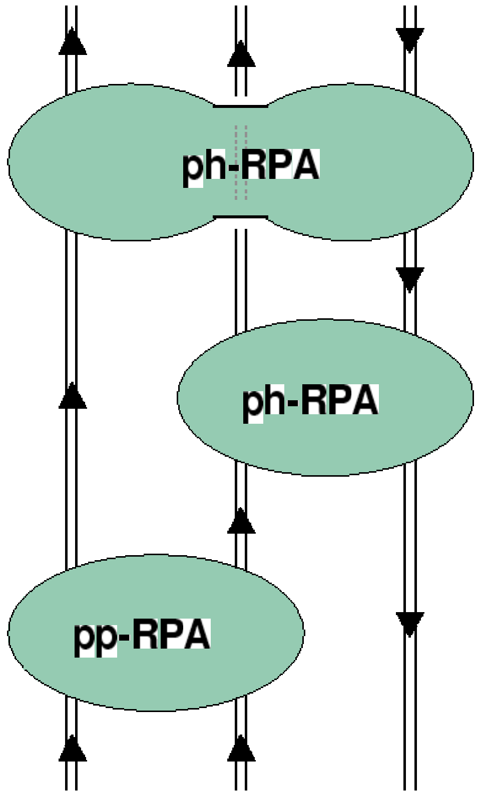
Some theoretical results for ^{16}O

	$S_{p1/2}$	$S_{p3/2}$		
• Experiment	0.63	0.67	±0.05	NIKHEF '94
• Short-range oriented methods				
VMC [Argonne, '94]	0.90			SRC 10%
GF(SRC) [St.Louis-Tübingen '95]	0.91	0.89		
FHNC/SOC [Pisa '00]	0.90			
• Including particle-phonon couplings				
GF(Faddeev) [St.Louis '01]	0.77	0.72		LRC rest
• → relevance of collective motion				

LRC ≈ particle-phonon (GR) coupling

Faddeev technique and Long-Range Correlations

- Both pp (hh) and ph phonons are collective in nuclei using RPA
- Faddeev technique allows correct summation to all orders of these phonons
- Formalism:
  Phys. Rev. C**63**, 034313 (2001)
- Results: for ^{16}O
  Phys. Rev. C**65**, 064313 (2002)

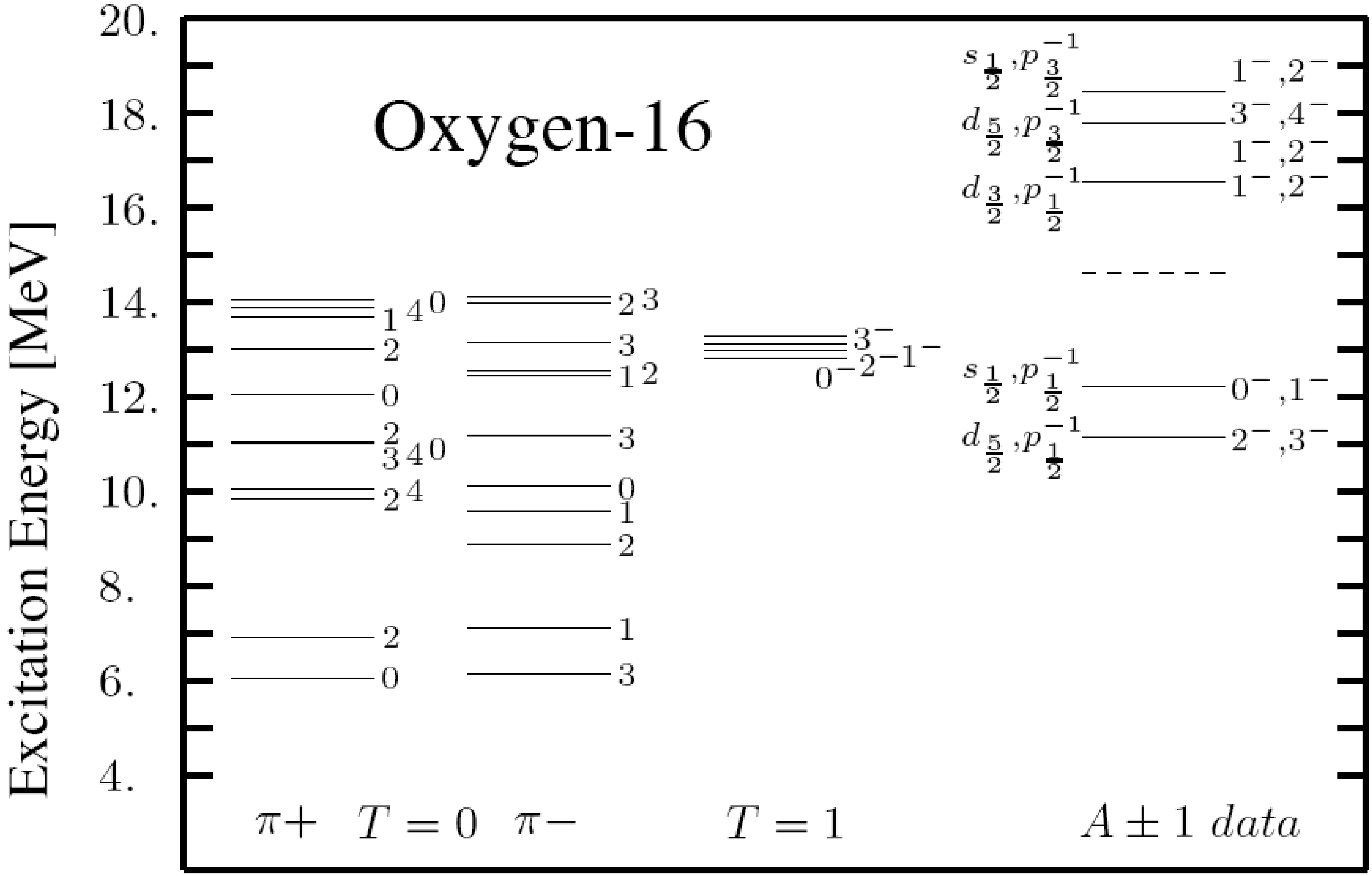


Faddeev results for Ne atom

	HF	Dyson(2)	F-TDA(3)	F-RPA(3)	Experiment
2p	-0.850	-0.763	-0.797	-0.790	-0.793
2s	-1.930	-1.750	-1.794	-1.785	-1.782

Small basis; large basis in progress (Barbieri, Van Neck, WD)

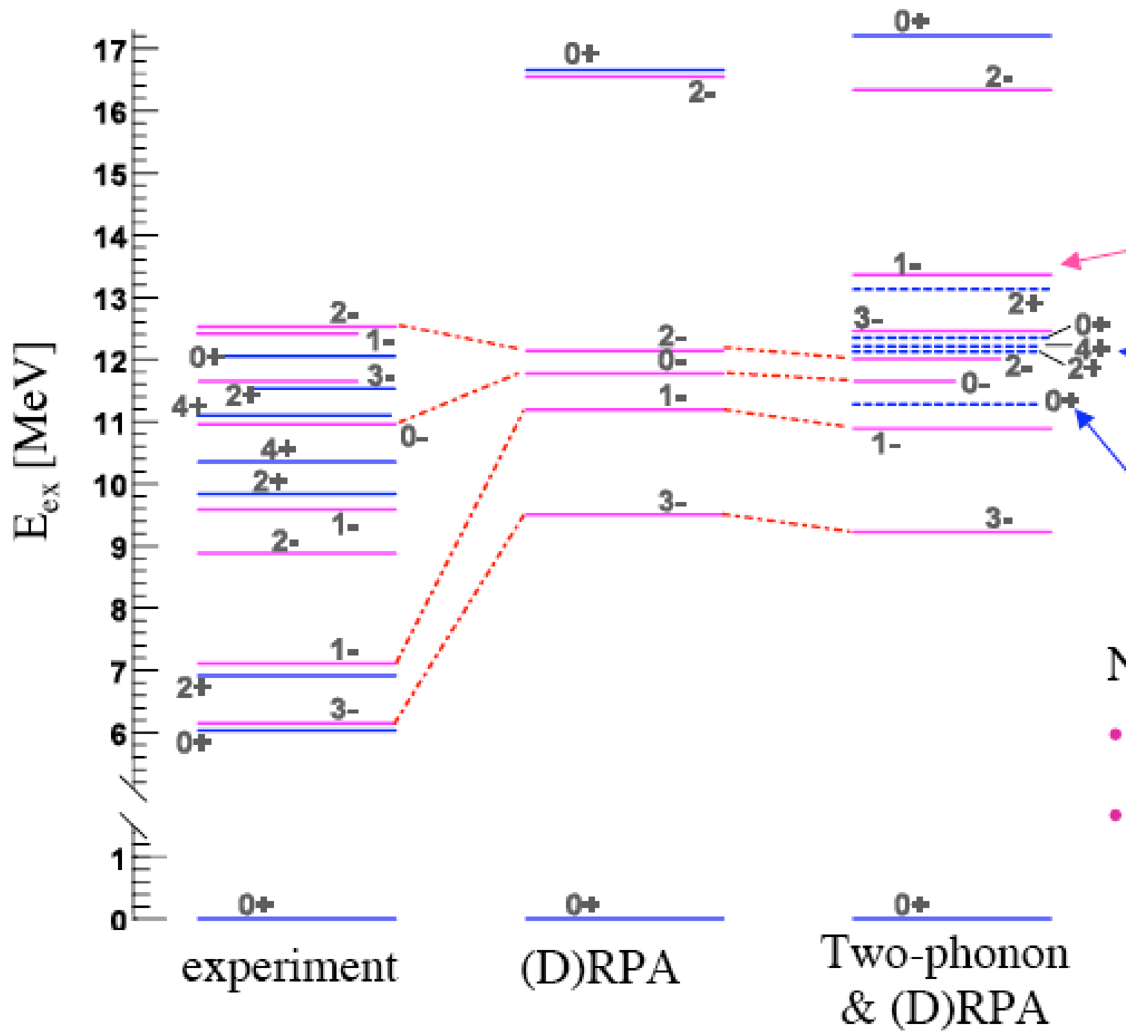
Excitation spectrum of ^{16}O



Improving excitation spectra beyond RPA

Coupling of two-phonons in ^{16}O

C.B., Dickhoff,
PRC68, 014311 (2003)



Roughly:

80% (0+)x(1-) + 20% ph

98% $(3\text{-})^2$

85% $(0+)^2$ + 15% ph

Need to do better:

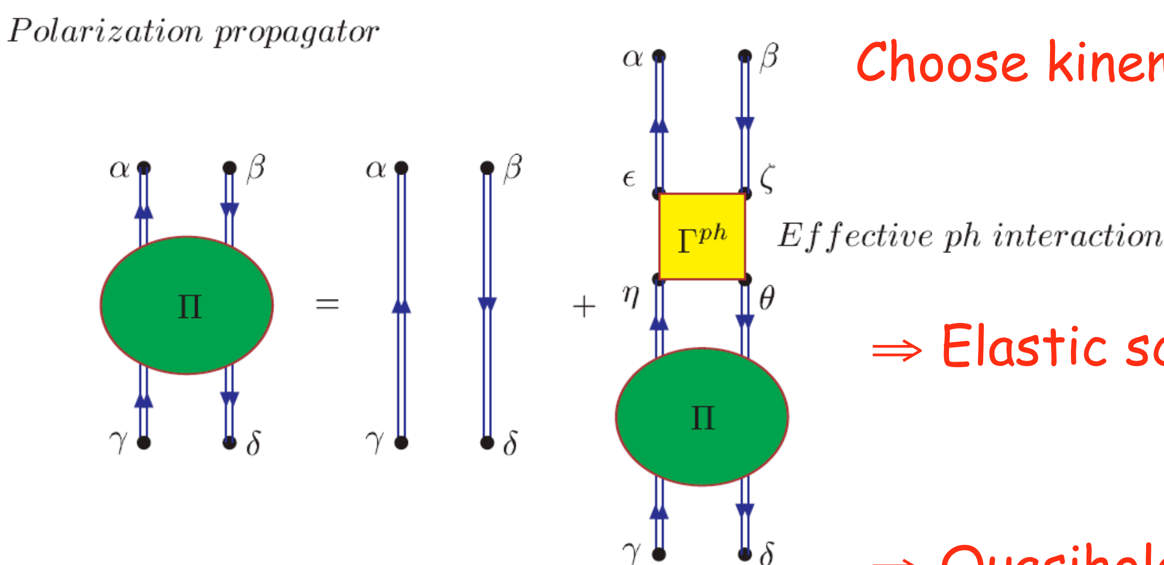
- pp(hh) interactions
- 4-phonon states
  [Feshbach & Iachello ('73)]

FSI and (e,e´p) $\Leftrightarrow$ analysis

$$\hat{O} = \sum_{\alpha\beta} \langle\alpha|O|\beta\rangle a_\alpha^+ a_\beta$$ Electron Scattering $\Rightarrow$ one-body operator

$$\left|\left\langle \Psi_n^A \middle| \hat{O} \middle| \Psi_0^A \right\rangle\right|^2 = \sum \langle\alpha|O|\beta\rangle^* \langle\gamma|O|\delta\rangle \left\langle \Psi_0^A \middle| a_\beta^+ a_\alpha \middle| \Psi_n^A \right\rangle \left\langle \Psi_n^A \middle| a_\gamma^+ a_\delta \middle| \Psi_0^A \right\rangle$$

Requires (imaginary part of) **exact** polarization propagator



Choose kinematics: $\Rightarrow$ only first term

$$\left\langle \Psi_m^{A+1} \middle| a_\alpha^+ \middle| \Psi_0^A \right\rangle$$

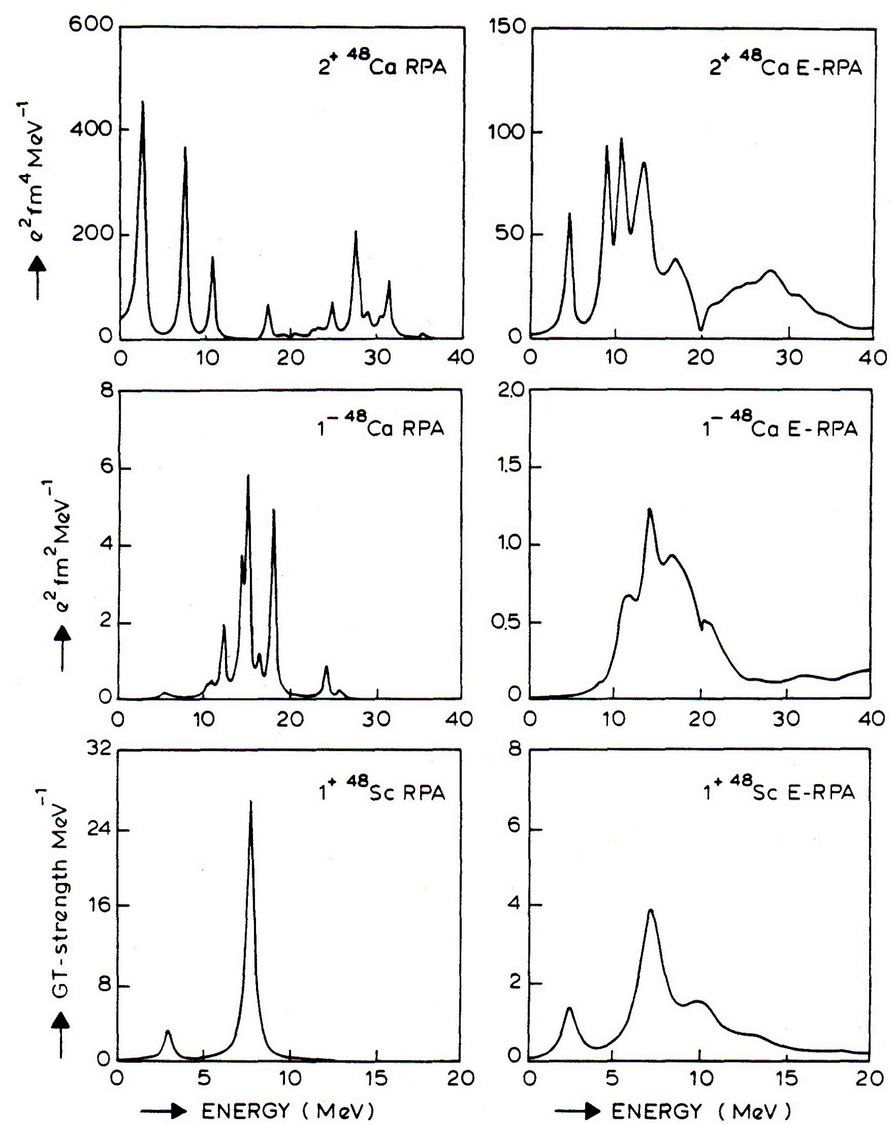
$\Rightarrow$ Elastic scattering (phenomenology)

$$\left\langle \Psi_n^{A-1} \middle| a_\beta \middle| \Psi_0^A \right\rangle$$

$\Rightarrow$ Quasihole wave function

"Absolute" spectroscopic factors √

Difference between RPA and ERPA



GQR

GDR

Gamow-Teller