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
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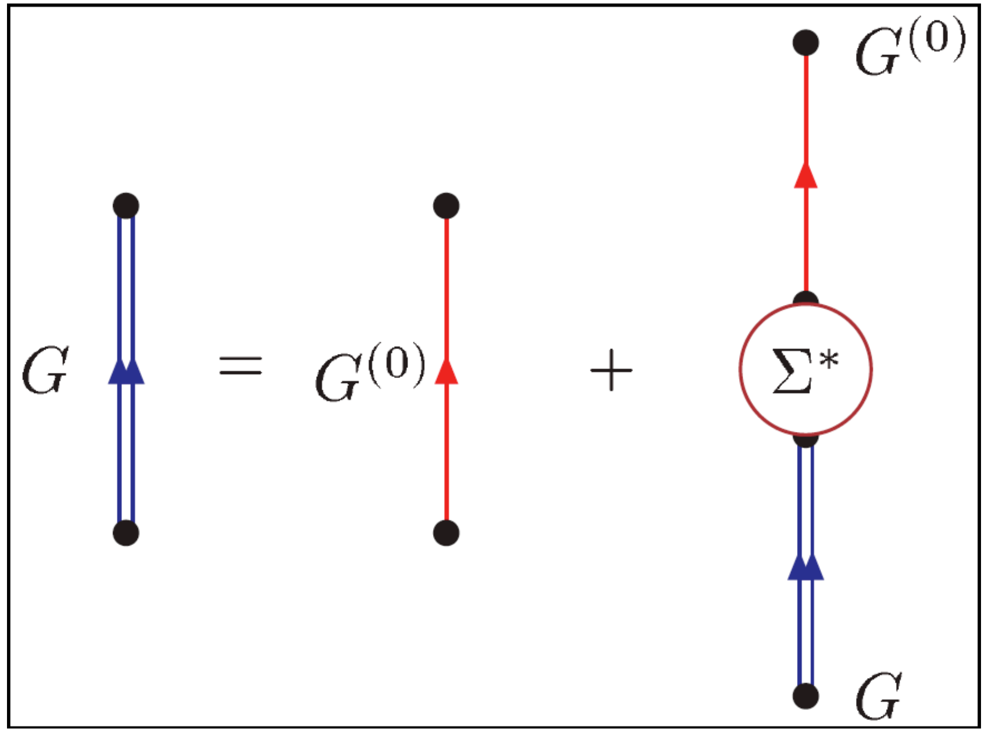
Outline

- 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 $\Leftrightarrow$ 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

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

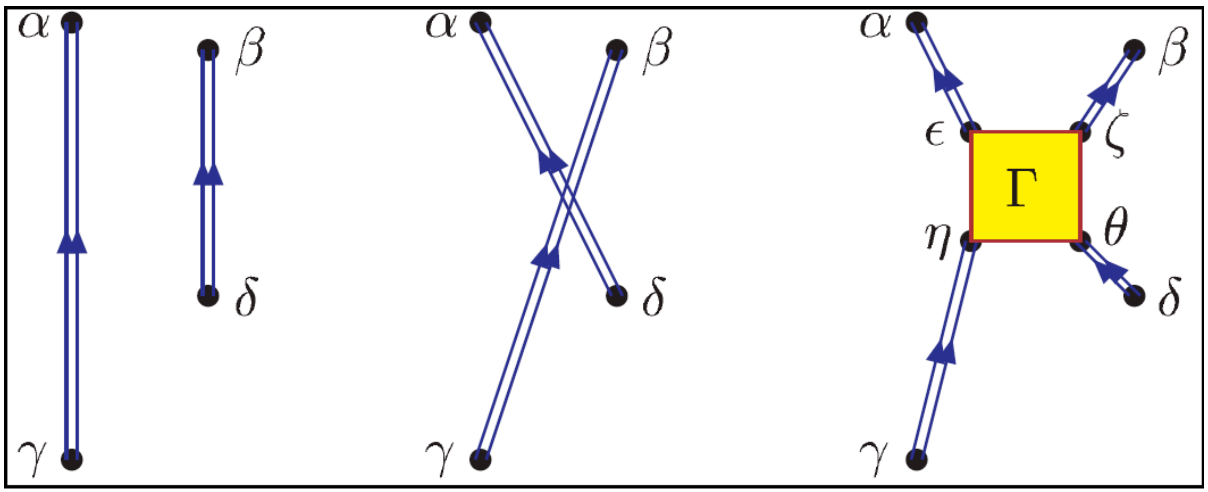
with the irreducible self-energy acting as the in-medium (complex) potential.

Link with two-particle propagator

Equation of motion for G

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

Diagrammatic analysis of G^{II} yields



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

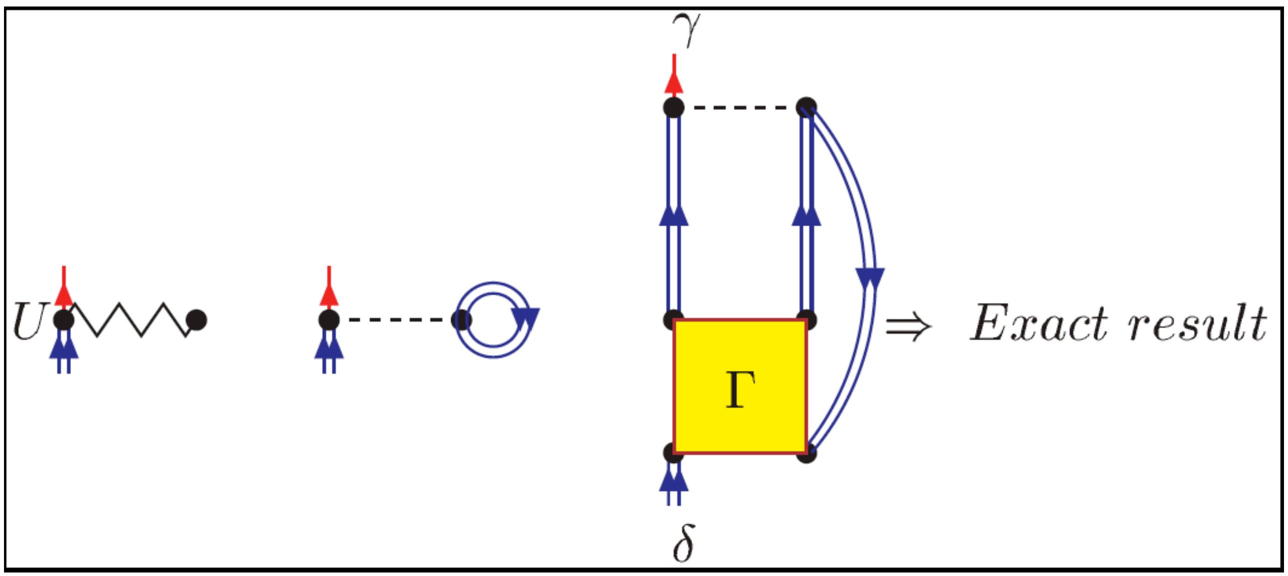
Dyson equation and vertex function

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

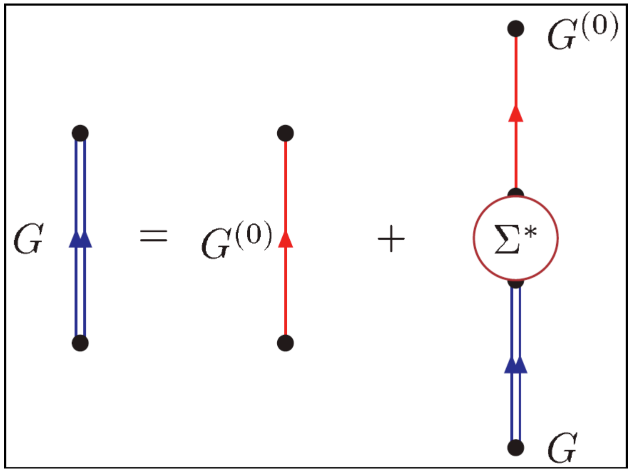
$$\Sigma^*(\gamma,\delta;E) = -\langle\gamma|U|\delta\rangle - i\int_{C\uparrow}\frac{dE'}{2\pi}\sum_{\mu\nu}\langle\gamma\mu|V|\delta\nu\rangle G(\nu,\mu;E')$$

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

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

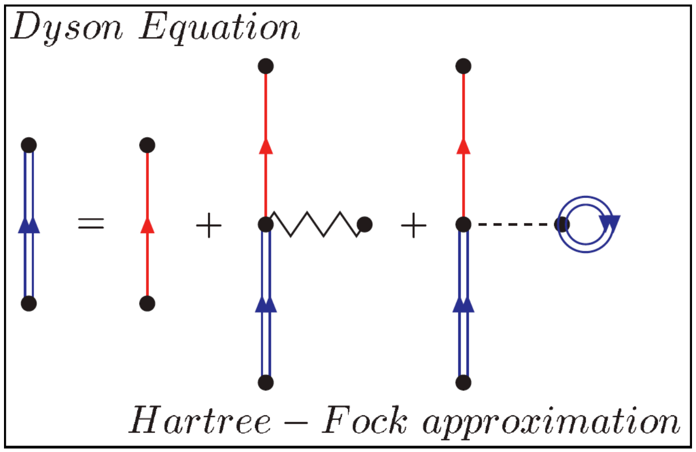
$$S = \left| \left\langle \Psi_n^{N-1}\middle| a_{\alpha_{qh}} \middle| \Psi_0^N \right\rangle \right|^2 = \frac{1}{1 - \left. \dfrac{\partial \Sigma'^{*}\left(\alpha_{qh}, \alpha_{qh}; E\right)}{\partial E} \right|_{E_n^-}}$$

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		

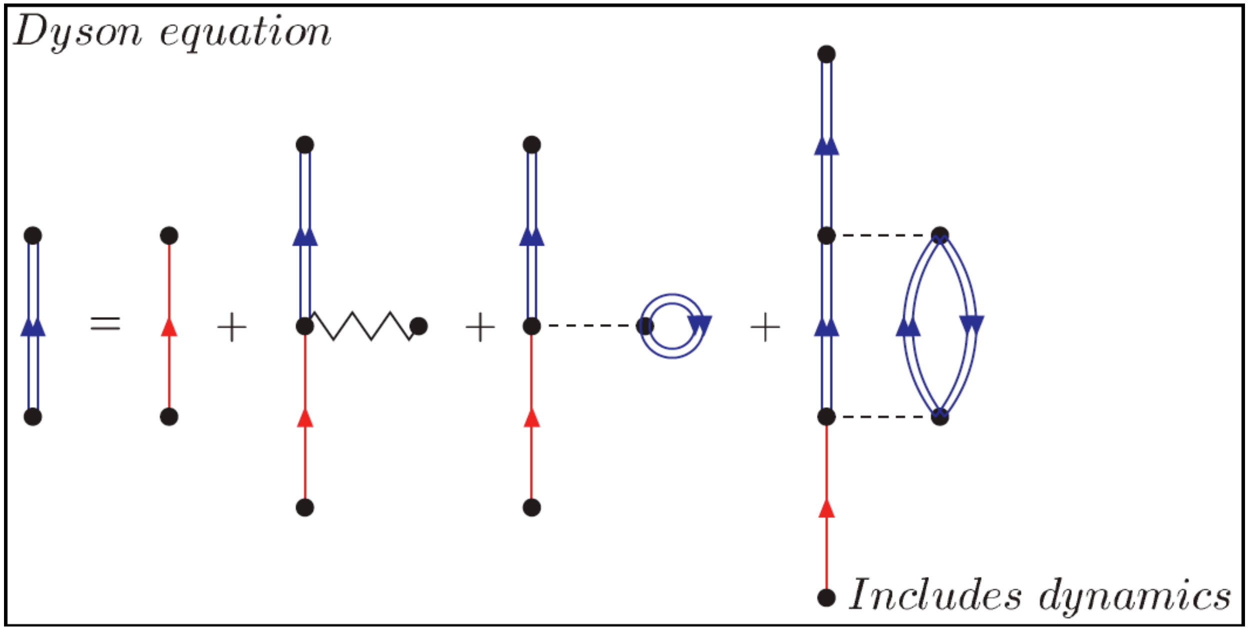
Energies in atomic units (Hartree)

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 ✓

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

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

Corresponding Dyson equation

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

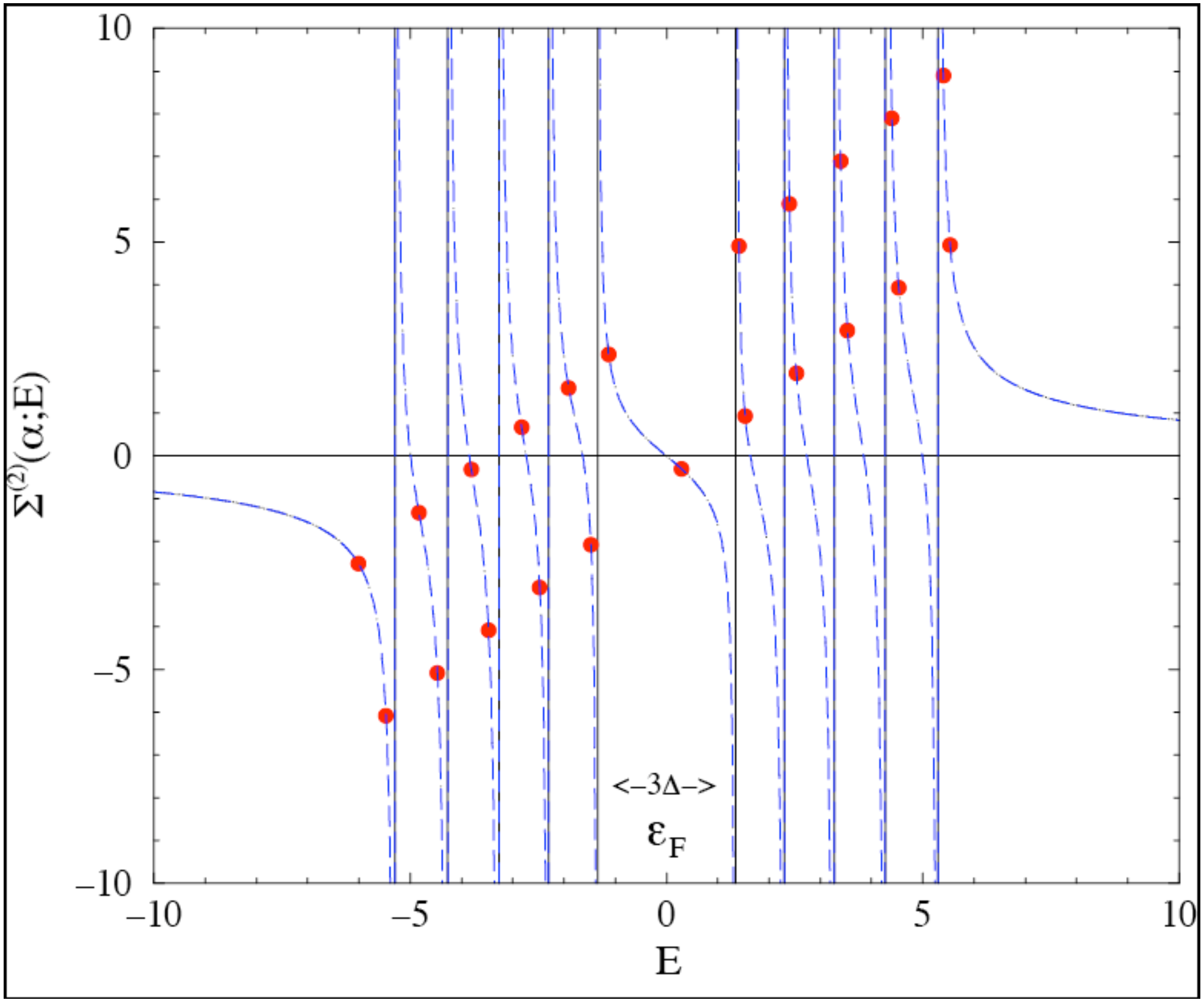
Assume discrete poles in Σ, then discrete solution (poles of G) for

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

With residue (spectroscopic factor)

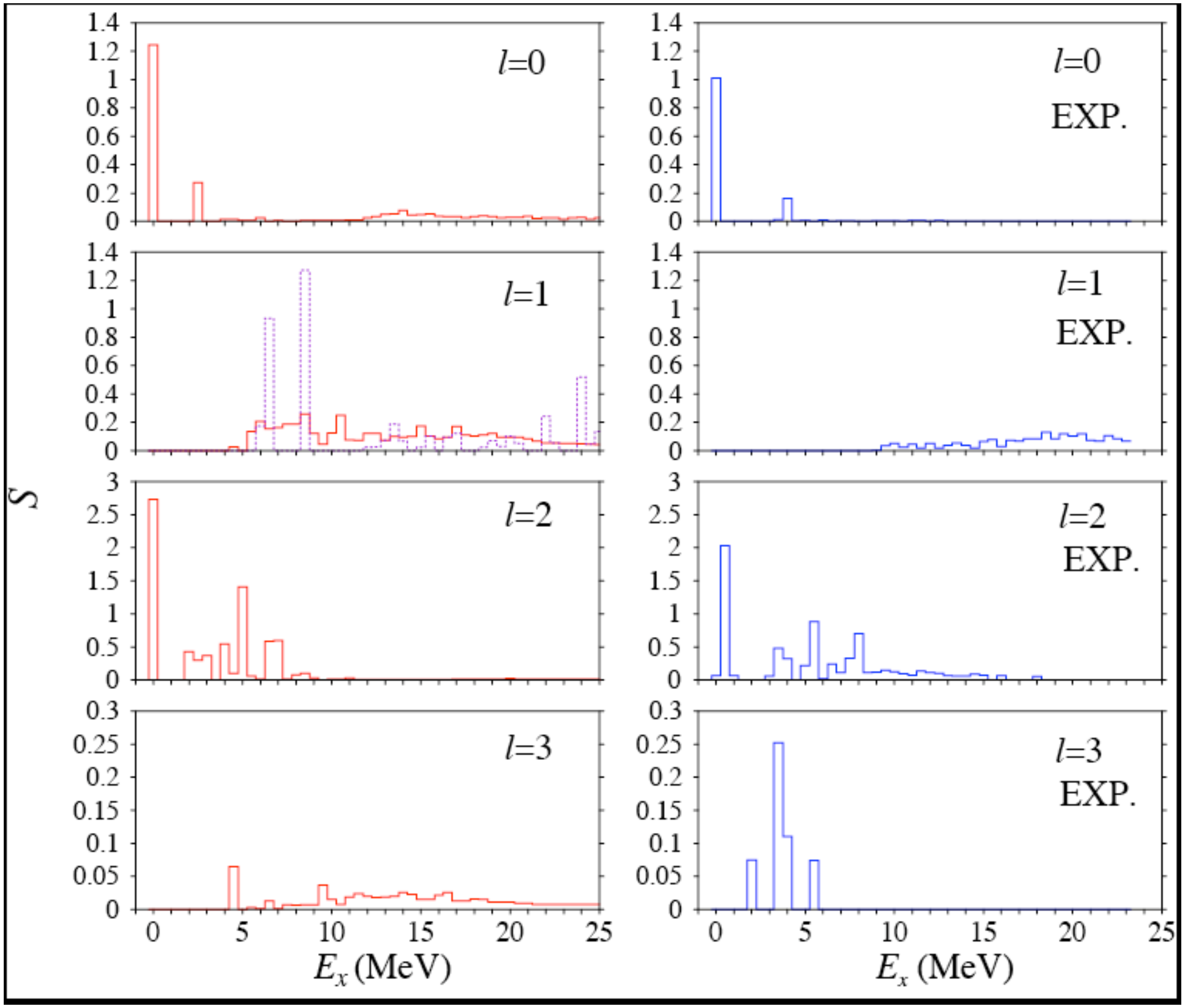
$$R_{n\alpha}=\frac{1}{1-\left.\frac{\partial\Sigma^{(2)}(\alpha;E)}{\partial E}\right|_{E_{n\alpha}}}$$

Solutions



Explains all qualitative features of sp strength distribution in nuclei!

Self-consistent calculation with Skyrme force

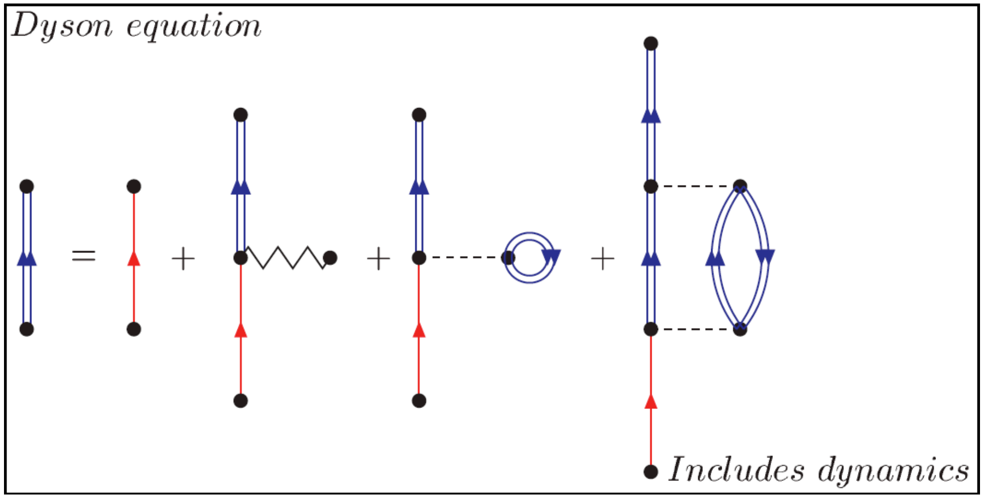


Data: ^{48}Ca(e,e´p)
Kramer NIKHEF
(1990)

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* ⇒ therefore this procedure doesn't **yet** completely include the effect of short-range and tensor correlations on sp motion.

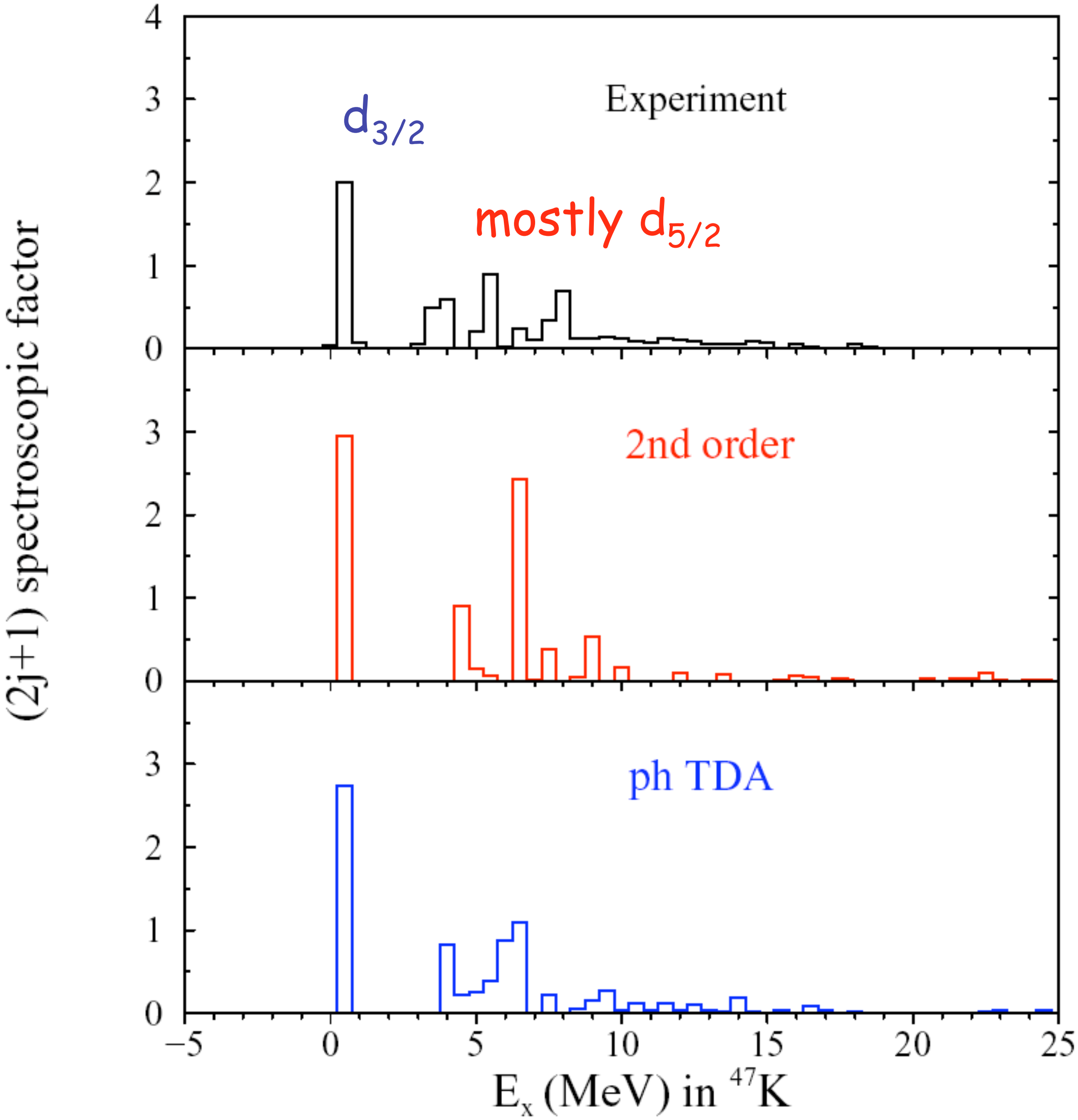
Neglect energy dependence of *G* then

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

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

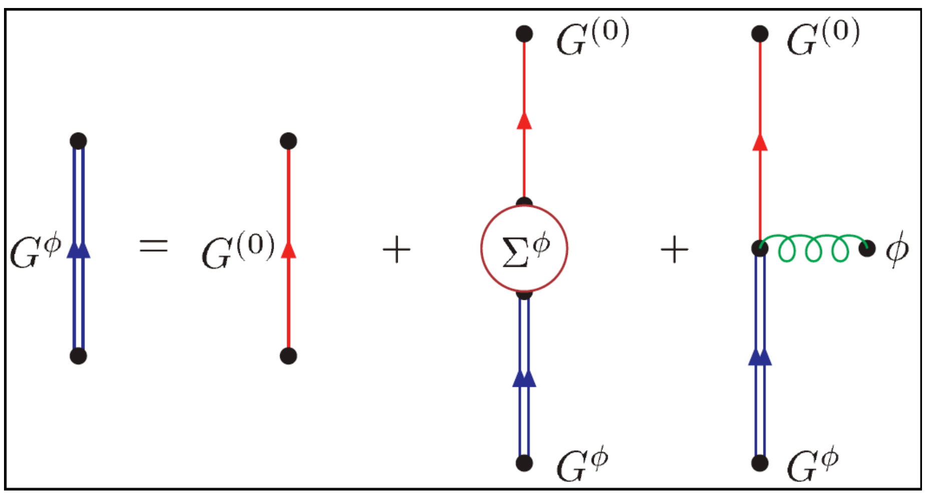
G-matrix strong enough to distribute strength in this interval

Excited states and G …
G and excited states …

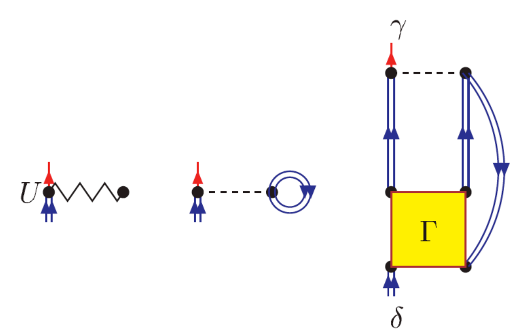
Before improving self-energy with a better description of the intermediate $2p1h$ and $2h1p$ states, it is instructive to clarify the deep relation between excited states and the sp propagator G.
$\Rightarrow$ Study time-dependent external fields that can probe excited states

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

In linear response (lowest order in ϕ):
Functional derivative of G^{ϕ} yields

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

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

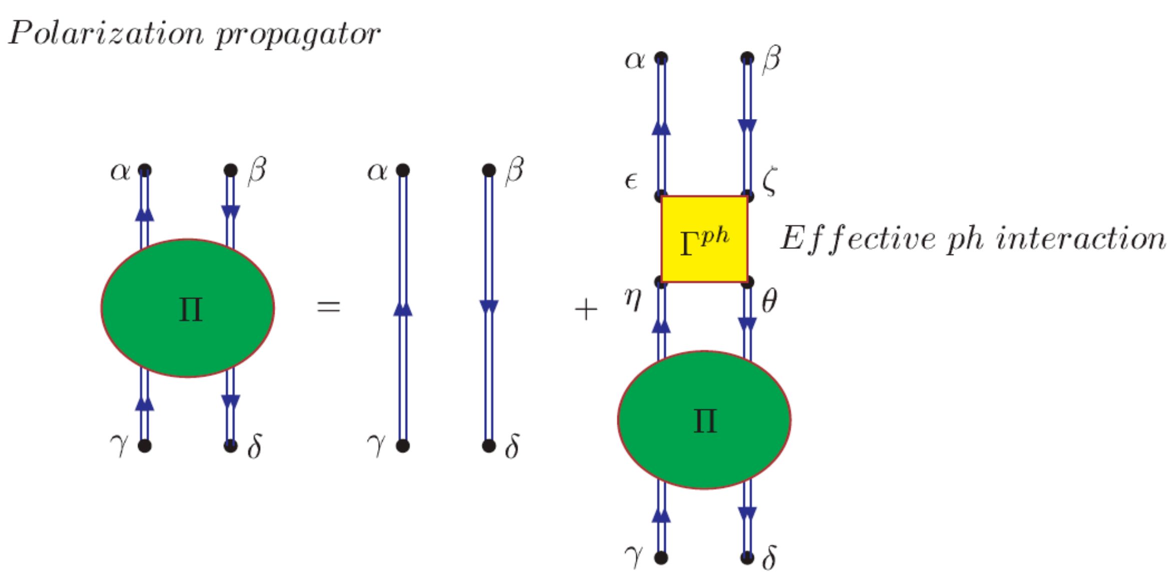
Conserving description of excited states

Fourier transform of two-time "polarization" propagator

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

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

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



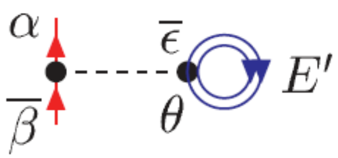
Propagators are dressed according to approximation (must be self-consistent)

Particle-hole interaction

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

If G is conserving, so is Π with this Γ^{ph}
Looks complicated … but …

Hartree-Fock and RPA



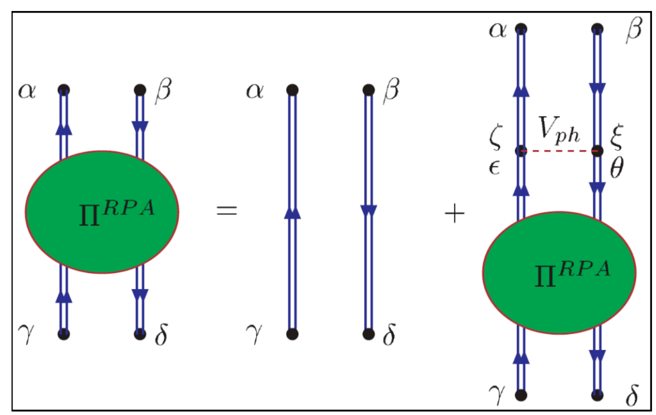
$$\Rightarrow \quad -i\hbar\delta(t - t') \sum_{\theta\overline{\epsilon}} \langle \alpha\overline{\epsilon} | V | \overline{\beta}\theta \rangle G^{HF}(\theta, \overline{\epsilon}; t - t^{+})$$

Functional derivative equivalent to breaking internal propagator line so

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

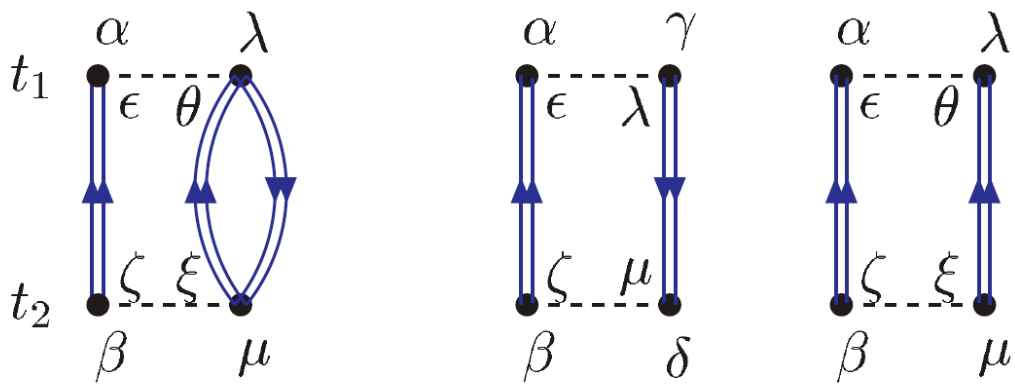
resulting in the RPA approximation to Π!!

sp propagators $\Rightarrow$ HF

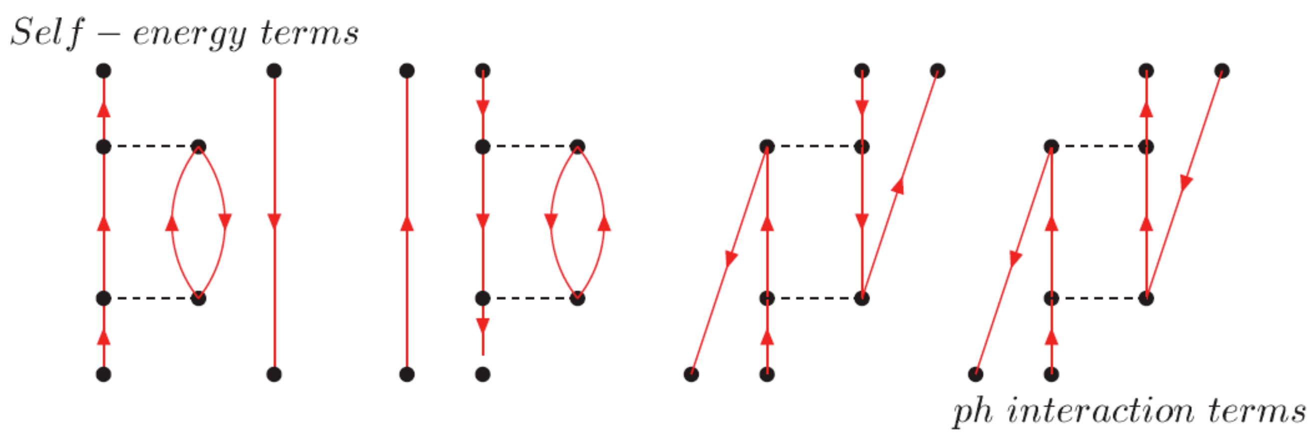


Beyond RPA = beyond mean-field for G

Second-order self-energy

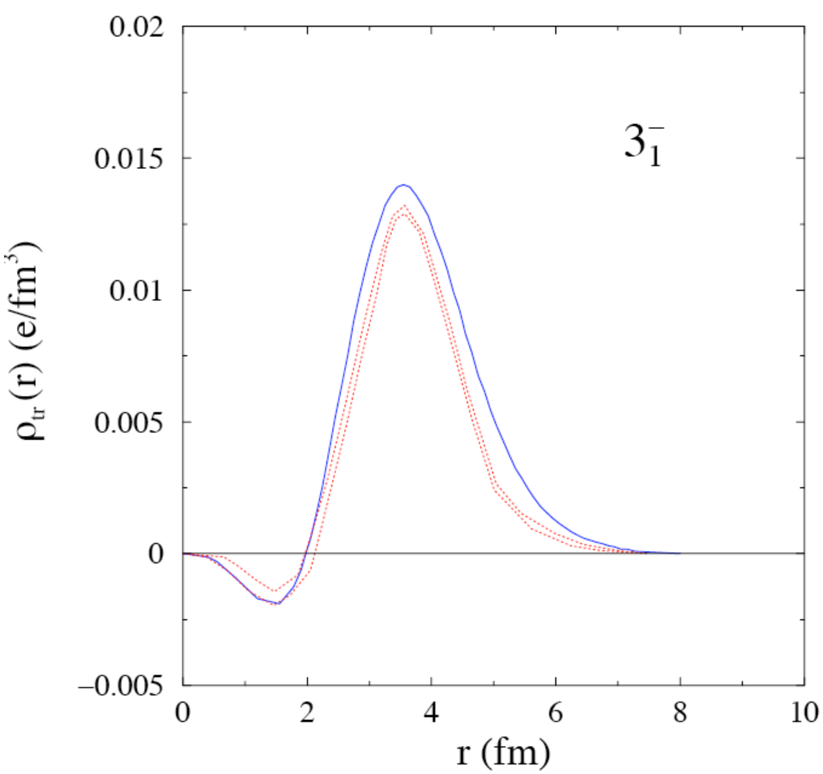


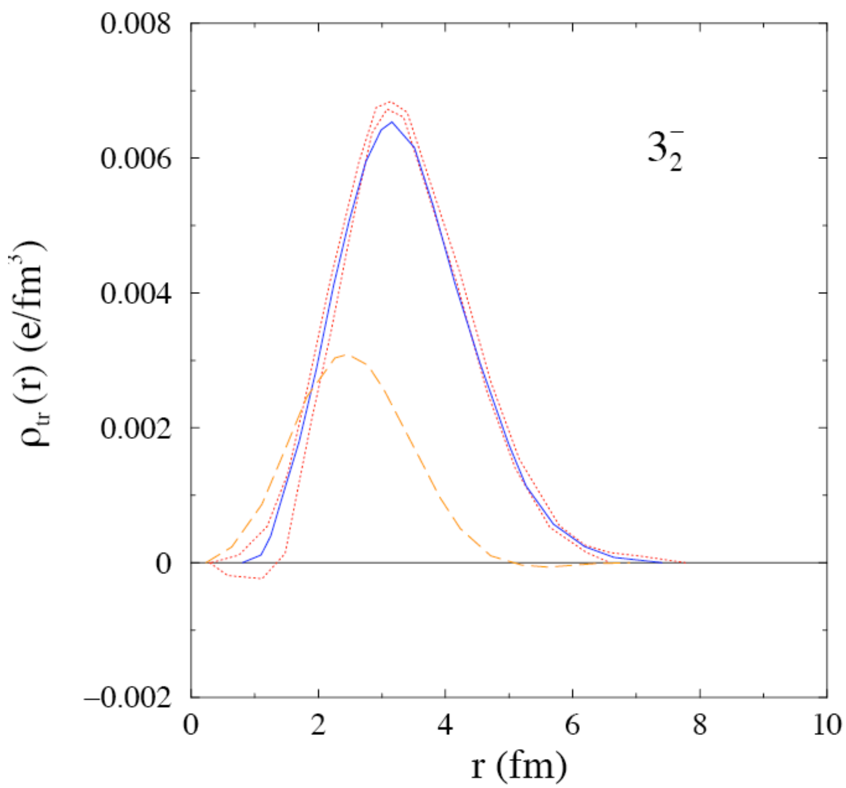
Leads to a consistent coupling of $1p1h$ to $2p2h$ configurations!



E(xtended)RPA results

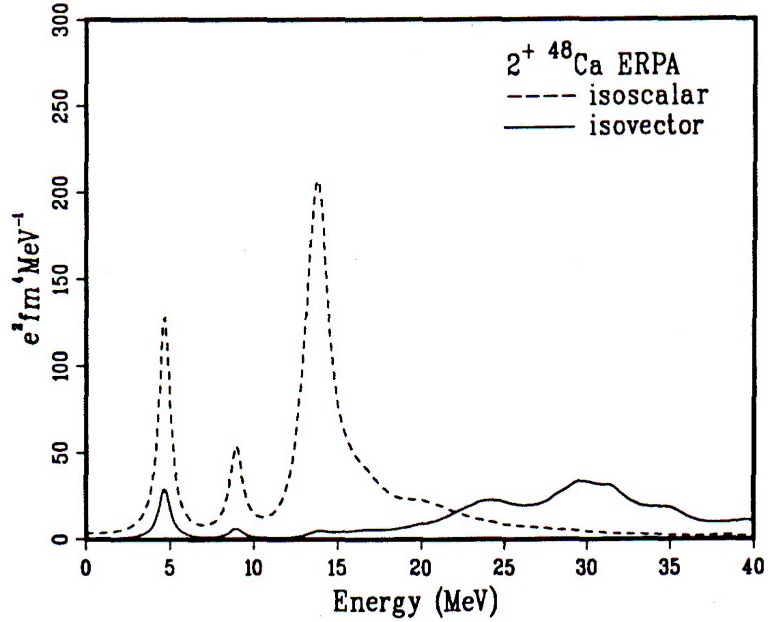
Transition densities in ^{48}Ca





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

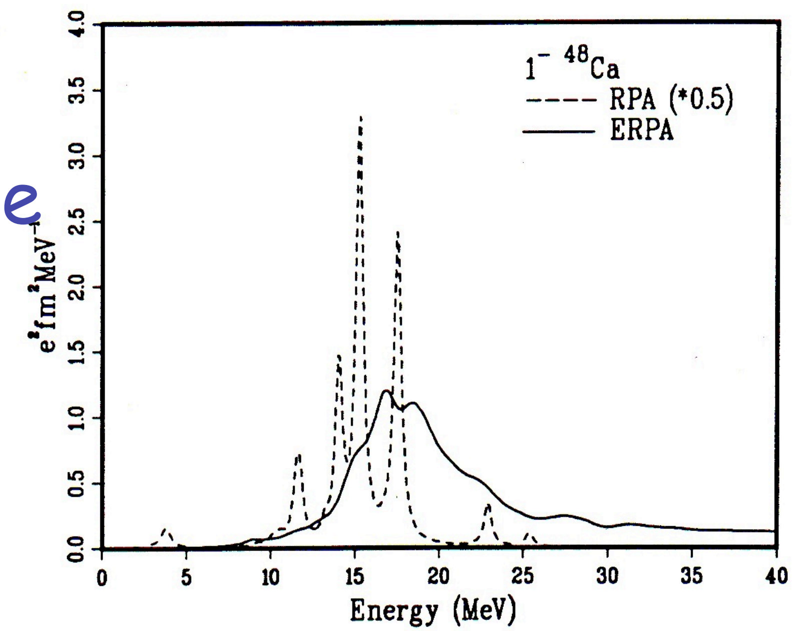
Giant Quadrupole



Giant Resonances
only correct when sp fragmentation is included!

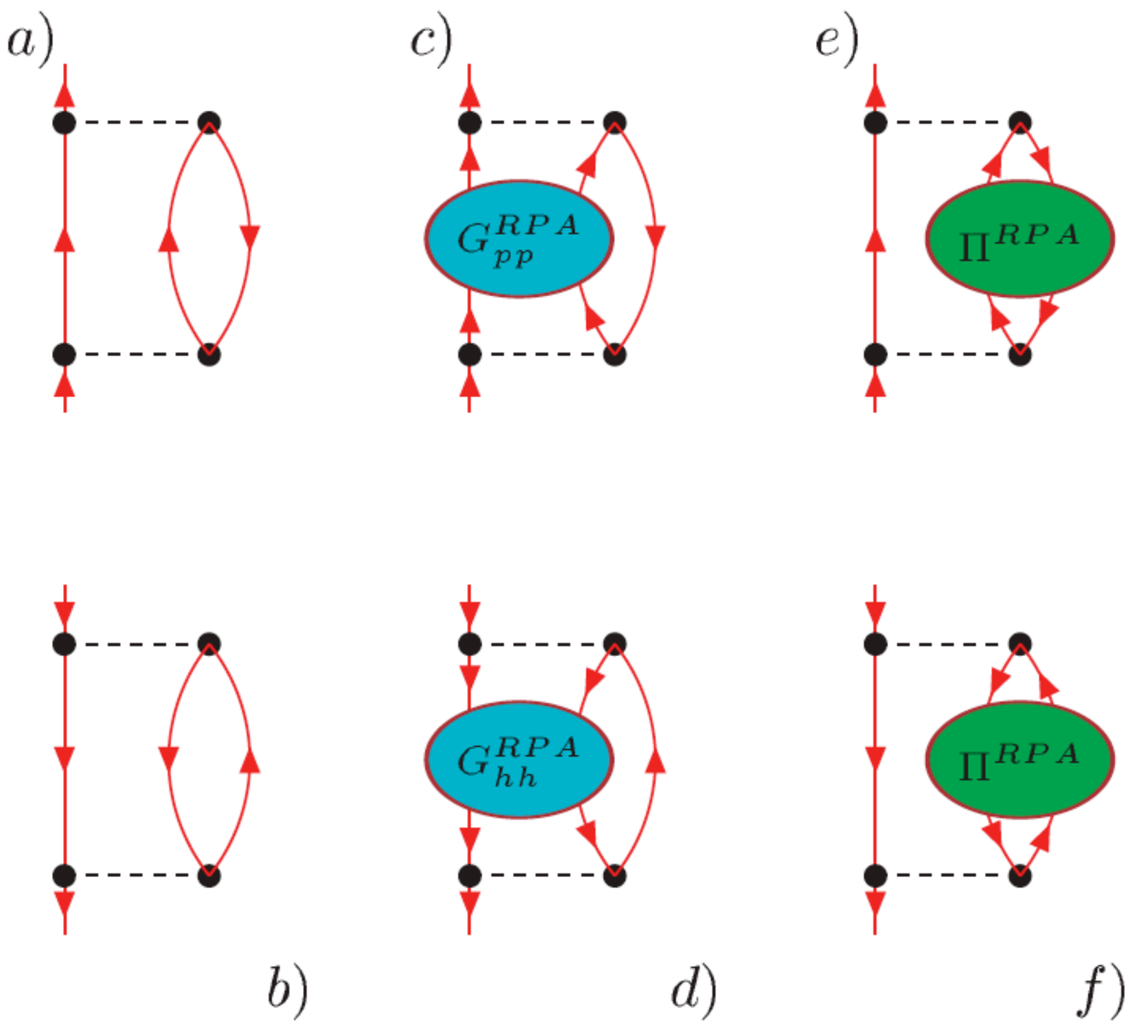
In turn:
Excited states
determine sp fragmentation

Giant Dipole



M. G. E. Brand, K. Allaart, and W. D. Dickhoff
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:

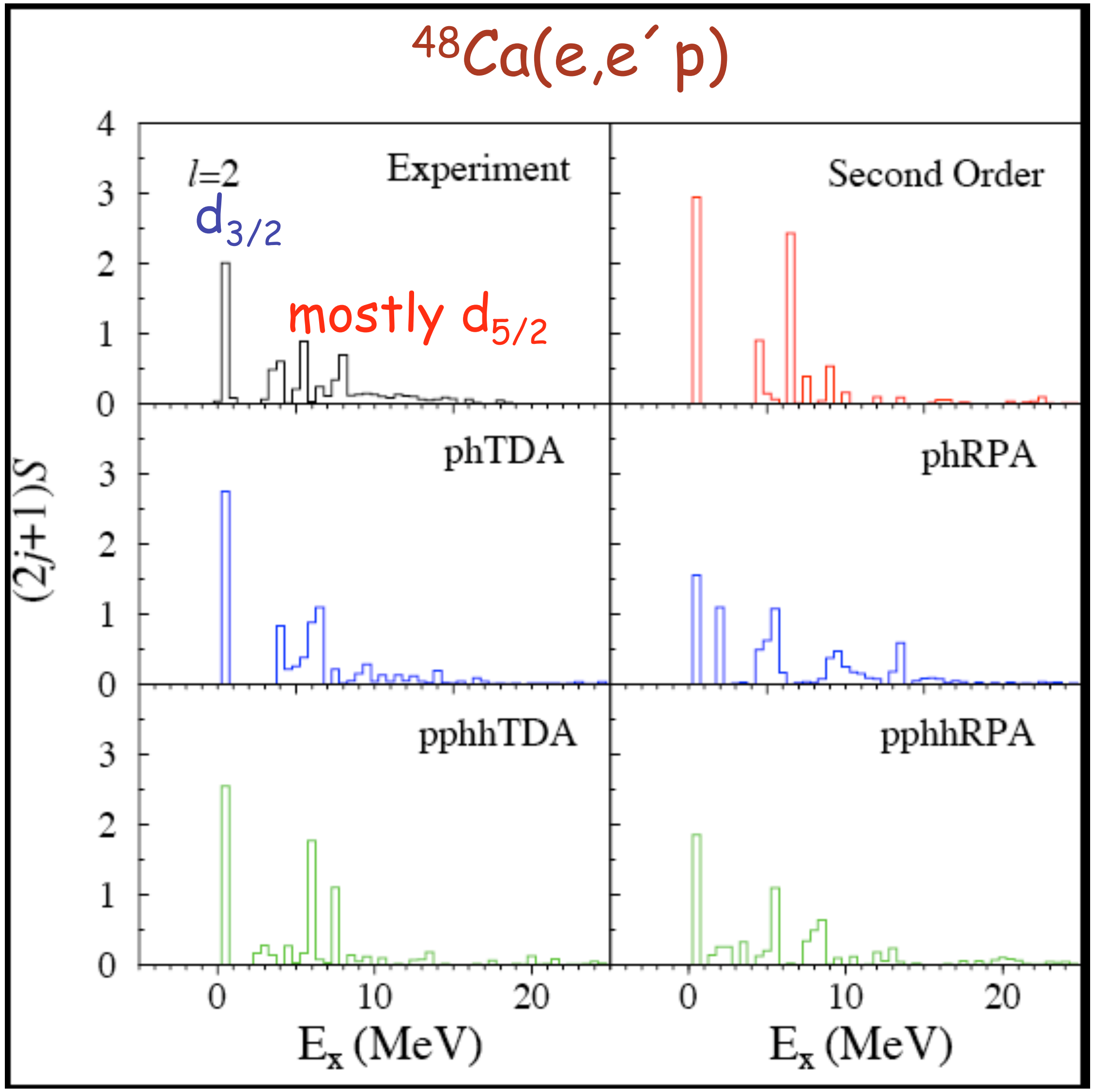
Better fragmentation at low energy
⇒ Excited states beyond RPA (unstable)

Less strength at low energy
⇒ Effect of SRC

Calculations yield:

10% strength at more bound energies!

10% depletion for states near the Fermi energy



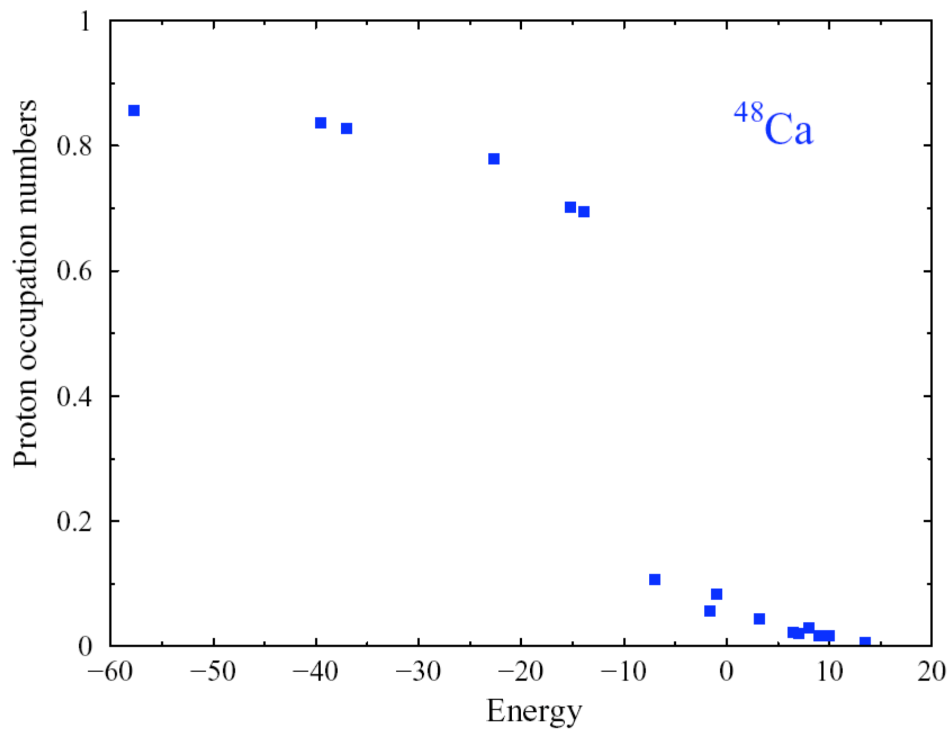
Occupation numbers ^{48}Ca

Shell	$\Sigma^{(2)}$	Σ_{ph}^{TDA}	Σ_{ph}^{RPA}	Σ_{pphh}^{TDA}	Σ_{pphh}^{RPA}
$0s\frac{1}{2}$	.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)

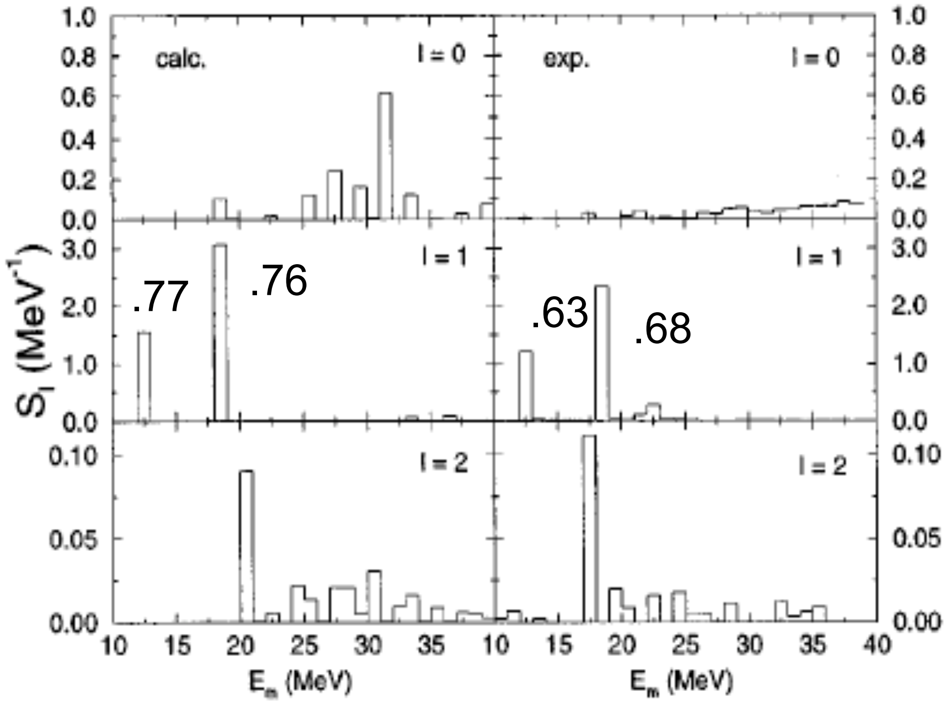
- Influence of LRC ✓✓

  RPA + Faddeev

  C. Barbieri and WHD,

  PRC**65**, 064313 (2002)

TDA

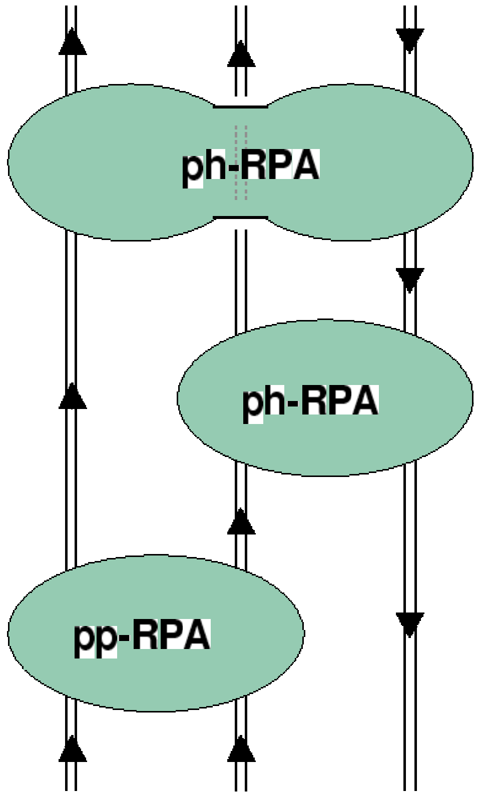


Shell	TDA	RPA
$d_{3/2}$	0.866	0.838
$s_{1/2}$	0.882	0.842
$d_{5/2}$	0.894	0.875
$p_{1/2}$	0.775	0.745
$p_{3/2}$	0.766	0.725

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

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)



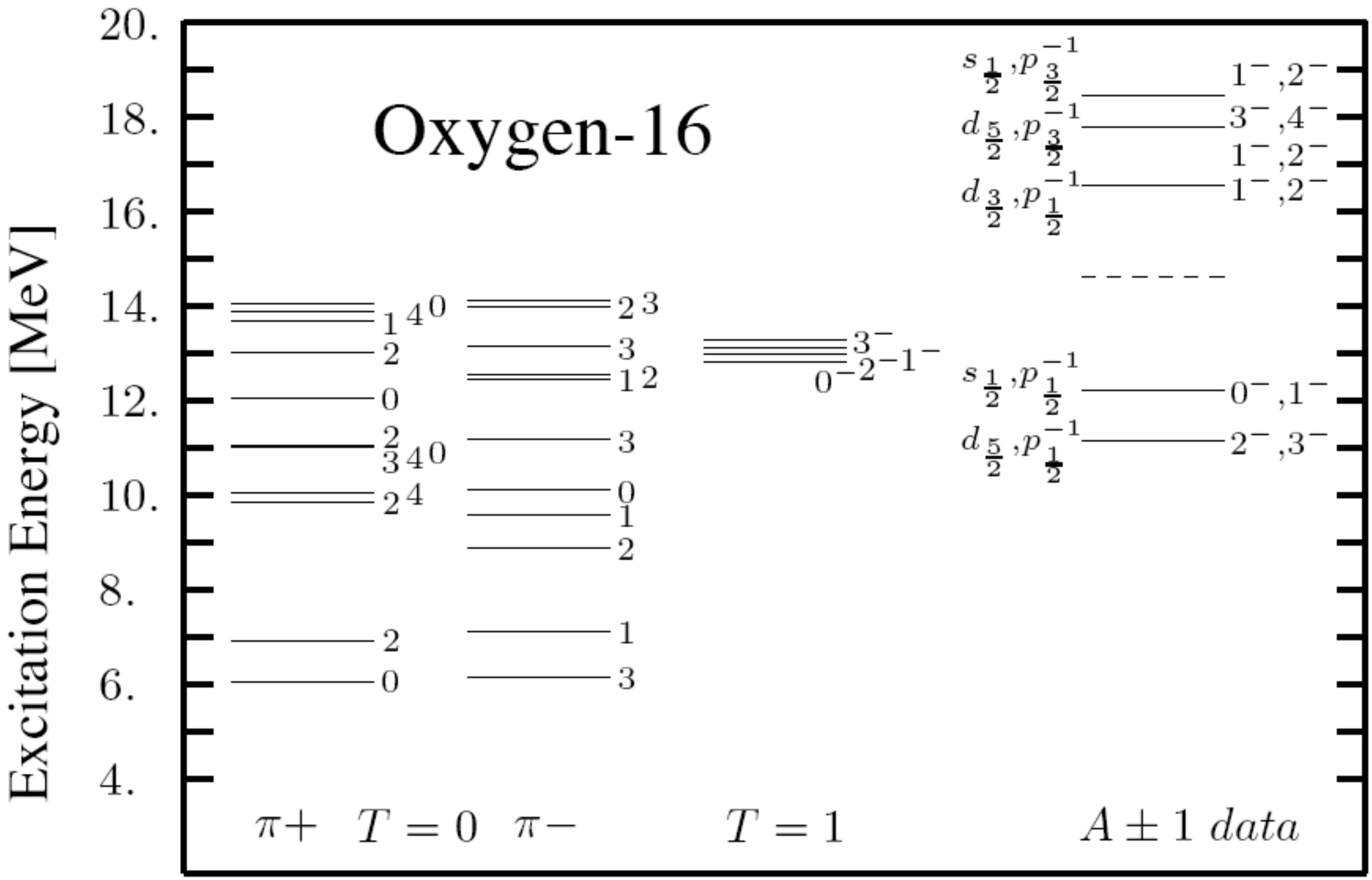
Some theoretical results for ^{16}O

	$S_{p1/2}$	$S_{p3/2}$		
• 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				LRC rest
GF(Faddeev) [St.Louis '01]	**0.77**	**0.72**		

- → relevance of collective motion

LRC ≈ particle-phonon (GR) coupling

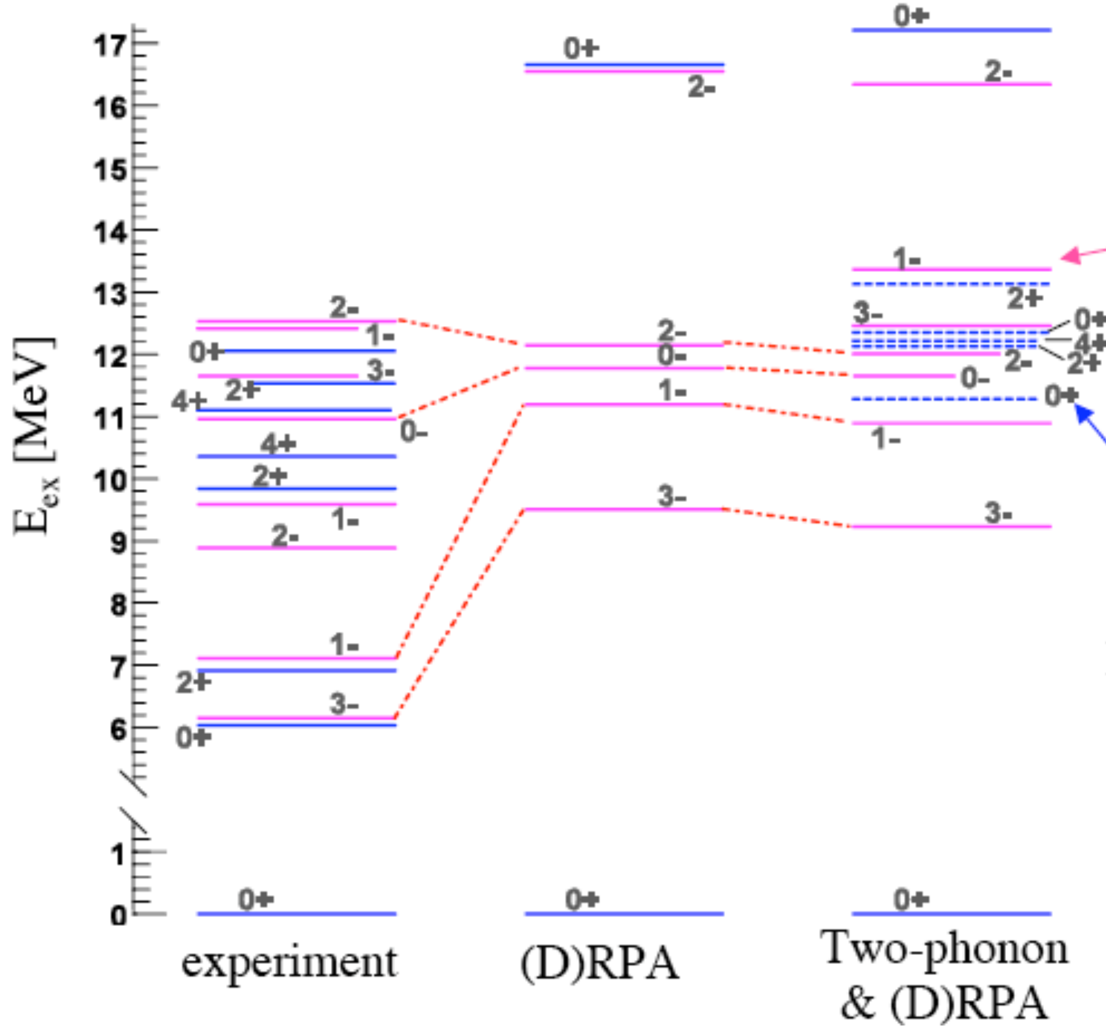
Excitation spectrum of ^{16}O



Improving excitation spectra beyond RPA

Coupling of two-phonons in ^{16}O

C.B., Dickhoff,
PRC**68**, 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)]

Faddeev results for Ne atom ionization energies

	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. PRA to be published

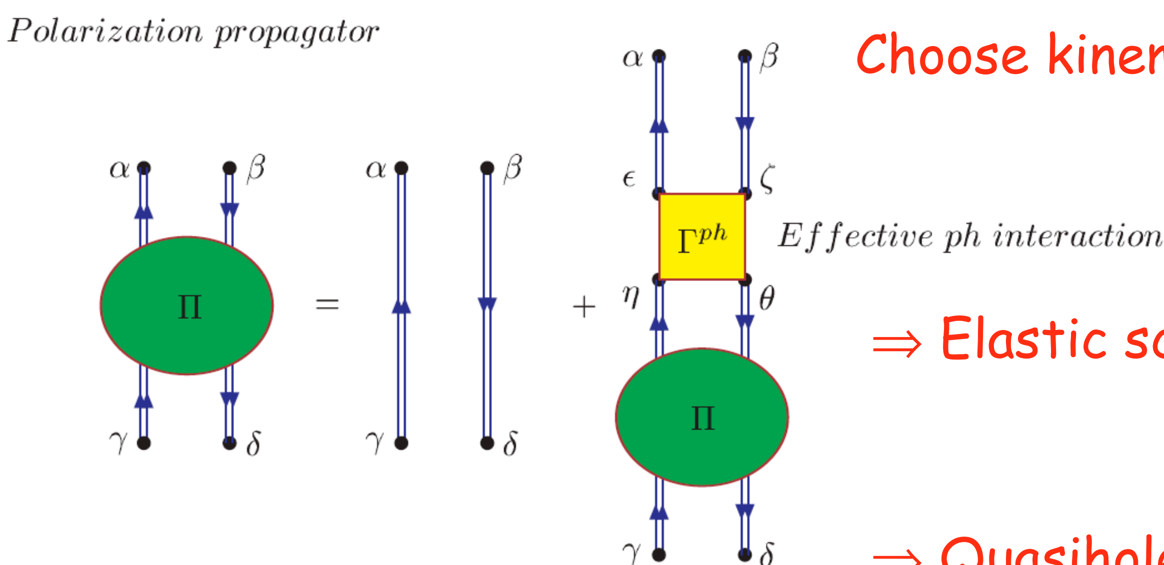
FSI and (e,e´p) $\Leftrightarrow$ analysis

$$\hat{O} = \sum_{\alpha\beta} \langle \alpha | O | \beta \rangle a^{+}_{\alpha} a_{\beta}$$

Electron Scattering $\Rightarrow$ one-body operator

$$\left| \left\langle \Psi^A_n \right| \hat{O} \left| \Psi^A_0 \right\rangle \right|^2 = \sum \langle \alpha | O | \beta \rangle^* \langle \gamma | O | \delta \rangle \left\langle \Psi^A_0 \right| a^{+}_{\beta} a_{\alpha} \left| \Psi^A_n \right\rangle \left\langle \Psi^A_n \right| a^{+}_{\gamma} a_{\delta} \left| \Psi^A_0 \right\rangle$$

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



Choose kinematics: $\Rightarrow$ only first term

$$\left\langle \Psi^{A+1}_m \middle| a^{+}_{\alpha} \middle| \Psi^A_0 \right\rangle$$

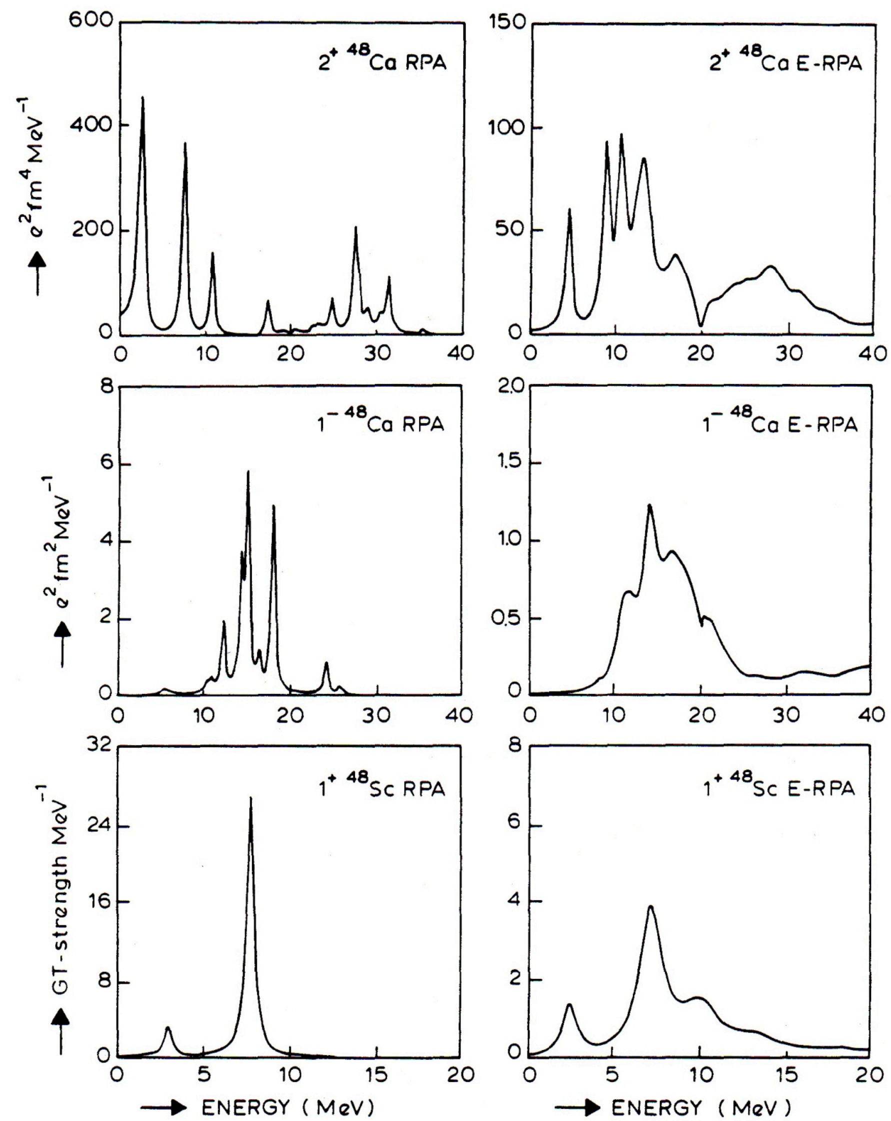
$\Rightarrow$ Elastic scattering (phenomenology)

$$\left\langle \Psi^{A-1}_n \middle| a_{\beta} \middle| \Psi^A_0 \right\rangle$$

$\Rightarrow$ Quasihole wave function

"Absolute" spectroscopic factors √

Difference between RPA and ERPA



GQR

GDR

Gamow-Teller