NSCL 7/19/05

Spectroscopic factors and the physics of the single-particle strength distribution in nuclei

Lecture 1: 7/18/05 Propagator description of single-particle motion and the link with experimental data

Lecture 2: 7/19/05 From diagrams to Hartree-Fock and spectroscopic factors < 1

Lecture 3: 7/20/05 Influence of long-range correlations and the relation to excited states

Lecture 4: 7/21/05 Role of short-range and tensor correlations associated with realistic interactions. Prospects for nuclei with N very different from Z.

Lecture 5: 7/22/05 Saturation problem of nuclear matter

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Outline

- Outline of perturbation theory
- Diagrams and diagram rules
- Self-energy and Dyson equation
- Link between sp and two-particle propagator
- Self-consistent Green's functions
- Hartree-Fock
- Dynamical self-energy and spectroscopic factors < 1

Many-body perturbation theory for *G*

- Identify solvable problem by considering $\hat{H}_0 = \hat{T} + \hat{U}$ where *U* is a suitable auxiliary potential.
- Develop expansion in $\hat{H}_1 = \hat{V} - \hat{U}$
- Employs time-evolution, Heisenberg, Schrödinger, and interaction picture of quantum mechanics.
- Once established, this expansion (expressed in Feynman diagrams) is organized in such a way that nonperturbative results can be obtained leading to the Dyson equation. The Dyson equation describes sp motion in the medium under the influence of the self-energy which is an energy-dependent complex sp potential.
- Further insight into the proper description of sp motion in the medium is obtained by studying the relation between sp and two-particle propagation. This allows the selection of appropriate choices of the relevant ingredients for the system under study.

How to calculate G?

Rearrange Hamiltonian $$\hat{H} = \hat{T} + \hat{V} = \left(\hat{T} + \hat{U}\right) + \left(\hat{V} - \hat{U}\right) = \hat{H}_0 + \hat{H}_1$$

Many-body problem with H_0 can be exactly solved
when U is a one-body potential like a Woods-Saxon or HO potential.
Corresponding sp propagator (replace H by H_0)

$$G^{(0)}(\alpha,\beta;E) = \sum_m \frac{\langle\Phi_0^N|a_\alpha|\Phi_m^{N+1}\rangle\langle\Phi_m^{N+1}|a_\beta^\dagger|\Phi_0^N\rangle}{E - \left(E_m^{A+1} - E_{\Phi_0^N}\right) + i\eta} + \sum_n \frac{\langle\Phi_0^N|a_\beta^\dagger|\Phi_n^{N-1}\rangle\langle\Phi_n^{N-1}|a_\alpha|\Phi_0^N\rangle}{E - \left(E_{\Phi_0^N} - E_n^{A-1}\right) - i\eta}$$

$$= \delta_{\alpha,\beta}\left[\frac{\theta(\alpha - F)}{E - \varepsilon_\alpha + i\eta} + \frac{\theta(F - \alpha)}{E - \varepsilon_\alpha - i\eta}\right]$$

using the sp basis associated with H_0. Note that

$$\hat{H}_0 a_\alpha^+|\Phi_0^N\rangle = \left(E_{\Phi_0^N} + \varepsilon_\alpha\right)a_\alpha^+|\Phi_0^N\rangle$$

$$\hat{H}_0 a_\alpha|\Phi_0^N\rangle = \left(E_{\Phi_0^N} - \varepsilon_\alpha\right)a_\alpha|\Phi_0^N\rangle$$

So that e.g. $$S_h^{(0)}(\alpha;E) = \frac{1}{\pi}\mathrm{Im}\,G^{(0)}(\alpha,\alpha;E) = \delta(E - \varepsilon_\alpha)\theta(F - \alpha)$$

and $$n^{(0)}(\alpha) = \int_{-\infty}^{\varepsilon_F^{(0)-}} dE\,\delta(E - \varepsilon_\alpha)\theta(F - \alpha) = \theta(F - \alpha)$$ ~ like in atoms

Perturbation expansion using $G^{(0)}$ and H_1

Use "interaction picture" $\hat{H}_1(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0 t}$

then ……

$$G(\alpha,\beta;t-t') = -\frac{i}{\hbar}\sum\left(\frac{-i}{\hbar}\right)^m \frac{1}{m!}\int dt_1\cdots\int dt_m \left\langle\Phi_0^N\left|T\left[\hat{H}_1(t_1)\cdots\hat{H}_1(t_m)a_\alpha(t)a_\beta^+(t')\right]\right|\Phi_0^N\right\rangle_{connected}$$

Can be calculated order by order using diagrams and Wick's theorem.
Yields expressions involving $G^{(0)}$ and matrix elements
of the two-body interaction V (and the auxiliary potential U)

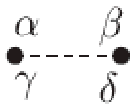
Simple diagram rules in time formulation.

For practical calculations use energy formulation. Diagrams

Diagram rules in energy formulation

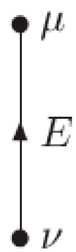
Rule 1 Draw all topologically distinct (direct) and connected diagrams with m horizontal interaction lines for V (dashed) and $2m+1$ directed (using arrows) Green's functions $G^{(0)}$

Rule 2 Label external points only with sp quantum numbers, *e.g.* α and β
Label each interaction with sp quantum numbers



$$\Rightarrow \langle\alpha\beta|\, V\, |\gamma\delta\rangle = (\alpha\beta|V|\gamma\delta) - (\alpha\beta|V|\delta\gamma)$$

For each arrow line one writes



$$\Rightarrow G^{(0)}(\mu,\nu;E)$$

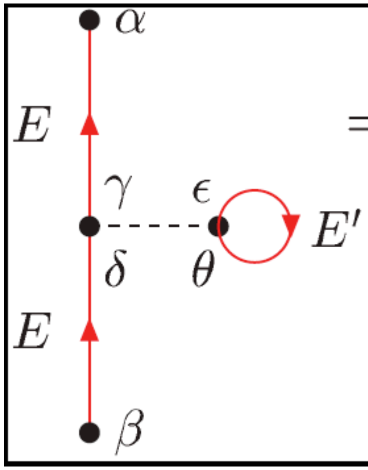
but in such a way that energy is conserved for each V

Rule 3 Sum (integrate) over all internal sp quantum numbers and integrate over all m internal energies
For each closed loop an independent energy integration occurs over the contour $C\uparrow$

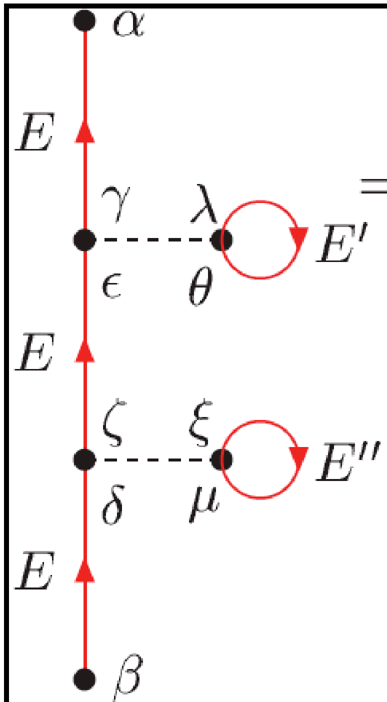
Rule 4 Include a factor $(i/2\pi)^m$ and $(-1)^F$ where F is the number of closed fermion loops

Rule 5 Include a factor of $\frac{1}{2}$ for each equivalent pair of lines

Examples of diagrams

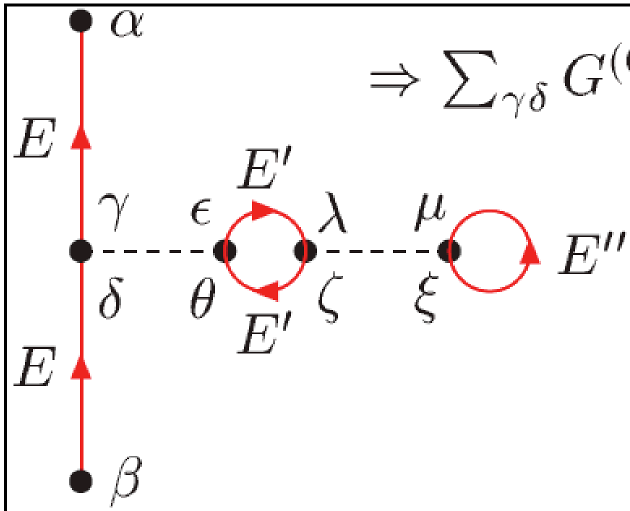


$$\Rightarrow \sum_{\gamma\delta} G^{(0)}(\alpha,\gamma;E)$$
$$\times \; -i\sum_{\epsilon\theta} \langle\gamma\epsilon|\, V\, |\delta\theta\rangle \int_{C\uparrow} \frac{dE'}{2\pi} G^{(0)}(\theta,\epsilon;E')$$
$$\times\; G^{(0)}(\delta,\beta;E)$$



$$\Rightarrow \sum_{\gamma\delta} G^{(0)}(\alpha,\gamma;E)$$
$$\times\; (-1)^2 i^2 \sum_{\epsilon,\zeta}\sum_{\lambda,\theta}\int_{C\uparrow}\frac{dE'}{2\pi}\langle\gamma\lambda|\, V\, |\epsilon\theta\rangle\, G^{(0)}(\theta,\lambda;E')$$
$$\times\; G^{(0)}(\epsilon,\zeta;E)\sum_{\xi,\mu}\int_{C\uparrow}\frac{dE''}{2\pi}\langle\zeta\xi|\, V\, |\delta\mu\rangle\, G^{(0)}(\mu,\xi;E'')$$
$$\times\; G^{(0)}(\delta,\beta;E)$$

More diagrams

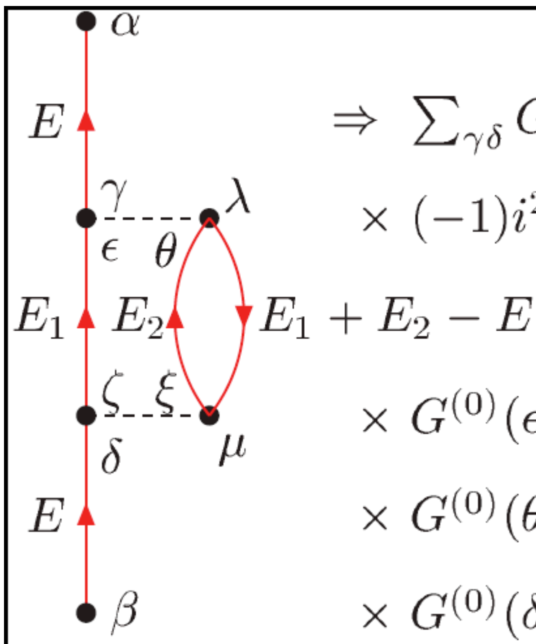


$$\Rightarrow \sum_{\gamma\delta} G^{(0)}(\alpha,\gamma;E) \times\ i^2 \sum_{\epsilon\theta}\sum_{\lambda\zeta}\int_{C\uparrow}\frac{dE'}{2\pi}$$

$$\times\ \langle\gamma\epsilon|\, V\, |\delta\theta\rangle\, G^{(0)}(\lambda,\epsilon;E')G^{(0)}(\theta,\zeta;E')$$

$$\times\ \sum_{\mu\xi}\int_{C\uparrow}\frac{dE''}{2\pi}\,\langle\zeta\xi|\, V\, |\lambda\mu\rangle\, G^{(0)}(\mu,\xi;E'')$$

$$\times\ G^{(0)}(\delta,\beta;E)$$



$$\Rightarrow\ \sum_{\gamma\delta} G^{(0)}(\alpha,\gamma;E)$$

$$\times\ (-1)i^2\frac{1}{2}\int\frac{dE_1}{2\pi}\int\frac{dE_2}{2\pi}\sum_{\lambda,\epsilon,\theta}\sum_{\zeta,\xi,\mu}\langle\gamma\lambda|\, V\, |\epsilon\theta\rangle$$

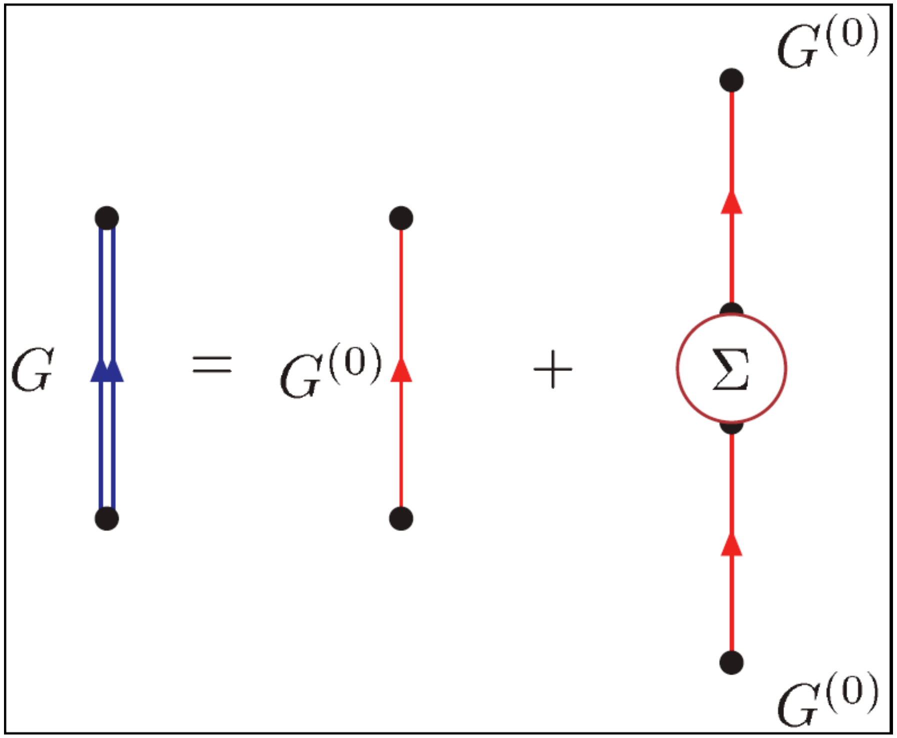
$$\times\ G^{(0)}(\epsilon,\zeta;E_1)G^{(0)}(\mu,\lambda;E_1+E_2-E)$$

$$\times\ G^{(0)}(\theta,\xi;E_2)\,\langle\zeta\xi|\, V\, |\delta\mu\rangle$$

$$\times\ G^{(0)}(\delta,\beta;E)$$

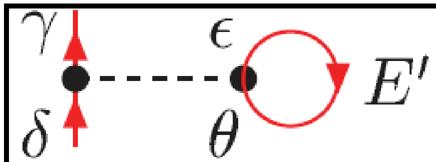
Diagram organization

Sum of all diagrams can be written as



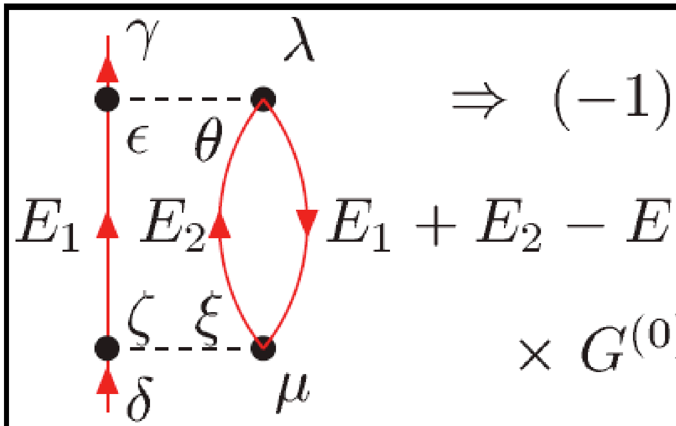
Introducing some self-energy diagrams

First order



$$\Rightarrow \; -i \sum_{\epsilon\theta} \langle \gamma\epsilon | V | \delta\theta \rangle \int_{C\uparrow} \frac{dE'}{2\pi} G^{(0)}(\theta, \epsilon; E')$$

One of the second order diagrams



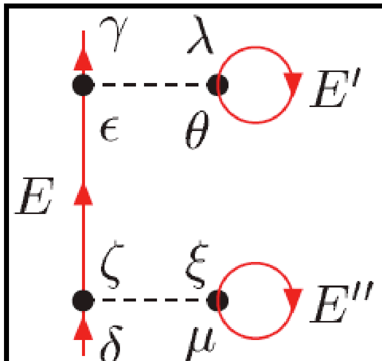
$$\Rightarrow \; (-1) i^2 \frac{1}{2} \int \frac{dE_1}{2\pi} \int \frac{dE_2}{2\pi} \sum_{\lambda,\epsilon,\theta} \sum_{\zeta,\xi,\mu} \langle \gamma\lambda | V | \epsilon\theta \rangle$$

$$\times \; G^{(0)}(\epsilon, \zeta; E_1) G^{(0)}(\mu, \lambda; E_1 + E_2 - E)$$

$$\times \; G^{(0)}(\theta, \xi; E_2) \langle \zeta\xi | V | \delta\mu \rangle$$

The irreducible self-energy

The following self-energy diagram is reducible (previous two were irreducible), *i.e*. can be obtained from lower order self-energy terms by iterating with $G^{(0)}$



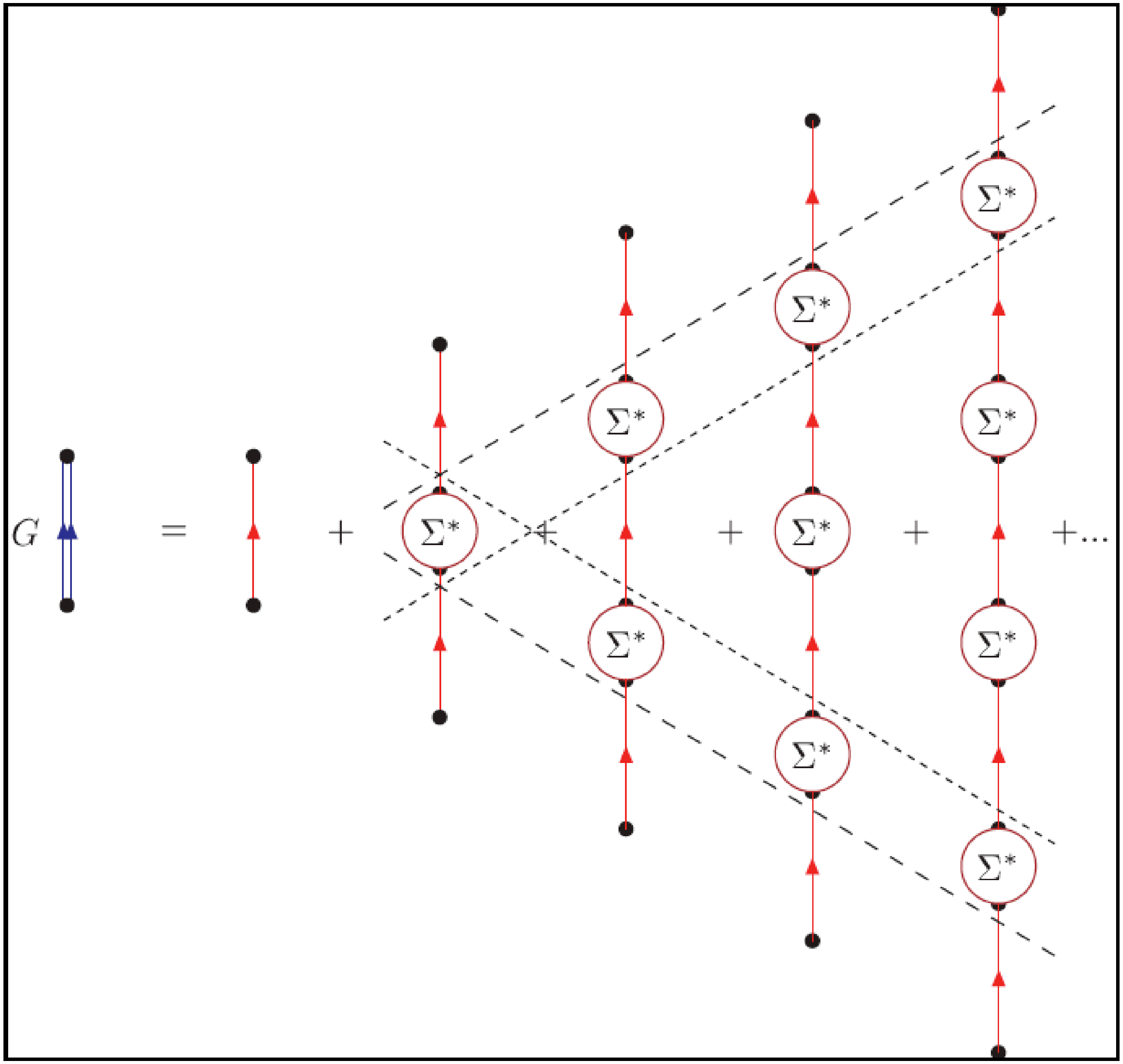
$$\Rightarrow \ (-1)^2 i^2 \sum_{\epsilon,\zeta} \sum_{\lambda,\theta} \int_{C\uparrow} \frac{dE'}{2\pi} \langle \gamma\lambda | V | \epsilon\theta \rangle \, G^{(0)}(\theta,\lambda;E') \times G^{(0)}(\epsilon,\zeta;E) \sum_{\xi,\mu} \int_{C\uparrow} \frac{dE''}{2\pi} \langle \zeta\xi | V | \delta\mu \rangle \, G^{(0)}(\mu,\xi;E'')$$

Sum of all irreducible diagrams is denoted by Σ^*.
All diagrams can then be obtained by summing

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

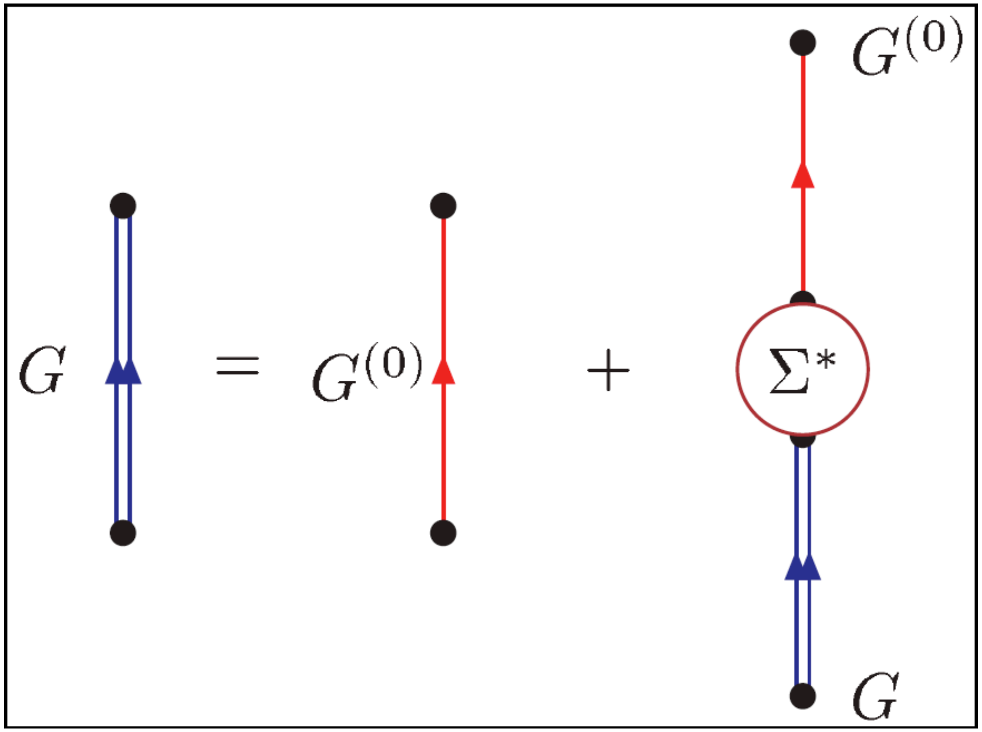
diagrammatically …

Towards the Dyson equation



Can be summed by

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.

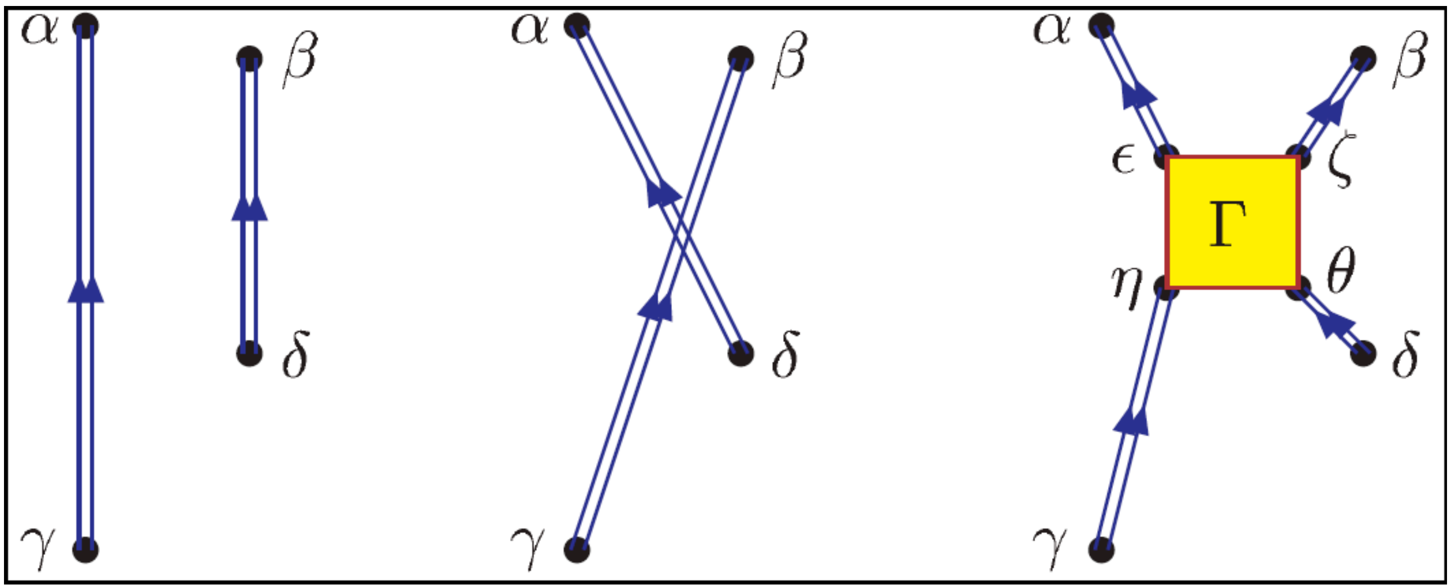
Link with two-particle propagator

Equation of motion for G

$$i\hbar\frac{\partial}{\partial t}G(\alpha,\beta;t-t') = \delta(t-t')\delta_{\alpha,\beta} + \varepsilon_\alpha G(\alpha,\beta;t-t') - \sum_\delta \langle\alpha|U|\delta\rangle G(\delta,\beta;t-t')$$

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

Diagrammatic analysis of G^{II} yields



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

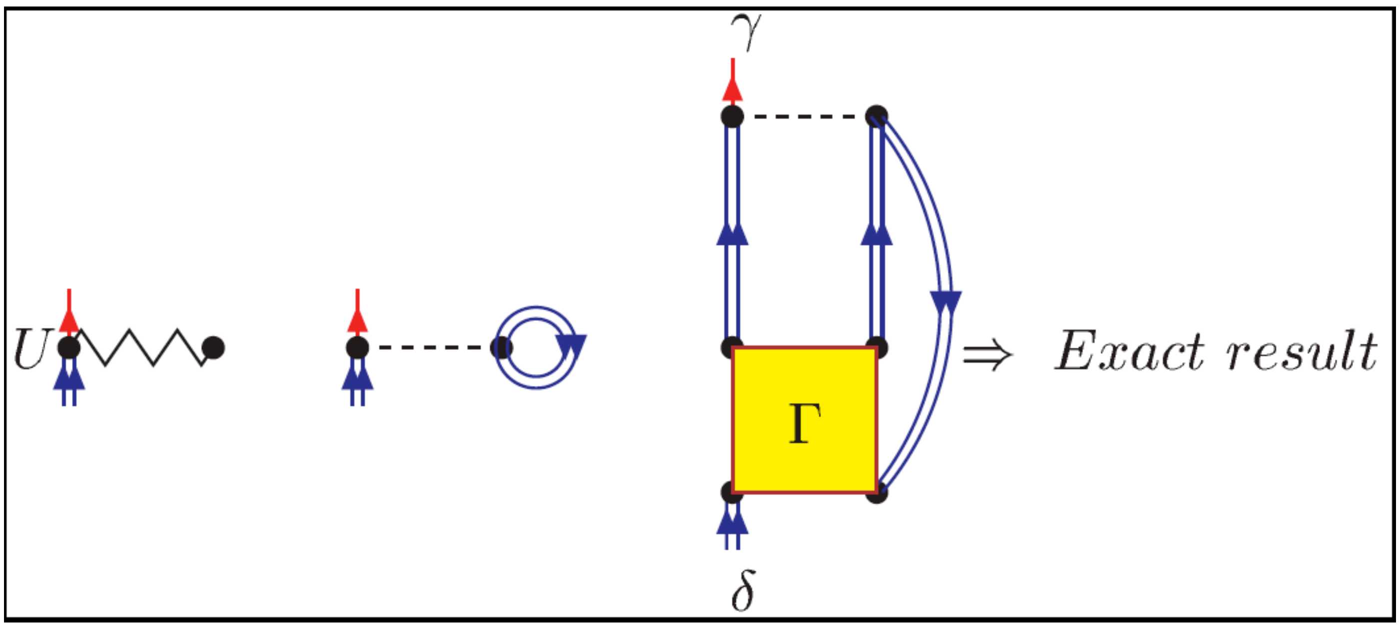
Dyson equation and vertex function

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

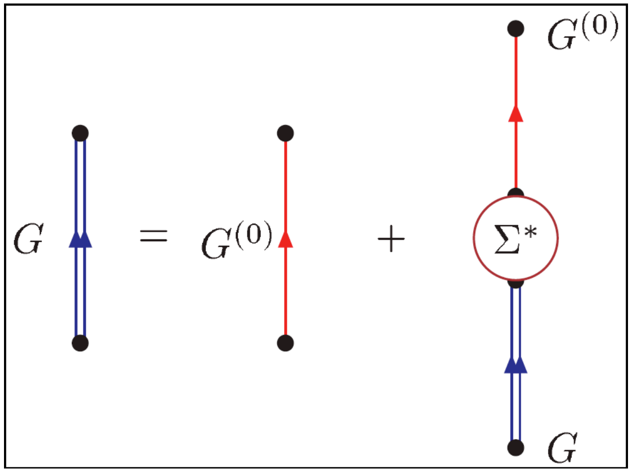
$$\Sigma^*(\gamma,\delta;E) = -\langle\gamma|U|\delta\rangle - i\int_{C\uparrow}\frac{dE'}{2\pi}\sum_{\mu\nu}\langle\gamma\mu|V|\delta\nu\rangle G(\nu,\mu;E')$$

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

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

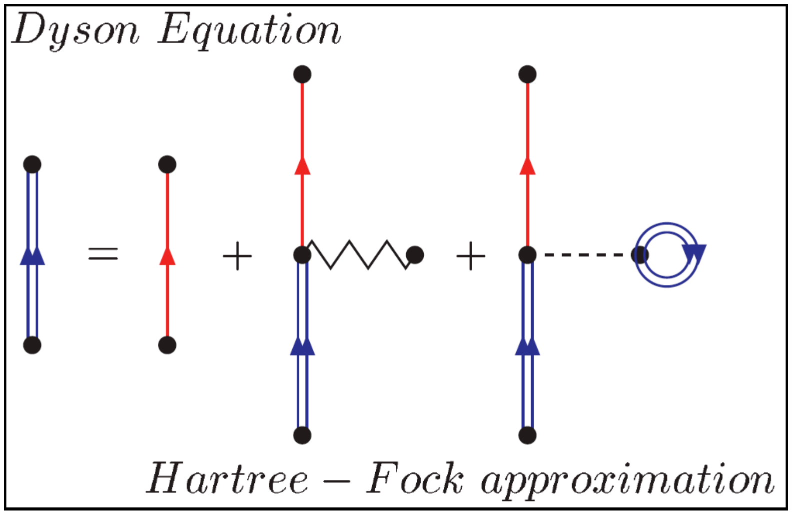
$$S = \left|\left\langle \Psi_n^{N-1}\middle| a_{\alpha_{qh}} \middle| \Psi_0^N \right\rangle\right|^2 = \frac{1}{1 - \left.\frac{\partial \Sigma'^{*}\left(\alpha_{qh},\alpha_{qh};E\right)}{\partial E}\right|_{E_n^-}}$$

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

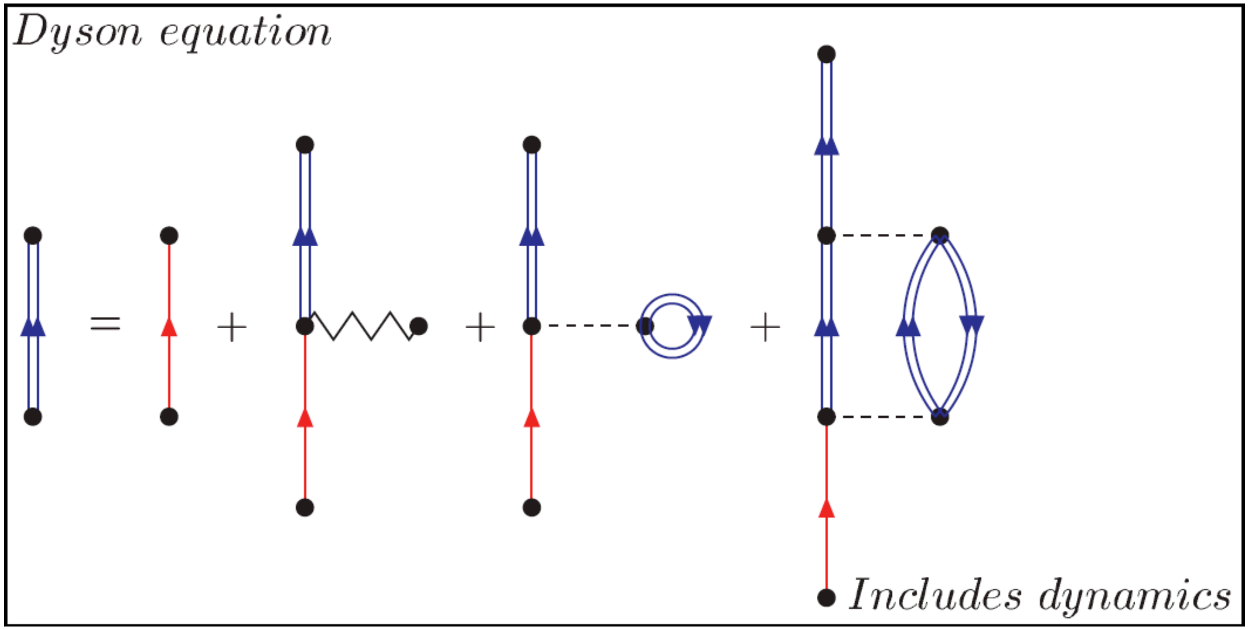
Energies in atomic units (Hartree)

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 $2p1h$ and $2h1p$ energies

Interesting consequences for solution of Dyson equation

Diagonal approximation

Further simplification: assume no mixing between major shells

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

Corresponding Dyson equation

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

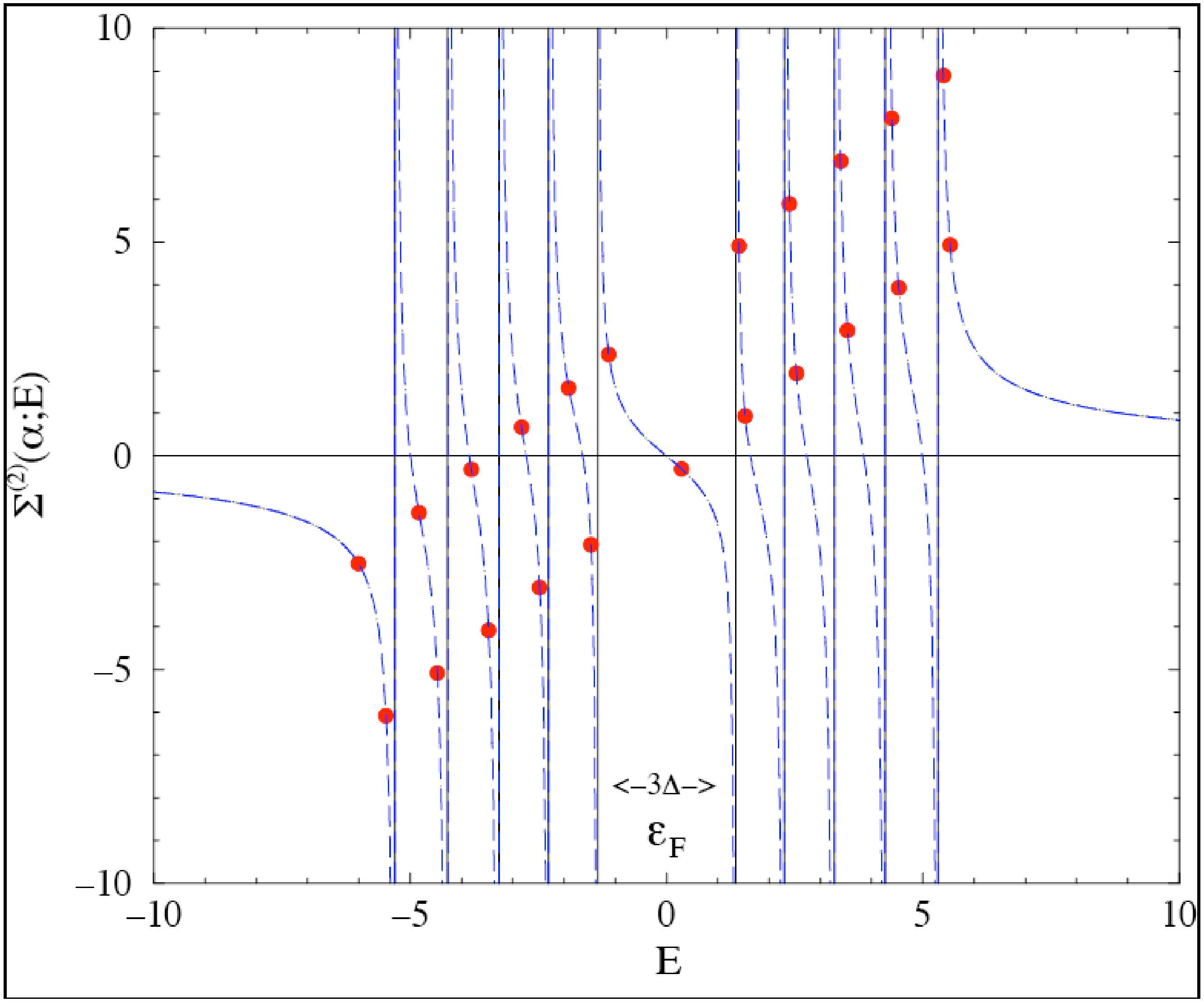
Assume discrete poles in Σ, then discrete solution (poles of *G*) for

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

With residue (spectroscopic factor)

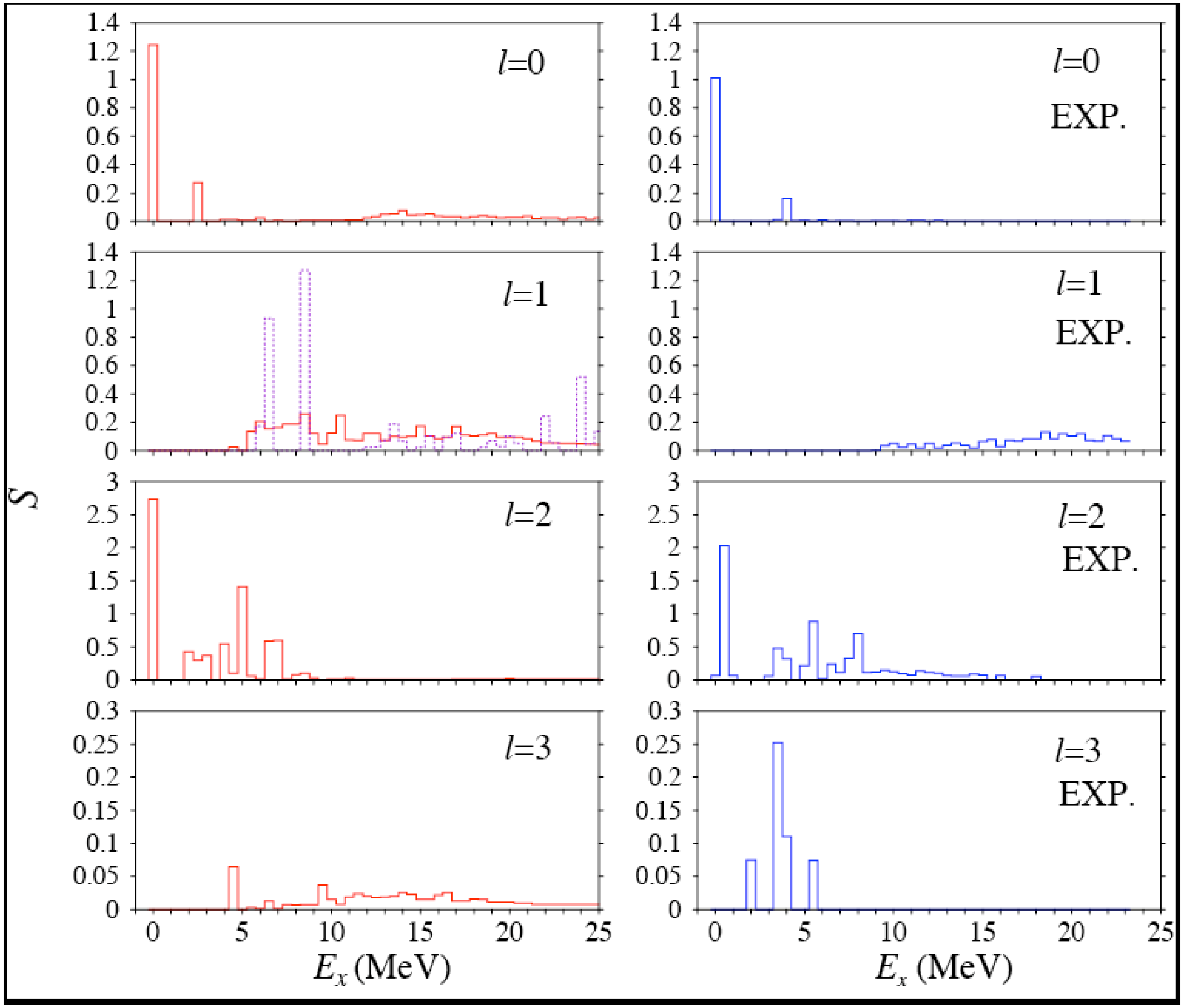
$$R_{n\alpha} = \frac{1}{1 - \left.\dfrac{\partial \Sigma^{(2)}(\alpha;E)}{\partial E}\right|_{E_{n\alpha}}}$$

Solutions



Explains all qualitative features of sp strength distribution in nuclei!

Self-consistent calculation with Skyrme force

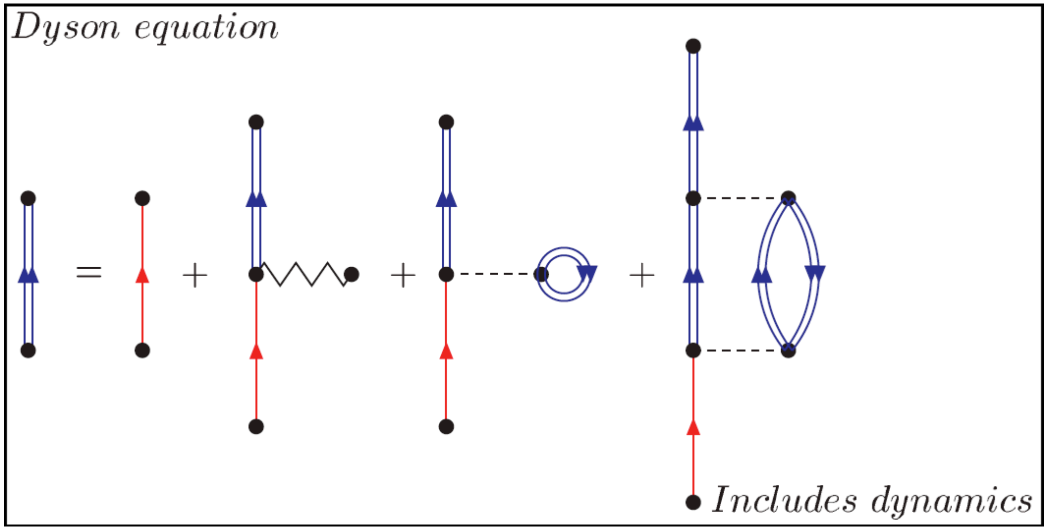


Data: ^{48}Ca(e,e´p) Kramer NIKHEF (1990)

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	-199.635	-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