Self-consistent Green's function in Finite Nucleai and related things…

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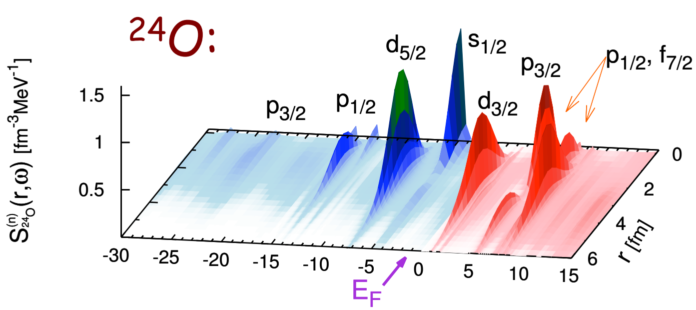

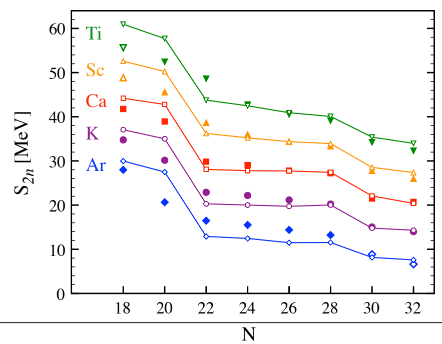

Literature

Recent reviews:

- F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. **61**, 237 (1998). → GW method
- G. Onida, L. Reining and A. Rubio, Rev. Mod. Phys. **74**, 601 (2002). → comparison of TDDTF and GF
- H. Müther and A. Polls, Prog. Part. Nucl. Phys. **45**, 243 (2000). → Applications to nuclear physics
- C.B. and W. H. Dickhoff, Prog. Part. Nucl. Phys. **52**, 377 (2004).

(Some) classic papers on formalism:

- G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961).
- G. Baym, Phys. Rev. **127**, 1391 (1962).
- L. Hedin, Phys. Rev. **139**, A796 (1965).

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Literature

Books on many-body Green's Functions:

- W. H. Dickhoff and D. Van Neck, *Many-Body Theory Exposed!*, 2nd ed. (World Scientific, Singapore, 2007)

- A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Physics,* (McGraw-Hill, New York, 1971)
- A. A. Abrikosov, L. P. Gorkov and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975)

- R. D. Mattuck, *A Guide to Feynmnan Diagrams in the Many-Body Problem,* (McGraw-Hill, 1976) [reprinted by Dover, 1992]
- J. P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems,* (MIT Press, Cambridge MA, 1986)
- J. W. Negele and H. Orland, *Quantum Many-Particle Systems,* (Benjamin, Redwood City CA, 1988)
- …

- Green's functions
- Propagators
- Correlation functions

names for the same objects

- Many-body Green's functions ← Green's functions applied to the MB problem

- Self-consistent Green's functions (SCGF) ← a particular approach to calculate GFs

Propagating a free particle

Consider a free particle with Hamiltonian

$h_1 = t + U(r)$

the eigenstates and egienenergies are $h_1|\phi_n\rangle = \varepsilon_n|\phi_n\rangle$

The time evolution is

$$i\hbar\frac{d}{dt}\,|\psi(t)\rangle = h_1\,|\psi(t)\rangle \quad \rightarrow \quad |\psi(t)\rangle = e^{-ih_1 t/\hbar}|\psi_{tr}\rangle$$

$$\begin{aligned}\langle\mathbf{r}|\psi(t)\rangle &= \langle\mathbf{r}|e^{-ih_1 t/\hbar}|\psi_{tr}\rangle \\ &= \int d\mathbf{r}'\langle\mathbf{r}|e^{-ih_1 t/\hbar}|\mathbf{r}'\rangle\langle\mathbf{r}'|\psi_{tr}\rangle\end{aligned}$$

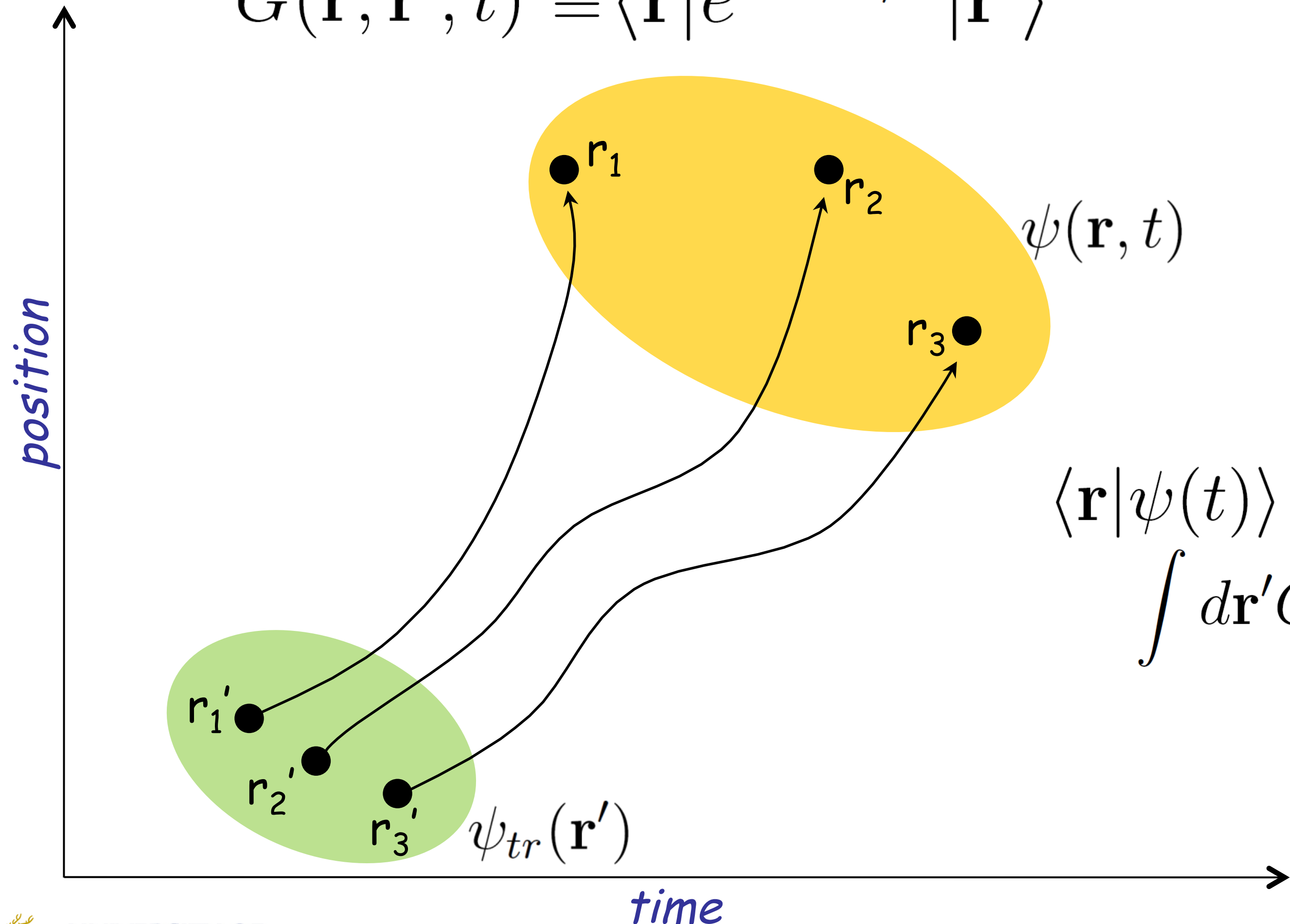
with: $\langle\mathbf{r}|\psi_{tr}\rangle$ wave fnct. at t=0

$\langle\mathbf{r}|\psi(t)\rangle$ wave fnct. at time t

Propagating a free particle

Green's function (=propagator) for a free particle:

$$G(\mathbf{r},\mathbf{r}';t) \equiv \langle \mathbf{r}| e^{-ih_1 t/\hbar} |\mathbf{r}'\rangle$$



$$\langle \mathbf{r}|\psi(t)\rangle = \int d\mathbf{r}' G(\mathbf{r},\mathbf{r}';t)\psi_{tr}(\mathbf{r}')$$

Propagating a free particle

Green's function (=propagator) for a free particle:

$$G(\mathbf{r},\mathbf{r}';t) \equiv \langle \mathbf{r}| e^{-ih_1 t/\hbar} |\mathbf{r}'\rangle$$

$$= \sum_n \underbrace{\langle \mathbf{r}|\phi_n\rangle e^{-i\varepsilon_n t/\hbar} \langle \phi_n|\mathbf{r}'\rangle}$$

Fourier transform
of the eigenspectrum!

$\langle \mathbf{r}|\phi_n\rangle$ → states

ε_n → energies

The spectrum of the Hamiltonian is separated by the FT because the time evolution is driven by H: $e^{-iH(t-t_0)/\hbar}$

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TALENT course on "Many Body Methods for NP"

July 2015 - Lectures I and II on SCGF for FN

- Fundamental equations & definitions of Green's function theory

Let's assume we know the solution of the A-body Schrödinger eq

$$E_0^A |\Psi_0^A\rangle = H |\Psi_0^A\rangle \qquad \text{"0" lables the g.s.}$$

And also for the (A-1)- and (A+1)-body states, for all the eigenstates and eigenvalues:

$$E_k^{A-1} |\Psi_k^{A-1}\rangle = H |\Psi_k^{A-1}\rangle \qquad k = 0, 1, 2, \ldots$$

$$E_n^{A+1} |\Psi_n^{A+1}\rangle = H |\Psi_n^{A+1}\rangle \qquad n = 0, 1, 2, \ldots$$

These actually lable the discreete and the continuum parts of the spectrum.

In Schödinger picture, the quantum state $|\Psi\rangle$ evolves in time as:

$$|\Psi(t)\rangle = e^{-iH(t-t_0)/\hbar}\,|\Psi\rangle_{t_0}$$

but we can also choose to keep $|\Psi\rangle$ constant and evolve in time the operators, instead. This is the Heisenberd picture:

$$a(t) = e^{iH(t-t_0)/\hbar}\, a\, e^{-iH(t-t_0)/\hbar}$$

The equation of motion is then.

$$\frac{d\,a(t)}{dt} = \frac{iH}{\hbar}\, e^{iH(t-t_0)/\hbar}\, a\, e^{-iH(t-t_0)/\hbar} + e^{iH(t-t_0)/\hbar}\, \overset{0}{\cancel{\frac{da}{dt}}}\, e^{-H(t-t_0)/\hbar} + e^{iH(t-t_0)/\hbar}\, a\, e^{-iH(t-t_0)/\hbar}\, \frac{-i}{\hbar} H$$

$$\Rightarrow \begin{cases} i\hbar \dfrac{d\,a(t)}{dt} = [a, H] \\[2ex] i\hbar \dfrac{d\,a^{\dagger}(t)}{dt} = [a^{\dagger}, H] \end{cases}$$

And of course: $i\hbar \dfrac{d\,H(t)}{dt} = [H, H] = 0 \iff H(t) = H_{t_0} \quad \forall t$

The hamiltonian is

$$H = \hat{T} + \hat{V} + \hat{W}$$

$$= \sum_{\alpha\beta} t_{\alpha\beta}\, a^\dagger_\alpha a_\beta + \frac{1}{4} \sum_{\substack{\alpha\beta \\ \gamma\delta}} v_{\alpha\beta,\gamma\delta}\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma +$$

$$+ \frac{1}{36} \sum_{\substack{\alpha\beta\gamma \\ \mu\nu\lambda}} w_{\alpha\beta\gamma,\mu\nu\lambda}\, a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma a_\lambda a_\nu a_\mu$$

$\hat{T}$: 1-body part of the hamiltonian (for nuclei: just the kinetic energy)

$\hat{V}, \hat{W}$: 2- and 3-body interactions (v and w: properly antisymmetrized mtx. els.)

<u>NOTE</u>: Here and in the following we use:

- $\alpha, \beta, \gamma, \ldots$ (greek) for the <u>1-body space</u> (our <u>s.p. basis</u>)
- n for (A+1)-body spectrum (the <u>quasiparticles</u>)
- k for (A-1)-body " (the <u>quasiholes</u>)

α, β, γ etc. can be any s-p. basis like coordinate space $\vec{r}$, momentum space $\vec{k}$, h.o. ... it also contains spin and isospin degrees of freedom.

- Second quantization exercise

Prove:

$$i\hbar \frac{da_\alpha(t)}{dt} = \sum_\beta t_{\alpha\beta}\, a_\beta(t) + \frac{1}{2}\sum_{\beta\gamma\delta} v_{\alpha\beta\gamma\delta}\, a^\dagger_\beta(t)\, a_\delta(t)\, a_\gamma(t)$$

$$+ \frac{1}{12}\sum_{\substack{\beta\gamma\\ \mu\nu\lambda}} w_{\alpha\beta\gamma,\mu\nu\lambda}\, a^\dagger_\beta(t)\, a^\dagger_\gamma(t)\, a_\lambda(t)\, a_\nu(t)\, a_\mu(t)$$

$$i\hbar \frac{d a^\dagger_\gamma(t)}{dt} = \sum_\alpha t_{\alpha\gamma}\, a^\dagger_\alpha(t) + \frac{1}{2}\sum_{\substack{\alpha\beta\\ \delta}} v_{\alpha\beta,\gamma\delta}\, a^\dagger_\alpha(t)\, a^\dagger_\beta(t)\, a_\delta(t)$$

$$+ \frac{1}{12}\sum_{\substack{\alpha\beta\delta\\ \nu\lambda}} w_{\alpha\beta\delta,\gamma\nu\lambda}\, a^\dagger_\alpha(t)\, a^\dagger_\beta(t)\, a^\dagger_\delta(t)\, a_\lambda(t)\, a_\nu(t)$$

Definition of "one-body propagator" (or "1-body GF", or "single particle GF/propagator").

Take the A-body g.s. $|\Psi_0^A(t)\rangle$ and add a particle in state β at time t':

$$a^\dagger_\beta e^{-iHt'}|\Psi_0^A\rangle$$

Evolve it for a time $\Delta t = t - t'$: $e^{-iH(t-t')/\hbar}$

Is this the same as adding a particle in state α at time t?
In other words, has the particle "travelled" from β to α?

$$\left(a^\dagger_\alpha e^{-iHt/\hbar}|\Psi_0^A\rangle \right)$$

The probability amplitude for this process is:

$$\langle\Psi_0^A| e^{iHt/\hbar} a_\alpha e^{-iH(t-t')/\hbar} a^\dagger_\beta e^{-iHt'/\hbar}|\Psi_0^A\rangle = \langle\Psi_0^A| a_\alpha(t)\, a^\dagger_\beta(t')|\Psi_0^A\rangle$$

↳ which is meaningful for $t > t'$, that is, when $\theta(t-t') \neq 0$

Likewise remove a particle from α at t and add it to β at t' (in this case, it must be $t < t'$...):

$$\langle\Psi_0^A| e^{iHt'/\hbar} a^\dagger_\beta e^{iH(t'-t)/\hbar} a_\alpha e^{-iHt/\hbar}|\Psi_0^A\rangle \times \theta(t'-t)$$

The one body propagator is then

$$i\hbar\, g_{\alpha\beta}(t,t') \equiv \langle \Psi_0^A | T[a_\alpha(t)\, a_\beta^\dagger(t')] | \Psi_0^A \rangle$$

$$= \vartheta(t-t') \langle \Psi_0^A | a_\alpha\, e^{-i(H-E_0)(t-t')/\hbar}\, a_\beta^\dagger | \Psi_0^A \rangle$$

$$- \vartheta(t'-t) \langle \Psi_0^A | a_\beta^\dagger\, e^{-i(H-E_0)(t'-t)/\hbar}\, a_\alpha | \Psi_0^A \rangle .$$

- $T[\dots]$ time ordering operator

- $\vartheta(\dots)$ the theta function enforces the causality principle

- The same as propagators in QFT for elementary particles. However, our "vacuum" is now the A-body g.s. $|\Psi_0^A\rangle$

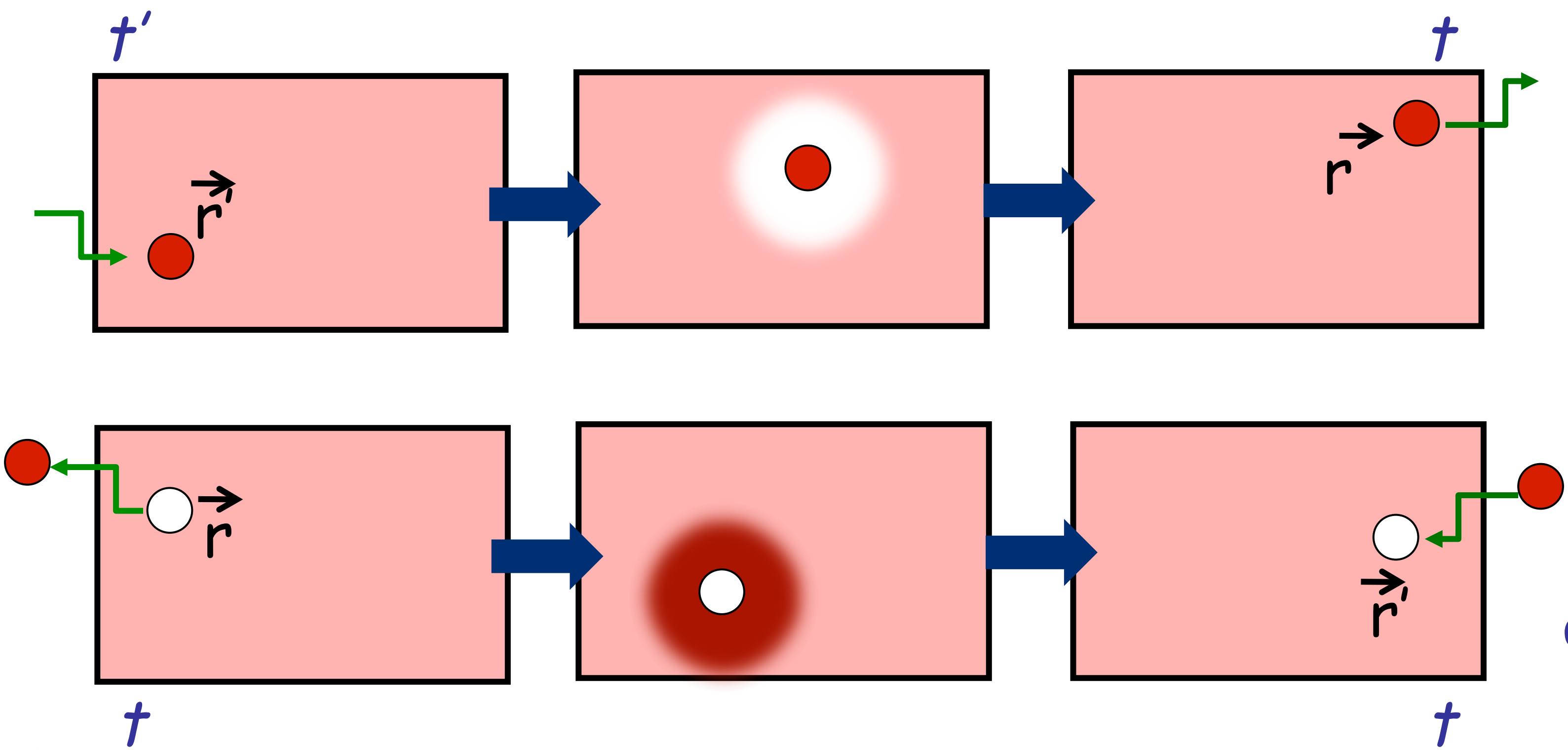
- We are non-relativistic, so we keep the time coordinate separated from the "spatial" ones ($\alpha, \beta, \dots$)

- $g_{\alpha\beta}(t,t') = g_{\alpha\beta}(t-t')$ depends on one time difference only!

Definition of one-body GF

With explicit time dependence:

$$
\begin{aligned}
g_{ss'}(\mathbf{r},\mathbf{r}';t-t') \quad = \quad & -\frac{i}{\hbar}\theta(t-t')\langle\Psi_0^N|\psi_s(\mathbf{r})e^{-i(H-E_0^N)(t-t')/\hbar}\psi_{s'}^\dagger(\mathbf{r}')|\Psi_0^N\rangle \\
& \mp\frac{i}{\hbar}\theta(t'-t)\langle\Psi_0^N|\psi_{s'}^\dagger(\mathbf{r}')e^{i(H-E_0^N)(t-t')/\hbar}\psi_s(\mathbf{r})|\Psi_0^N\rangle
\end{aligned}
$$



$t > t'$
adds a particle

$t' > t$
removes a particle

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One can Fourier transform time 't' to energy 'ω'

$$g_{\alpha\beta}(\omega) \equiv \int d\tau \, e^{i\omega\tau} g_{\alpha\beta}(\tau)$$

$$\left(\begin{array}{l} \text{Using} \\ \theta(\pm\tau) = \mp \lim_{\eta\to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{-i\tilde{\omega}\tau}}{\tilde{\omega} \pm i\eta} \end{array} \right)$$

$$g_{\alpha\beta}(\omega) = \int d\tau \frac{e^{i\omega\tau}}{i\hbar} (-) \lim_{\eta\to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{e^{-i\tilde{\omega}\tau}}{\tilde{\omega} + i\eta} \langle \Psi_0^A | a_\alpha \, e^{-i(H-E_0)\tau/\hbar} a_\beta^\dagger | \Psi_0^A \rangle d\tilde{\omega}$$

$$- \int d\tau \frac{e^{i\omega\tau}}{i\hbar} + \lim_{\eta\to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{e^{-i\tilde{\omega}\tau}}{\tilde{\omega} - i\eta} \langle \Psi_0^A | a_\beta^\dagger \, e^{-i(E_0-H)\tau/\hbar} a_\alpha | \Psi_0^A \rangle d\tilde{\omega}$$

$$= \lim_{\eta\to 0^+} \int_{-\infty}^{+\infty} d\tilde{\omega} \langle \Psi_0^A | a_\alpha \frac{-1}{i^2} \frac{1}{2\pi\hbar} \int dt \frac{e^{i[\omega - \tilde{\omega} - (H-E_0)/\hbar]\tau}}{\tilde{\omega} + i\eta} a_\beta^\dagger | \Psi_0^A \rangle$$

$$+ \lim_{\eta\to 0^+} \int d\tilde{\omega} \langle \Psi_0^A | a_\beta^\dagger \frac{-1}{(i)^2} \frac{1}{\tilde{\omega} - i\eta} \frac{1}{2\pi\hbar} \int d\tau \, e^{i[\omega - \tilde{\omega} + (H-E_0)/\hbar]\tau} a_\alpha | \Psi_0^A \rangle$$

$$= \lim_{\eta\to 0^+} \int d\tilde{\omega} \left\{ \frac{1}{\hbar} \langle \Psi_0^A | a_\alpha \frac{\delta[\omega - \tilde{\omega} - (H-E_0^A)/\hbar]}{\tilde{\omega} + i\eta} a_\beta^\dagger | \Psi_0^A \rangle + \right.$$

$$\left. + \langle \Psi_0^A | a_\beta^\dagger \frac{\delta[\omega - \tilde{\omega} + (H-E_0^A)/\hbar]}{\tilde{\omega} - i\eta} a_\alpha | \Psi_0^A \rangle \right\} \Rightarrow$$

Thus:

$$g_{\alpha\beta}(\omega) = \int_{-\infty}^{+\infty} d\tau \, e^{i\omega\tau} \, g_{\alpha\beta}(\tau)$$

$$= \langle \Psi_0^A | Q_\alpha \frac{1}{\hbar\omega - (H - E_0^A) + i\eta} Q_\beta^\dagger | \Psi_0^A \rangle$$

$$+ \langle \Psi_0^A | Q_\beta^\dagger \frac{1}{\hbar\omega + (H - E_0^A) \pm i\eta} Q_\alpha | \Psi_0^A \rangle$$

Expectation values

For one-body operators: $\hat{O} = \sum_{\alpha\beta} O_{\alpha\beta}\, a^\dagger_\alpha a_\beta$

$$\langle \hat{Q} \rangle = \langle \Psi_0^A | \hat{O} | \Psi_0^A \rangle = \sum_{\alpha\beta} O_{\alpha\beta} \langle \Psi | a^\dagger_\alpha a_\beta | \Psi_0^A \rangle$$

$$= \sum_{\alpha\beta} O_{\alpha\beta}\, \rho_{\beta\alpha} = Tr\{\hat{O}\rho\}$$

I define the one-body density matrix as

$$\rho_{\alpha\beta} \equiv \langle \Psi_0^A | a^\dagger_\beta a_\alpha | \Psi_0^A \rangle$$

(someone inverts $\alpha \leftrightarrow \beta$)

$$\lim_{\tau \to 0^-} -i\hbar\, g_{\alpha\beta}(\tau) = \lim_{t \to t' - i\eta} -\langle \Psi_0^A | T[a_\alpha(t)\, a^\dagger_\beta(t')] | \Psi_0^A \rangle = \rho_{\alpha\beta}$$

Thus

$$\langle \hat{O} \rangle = -i\hbar \lim_{\tau \to 0^-} Tr\{\hat{O}\, g_{\alpha\beta}(\tau)\}$$

$$\langle \hat{T} \rangle = -i\hbar \lim_{\tau \to 0^-} \sum_{\alpha,\beta} t_{\beta\alpha}\, g_{\alpha\beta}(\tau) =$$

$$-i\hbar \lim_{\tau\to 0^-} \mathrm{Tr}\{ g_{\alpha\alpha}(\tau)\} = \langle \Psi_0^A | \sum_\alpha a_\alpha^\dagger a_\alpha | \Psi_0^A \rangle = A$$

number of particles.

Likewise, defining a 2-particle/2-hole (pp/hh) propagator:

$$i\hbar\, g^{II}_{\alpha\beta,\gamma\delta}(t,t') \equiv \langle \Psi_0^A | T\left[a_\beta(t)\, a_\alpha(t)\, a_\gamma^\dagger(t')\, a_\delta^\dagger(t')\right] | \Psi_0^A \rangle$$

hence:

$$\langle \hat{V} \rangle = \frac{1}{4} \sum_{\substack{\alpha\beta\\ \gamma\delta}} v_{\alpha\beta,\gamma\delta} \langle \Psi_0^A | a_\alpha^\dagger\, a_\beta^\dagger\, a_\delta\, a_\gamma | \Psi_0^A \rangle =$$

$$= \frac{1}{4} \sum_{\substack{\alpha\beta\\ \gamma\delta}} v_{\alpha\beta,\gamma\delta}\, \Gamma_{\gamma\delta,\alpha\beta} = \frac{-i\hbar}{4} \sum v_{\alpha\beta,\gamma\delta}\, g^{II}_{\gamma\delta,\alpha\beta}(0^-)$$

$$= -i\hbar \lim_{\tau\to 0^-} \mathrm{Tr}\left\{ \hat{V}\, g^{II} \right\}$$

And a 3p/3h GF yields $\langle W \rangle$ ...

Some "magic":

$$(i\hbar)^2 \frac{d}{dt} g_{\alpha\zeta}(t,t') = \langle \Psi_0^A | T\left[i\hbar \frac{dQ_\alpha(t)}{dt} Q_\zeta^\dagger(t') \right] | \Psi_0^A \rangle$$

$$= -\langle \Psi_0^A | T\Big[Q_\zeta^\dagger(t)\, t_{\alpha\beta}\, Q_\beta(t') +$$

$$+ 2\, Q_\zeta^\dagger(t) \frac{V_{\alpha\beta,\gamma\delta}}{4} Q_\beta^\dagger(t') Q_\delta(t') Q_\gamma(t) +$$

$$+ 3\, Q_\zeta^\dagger(t) \frac{W_{\alpha\beta\gamma,\mu\nu\lambda}}{36} Q_\beta(t') Q_\gamma(t') Q_\lambda(t') Q_\nu(t') Q_\mu(t') \Big] | \Psi_0^A \rangle$$

Thus:

$$(-i\hbar) \lim_{t' \to t^+} \sum_\alpha \left\{ i\hbar \frac{d}{dt} g_{\alpha\alpha}(t,t') \right\} = \langle \hat{T} \rangle + 2\langle \hat{V} \rangle + 3 \langle \hat{W} \rangle$$

Which leads to two forms of the Koltun sum rule

$$\frac{-i\hbar}{2} \lim_{\tau \to 0^-} \mathrm{Tr}\left\{ i\hbar \frac{d}{d\tau} g(\tau) + \hat{T} g(\tau) \right\} = E_0^A + \frac{1}{2} \langle \hat{W} \rangle$$

$$\frac{-i\hbar}{2} \lim_{\tau \to 0^-} \mathrm{Tr}\left\{ i\hbar \frac{d}{d\tau} g(\tau) + 2 \hat{T} g(\tau) \right\} = E_0^A - \frac{1}{3} \langle \hat{V} \rangle$$

Lehman representation

Use the completnes relations:

$$\mathbb{1} = \sum_n |\Psi_n^{A+1}\rangle\langle\Psi_n^{A+1}| + \int d\nu_n |\Psi_{\nu_n}^{A+1}\rangle\langle\Psi_{\nu_n}^{A+1}|$$

$$\mathbb{1} = \sum_K |\Psi_K^{A-1}\rangle\langle\Psi_K^{A-1}| + \int d\nu_k |\Psi_{\nu_k}^{A-1}\rangle\langle\Psi_{\nu_k}^{A-1}|$$

Substitute in $g_{\alpha\beta}(\omega)$ on page 8:

$g_{\alpha\beta}(\omega) =$

For shortness of notation, it is useful to introduce:

$$\begin{cases} \chi_\alpha^n \equiv \langle \Psi_n^{A+1} | a_\alpha^\dagger | \Psi_0^A \rangle \\ \varepsilon_n^+ \equiv E_n^{A+1} - E_0^A \end{cases}$$

$$\begin{cases} \mathcal{Y}_\alpha^n \equiv \langle \Psi_k^{A-1} | a_\alpha | \Psi_0^A \rangle \\ \varepsilon_k^- \equiv E_0^A - E_k^{A-1} \end{cases}$$

Then:

$$g_{\alpha\beta}(\omega) = \sum_n \frac{(\chi_\alpha^n)^* \chi_\beta^n}{\hbar\omega - \varepsilon_n^+ + i\eta} + \sum_k \frac{\mathcal{Y}_\alpha^k (\mathcal{Y}_\beta^k)^*}{\hbar\omega - \varepsilon_k^- - i\eta}$$

$$= g_{\alpha\beta}^{(p)}(\omega) + g_{\alpha\beta}^{(h)}(\omega)$$

$\Rightarrow$ $\pm i\eta$ comes from $\theta(\pm\tau)$ and it reflects the causality principle...

Spectral functions

$$\frac{1}{x \pm i\eta} = \frac{P}{x} \mp \pi i \delta(x)$$

Particle spectral function

$$S^{(p)}_{\alpha\beta}(\omega) = \frac{-1}{\pi} \operatorname{Im}\left\{ g^{(p)}_{\alpha\beta}(\omega) \right\}$$

$$= \sum\!\!\!\!\!\!\int_n \langle \Psi_0^A | a_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | a_\beta^\dagger | \Psi_0^A \rangle \, \delta(\omega - [E_n^{A+1} - E_0^A])$$

$$= \sum\!\!\!\!\!\!\int_n (\chi_\alpha^n)^* \chi_\beta^n \, \delta(\omega - \varepsilon_n^+)$$

Hole spectral function

$$S^{(h)}_{\alpha\beta}(\omega) = \frac{1}{\pi} \operatorname{Im}\left\{ g^{(h)}_{\alpha\beta}(\omega) \right\}$$

$$= \sum\!\!\!\!\!\!\int_k \langle \Psi_0^{A-1} | a_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | a_\alpha | \Psi_0^A \rangle \, \delta(\omega - [E_0^A - E_0^{A-1}])$$

$$= \sum\!\!\!\!\!\!\int_k \mathcal{Y}_\alpha^k (\mathcal{Y}_\beta^k)^* \, \delta(\omega - \varepsilon_k^-)$$

Interpretation of $S^{(p)}$ and $S^{(h)}$

Consider diagonal elements in coordinate space:

$$S^{p}(\vec{r},\omega) = \sum_n |\langle \Psi_n^{A+1} | \hat{\psi}^{\dagger}(\vec{r}) | \Psi_0^{A} \rangle| \, \delta(\hbar\omega - \varepsilon_n^{+})$$

Probability of adding a nucleon at $\vec{r}$ and...

$$S^{(h)}(\vec{r},\omega) = \sum_n |\langle \Psi_k^{A-1} | \hat{\psi}(\vec{r}) | \Psi_0^{A} \rangle| \, \delta(\hbar\omega - \varepsilon_k^{-})$$

Dispersion relation

$$g_{\alpha\beta}(\omega) = \int_{\varepsilon_0^+}^{\infty} \frac{S^{(p)}_{\alpha\beta}(\tilde{\omega})}{\omega - \tilde{\omega} + i\eta} \, d(\hbar\tilde{\omega}) - \int_{-\infty}^{\varepsilon_0^-} \frac{S^{(h)}_{\alpha\beta}(\tilde{\omega})}{\omega - \tilde{\omega} - i\eta} \, d(\hbar\tilde{\omega})$$

$g_{\alpha\beta}(\omega)$ is completely defined by its imaginary parts (which reflects causality).

Expectation values and sum rules revisited:

$$\langle U \rangle = \sum_{\alpha\beta} \int_{-\infty}^{\varepsilon_0^-} u_{\alpha\beta}\, S^{(h)}_{\beta\alpha}(\omega)\, d(\hbar\omega)$$

$$\sum_{\alpha} \int d(\omega\hbar)\, S^{(h)}_{\alpha\alpha}(\omega) = \int d\vec{r} \int_{-\infty}^{\varepsilon_0^-} d(\hbar\omega)\, S^{(h)}(r;\omega) = A$$

$$\int_{-\infty}^{\varepsilon_0^-} d(\hbar\omega)\, S^{(h)}(r,\omega) = \rho(r)$$

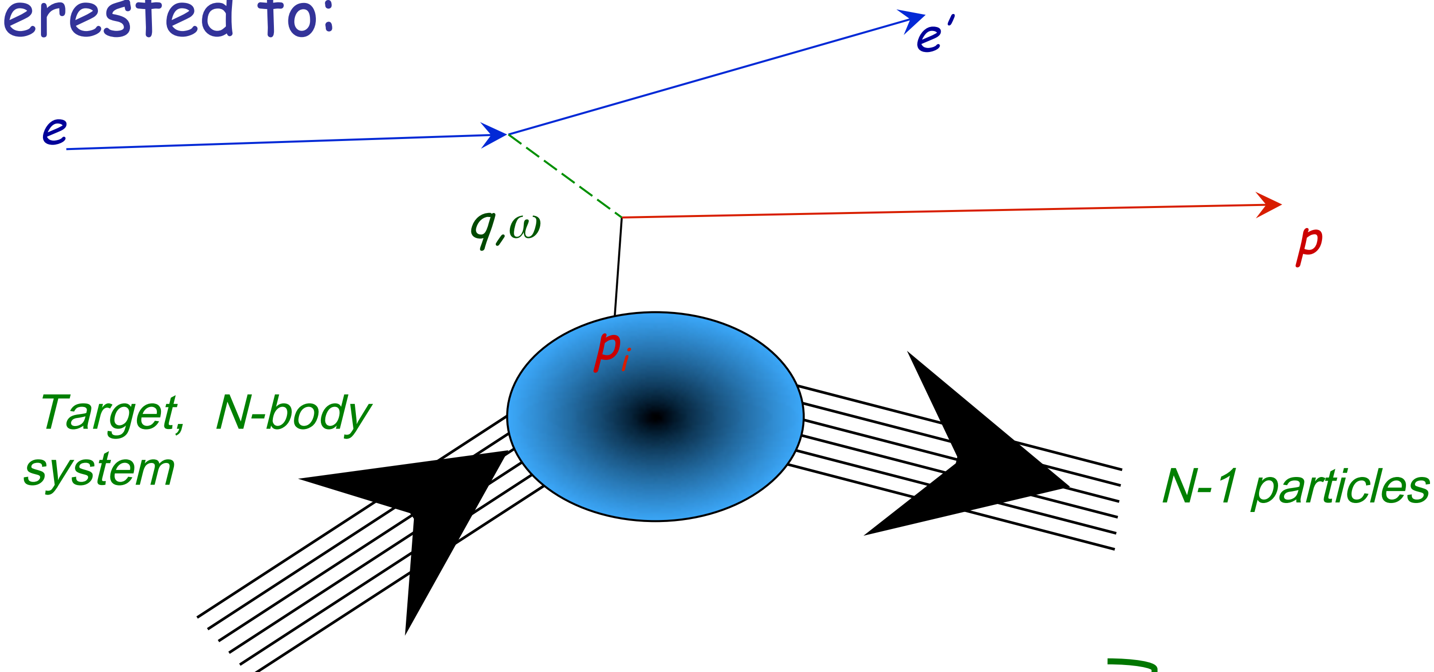
$$\int d\vec{r}\, S^{(h)}(r;\omega) = SF(\omega)$$

KGM sum rule:

$$\sum_{\alpha\beta} \int_{-\infty}^{\varepsilon_0^-} d(\hbar\omega) \frac{1}{2} \left\{ t_{\alpha\beta} + \hbar\omega\, \delta_{\alpha\beta} \right\} S^{(h)}_{\beta\alpha}(\omega) = E_0^A + \frac{1}{2} \langle \hat{W} \rangle$$

Spectroscopy via knock out reactions-basic idea

Use a probe (ANY probe) to eject the particle we are interested to:



Basic idea:

- we know, e, e' and p
- "get" *energy and momentum* of p_i: $p_i = k_e' + k_p - k_e$
  $E_i = E_e' + E_p - E_e$

Better to choose large transferred momentum and weak probes!!!

Knock-out processes

- Initial state: $|\Psi_i\rangle = |\Psi_0^N\rangle$
- Final state: $|\Psi_f\rangle = a^\dagger_{\boldsymbol{p}} |\Psi_n^{N-1}\rangle$ ← particle flying out, better if interacting as little as possible with the rest of the system
- Prob $\rho(\boldsymbol{q}) = \sum_{j=1}^{N} \exp\left(i\boldsymbol{q}\cdot\boldsymbol{r}_j\right)$ ← This can be anything: it *transfers* energy, and momentum q to the system; it's the simplest model for such a probe

$$\hat\rho(\boldsymbol{q}) = \sum_{\boldsymbol{p},\boldsymbol{p}'} \langle \boldsymbol{p}| \exp\left(i\boldsymbol{q}\cdot\boldsymbol{r}\right) |\boldsymbol{p}'\rangle a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{p}'} = \sum_{\boldsymbol{p}} a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{p}-\boldsymbol{q}} \quad ; \qquad \langle \mathbf{r}|\mathbf{p}\rangle = \frac{1}{(2\pi)^{3/2}} e^{-i\mathbf{r}\mathbf{p}/\hbar}$$

Knock-out processes

$$\hat{\rho}(\boldsymbol{q}) = \sum_{\boldsymbol{p},\boldsymbol{p}'} \langle \boldsymbol{p} | \exp{(i\boldsymbol{q}\cdot\boldsymbol{r})} | \boldsymbol{p}' \rangle a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{p}'} = \sum_{\boldsymbol{p}} a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{p}-\boldsymbol{q}}$$

- Transition matrix element:

$$\begin{aligned}
\langle \Psi_f | \hat{\rho}(\boldsymbol{q}) | \Psi_i \rangle &= \sum_{\boldsymbol{p}'} \langle \Psi_n^{N-1} | a_{\boldsymbol{p}} a^\dagger_{\boldsymbol{p}'} a_{\boldsymbol{p}'-\boldsymbol{q}} | \Psi_0^N \rangle \\
&= \sum_{\boldsymbol{p}'} \langle \Psi_n^{N-1} | \delta_{\boldsymbol{p}',\boldsymbol{p}} a_{\boldsymbol{p}'-\boldsymbol{q}} + \underbrace{a^\dagger_{\boldsymbol{p}'} a_{\boldsymbol{p}'-\boldsymbol{q}} a_{\boldsymbol{p}}}_{} | \Psi_0^N \rangle \\
&\approx \langle \Psi_n^{N-1} | a_{\boldsymbol{p}-\boldsymbol{q}} | \Psi_0^N \rangle .
\end{aligned}$$

Impulse Approximation (IA) means throwing away this part. If the particle is ejected with very high momentum transfer, it is usually a good approximation

Knock-out processes

$$H_N = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i<j=1}^{N} V(i,j) = H_{N-1} + \frac{\boldsymbol{p}_N^2}{2m} + \underbrace{\sum_{i=1}^{N-1} V(i,N)}$$

$$|\Psi_f\rangle = a^\dagger_{\boldsymbol{p}} |\Psi_n^{N-1}\rangle$$

← The plane wave approximation assumes the flies out without interacting with the rest of the system. This is OK in some cases. In others, one has to worry about the distortion due to final state interactions.

Knock-out processes

- Use the Fermi Golden rule:

$$d\sigma \sim \sum_n \delta(\omega + E_i - E_f) |\langle \Psi_f | \hat{\rho}(\boldsymbol{q}) | \Psi_i \rangle|^2$$

- "missing" moment $\boldsymbol{p}_{miss} = \boldsymbol{p} - \boldsymbol{q}$
- "missing" energy $E_{miss} = \boldsymbol{p}^2/2m - \omega = E_0^N - E_n^{N-1}$

Interpreted as *energy* and *momentum* of initial particle!!

- In plane wave impulse approximation (PWIA):

$$d\sigma \sim \sum_n \delta(E_{miss} - E_0^N + E_n^{N-1}) |\langle \Psi_n^{N-1} | a_{\boldsymbol{p}_{miss}} | \Psi_0^N \rangle|^2$$

$$d\sigma = \sigma_{probe}\, S^h(\boldsymbol{p}_{miss}, E_{miss})$$

PWIA is not always justified, but it is all OK for our display purposes:
Can "see" the spectral fnct.!!!

One-hole spectral function

Overlap function:

$$\psi_k^{overlap}(\mathbf{r}) \quad = \quad \langle \Psi_k^{N-1} | \psi_s(\mathbf{r}) | \Psi_0^N \rangle$$

Spectroscopic factor:

$$S_k = \int d\mathbf{r} |\psi_k^{overlap}(\mathbf{r})|^2$$

= 1 , for free fermions
< 1 , for interacting particles (correlations!!)

$$S^h(\mathbf{p},\omega) = \sum_k \left| \langle \Psi_k^{N-1} | \psi_k(\mathbf{p}) | \Psi_0^N \rangle \right|^2 \; \delta\left(\hbar\omega - (E_0^N - E_k^{N-1})\right)$$

Integrate S^h over p : → spectral strength distribution

Integrate S^h over ω : → momentum distribution

Knock-out processes

So, I can "see" $S^h(\mathbf{p},\omega)$:

$$d\sigma = \sigma_{probe}\, S^h(\boldsymbol{p}_{miss}, E_{miss})$$

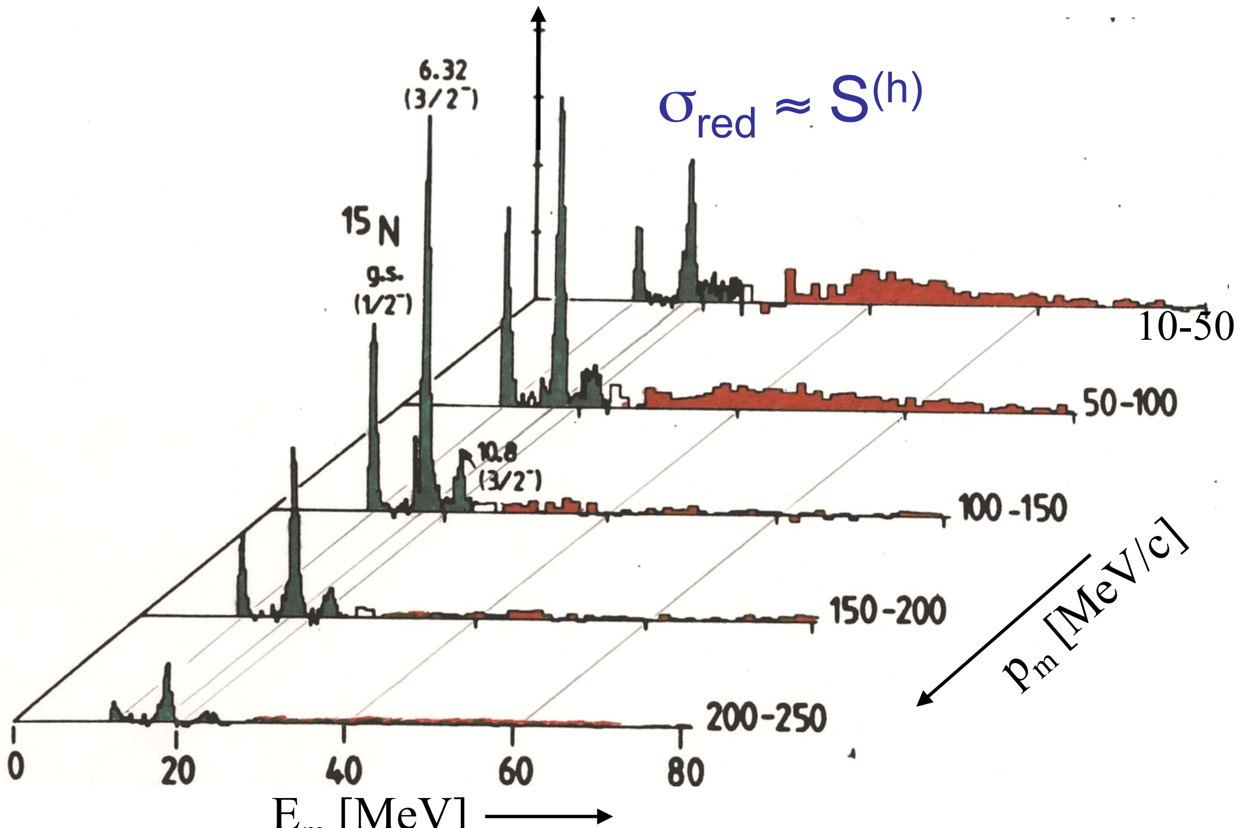
x-sec for scattering on a free particle

PWIA is not always justified, but it is all OK for our display purposes:
Can "see" the spectralfnct.!!!

…does it really work ?!?!?!?

Concept of correlations

Spectral function: distribution of momentum (p_m) and energies (E_m)



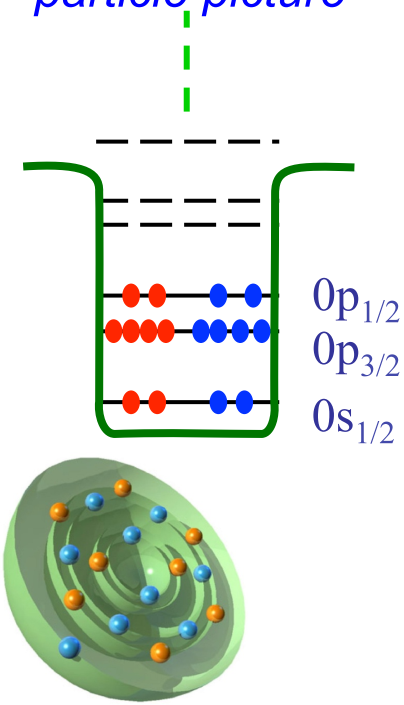
Saclay data for $^{16}O(e,e'p)$

[Mougey et al., Nucl. Phys. A335, 35 (1980)]

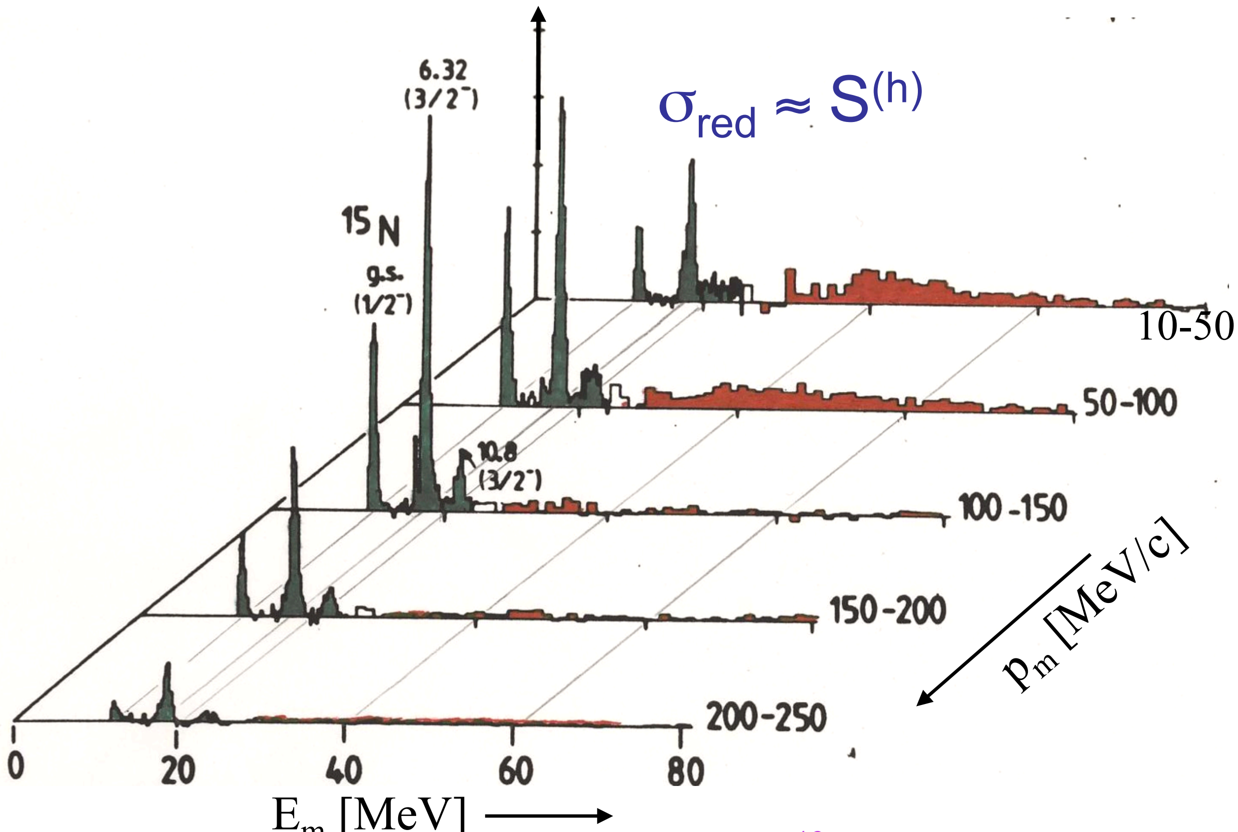
$$S^{(h)}(p_m, E_m) = \sum_n \left| \langle \Psi_n^{A-1} | c_{\vec{p}_m} | \Psi_0^A \rangle \right|^2 \delta(E_m - (E_0^A - E_n^{A-1}))$$

Concept of correlations

independent particle picture



Spectral function: distribution of momentum (p_m) and energies (E_m)



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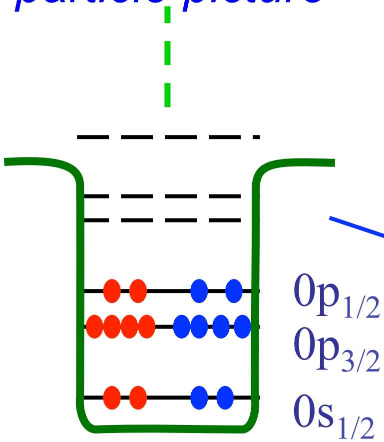
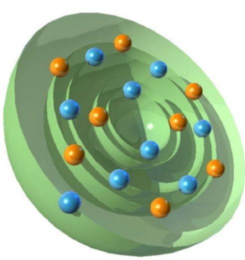
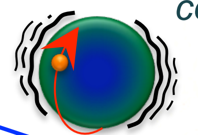
Concept of correlations

independent particle picture

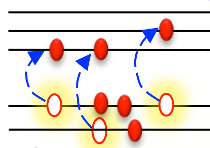




Particle-vibration coupling (PV)

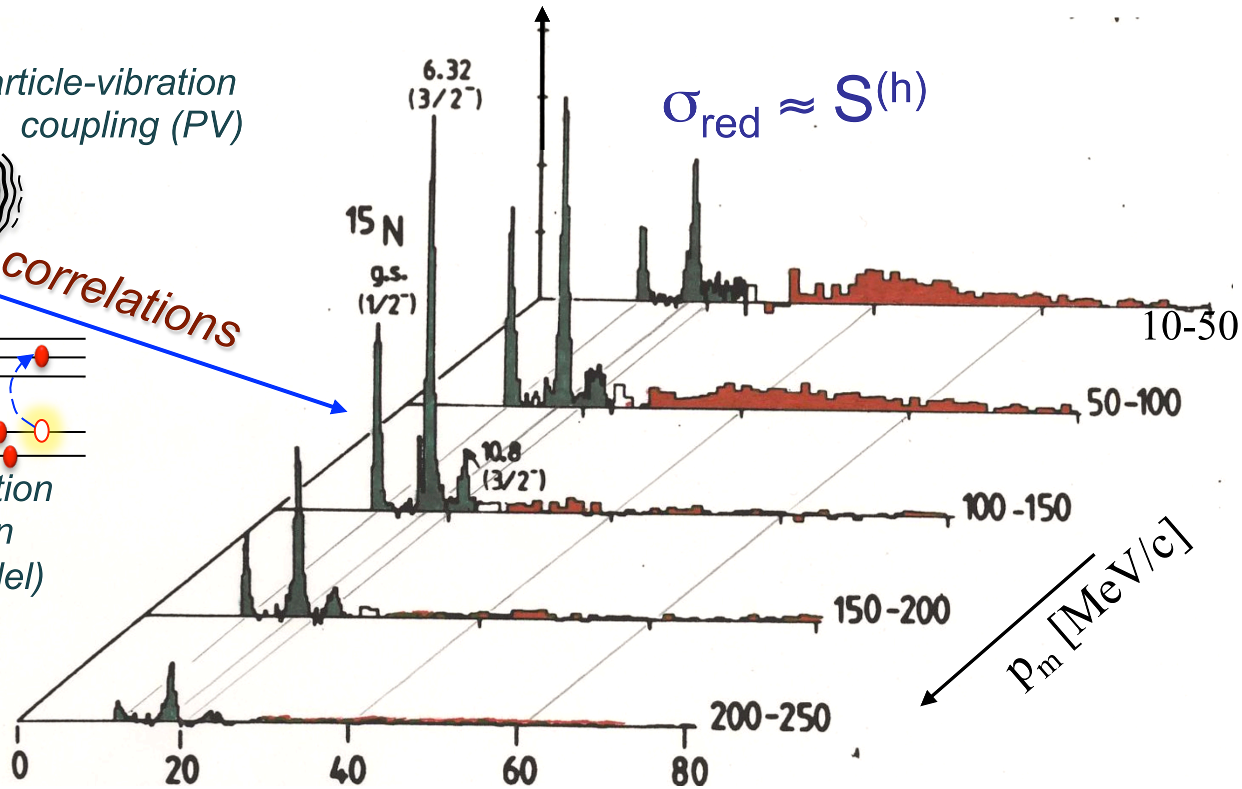


correlations



Configuration interaction (shell model)

Spectral function: distribution of momentum (p_m) and energies (E_m)



Saclay data for $^{16}O(e,e'p)$

[Mougey et al., Nucl. Phys. A335, 35 (1980)]

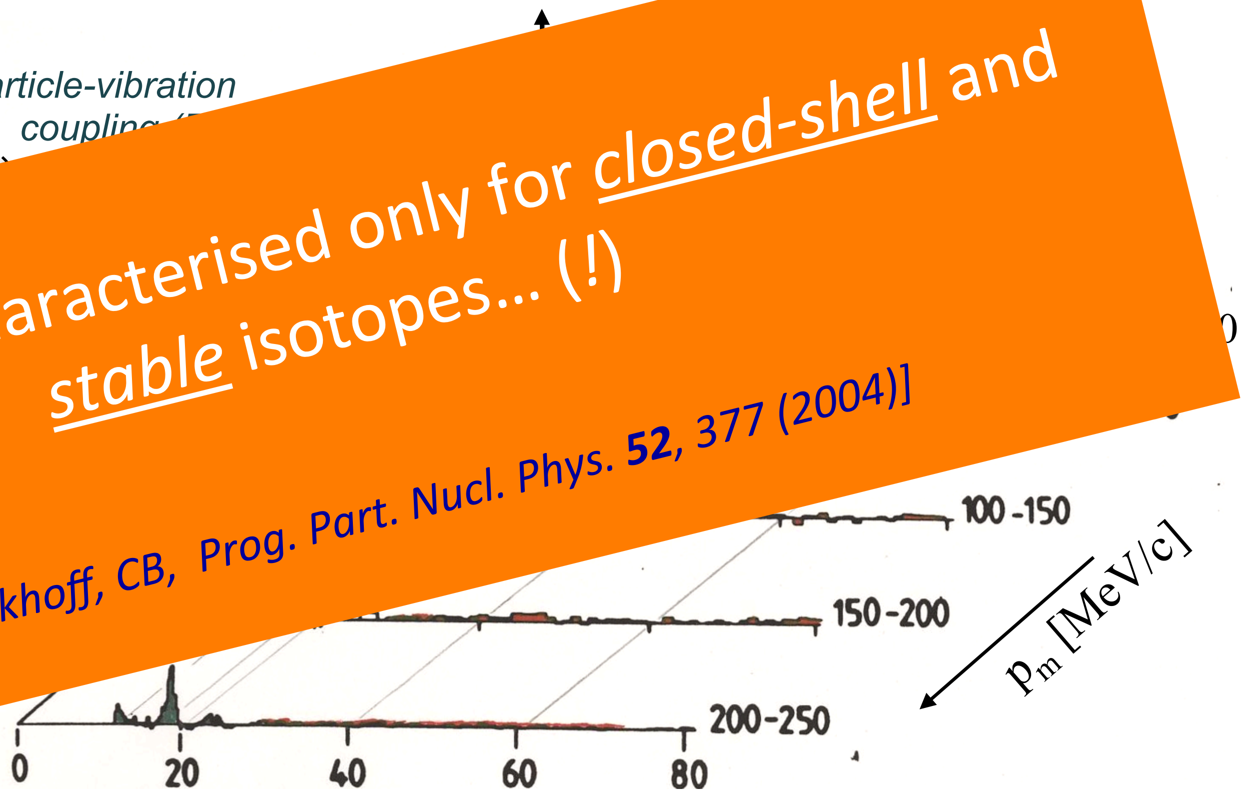
$$S^{(h)}(p_m, E_m) = \sum_n \left| \langle \Psi_n^{A-1} \,|\, c_{\vec{p}_m} \,|\, \Psi_0^A \rangle \right|^2 \delta(E_m - (E_0^A - E_n^{A-1}))$$

Concept of correlations

independent particle picture

Particle-vibration coupling (...)

Spectral function: distribution of momentum (p_m) and en...)



So far, fully characterised only for <u>closed-shell</u> and <u>stable</u> isotopes... (!)

[W. Dickhoff, CB, Prog. Part. Nucl. Phys. **52**, 377 (2004)]

Saclay data for $^{16}O(e,e'p)$

[Mougey et al., Nucl. Phys. A335, 35 (1980)]

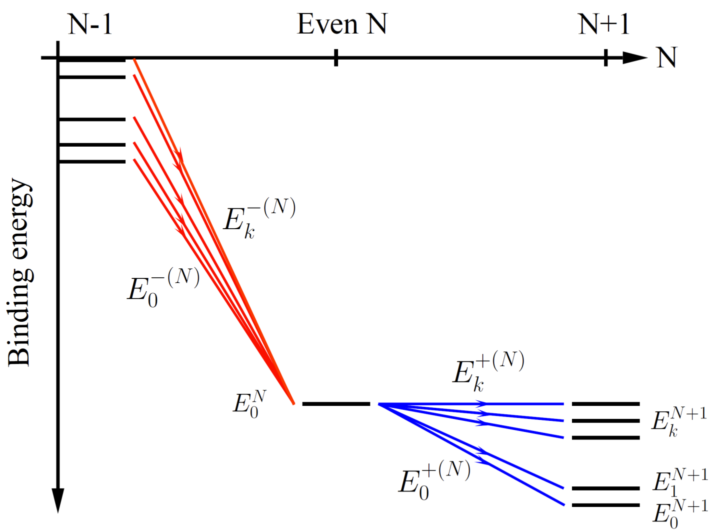
$$S^{(h)}(p_m, E_m) = \sum_n \left| \langle \Psi_n^{A-1} | c_{\vec{p}_m} | \Psi_0^A \rangle \right|^2 \delta(E_m - (E_0^A - E_n^{A-1}))$$

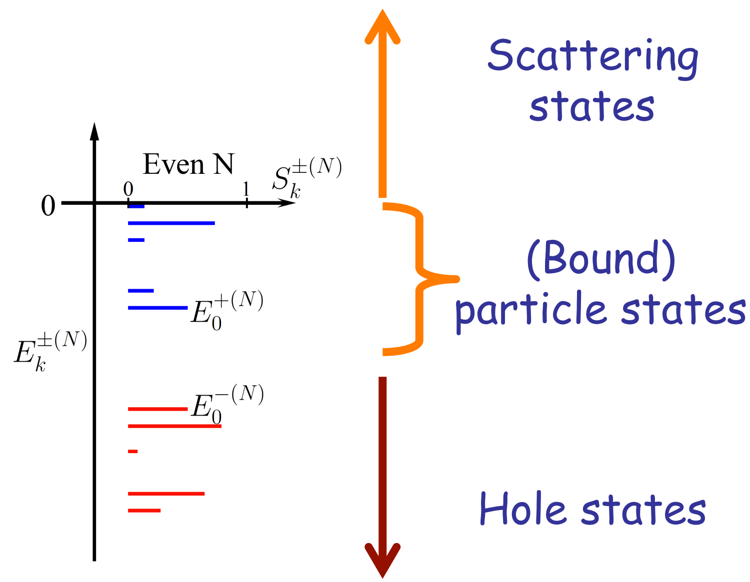
Green's functions in many-body theory

One-body Green's function (or propagator) describes the motion of quasi-particles and holes:

$$g_{\alpha\beta}(E) = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{E - (E_n^{A+1} - E_0^A) + i\eta} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle}{E - (E_0^A - E_k^{A-1}) - i\eta}$$

…this contains all the structure information probed by nucleon transfer (spectral function):





Separation energies and transfer strengths

[pic. J. Sadoudi]

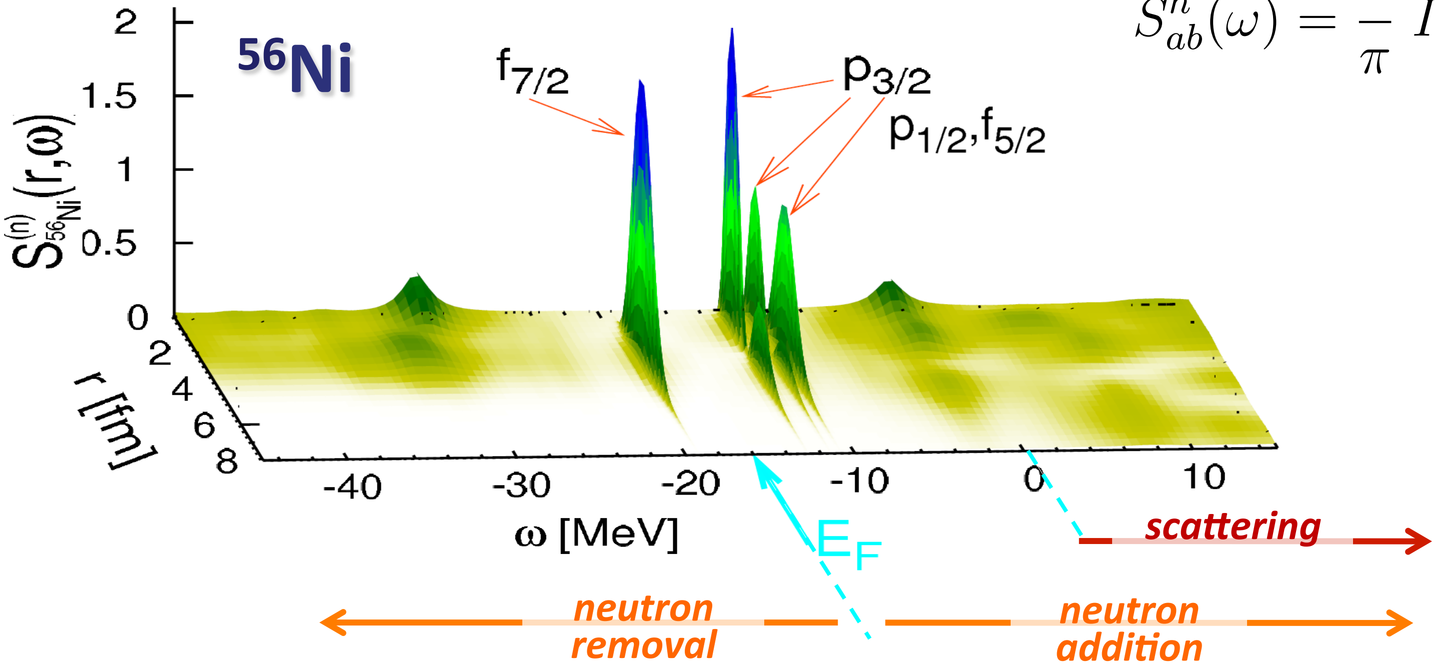
Example of spectral function ^{56}Ni

One-body Green's function (or propagator) describes the motion of quasi-particles and holes:

$$g_{\alpha\beta}(E) = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{E - (E_n^{A+1} - E_0^A) + i\eta} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle}{E - (E_0^A - E_k^{A-1}) - i\eta}$$

…this contains <u>all the structure information</u> probed by nucleon transfer (spectral function):

$$S_{ab}^h(\omega) = \frac{1}{\pi} Im\, g_{ab}(\omega)$$



[CB, M.Hjorth-Jensen, Pys. Rev. C**79**, 064313 (2009); CB, Phys. Rev. Lett. **103**, 202502 (2009)]

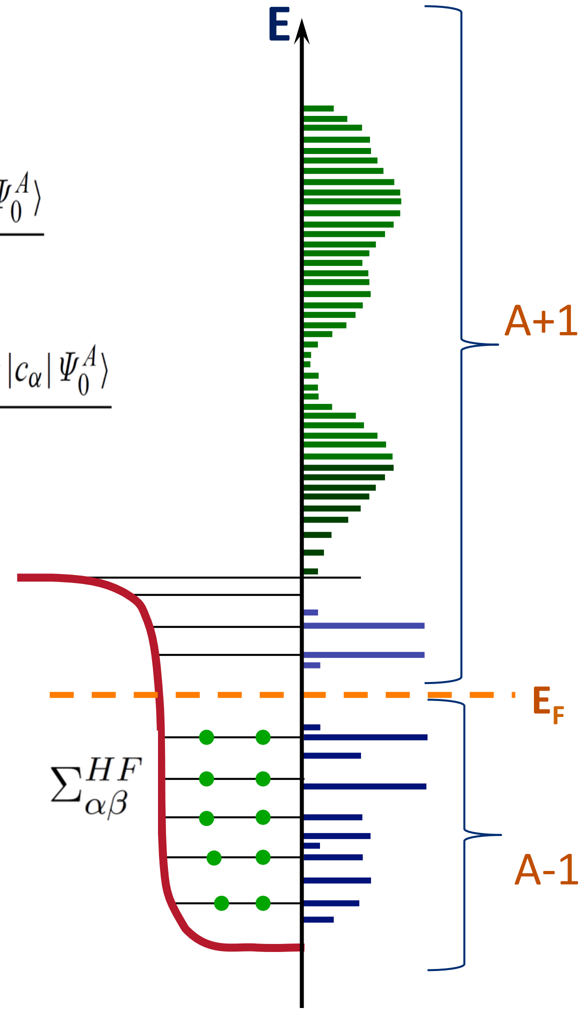
Nucleon elastic scattering

The full Lehmann representation of the single particle propagator is

$$g_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{\hbar\omega - \varepsilon_n^+ + i\eta} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle}{\hbar\omega - \varepsilon_k^- - i\eta}$$

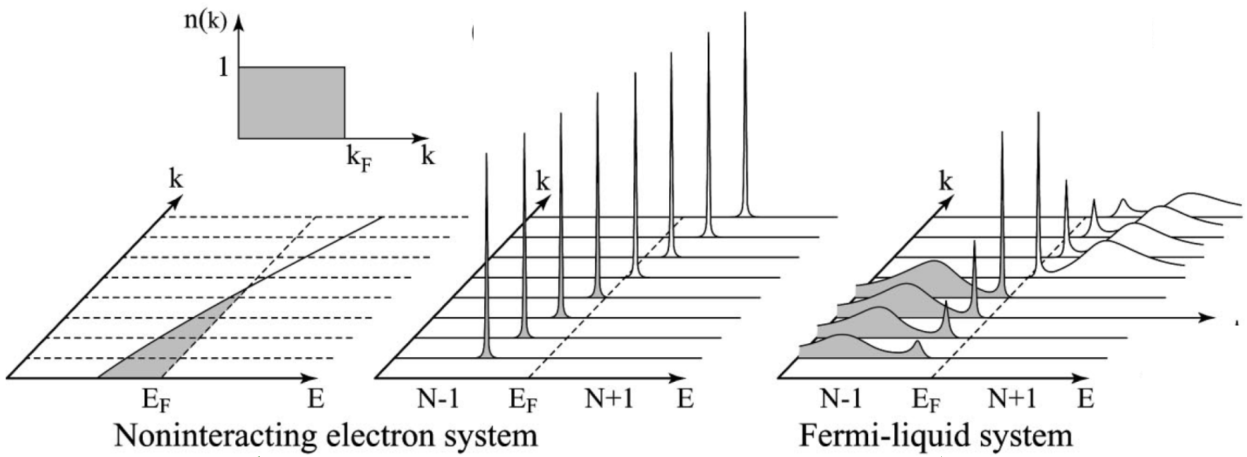
$$+ \int_{\varepsilon_T^+}^{\infty} \mathrm{d}\varepsilon_\nu^+ \frac{\langle \Psi_0^A | c_\alpha | \Psi_\nu^{A+1} \rangle \langle \Psi_\nu^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{\hbar\omega - \varepsilon_\nu^+ + i\eta} + \int_{-\infty}^{\varepsilon_T^-} \mathrm{d}\varepsilon_\kappa^- \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_\kappa^{A-1} \rangle \langle \Psi_\kappa^{A-1} | c_\alpha | \Psi_0^A \rangle}{\hbar\omega - \varepsilon_\kappa^- - i\eta}$$

→ In real systems these is always a continuum for large particle and hole energies—The one body equation for the residues is the same in both discrete and continuum spectrum



One-hole spectral function

Spectral function of infinite fermion systems

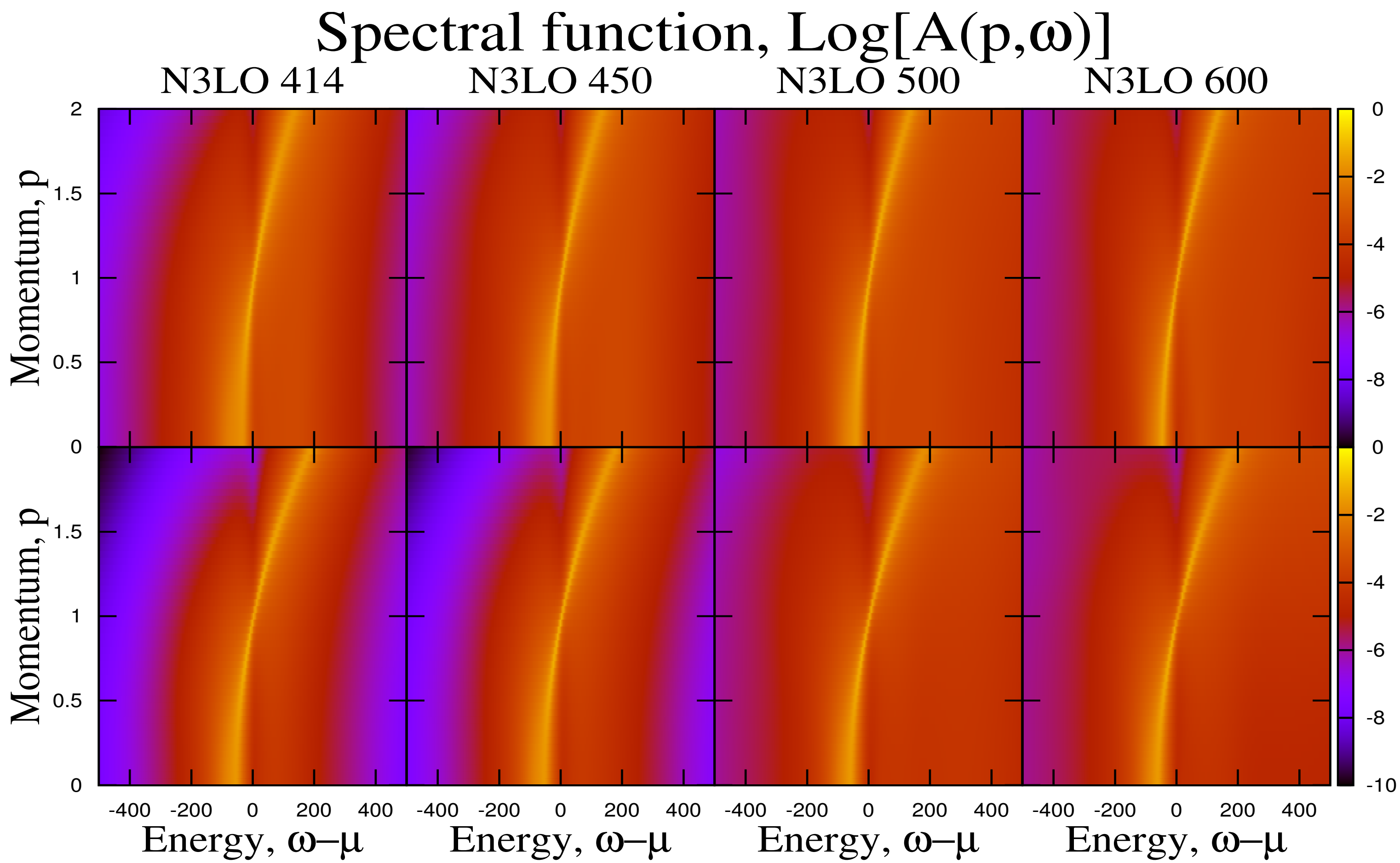


$$S(\mathbf{p},\omega) = \theta(|\mathbf{p}| - k_F)\delta\left(\hbar\omega - \frac{p^2}{2m}\right) + \theta(k_F - |\mathbf{p}|)\delta\left(\hbar\omega - \frac{p^2}{2m}\right)$$

$$S^h(\mathbf{p},\omega) = \sum_k \left|\langle \Psi_k^{N-1} | \psi_k(\mathbf{p}) | \Psi_0^N \rangle\right|^2 \delta\left(\hbar\omega - (E_0^N - E_k^{N-1})\right)$$

[Picture credit: A. Damascelli, Rev. Mod. Phys. 75, 473 (2003)]

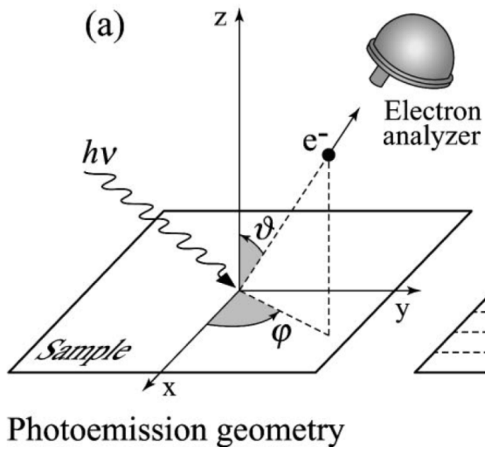
Spectral function in asymm. matter



A. Carbone, priv. comm.

Angle Resolved Photon Emission Spectroscopy (ARPES)

An ARPES setup – spectroscopy at the Fermi surface



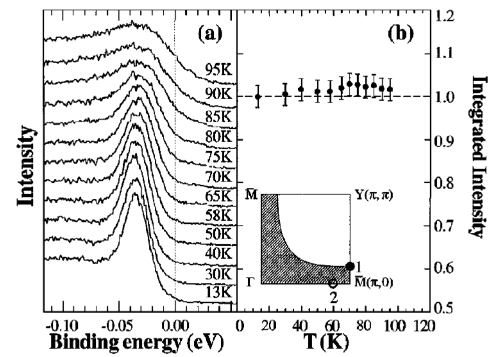


FIG. 4. Temperature dependence of the photoemission data from $Bi_2Sr_2CaCu_2O_{8+\delta}$ (T_c=87 K): (a) ARPES spectra measured at $\mathbf{k}=\mathbf{k}_F$ (point 1 in the Brillouin-zone sketch); (b) integrated intensity. From Randeria *et al.*, 1995.

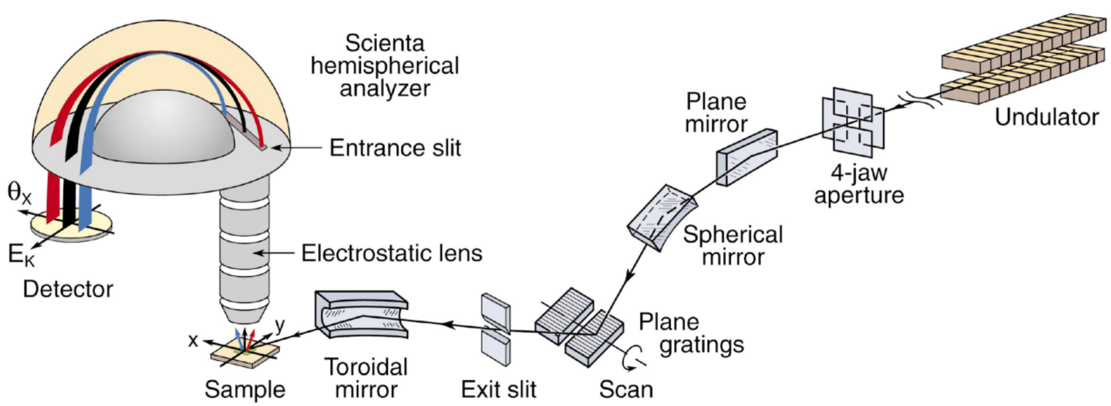


FIG. 6. Generic beamline equipped with a plane grating monochromator and a Scienta electron spectrometer (Color).

- Incoming beam of real photons
- Measure the emitted electron
- From angle and energy recover the momentum of the ejected particle + separation energy

UNIVERSITY OF SURREY

[Pictures credit: A. Damascelli, et. al, Rev. Mod. Phys. 75, 473 (2003)]

Angle Resolved Photon Emission Spectroscopy (ARPES)

An ARPES setup – spectroscopy at the Fermi surface

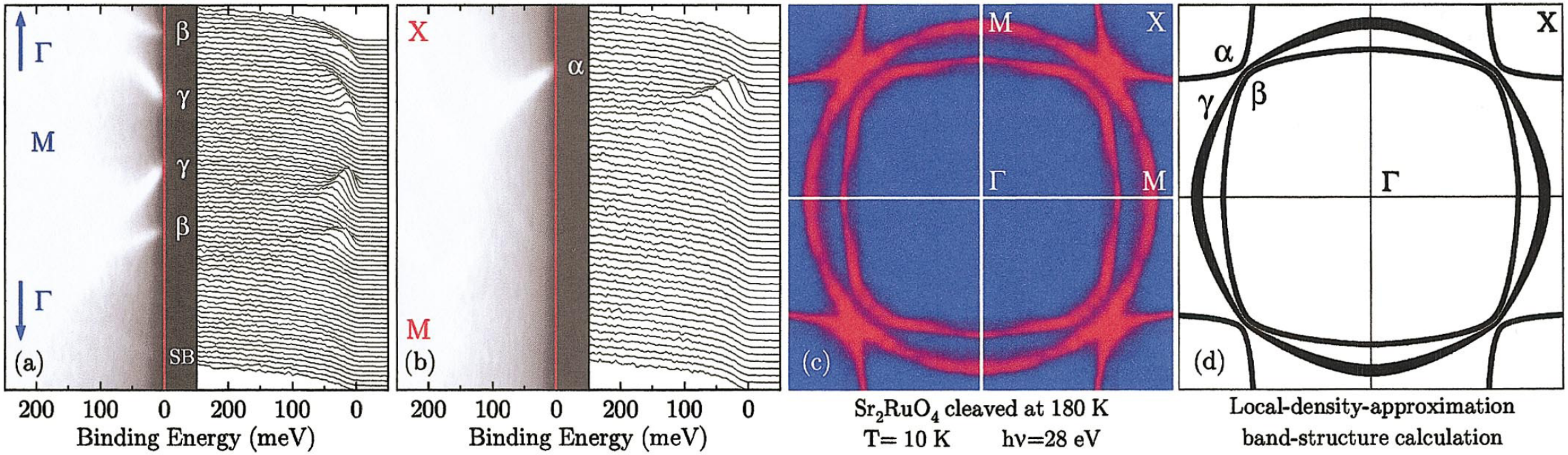


FIG. 9. Photoemission results from Sr_2RuO_4: ARPES spectra and corresponding intensity plot along (a) Γ-*M* and (b) *M*-*X*; (c) measured Fermi surface; (d) calculated Fermi surface (Mazin and Singh, 1997). From Damascelli *et al.*, 2000 (Color).

→ can "see" the Fermi surface!!

[Rev. Mod. Phys. 75, 473 (2003)]