One-body descriptions of many-body problems and the role of spectroscopic factors

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Spectroscopic factors

…contain valuable information on the structure of the nuclear many-body system.

…are defined as the norms of one-body overlap functions:

$$S^A_{nm} = \int d\boldsymbol{r} |\phi^A_{nm}(\boldsymbol{r})|^2$$

$$\phi^A_{nm}(\boldsymbol{r}) = \langle \Psi^n_{A-1} | a(\boldsymbol{r}) | \Psi^m_A \rangle$$

and, similarly:

$$\phi^{A+1}_{mk}(\boldsymbol{r}) = \langle \Psi^m_A | a(\boldsymbol{r}) | \Psi^k_{A+1} \rangle$$

…provide the link between an effective one-body picture and the full nuclear many-body problem:

- Nucleon capture reactions:

$$\sigma_{(\mathrm{exp})} = S_0 \, \sigma_{(\mathrm{calc})}$$

- Proton emission:

$$\Gamma^{(\mathrm{exp})} = S_0 \, \Gamma^{(\mathrm{calc})}$$

calculated in a single-particle model

Spectroscopic factors in capture reactions

Reduction from a many-body approach to a one-body description is fairly straight-forward…

Exact many-body transition matrix element:

$$\begin{aligned}\mathcal{M} &= \langle \Psi_A^m | \mathcal{F} | \Psi_A^{m'} \rangle \\ &= \int d\boldsymbol{r} d\boldsymbol{r}' F(\boldsymbol{r}, \boldsymbol{r}') \rho_{mm'}(\boldsymbol{r}, \boldsymbol{r}') \\ &= \sum_n \int d\boldsymbol{r} d\boldsymbol{r}' \phi_{nm}^{A*}(\boldsymbol{r}) F(\boldsymbol{r}, \boldsymbol{r}') \phi_{nm'}^{A}(\boldsymbol{r}')\end{aligned}$$

When the (A-1)-body system remains in the ground state (here for radiative capture):

$$\mathcal{M} \approx \sqrt{S_{0m}^A} \int d\boldsymbol{r}\ \tilde{\phi}_{0m}^{A*}(\boldsymbol{r}) \exp[i\boldsymbol{k}\cdot\boldsymbol{r}] \phi_{0m}^{A}(\boldsymbol{r})$$

where $\phi = \sqrt{S_0}\,\tilde{\phi}$

Since $\sigma \sim \mathcal{M}^2$, it is reasonable to write:

$$\sigma_{(\mathrm{exp})} = S_0\, \sigma_{(\mathrm{calc})}$$

Spectroscopic factors in proton emission?

Situation not straight-forward…

To understand the role of spectroscopic factors in cross sections, one needs to start with a many-body approach and reduce the problem to a one-body case.

Our study

Revisiting the issue for proton emission…

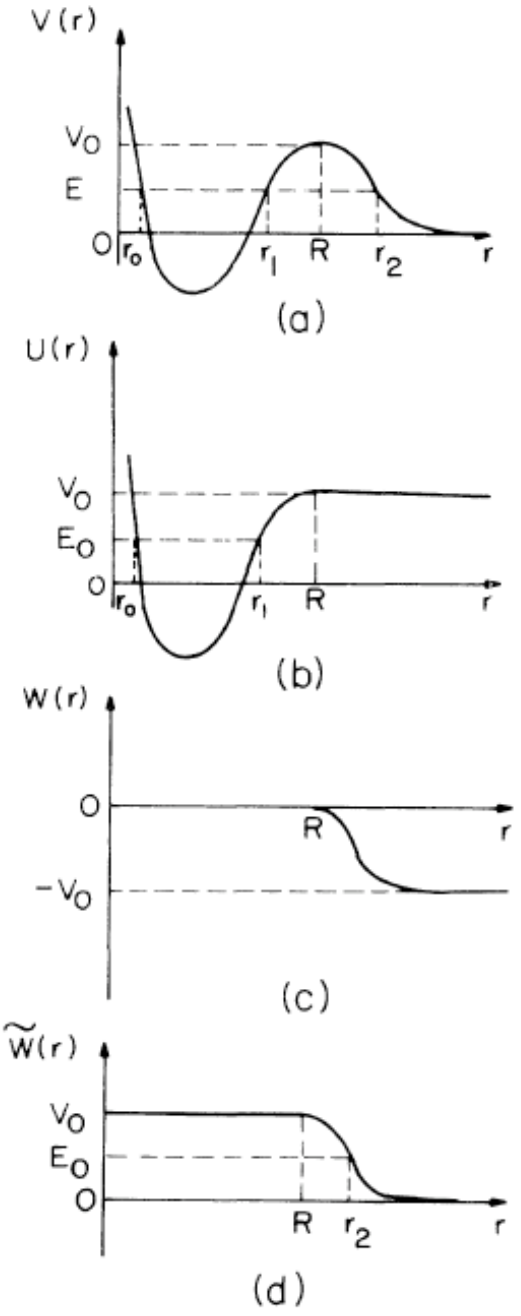
- derive expressions for the decay width in a many-body formalism
- use a formalism based on the two-potential perturbative approach of Gurvitz and Kalbermann
- reduce the problem to an effective one-body problem through an appropriate choice of the perturbing potential

We find…

- ambiguities in the interpretation of the normalization factor obtained from experiments.

Two potential approach

Gurvitz & Kalbermann, PRL **59** (1987) 262;
Gurvitz, PRL **59** (1987) 262



Goal: calculate decay width for a quasistationary state

Approach:

- split the potential

$$V(r) = U(r) + W(r)$$

- start with a bound state ψ_0

$$H_0 = T + U$$

$$H_0\,\varphi_0 = E_0\,\varphi_0$$

- add a perturbation W(r)
- calculate the energy shift and decay width

$$\Gamma = \frac{4m}{\hbar^2 k}\left|\int_R^\infty \varphi_0(r) W(r) \chi_k(r) dr\right|^2$$

- Simplify via integration by parts

$$\Gamma = \frac{4\hbar^2\alpha^2}{mk}\,|\,\varphi_0(R)\chi_k(R)\,|^2$$

Many-body implementation

Start with the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

Use Laplace transform and solve for probability amplitude:

$$\langle \psi_0|\psi(t)\rangle = \frac{i}{2\pi}\int_{-\infty}^{\infty} dE e^{-iEt/\hbar}\langle \psi_0|\frac{1}{E-H+i\epsilon}|\psi_0\rangle$$

where $\psi(t=0)= \psi_0$. The decay rate can be extracted from imaginary part of the pole location (if one pole dominates).

-> Task: Determine the matrix element of the Green's function.

Many-body implementation - projection operator formalism

-> Approach: Use projection operator formalism to obtain

$$\left[E - \langle \psi_0 | \left(H + HQ \frac{1}{E - QHQ + i\epsilon} QH \right) | \psi_0 \rangle \right] \langle \psi_0 | G | \psi_0 \rangle = 1$$

where $P = | \psi_0 \rangle \langle \psi_0 |$ and $Q = 1 - P$.

-> The poles of the Green's function are found by solving:

$$E = \langle \psi_0 | H | \psi_0 \rangle + \int_{-\infty}^{\infty} dE' \frac{|\langle \psi_0 | HQ | \zeta_{E'} \rangle|^2}{E - E' + i\epsilon}$$

where $E' | \zeta_{E'} \rangle = QHQ | \zeta_{E'} \rangle$.

Many-body implementation - perturbative approximation

Introduce a Hermitean Hamiltonian H_0 with

$$H = H_0 + \delta H$$
$$H_0 \mid \psi_0 > = E_0 \mid \psi_0 >$$

and derive:

$$E \approx E_0 + \langle \psi_0 | \delta H | \psi_0 \rangle + \int_{-\infty}^{\infty} dE' \frac{|\langle \psi_0 | \delta H Q | \zeta_{E'} \rangle|^2}{E_0 - E' + i\epsilon}$$

➠ still a many-body problem!

Reduction to an effective one-body problem

Criteria for selecting H_0 (and δH) in $H = H_0 + \delta H$:

H_0 needs to produce a bound initial state with energy E_0 .

After the decay, the wave function of the system describes a free proton and the bound (A-1)-body system.

Our choice:

$$\delta H = -\int d\mathbf{r} a^{\dagger}(\mathbf{r}) |\Phi_{A-1}\rangle V(\mathbf{r}) \langle \Phi_{A-1}| a(\mathbf{r})$$

$|\Phi_{A\text{-}1}\rangle$ is the (A-1)-body ground state,

r is the relative coordinate of the proton and the (A-1)-body system,

V(**r**) is larger than E_0 outside the range of the nuclear potential and zero inside.

An effective one-body problem

Consequence of our particular choice of δH :

$$E \approx E_0 - \int d\mathbf{r}\phi_0^*(\mathbf{r})V(\mathbf{r})\phi_0(\mathbf{r})$$

$$+ \int_{-\infty}^{\infty} dE' \frac{\left| \int d\mathbf{r}\phi_0^*(\mathbf{r})V(\mathbf{r})\phi_{E'}(\mathbf{r}) \right|^2}{E_0 - E' + i\epsilon}$$

We have an effective one-body problem!

The many-body aspects of the problem are contained in the overlap functions $\phi_0(\mathbf{r})$ and $\phi_{E'}(\mathbf{r})$.

Only assumption made so far: 2nd order perturbation is valid (E has been replaced by E_0). Should be valid for narrow states.

The decay width can be determined from the equation above!

Expression for the decay width

We find : $$\Gamma_0 \approx 2\pi \left| \int d\mathbf{r} \phi_0^*(\mathbf{r}) V(\mathbf{r}) \phi_{E_0}(\mathbf{r}) \right|^2$$

$$\approx 2\pi S_0 \left| \int d\mathbf{r} \hat{\phi}_0^*(\mathbf{r}) V(\mathbf{r}) \phi_{E_0}(\mathbf{r}) \right|^2 \qquad (*)$$

where $\phi_0 = \sqrt{S_0}\hat{\phi}_0(\mathbf{r})$ is the solution of

$$E\phi_0(\mathbf{r}) = \int d\mathbf{r}' [\mathcal{H}_{\mathcal{M}}(\mathbf{r},\mathbf{r}') + \delta(\mathbf{r},\mathbf{r}')V(\mathbf{r}')]\phi_0(\mathbf{r}')$$

and $\mathcal{H}_{\mathcal{M}}(\mathbf{r},\mathbf{r}')$ is the mass operator.

When $\mathcal{H}_{\mathcal{M}}(\mathbf{r},\mathbf{r}')$ is approximately local, the integral in (*) can be evaluated via integration by parts

$$I = \frac{\hbar^2}{2m_k(r_0)} [\hat{\phi}_{r0}^*(r_0)\phi'_{rE_0}(r_0) - \phi_{rE_0}(r_0)\hat{\phi}'^*_{r0}(r_0)]$$

Spectroscopic factor and the decay width

In practical applications, the one-body functions are taken to be solutions of a potential model and are normalized to 1.

It seems to follow that indeed

$$\Gamma^{(\mathrm{exp})} = S_0 \, \Gamma^{(\mathrm{calc})}$$

where $\Gamma^{(\mathrm{calc})}$ is calculated using a potential model.

However…

Alternative expression for the decay width

We also find : $$\Gamma_0 \approx 2\pi \left| \int d\mathbf{r} \bar{\phi}_0^*(\mathbf{r}) \bar{V}(\mathbf{r}) \bar{\phi}_{E_0}(\mathbf{r}) \right|^2$$

$$\approx 2\pi \bar{S}_0 \left| \int d\mathbf{r} \hat{\bar{\phi}}_0^*(\mathbf{r}) \bar{V}(\mathbf{r}) \bar{\phi}_{E_0}(\mathbf{r}) \right|^2 \quad (**)$$

where $\bar{\phi}(\mathbf{r}) = \int d\mathbf{r}' \mathcal{N}(\mathbf{r},\mathbf{r}')^{-1/2} \phi(\mathbf{r}')$ is the solution of

$$E\bar{\phi}_0(\mathbf{r}) = \int d\mathbf{r}' [\bar{\mathcal{H}}(\mathbf{r},\mathbf{r}') + \delta(\mathbf{r},\mathbf{r}') \bar{V}(\mathbf{r}')] \bar{\phi}_0(\mathbf{r}')$$

with

$$\bar{\mathcal{H}}(\mathbf{r},\mathbf{r}') = \int d\mathbf{r}'' d\mathbf{r}''' \mathcal{N}(\mathbf{r},\mathbf{r}'')^{-1/2} \mathcal{H}(\mathbf{r}'',\mathbf{r}''') \mathcal{N}(\mathbf{r}''',\mathbf{r}')^{1/2}$$

$$\mathcal{N}(\mathbf{r},\mathbf{r}') = \langle \Phi_{A-1} | a(\mathbf{r}) a^\dagger(\mathbf{r}') | \Phi_{A-1} \rangle$$

$$\bar{\phi}_0(\mathbf{r}) = \sqrt{\bar{S}_0} \hat{\bar{\phi}}_0(\mathbf{r})$$

When $\bar{\mathcal{H}}(\mathbf{r},\mathbf{r}')$ is approximately local, the integral in (**) can be evaluated via integration by parts:

$$I = \frac{\hbar^2}{2\bar{m}_k(r_0)} [\hat{\bar{\phi}}_{r0}^*(r_0) \bar{\phi}'_{rE_0}(r_0) - \hat{\bar{\phi}}_{rE_0}(r_0) \bar{\phi}'^*_{r0}(r_0)]$$

Two valid expressions for the decay width

The previous derivations show:

$$\Gamma^{(\mathrm{exp})} \approx 2\pi S_0 \left| \int d\mathbf{r} \hat{\phi}_0^*(\mathbf{r}) V(\mathbf{r}) \phi_{E_0}(\mathbf{r}) \right|^2$$

and

$$\Gamma^{(\mathrm{exp})} \approx 2\pi \bar{S}_0 \left| \int d\mathbf{r} \hat{\bar{\phi}}_0^*(\mathbf{r}) \bar{V}(\mathbf{r}) \bar{\phi}_{E_0}(\mathbf{r}) \right|^2$$

→Do we know which normalization factor we extract?

$$S_0 = \Gamma^{(\mathrm{exp})} / \Gamma^{(\mathrm{calc})} \quad ?$$

or

$$\bar{S}_0 = \Gamma^{(\mathrm{exp})} / \Gamma^{(\mathrm{calc})} \quad ?$$

or possibly yet another factor?

Three questions…

…we should ask:

- What are we approximating when we use a potential model and potential-model wave functions?
- Do we need to care? (How much difference is there between S_0 and $\overline{S_0}$?)
- What are these $\overline{\phi}(\mathrm{r})$?

What are we approximating?

This needs to be studied further…

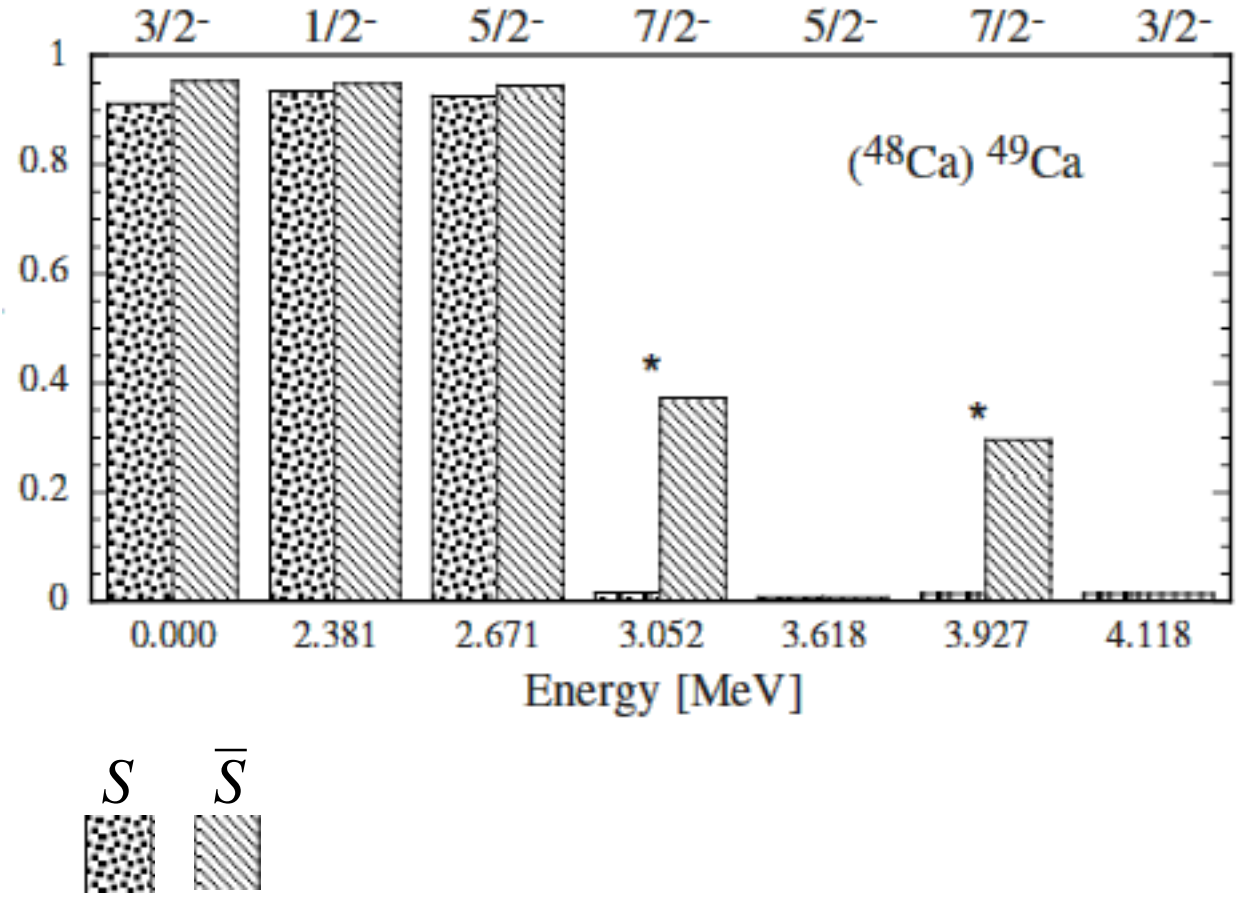
Does the difference matter?

It depends!

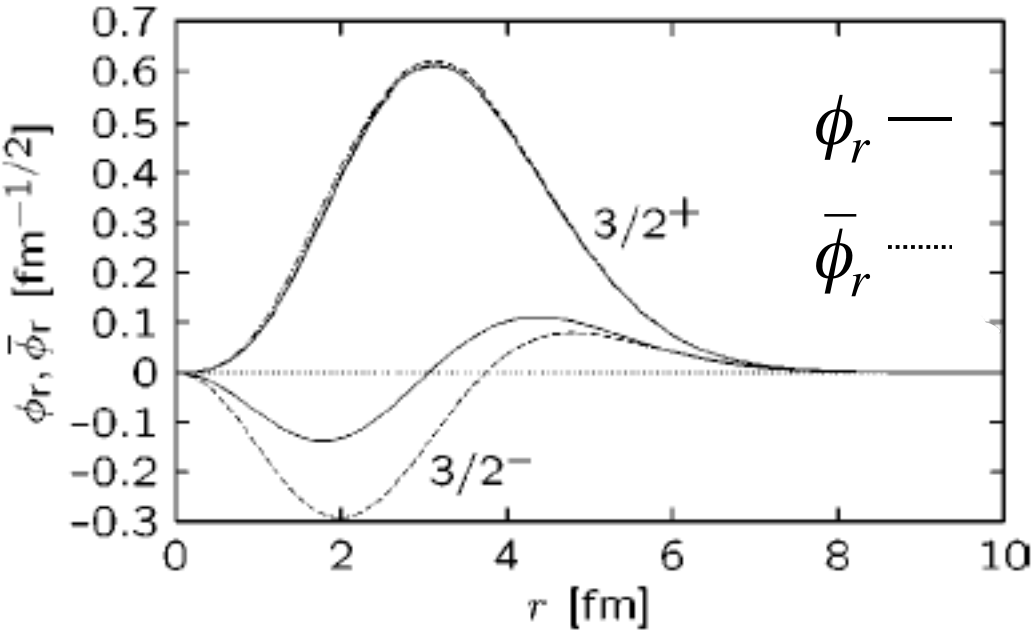
$$S_0 \leq \bar{S}_0 \leq 1$$

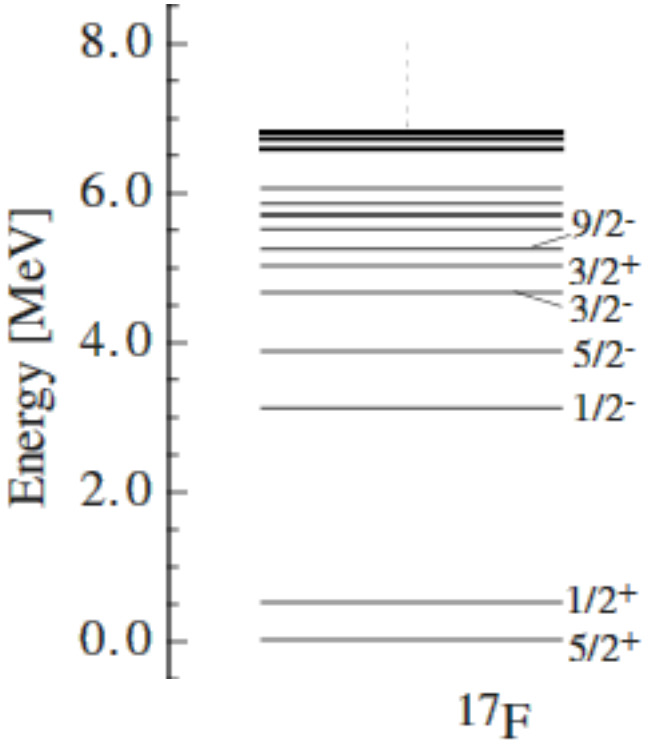
For states with a large spectroscopic factor ($S_0 \approx 1$): Not really!

For states with a small spectroscopic factor ($S_0 < 1$): Yes!



ϕ(r) and $\bar{\phi}$(r) for (^{16}O)^{17}F





Interpretation of the one-body functions

The function $\phi(r)$

We have a good intuitive understanding of the one-body overlap functions. They play an important role in capturing certain aspects of the complex many-body system.

The function $\bar{\phi}(r)$

How should the auxiliary functions be interpreted?

Do they have any useful application?

Fliessbach's auxiliary functions

Definition of the auxiliary functions $\bar{\phi}$(r):

- For the hole case A-1:

$$\bar{\phi}^A_{nm}(\boldsymbol{r}) \equiv \int d\boldsymbol{r}' \rho^A(m,\boldsymbol{r},m,\boldsymbol{r}')^{-1/2}\phi^A_{nm}(\boldsymbol{r}')$$

$$\rho^A(m,\boldsymbol{r},m,\boldsymbol{r}') = \langle \Psi^m_A | a^\dagger(\boldsymbol{r}) a(\boldsymbol{r}') | \Psi^m_A \rangle$$

- For the particle case A+1:

$$\bar{\phi}^{A+1}_{mk}(\boldsymbol{r}) \equiv \int dr' \mathcal{N}^A(m,\boldsymbol{r},m,\boldsymbol{r}')^{-1/2}\phi^{A+1}_{mk}(\boldsymbol{r}')$$

$$\mathcal{N}^A(m,\boldsymbol{r},m,\boldsymbol{r}') = \langle \Psi^m_A | a(\boldsymbol{r}) a^\dagger(\boldsymbol{r}') | \Psi^m_A \rangle$$

The norm:

$$\bar{S}^{A+1}_{mk} \equiv \int d\boldsymbol{r} |\bar{\phi}^{A+1}_{mk}(\boldsymbol{r})|^2$$

Completeness and sum rules

Completeness relation for the auxiliary functions:

$$\delta_{mm'}\delta(\boldsymbol{r}-\boldsymbol{r}') \quad = \quad \sum_{k=0}^{\infty} \bar{\phi}^{A+1}_{mk}(\boldsymbol{r})\bar{\phi}^{(A+1)*}_{m'k}(\boldsymbol{r}')$$

Sum rule for the auxiliary functions:

$$1 \quad = \quad \sum_{k=0}^{\infty} |\langle \bar{\phi}^{A+1}_{mk}|\varphi_\alpha\rangle|^2$$

Note:

- The $\bar{\phi}^{A+1}_{mk}(\boldsymbol{r})$ are complete in the 'particle-only' space, whereas the standard overlaps require the complete 'particle-hole' space.
- Analogous equations can be derived for the $\bar{\phi}^{A}_{nm}(\boldsymbol{r})$. These functions are complete in the 'hole-only' space.

Completeness and sum rules for the one-body overlap functions

The combination of overlap functions $\{\phi^A_{nm}(\boldsymbol{r})\}_{n=0,1,2,\ldots}$ and $\{\phi^{A+1}_{mk}(\boldsymbol{r})\}_{k=0,1,2,\ldots}$ forms a complete set:

$$\delta_{mm'}\delta(\boldsymbol{r}-\boldsymbol{r}') = \sum_{n=0}^{\infty} \phi^{A*}_{nm}(\boldsymbol{r}')\phi^{A}_{nm'}(\boldsymbol{r}) + \sum_{k=0}^{\infty} \phi^{A+1}_{mk}(\boldsymbol{r}')\phi^{(A+1)*}_{m'k}(\boldsymbol{r})$$

where the sums involve both bound and continuum states.

The closure relation yields the sum rule

$$\begin{aligned} 1 &= \sum_{n=0}^{\infty} |\langle \Psi^m_A | a^\dagger_\alpha | \Psi^n_{A-1}\rangle|^2 + \sum_{k=0}^{\infty} |\langle \Psi^m_A | a_\alpha | \Psi^k_{A+1}\rangle|^2 \\ &= \sum_{n=0}^{\infty} |\langle \phi^A_{nm} | \varphi_\alpha\rangle|^2 + \sum_{k=0}^{\infty} |\langle \phi^{A+1}_{mk} | \varphi_\alpha\rangle|^2 \end{aligned}$$

where $\varphi_\alpha(\boldsymbol{r})$ denotes the single-particle orbital with quantum numbers $\alpha = \{n, l, j, t, t_z\}$.

Fliessbach's auxilliary functions -- physical interpretation

Trick: Expand the auxiliary functions in terms of natural orbitals.

The natural orbitals $\{\hat{\varphi}_l(\boldsymbol{r})\}_{l=1,2,...}$ diagonalize the density matrix operator: $\int d\boldsymbol{r}\rho^A(m,\boldsymbol{r},m,\boldsymbol{r}')\hat{\varphi}_l(\boldsymbol{r}') = \lambda_l\hat{\varphi}_l(\boldsymbol{r})$, where λ_l is the occupancy of $\hat{\varphi}_l(\boldsymbol{r})$ in Ψ_A^m. They also diagonalize $\hat{\mathcal{N}}^A(m,\boldsymbol{r},m,\boldsymbol{r}')$, with eigenvalues $(1-\lambda_l)$.

The expansion coefficients are:

$$\langle\hat{\varphi}_l|\bar{\phi}_{mk}^{A+1}\rangle = \frac{1}{\sqrt{1-\lambda_l}}\langle\hat{\varphi}_l|\phi_{mk}^{A+1}\rangle$$

Fliessbach's auxilliary functions -- physical interpretation

One can show:

$$|\langle\hat{\varphi}_l|\phi^{A+1}_{mk}\rangle| = |\langle\Psi^m_A|a_{\hat{\varphi}_l}|\Psi^k_{A+1}\rangle| = \sqrt{1-\lambda_l}|\langle\chi^{ml}_A|a_{\hat{\varphi}_l}|\Psi^k_{A+1}\rangle|$$
$$|\langle\hat{\varphi}_l|\bar{\phi}^{A+1}_{mk}\rangle| = |\langle\chi^{ml}_A|a_{\hat{\varphi}_l}|\Psi^k_{A+1}\rangle|$$

χ^{ml}_A is the component in the wave function Ψ^m_A in which $\hat{\varphi}_l(\boldsymbol{r})$ is empty $[\langle\chi^{ml}_A|\chi^{ml}_A\rangle = 1]$.

$$\left|\Psi^m_A\right\rangle = a_A{}^{ml}\left|\vartheta^{ml}_A\right\rangle + b_A{}^{ml}\left|\chi^{ml}_A\right\rangle$$

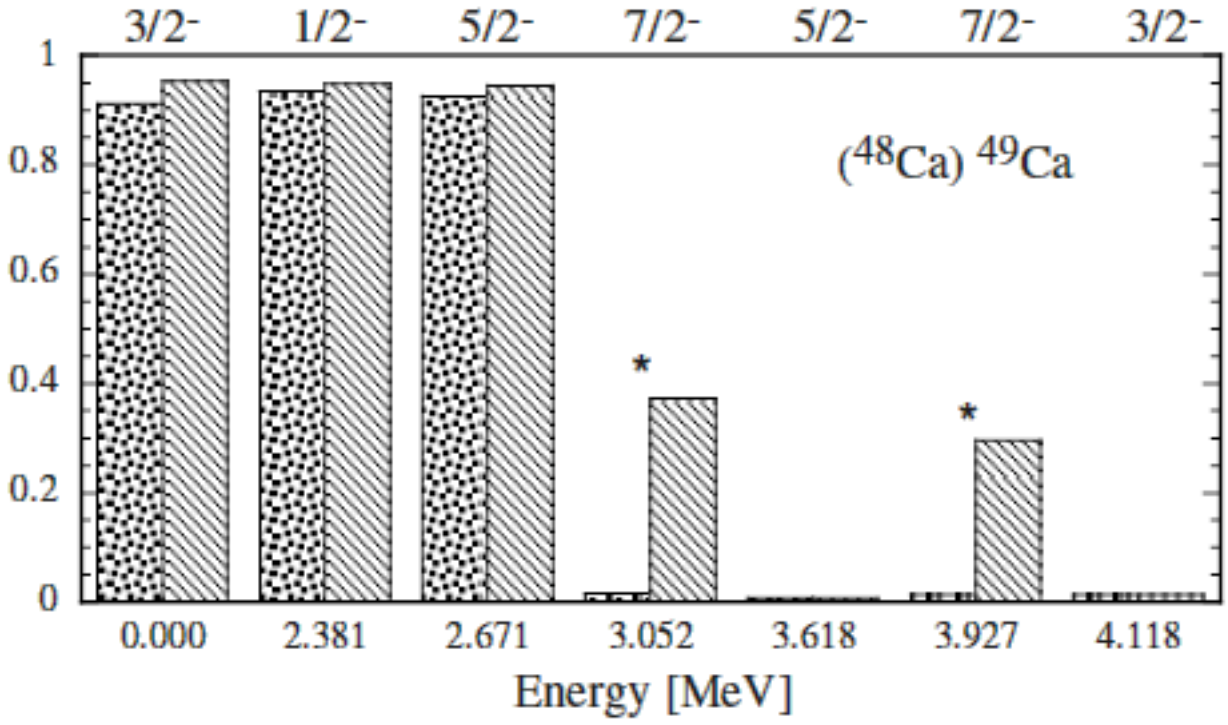
Meaning of the norms:

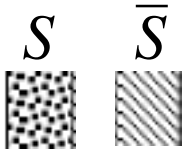
$$S^{A+1}_{mk} = \sum_l |\langle\Psi^m_A|a_{\hat{\varphi}_l}|\Psi^k_{A+1}\rangle|^2$$

$$\bar{S}^{A+1}_{mk} = \sum_l |\langle\chi^{ml}_A|a_{\hat{\varphi}_l}|\Psi^k_{A+1}\rangle|^2$$

S^{A+1}_{mk} gives the overall probability of obtaining Ψ^k_{A+1} by adding a nucleon to Ψ^m_A. $\bar{S}^{A+1}_{mk}$ measures the probability of obtaining Ψ^k_{A+1} when adding a nucleon to a particular component of Ψ^m_A. The relevant component decribes the part of Ψ^m_A which is not Pauli-blocked.

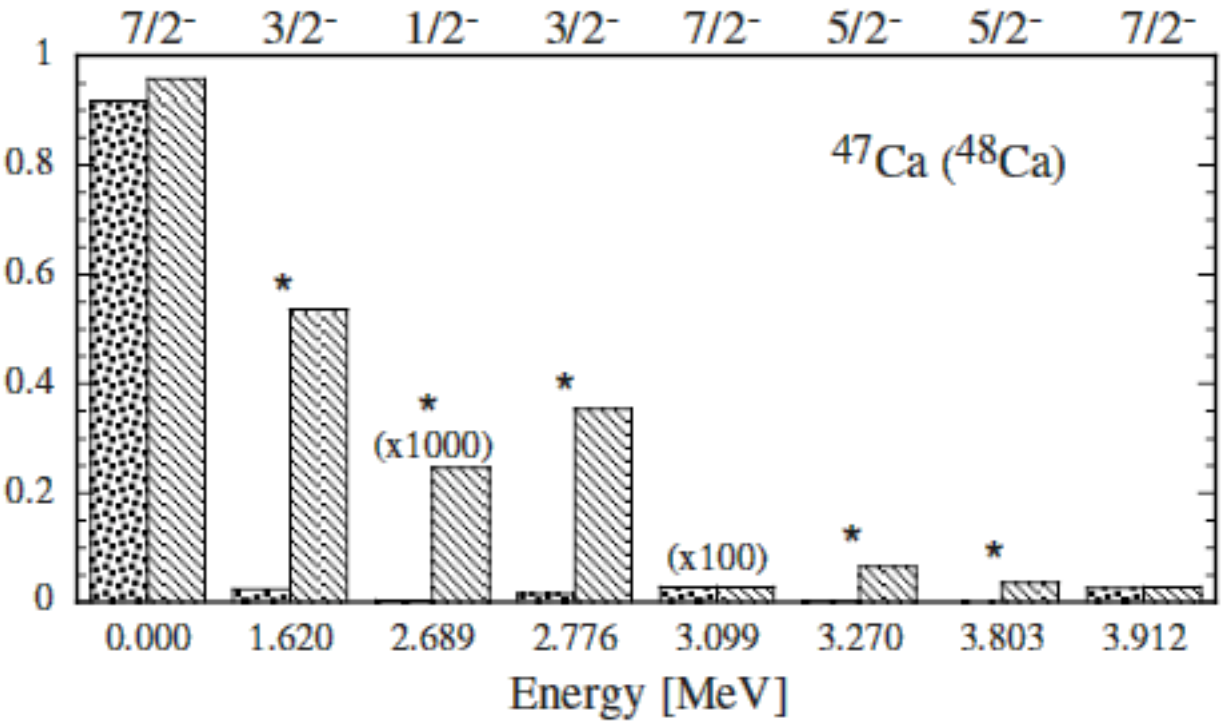
S and $\bar{S}$ for $(^{48}Ca)^{49}Ca$

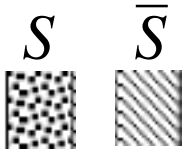




The calculated values of S and $\bar{S}$ can be understood in terms of a sharp Fermi surface.

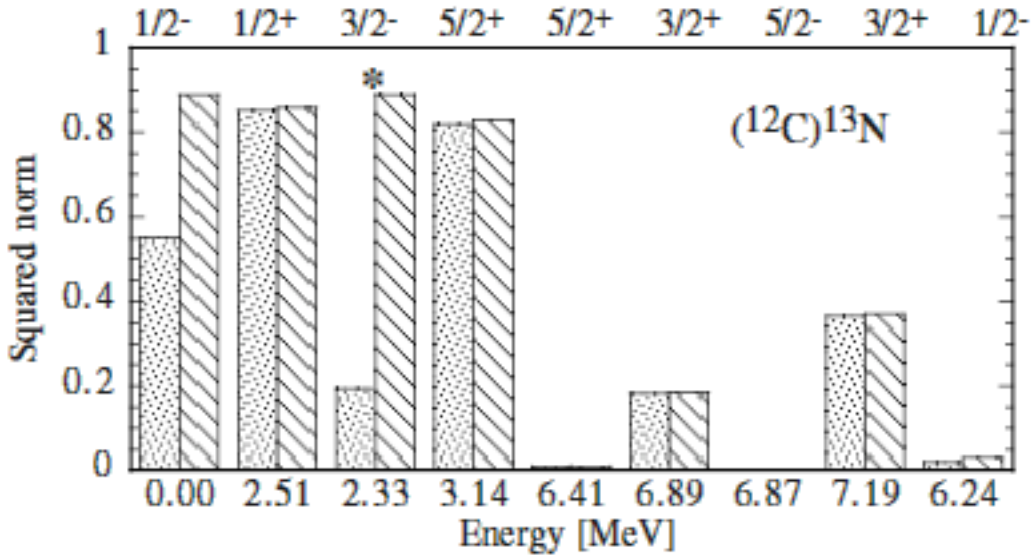
S and $\bar{S}$ for ^{47}Ca(^{48}Ca)

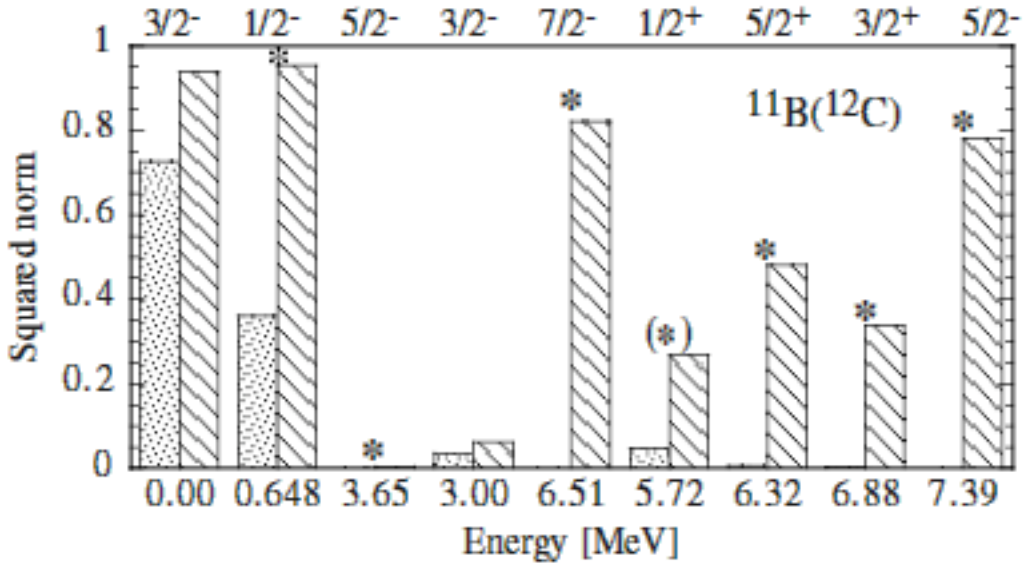


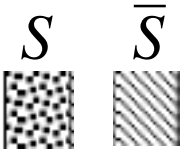


The calculated values of S and $\bar{S}$ can be understood in terms of a sharp Fermi surface.

S and $\bar{S}$ for (^{12}C)







Summary

Spectroscopic factors provide the link between an effective one-body picture and the full nuclear many-body problem.

Our formal study of the proton emission process demonstrates:

- The two-potential (perturbative) approach of Gurvitz and Kalbermann can be used in a many-body picture
- An appropriate choice of the perturbing potential allows for a reduction to an effective one-body problem
- The many-body effects are contained in the normalization of the proton decay width
- It is not clear whether this normalization coincides with the spectroscopic factor

One-body functions can be defined in various ways…

- The different functions carry complementary nuclear structure information
- One has to be careful when using a single-particle approximation

Appendix

Small spectroscopic factors

What can we infer from a small spectroscopic factor?

$$S^{A+1}_{mk} = \sum_\alpha |\langle \Psi^m_A | a_\alpha | \Psi^k_{A+1} \rangle|^2$$

$$S^{A}_{nm} = \sum_\alpha |\langle \Psi^m_A | a^\dagger_\alpha | \Psi^n_{A-1} \rangle|^2$$

$|\langle \Psi^m_A | a_\alpha | \Psi^k_{A+1} \rangle| = |\langle \Psi^k_{A+1} | a^\dagger_\alpha | \Psi^m_A \rangle|$ is small when:

a) the norm of $a^\dagger_\alpha |\Psi^m_A\rangle$, namely $|\langle \Psi^m_A | a_\alpha a^\dagger_\alpha | \Psi^m_A \rangle|^{1/2}$, is small (Pauli blocking); or

b) the states $|\Psi^k_{A+1}\rangle$ and $a^\dagger_\alpha |\Psi^m_A\rangle$ differ significantly, i.e. $\langle \Psi^k_{A+1} | a^\dagger_\alpha | \Psi^m_A \rangle / |\langle \Psi^m_A | a_\alpha a^\dagger_\alpha | \Psi^m_A \rangle|^{1/2}$ is small (structural difference); or

c) both a) and b) apply.

[Similar considerations apply to S^A_{nm}.]