Effective single-particle energies in correlated many-nucleon systems

An ab-initio take on academic, though recurring, questions

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Disclaimer

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- Old question, i.e. everyone has some sort of (a different) view on it
- The main objective of the present study is simply to
  1. Clarify certain key concepts that are often mixed up
  2. Profit by the availability of ab-initio calculations of medium-mass nuclei
  3. Connect to effective SM and EDF approaches
- Knowledge mostly exists; i.e. do not be surprised if parts are known to you

Outline

1. Context and basic ingredients
2. Effective single-particle energies
3. Results from CCSD calculations
4. Extension to particle-number breaking theories
5. Take away messages

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Problem

Context

- **Single-nucleon shells** = pillar of our understanding of nuclear structure
- Evolution of shells drives the physics of exotic nuclei
- However the only thing one can solve is a A-body problem

$$H|\Psi_k^{\mathrm{A}}\rangle = E_k^{\mathrm{A}}|\Psi_k^{\mathrm{A}}\rangle$$

- One-nucleon pick-up and stripping reactions give access to

$$E_k^{\pm} \equiv \pm\left(E_k^{\mathrm{A}\pm 1} - E_0^{\mathrm{A}}\right) \text{ and } \sigma_k^{\pm}$$

The nucleus is a **correlated system**

- ✗ Is $\{E_k^{\pm}\}$ related to a set of **uniquely defined** single-particle energies $\{\epsilon_p\}$?
- ✗ If yes, to which **independent-particle problem h** are the $\{\epsilon_p\}$ associated?
- ✗ If yes, is the single-nucleon shell structure $\{\epsilon_p\}$ of any practical use, i.e.
  - ✗ Is a simplified picture needed and beneficial or potentially misleading?
  - ✗ Is any variant of ϵ_p more or less equivalent?
  - ✗ Is inferring behavior of observable $E_k^{\pm}, 2_1^{+}, \ldots$ from $\{\epsilon_p\}$ safe and easy?

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Basic ingredients (1)

Elements from one-nucleon addition and removal processes

1. Spectroscopic amplitudes (= overlap functions) in basis $\{a_p^\dagger\}$ of $\mathcal{H}_1$

$$\langle \Psi_\mu^{\text{A+1}} | a_p^\dagger | \Psi_0^{\text{A}} \rangle \equiv U_\mu^{p*} \quad , \quad \langle \Psi_\nu^{\text{A-1}} | a_p | \Psi_0^{\text{A}} \rangle \equiv V_\nu^{p*}$$

2. Spectroscopic "probability" matrix in basis $\{a_p^\dagger\}$

$$\begin{aligned} S_\mu^{+pq} &\equiv \langle \Psi_0^{\text{A}} | a_p | \Psi_\mu^{\text{A+1}} \rangle \langle \Psi_\mu^{\text{A+1}} | a_q^\dagger | \Psi_0^{\text{A}} \rangle \\ S_\nu^{-pq} &\equiv \langle \Psi_0^{\text{A}} | a_q^\dagger | \Psi_\nu^{\text{A-1}} \rangle \langle \Psi_\nu^{\text{A-1}} | a_p | \Psi_0^{\text{A}} \rangle \end{aligned}$$

3. Spectroscopic factors (basis independent)

$$SF_\mu^+ \equiv \sum_{p \in \mathcal{H}_1} S_\mu^{+pp} \quad , \quad SF_\nu^- \equiv \sum_{p \in \mathcal{H}_1} S_\nu^{-pp}$$

provide the norm of one-nucleon overlap functions

Basic ingredients (2)

One-nucleon transfer spectral-function $\mathbb{S}(\omega) = \mathbb{S}^{+}(\omega) + \mathbb{S}^{-}(\omega)$

- Defines an energy-*dependent* matrix on $\mathcal{H}_1$

$$\mathbb{S}_{pq}(\omega) \quad \equiv \quad \sum_{\mu \in \mathcal{H}_{A+1}} S_{\mu}^{+pq}\, \delta(\omega - E_{\mu}^{+}) + \sum_{\nu \in \mathcal{H}_{A-1}} S_{\nu}^{-pq}\, \delta(\omega - E_{\nu}^{-})$$

containing the same information as the dressed one-body Green's function

$$i\mathbb{G}_{pq}(t - t') \equiv \langle \Psi_0^{\mathrm{A}} | T\{a_p(t)\, a_q^{\dagger}(t')\} | \Psi_0^{\mathrm{A}} \rangle$$

- Moments of the spectral-function

$$\mathbb{M}^{(n)} \equiv \int_{-\infty}^{+\infty} \omega^n\, \mathbb{S}(\omega)\, d\omega$$

  - Defines an energy-*independent* matrix on $\mathcal{H}_1$
  - Diagonal element $S_{pp}(\omega)$ has the meaning of a PDF as $\mathbb{M}^{(0)} = \mathbb{1}_1$

Basic ingredients (3)

Spectral-strength distribution $\mathcal{S}(\omega) = \mathcal{S}^{+}(\omega) + \mathcal{S}^{-}(\omega)$

$$\mathcal{S}(\omega) \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbb{S}(\omega)\right] = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+}\, \delta(\omega - E_{\mu}^{+}) + \sum_{\nu \in \mathcal{H}_{A-1}} SF_{\nu}^{-}\, \delta(\omega - E_{\nu}^{-})$$

- Defines a (basis-independent) function of energy
- May define $\mathcal{S}^{J^{\pi}}(\omega)$ by only tracing over (l, j) symmetry sub-block

Uncorrelated system

- $SF_{\mu}^{\pm} = 0$ or 1
- $\mathrm{Card}\{SF_{\mu}^{\pm} \neq 0\} = \dim_{\mathcal{H}_1}$

Correlated system

- $0 < SF_{\mu}^{\pm} < 1$
- $\mathrm{Card}\{SF_{\mu}^{\pm} \neq 0\} > \dim_{\mathcal{H}_1}$

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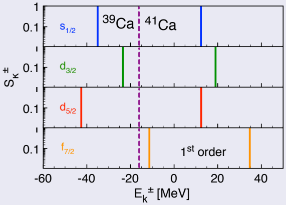

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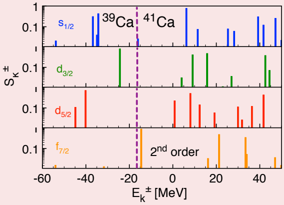

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Conclusions and questions

1. Direct addition and removal populate more states than $\dim_{\mathcal{H}_1}$
2. $E^{\pm}_{\mu}$ spectrum does not possess features of single-particle spectrum
3. Can one meaningfully extract an effective single-particle energy spectrum?

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Effective single-particle energies

Centroid energies

1. Compute centroid matrix [M. Baranger, NPA149, 225 (1970)]

$$h_{pq}^{\text{cent}} \equiv \sum_{\mu \in \mathcal{H}_{A+1}} S_{\mu}^{+pq} E_{\mu}^{+} + \sum_{\nu \in \mathcal{H}_{A-1}} S_{\nu}^{-pq} E_{\mu}^{-} = \mathbb{M}_{pq}^{(1)}$$

which requires information from both stripping *and* pick-up

2. Effective Single Particle Energies $\equiv$ eigenvalues of h^{cent}

$$h^{\text{cent}} \psi_{p}^{\text{cent}} = e_{p}^{\text{cent}} \psi_{p}^{\text{cent}}$$

- e_{p}^{cent} is the mean of the PDF $\mathbb{S}_{pp}(\omega)$
- Reduce to eigenvalues of h for uncorrelated A-body problem

3. Basis-independent definition valid for any correlated system
   - Different from computing h_{pp}^{cent} in an arbitrarily chosen, e.g. HO, basis
   - Different from guessing an unperturbed reference a priori

4. Two sets of connected but different wave functions and energies
   - Overlap functions $\{U_{\mu}(\vec{r}\sigma\tau), V_{\nu}(\vec{r}\sigma\tau)\}$ decaying with $\{E_{\mu}^{+}, E_{\nu}^{-}\}$
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Effective single-particle energies

Sum rule and correlations

1. Identity for n$^{\text{th}}$ moment of $\mathbb{S}(\omega)$

$$\mathbb{M}_{pq}^{(n)} = \langle \Psi_0^{\mathrm{A}} | \{ \overbrace{[\ldots[[a_p, H], H], \ldots]}^{n\,\text{commutators}}, a_q^\dagger \} | \Psi_0^{\mathrm{A}} \rangle$$

provides for $n = 1$ [M. Baranger, NPA149, 225 (1970)]

$$h_{pq}^{\text{cent}} = T_{pq} + \sum_{rs} \bar{V}_{prqs}^{2\mathrm{N}} \rho_{sr}^{[1]} + \frac{1}{4} \sum_{rstv} \bar{V}_{prtqsv}^{3\mathrm{N}} \rho_{svrt}^{[2]} = h_{pq}^{\infty}$$

- $\rho^{[k]}$ is the k-body density matrix of $|\Psi_0^{\mathrm{A}}\rangle$
- Accessing ESPEs only require to compute $|\Psi_0^{\mathrm{A}}\rangle$
- $e_p^{\text{cent}} - \epsilon_p^{\text{HF}} \neq 0$ due to correlations in $\rho^{[k]}$
- $h^{\infty} \equiv$ energy-independent part of one-body $\Sigma(\omega)$ in Dyson-SCGF

2. Centroids do screen out most of the correlations
   - h^{cent} involves monopole part of the interaction $V^{\text{mon}} \equiv \sum_J (2J+1)\, V^J$
   - Higher multipoles responsible for genuine correlation effects

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Conclusions

- ✓ ESPE extract meaningful s.p. shell structure from correlated nuclei
- ✓ $e_p^{\text{cent}} =$ centroid of E_μ^+/E_ν^- weighted by $|\langle\Psi_\mu^{A+1}|b_p^\dagger|\Psi_0^A\rangle|^2/|\langle\Psi_\nu^{A-1}|b_p|\Psi_0^A\rangle|^2$
- ✓ Require both stripping and pick-up reactions experiment
- ✓ Is it useful? It depends
  - ✓ Yes $=$ analyze shell-structure evolution via e_p^{cent} (NOT via E_μ^+/E_ν^-)
  - ✓ No $=$ may not reflect actual physics, i.e. E_μ^+/E_ν^-, 2_1^+, drip-line position

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Calculation setting

EOM-CCSD method in (Gamow) HF basis

1. V^{2N} = Chiral N^3LO (Λ_χ =500 MeV) + RG ($V_{\text{low k}}$) down to Λ_{RG} =2.4 fm^{-1}
2. Harmonic oscillator model space
   - O: $n_{\text{max}} = 12$; $\hbar\omega$ =16 MeV + 30 WS orbitals for "valence" neutron PW
   - Ca: $n_{\text{max}} = 12$; $\hbar\omega$ =16 MeV

Probing the effect of correlations

1. Normal-ordered form of H with respect to $|\Phi_0^{\text{HF}}\rangle$ in HF single-particle basis

$$H = E_0^{\text{HF}} + \sum_p \epsilon_p^{\text{HF}} : b_p^\dagger b_p : + \frac{1}{4} \sum_{pqrs} \bar{V}_{pqrs}^{2N} : b_p^\dagger b_q^\dagger b_s b_r : \quad \equiv \quad h^{\text{HF}} + V_{\text{res}}$$

$$\epsilon_p^{\text{HF}} = T_{pp} + \sum_{q=1}^{A} \bar{V}_{pqpq}^{2N}$$

2. Define $V_{\text{res}}(\lambda) \equiv \lambda\, V_{\text{res}}$ such that $H(0) = h^{\text{HF}}$ and $H(1) = H$
3. Solve EOM-CCSD to extract $e_p^{\text{cent}}(\lambda)$ and $(E_\mu^+(\lambda), E_\nu^-(\lambda))$ for $\lambda \in [0,1]$

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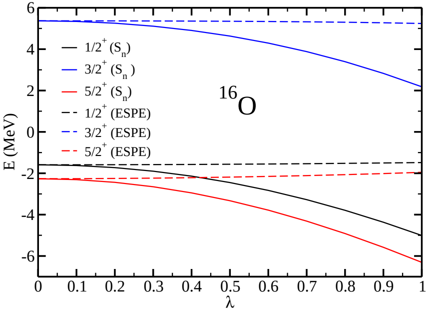
From an uncorrelated to a correlated system



Correlations in doubly-magic ^{16}O

1. Neutron $E^+_\mu(\lambda)$ in ^{17}O
2. Neutron centroid energies $e^{\text{cent}}_p(\lambda)$

Switching on correlations in doubly-magic ^{16}O

1. Uncorrelated limit: $e^{\text{cent}}_p(0) = E^+_\mu(0) = \epsilon^{\text{HF}}_p$ (Koopman's theorem)
2. Strongly correlated system as $E^+_\mu(1) - e^{\text{cent}}_p(1) \approx -3\,\text{MeV}$
3. Centroid energies almost untouched by correlations as $\partial_\lambda\, e^{\text{cent}}_p(\lambda) \approx 0$
4. Both would be significantly more affected in open-shell nucleus

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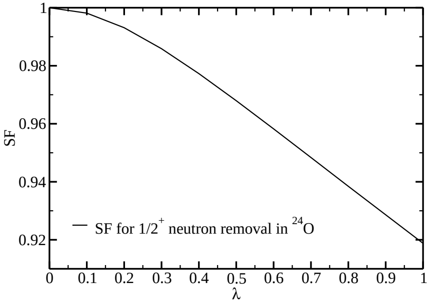

$J^\pi = 1/2^+$ neutron removal in ^{24}O

1. $SF^-_{1/2+}(\lambda)$
2. $E^-_{1/2+}(\lambda)$ versus $e^{\text{cent}}_{2\,1/2+}(\lambda)$
3. Overlap function $|V_{1/2+}(\vec{r};\lambda)|^2$
4. Centroid function $|\psi^{\text{cent}}_{2\,1/2+}(\vec{r};\lambda)|^2$

Switching on correlations in doubly-magic ^{24}O

1. Based on $SF^-_{1/2+}(1)$ looks like a good single-particle state
2. Correlation energy is however significant $E^-_{1/2+}(1) - e^{\text{cent}}_{2\,1/2+}(1) \approx -1.7\,\text{MeV}$
3. Asymptotic/norm of $|V_{1/2+}(\vec{r};\lambda)|^2$ changes while $\partial_\lambda|\psi^{\text{cent}}_{2\,1/2+}(\vec{r};\lambda)|^2 \approx 0$
4. $|\psi^{\text{cent}}_{2\,1/2+}(\vec{r};0.9)|^2$ decays according to $e^{\text{cent}}_{2\,1/2+}(0.9) = -7.65\,\text{MeV}$

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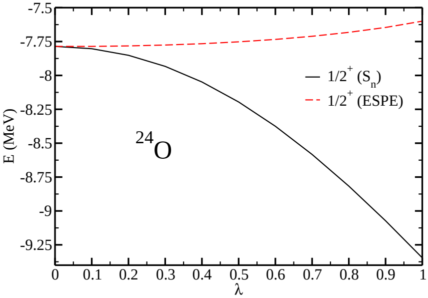

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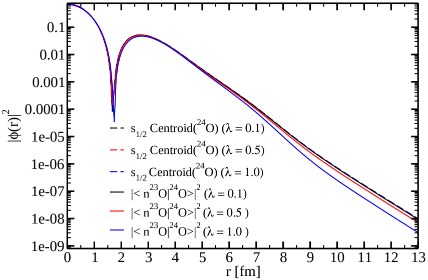

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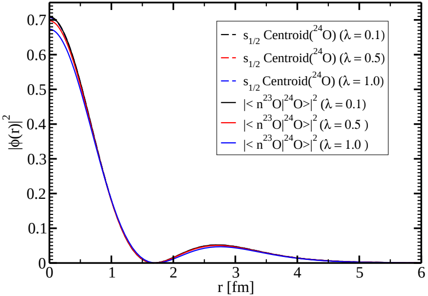
2. Correlation energy is however significant $E^-_{1/2+}(1) - e^{\text{cent}}_{2\,1/2+}(1) \approx -1.7\,\text{MeV}$
3. Asymptotic/norm of $|V_{1/2+}(\vec{r};\lambda)|^2$ changes while $\partial_\lambda|\psi^{\text{cent}}_{2\,1/2+}(\vec{r};\lambda)|^2 \approx 0$
4. $|\psi^{\text{cent}}_{2\,1/2+}(\vec{r};0.9)|^2$ decays according to $e^{\text{cent}}_{2\,1/2+}(0.9) = -7.65\,\text{MeV}$

From an uncorrelated to a correlated system



$J^\pi = 1/2^+$ neutron removal in ^{24}O

1. $SF^{-}_{1/2+}(\lambda)$
2. $E^{-}_{1/2+}(\lambda)$ versus $e^{\text{cent}}_{2\,1/2+}(\lambda)$
3. Overlap function $|V_{1/2+}(\vec{r};\lambda)|^2$
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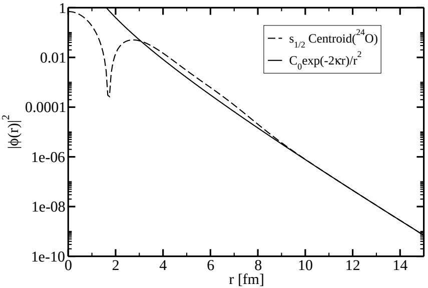

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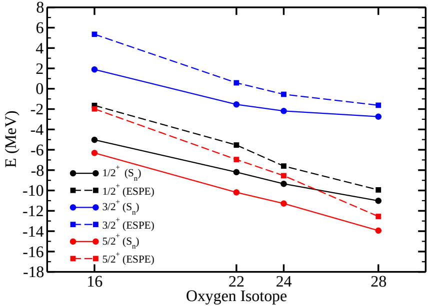
Single-nucleon shell structure in O isotopes



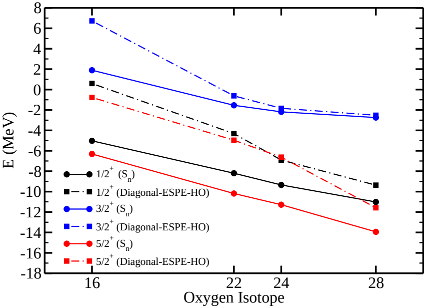
Doubly-closed shell O isotopes

1. Neutron E_μ^+, E_ν^-
2. Neutron centroid energies e_p^{cent}

Evolution of neutron states

1. (E_μ^+, E_ν^-) differ significantly from e_p^{cent} in "good-closed-shell" nuclei
   - Care to be taken when inferring physics from e_p^{cent} only
   - Difference is not the same in various "good-closed-shell" nuclei
2. SM postulates core to be a perfect closed-shell nucleus, i.e. $e_p^{\text{core}} \equiv E_\mu^+ \delta_{pk}$
   - Wrong but ok in view of large SF_μ^+ = good effective low-energy d.o.f.

Approximate computation of ESPE



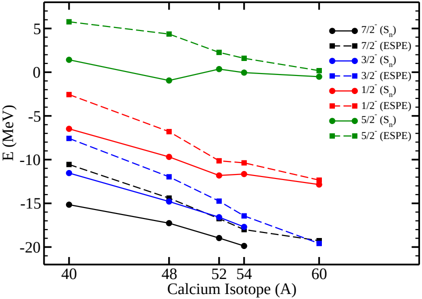
Doubly-closed shell O isotopes

1. Neutron E_μ^+, E_ν^-
2. Neutron "SM-like" centroids
   - Diagonal h_{pp}^{cent} in HO basis
   - Naive uncorrelated filling

Difference with "SM-like" definition of ESPE

1. Significant impact but general trend unclear
   - Continuum states and states away from ϵ_F are the most affected
   - Must decouple effect from (i) self-consistency (ii) correlated ρ[1]
2. Full e_p^{cent} follow better (E_μ^+, E_ν^-) overall
3. More systematic investigations necessary

Single-nucleon shell structure in Ca isotopes



Doubly-closed shell Ca isotopes

1. Neutron E_μ^+, E_ν^-
2. Neutron centroid energies e_p^{cent}

Evolution of neutron states

1. (E_μ^+, E_ν^-) differ significantly from e_p^{cent} in "good-closed-shell" nuclei
   - Difference diminishes strongly going from ^{40}Ca to ^{60}Ca
   - Reflects specificity of $N \approx Z$ or smooth trend with $N - Z$?
2. Perform systematic study of correlation between $(\Delta e_p^{\text{cent}})_{\text{F}}$ and 2_1^+
3. Extend analysis to mid-shell nuclei

Outline

1. Context and basic ingredients
2. Effective single-particle energies
3. Results from CCSD calculations
4. Extension to particle-number breaking theories
5. Take away messages

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Take away messages

The nucleus is a **correlated system**

1. Is $\{E_k^{\pm}\}$ related to a set of uniquely defined single-particle energies $\{\epsilon_p\}$?
   - $\rightsquigarrow$ **Yes, the so-called centroid energies $\{\mathbf{e_p^{cent}}\}$**
2. To which independent-particle problem **h** are the ϵ_p associated?
   - $\rightsquigarrow$ **$\{\mathbf{e_p^{cent}}\}$ are eigenvalues of $\mathbf{h^{cent} = h^{\infty}}$**
   - $\rightsquigarrow$ **Associated $|\Phi^{\mathbf{cent}}\rangle$ can be further characterized (not done here)**
3. Is approximating $\{e_p^{\text{cent}}\}$ safe?
   - $\rightsquigarrow$ **No as self-consistency and continuum effects may be significant**
4. Is an effective s.p. picture needed and beneficial or potentially misleading?
   - $\rightsquigarrow$ **A simplified picture is helpful but has to be used with care**
   - $\rightsquigarrow$ **Provides a $\Lambda_{\mathbf{RG}}$-dependent analysis tool given $\mathbf{H}(\Lambda_{\mathbf{RG}})$**
5. Is inferring behavior of $\{E_k^{\text{A}}\}$ and $\{E_k^{\pm}\}$ from $\{e_p^{\text{cent}}\}$ safe and easy?
   - $\rightsquigarrow$ **No as they may be remote even in "good-closed-shell" nuclei**

Thank you !