Open-shell nuclei from first principles \mathbf{f} <u>l from fi</u> + \mathbf{r} t princi $x = 3$ \mathbf{S}

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✺ Introduction

✺ Gorkov-Green's functions approach

✺ Results: benchmarks, calcium chain, 74Ni

✺ Outlook

Introduction

Towards a unified description of nuclei

Towards a unified description of nuclei

Main challenges:

- ✔ Good nuclear Hamiltonians
- \vee Proper treatment of continuum
- ✘ Connection to reactions
- ✘ Extension to open-shell systems

Medium-mass ab-initio nuclear structure

- ✺ Configuration interaction techniques become unfeasible in large spaces
	- **■→ Solution of the nuclear many-body problem has to be approximated**
- ✺ Ab-initio approaches to medium-mass nuclei
	- **→ No core, all nucleons active**
	- ^{■→} Only inputs are NN & NNN interactions
	- **Rely on a controlled expansion**
- ✺ Examples:
	- Self-consistent Dyson-Green's function [Barbieri, Dickhoff, ...]
	- Coupled-cluster [Dean, Hagen, Hjorth-Jensen, Papenbrock, ...]
	- In-medium similarity renormalization group [Bogner, Hergert, Schwenk, Tsukiyama,...]
	- \rightarrow But limited to to doubly-closed-shell \pm 1 and \pm 2 nuclei

✺ Beams of exotic isotopes becoming available worldwide

➟ Predictive theoretical models needed

✺ Nuclear interactions from chiral EFT

- ➟ Consistent many-body forces
- **A way to quantify theoretical errors**

✺ Renormalization group techniques for NN and 3N forces

➟ Many-body problem more perturbative

✺ Benchmarks for more phenomenological methods **■ Non-empirical EDF, (microscopic) shell model, ...**

Gorkov-Green's function approach

which follows from Eqs. (15).

^k [|]aa[|] ^A

One introduces a set of four Green's functions, known

 \mathbf{r} he simplicity of a single-reference $\frac{d\mathbf{r}}{dt}$ $\frac{1}{2}$ follows from Eqs. (15) and $\frac{1}{2}$ and $\frac{1}{2}$ ✺ Keep the simplicity of a single-reference

^Gab(!) = ^X

the system, one considers a system, one considers a form ress explicitly the non-perturbative formation of Cooj $*$ Address s $\rho x n!$ *** Audiess expl** C. Gorkov propagators ✺ Address explicitly the non-perturbative formation of Cooper pairs

⁰ *[|]aa[|] ^A*+1

fashion for the appearance and destruction for the appearance and destruction of condensed of condensed of con
The appearance and destruction of condensed of condensed of condensed of condensed of condensed of condensed o

- Γ consider the proposition selection systems, Γ $\sum_{i=1}^n$ \longrightarrow Formul **••** Formulate the expansion scheme around a Bogoliubov vacuum $\frac{1}{1}$ μ nd a Bogoliubov vacuum ⇡
	- ticle-number conservation (eventually restored) \mathbf{H}^{N} Inticle-pumber conservation (eventually restored) \mathbf{F} , one must generally denote the single-particle propaga-particle propaga-➟ Breaking of particle-number conservation (eventually restored)

^k ih *^A*+1

* Auxiliary many-body state take into account the formation and destruction of pairs. \sqrt{S} is take intervals functions, \sqrt{S} four \sqrt{S} *k*

⁰ !, (15)

 \mathbf{M}_{ivee} ven • Mixes various particle numbers $|\Psi_0\rangle = \sum c_A |\psi_0\rangle$ $m \rightarrow$ Mixes to parity quantum number. Together with such a state, one $\overline{27}$ $\begin{array}{cccc} \text{if } A & A \\ & \text{if } A \end{array}$ \rightarrow Mixes various particle numbers $|\Psi_0\rangle \equiv$ even \sum $c_A \, |\psi_0^A\>$ $\begin{pmatrix} A \\ 0 \end{pmatrix}$ even
 \bullet 1.41

^h *^A*

- ➟ Introduce a "grand-canonical" potential number operator, in place of H [26]. The state |Ψ0! is ^{"→} Introduce a "gran $\begin{pmatrix} A \\ C \end{pmatrix}$ \mathcal{A} *A* $\Omega = H - \mu A$ *A* = h ⁰*|A|* ⁰i (20)
- $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$ under the constra $\mathcal{L} \left(\left| \mathcal{L} \right| \mathcal{L} \right) \mathcal{L} \left| \mathcal{L} \right|$) ≡ \$Ψ0|T $\Rightarrow |\Psi_0\rangle$ minimizes $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$ under the constraint $A = \langle \Psi_0 | A | \Psi_0 \rangle$ Ψ_0 minimizes $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$ under the constraint $A = \langle \Psi_0 | A | \Psi_0 \rangle$

to define diagonal in $\mathcal{O}(1)$ by introducing additional objects that $\mathcal{O}(1)$

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 $\frac{X}{X}$

^h *^A*

⁰ *|a†*

*a[|] ^A*¹

^k ih *^A*¹

^k |a†

•• Observables of the N system $\Omega_0 = \sum |c_{A'}|^2 \Omega_0^{A'}$ $\frac{c}{A'}$ in the asymptotic behaviour of $\frac{A'}{A'}$ the former is driven by the latter, e.g. for *e*cent $\Omega_0 = \sum |c_{A^\prime}|^2 \,\Omega_0^{A^\prime} \approx E_0^A - \mu A$ $\overline{0}$ $A[′]$ $|c_{A'}|^2 \Omega_0^{A'} \approx E_0^A - \mu A$

Gorkov equations techniques and many-body perturbation theory, which $\sum_{i=1}^{n}$ \mathbf{V} equations GOTKOV equations. $\mathcal C$ \mathcal{L} $\mathcal{L}(\mathcal{L})$

After this distinction one can work out that the com-

(21), together with the normalization condition condition condition condition condition condition condition co

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✺ Set of 4 Green's functions $H = \frac{1}{2}$ to define the distribution of \mathcal{A} introducing additional objects that \mathcal{A} $\mathcal K$ bet of 4 Green's functions. $\frac{1}{2}$ Set of 4 Green's functions $\mathscr W$ det di τ diterminal objectives ‱ Set of 4 Green's functions $w = 0$ being the chemical potential potential potential and N

where c^N denote complex coefficients. The sum over even

particle number is said to respect the (even) number-

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| World - particle particle propaga-particle propaga-particle propaga-particle propaga-particle propaga-particle

In order to access all one-body information contained a strategies all one-body information contained a strategies

$$
i G_{ab}^{11}(t, t') \equiv \langle \Psi_0 | T \left\{ a_a(t) a_b^{\dagger}(t') \right\} | \Psi_0 \rangle = \begin{pmatrix} a \\ b \end{pmatrix} \qquad i G_{ab}^{21}(t, t') \equiv \langle \Psi_0 | T \left\{ \bar{a}_a^{\dagger}(t) a_b^{\dagger}(t') \right\} | \Psi_0 \rangle = \begin{pmatrix} \bar{a} \\ \bar{a}_b^{\dagger}(t, t') \end{pmatrix} \begin{pmatrix} \bar{a}_b(t) a_b(t') \end{pmatrix} | \Psi_0 \rangle = \begin{pmatrix} \bar{a} \\ \bar{b} \end{pmatrix}
$$

$$
i G_{ab}^{12}(t, t') \equiv \langle \Psi_0 | T \left\{ a_a(t) \bar{a}_b(t') \right\} | \Psi_0 \rangle = \begin{pmatrix} \bar{a} \\ \bar{b} \end{pmatrix}
$$

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[Gorkov 1958] $\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$ [Gorkov 1958] \Box \mathbf{t} difference that \mathbf{t} C_{cubic} 1050] $\left[$ GOTKOV 1958]

$$
G_{ab}(\omega) = G_{ab}^{(0)}(\omega) + \sum_{cd} G_{ac}^{(0)}(\omega) \Sigma_{cd}^{\star}(\omega) G_{db}(\omega)
$$

^a(t)¯ab(t

Finally, Dyson's equation is generalized as set of coupled

equations in the two types of propagators in the two types of propagators and self-two types of propagators and

energies. These are known as Gores are known as Gores are known as Gores and \downarrow

^a(t)¯ab(t

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where single-particle operators associated with the dual design of the dual design of the dual design of the du

basis are as defined in Eq. (1) and where the modified in Eq. (1) and where the modified in Eq. (1) and where the modified in \mathcal{L}

Gorkov equations **Gorkov** equations lem of solving the many-body system with \mathbf{A} nucleons is \mathbf{A} nucleons is \mathbf{A} tions represent an expansion of interactions representation of interactions of interactions of interactions or
The contractions of interactions of interactions of interactions of interactions of interactions of interactio

One-nucleon spectral function S_{the flu} *h*cent cent *p*

Saclay data for ¹⁶O(e,e'p) [Mougey et al. 1980] which, as already pointed out before, is *not* the case of

✺ Spectral function correlated one-nucleon separation energies with non-zero spectroscopic strength.

$$
S_p^-(\omega) \equiv \sum_k |\langle \psi_k^{A-1} | a_p | \psi_0^A \rangle|^2 \delta(\omega - (E_0^A - E_k^{A-1}))
$$

 \rightarrow distribution of momenta and energies consistent in the sense that the sense that the asymptotic behaviour of the asympt spectroscopic strength.
Spectroscopic strength of the strength of the strength of the strength of the strength.

✺ Spectral function

spectroscopic strength.
Spectroscopic strength of the strength of the strength of the strength of the strength.

✺ Spectral function

particle energy levels that (i) are in one-to-one correspon-

$$
S_a^-(\omega) \equiv \sum_k |\langle \psi_k^{A-1} | a_a | \psi_0^A \rangle|^2 \delta(\omega - (E_0^A - E_k^{A-1})) = \frac{1}{\pi} \text{Im} \, G_{aa}(\omega)
$$

spectroscopic strength.

✺ Green's function \mathscr{C} roon's $\frac{1}{2}$ and $\frac{1}{2}$ correlated many-nucleon systems. $\mathbf{F}_{\mathbf{q}}$ constant in the sense that the sense that the sense that the asymptotic behaviour of the asymptotic behaviour o

$$
G_{ab}(\omega)=\sum_k\frac{\langle\psi_0^A|a_a|\psi_k^{A+1}\rangle\langle\psi_k^{A+1}|a_a^\dagger|\psi_0^A\rangle}{\omega-(E_k^{A+1}-E_0^A)+i\eta}+\sum_k\frac{\langle\psi_0^A|a_a^\dagger|\psi_k^{A-1}\rangle\langle\psi_k^{A-1}|a_a|\psi_0^A\rangle}{\omega-(E_0^A-E_k^{A-1})-i\eta}
$$

- ➟ Contains all structure information probed by nucleon transfer *r*ucture inform ror*i* $\dot{1}$ O *e*⇠*^p ^r* ⇠*^p r* ^d by nucleon
- **™** Gives access to:
	- \blacktriangleright all one-body observables of the A system \sim ϵ then \overline{a} e A system
	- If the total energy of the A system via Koltun's sumrule

$$
\langle \hat{H} \rangle = E_0 = \sum_{ab} \int \frac{d\omega}{2\pi} \left[t_{ab} + \omega \, \delta_{ab} \right] G_{ab}(\omega)
$$

Spectrum and spectroscopic factors nd spectroscopic factor) + iθ(t =
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| + ! #Ψ0|a† b|<u>|</u>
|<u>|Ψk" = international population</u>
|) . \overline{C} which is given by decay constant in \overline{C} Spectrum and spectroscopic factor A similar result can, of course, be obtained for *V*⌫(*r*⌧) $\frac{1}{2}$ ⌫ *,* (15) Croachurus, and an ochuseasais fosters. spectrum and sp

One can proceed similarly for the other three Gorkov-

✺ Separation energy spectrum $G = \mathbf{f}^*$ ϵ beparation energy s k ⌫ relates to *E* F eparation energy spectrum *ration* energy \overline{a} and \overline{b} and \overline{c} and \overline{c} and \overline{c} *H*_{OJ} \overline{p} ⌫2*HA*¹

$$
G_{ab}^{11}(\omega) = \sum_{k} \left\{ \frac{\mathcal{U}_a^k \mathcal{U}_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\bar{\mathcal{V}}_a^{k*} \bar{\mathcal{V}}_b^k}{\omega + \omega_k - i\eta} \right\}
$$

Lehmann representation ^a ^Vk[∗] V¯k∗ ^a ^U¯^k <u>u</u> *I* Lehmann representation respondence with states of a single-particle basis of *H*¹ ing) a nucleon to I a nucleon to I

 \overline{a}

where
$$
\begin{cases} \mathcal{U}_a^{k*} \equiv \langle \Psi_k | a_a^{\dagger} | \Psi_0 \rangle \\ \mathcal{V}_a^{k*} \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}
$$

and

and
$$
\begin{cases} E_k^{+(A)} \equiv E_k^{A+1} - E_0^A \equiv \mu + \omega_k \\ E_k^{-(A)} \equiv E_0^A - E_k^{A-1} \equiv \mu - \omega_k \end{cases}
$$

✺ Spectroscopic factors from which follows that $\mathcal{L}_{\mathcal{A}}$ follows that $\mathcal{L}_{\mathcal{A}}$ ^DIC TACLOTS over the one-body Hilbert space *H*¹ gives access to spectroscopic *factors* the formulation of ϵ for ϵ . For ϵ \mathbf{r} and \mathbf{r} the wave function behaves as \mathbf{r} \mathbf{E} \ast Spectroscopic factors

$$
SF_k^+ \equiv \sum_{a \in \mathcal{H}_1} |\langle \psi_k | a_a^\dagger | \psi_0 \rangle|^2 = \sum_{a \in \mathcal{H}_1} |U_a^k|^2
$$

$$
SF_k^- \equiv \sum_{a \in \mathcal{H}_1} |\langle \psi_k | a_a | \psi_0 \rangle|^2 = \sum_{a \in \mathcal{H}_1} |V_a^k|^2
$$

[figure from Sadoudi]

Self-energy truncation nerow tru C↑ **C** \mathbf{V} $\frac{1}{2}$ runc −
− internet ! dω" ^Uk[∗] ^c ^V^k $\overline{10}$ norav truncati ! dω" ^Vk[∗] ^c ^U^k \bullet ^Vk[∗] ^d ^V^k c elf-energ for the unperturbed propagator, lead to ^I(E) = ! ⁺[∞] −∞ **T7** # F¹ truncatio et10n <u>Fib2</u> + in the fact of the fact of $\overline{}$

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expression now evaluated at ω = ωk, which can be rewritten as

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This subsection addresses the calculation of the first-

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nder •• energy-independent se $\frac{1}{\sqrt{d}}$ [\] \ 1st order [{] normal energy-independent self-energ $\sqrt{2}$ diard chargy $\frac{1}{2}$ [•] 1st order ^{™→} energy-independent self-energy $\overline{2}$ " 1ϵ ^V¯cd¯ ab¯ ^Uk[∗] ^c ^V^k d $\frac{1}{2}$ 1st order \blacksquare energy independent solf energy $\overline{1}$ V¯ ∩r ⊪⇒ c $\mathbf{r} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ \mathbf{p} $\frac{1}{2}$ + $\frac{1}{2}$ $\hat{=}$ \cap P^1 g_V $*$ 1st order \rightarrow energy independent solf energy $\mathcal F$ is order $\mathcal F$ energy-independent self-energy \mathcal{O}_s in the same and \mathcal{O}_s

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This subsection addresses the calculation addresses the calculation of the first-

 $\frac{1}{\sqrt{2}}$

$$
\Sigma_{ab}^{11\,(1)} = \qquad \begin{array}{c} a \\ \bullet \\ b \end{array} = -\frac{c}{d} \bigodot \downarrow \omega' \qquad \qquad \Sigma_{ab}^{12\,(1)} = \qquad \begin{array}{c} a \\ c \\ \leftarrow \omega' \end{array}
$$

E − (f² − b1) − iη

 $\leftarrow \omega'$

^d order ™ er $\overline{1}$.
ነተ*ር* \mathcal{L} $\frac{1}{2}$ dependent colf energy $\overline{\text{R}}$ [‰] 2nd order ™ energy-dependent self-energy order contributions. The first term is the standard standard standard standard standard standard standard stand \mathbb{R}^d [•] 2nd order → energy-dependent self-ene \mathbf{R} \mathbb{Z} onder the \mathbb{Z} acpendent sen-energy $\overline{1}$. \mathbf{r} \sim ci exect deceasedere tool <u>ependent</u> sel \int c $\cos \theta$ energy

b

which can be written, using properties (90) and (91), as Σ11 (2) ab (ω) = ¹ ! k1k2k³ ^Mk1k2k³ ^a (Mk1k2k³ ^b ⁺ ^Pk1k2k³ ^b ⁺ ^Rk1k2k³ ^b)† ω − E^k1k2k³ + iη + ^N ^k1k2k³ a (^N ^k1k2k³ ^b ⁺ ^Qk1k2k³ ^b ⁺ ^Sk1k2k³ ^b) ω + E^k1k2k³ − iη # (Mk1k2k³ ^a ⁺ ^Pk1k2k³ ^a ⁺ ^Rk1k2k³ ^a) (Mk1k2k³ ^b ⁺ ^Rk1k2k³ ^b)† # which can be written, using properties (90) and (91), as Σ12 (2) ab (ω) = ¹ ! k1k2k³ " ^M^k1k2k³ ^a (M^k1k2k³ ^b ⁺ ^P^k1k2k³ ^b ⁺ ^R^k1k2k³ ω − Ek1k2k³ + iη " (M^k1k2k³ ^a ⁺ ^P^k1k2k³ ^a ⁺ ^R^k1k2k³ ^a) (M^k1k2k³ Σ11 (2!) ab (ω) = [↑] ^ω" [↑] ^ω"" d g [↓] ^ω""" c f b a h e (C25) C↑ 2π V¯cd¯ ab¯ V¯k ^c ^U¯k[∗] ω" − ω^k + iη ^Uk[∗] c¯ [↓] ^ω" , ⁼ [−] ⁱ C↑ 2π V¯cd¯ ab¯ V¯k ^c ^U¯k[∗] ω" − ω^k + iη V¯cd¯ ab¯ ^Uk[∗] ^c ^V^k ω" + ω^k − iη ω ^Uk[∗] a % = " \$ ^tab [−] ^µab ⁺ ^Σ¹¹ ab(ω) Σ¹² ab(ω) Σ²¹ ab(ω) [−]tab ⁺ ^µab ⁺ ^Σ²² ab(ω) % \$ ^Vk[∗] b ^Uk[∗] b , (64) where the two sides are evaluated at ω = −ωk. Computing the residue at ω^k one similarly obtains G²¹ ab(ω) = ! " ^V¯^k ^a ^U¯k[∗] b ω − ω^k + iη ab(ω) = ! " ^V¯^k ^a ^V¯k[∗] b [←] ^ω! Σ12 (2!) ab (ω) = ^h ¯^b [←] ^ω! [↑] ^ω!! [↓] ^ω!!! c f a ¯ g d e , (C22) With the same technique we can evaluate all other terms contributing to the second order self-energy. We have ^Σ11 (2!!) ab (ω) = [↑] ^ω! d g¯ c f [↑] ^ω!!! [↑] ^ω!! b a h¯ e (C16) ^Σ12 (2!!) ab (ω) = c f [↓] ^ω!!! h¯ ¯b % ^ω!! a ¯ g¯ d

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Lehmann representations

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^g ^U¯k3[∗] ^e $\frac{b}{1}$

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 \cdot – – – – \oplus \bar{d}

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 $\leftarrow \omega'$

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 $c \bullet - - - - - \bullet \bar{d}$

- - - -

 \mathbb{R} + \mathbb{R}

 $-\omega'$

 \overline{I} $c4$ → energ $\overline{1}$ \overline{r} .
1999 - Carl III
1999 - Carl III μ cig \mathbb{R}^2 a $\frac{1}{2}$ ^a ⁺ ^S^k1k2k³ $\mathbb{E} \left[\mathbb{E} \left[\mathbb{$ _☀ Gorkov equations Pr \mathbf{e} ∙gy dependent e $\ddot{}$ $\overline{\mathcal{L}}$ v equat ab(ω) [−]tab ⁺ ^µab ⁺ ^Σ²² ab(ω) V¯k b energy *dependent* eigenvalue problem LUI 15 \mathcal{L}^{max} \longrightarrow energy dependent eig $\mathbb{R}^2 \times \mathbb{R}^2$ \sim dex \sim \mathbf{r} \overline{a} \overline{a} 114 problem

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$$
\sum_{b} \left(t_{ab} - \mu_{ab} + \Sigma_{ab}^{11}(\omega) \frac{\Sigma_{ab}^{12}(\omega)}{-t_{ab} + \mu_{ab} + \Sigma_{ab}^{22}(\omega)} \right) \Big|_{\omega_k} \left(\frac{\mathcal{U}_b^k}{\mathcal{V}_b^k} \right) = \omega_k \left(\frac{\mathcal{U}_a^k}{\mathcal{V}_a^k} \right) \qquad \mathcal{U}_a^{k*} \equiv \langle \Psi, \rangle
$$

a

$$
\mathcal{U}_a^{k*} \equiv \langle \Psi_k | \bar{a}_a^{\dagger} | \Psi_0 \rangle
$$

$$
\mathcal{V}_a^{k*} \equiv \langle \Psi_k | a_a | \Psi_0 \rangle
$$

Scaling of Gorkov's problem # and \mathbf{v} theorem has been used, i.e. the first set of \mathbf{v} a lino of Larkov's n and up the upper plane and the standard plane and the standard plane and the standard plane and the standard p case the Hartree-Fock self-energy is energy independent. prol 2 <u>In</u> <u>em</u>

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Similarly one computes the other normal self-energy

✺ Transformed into an energy *independent* eigenvalue problem which grouped to group with example a set of the set of the four couples with Eq. (98) provide a set of the Transformal eq. (98) μ and μ \mathcal{R} in a matrix and a matrix \mathcal{R} nsi C↑ 2π \mathbf{r} d into nto ai $\sum_{i=1}^{n} a_i$ **hato** $\overline{}$ nd \mathbf{r} t^- " $-1,$ ropralı าvalu $\frac{1}{2}$ $\iota\iota$ <u>ን1ና</u> envalue pro probl $n \sim$ \overline{C}

Σ21 (1)

formula

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1920 - Paul Barnett, politik eta poli
1921 - Paul Barnett, politik eta poli

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 $\frac{1}{\sqrt{2}}$)

Coupling to 2p1h / 2h1p Coupling to 3qp whose eigenvalues and eigenvectors yield the complete set of poles of one-body Green's functions. The solution of this \mathbf{r} and \mathbf{r} the standard is the standard is the standard is the standard is the standard in \mathbf{r} $\mathsf{L}\Omega$ \overline{Q} \overline{Q} \overline{Q} $\overline{0}$ $\overline{1}$

b

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Σ21 (1)

 $\frac{1}{\sqrt{2}}$

Let us proceed now the computation of the secondorder contributions. The first term is the standard term in the standard standard in the standard standard in
The standard in the standard i $\mathbf{1}$ + $\mathbf{0}$ Couping to $\mathcal C$ cuptu, α oupling to 3qp m $\sum_{i=1}^n$.
in 2π to 3qp -

b

(161<u>a)</u>
161a - Johann John Barn, amerikanischer Politiker
161a - Johann John Barn, amerikanischer Politiker († 1610)

*** Transformed into an energy independent eigenvalue problem** $\frac{1}{2}$ \mathbb{R} Iransformed mito and \mathbb{R} d into an energy *independent* eigenvalue problem $m_{\rm H}$ \sim 2 μ $\$ and using Eqs. (144), (144), (144), (147), (147), (147), (147), (147), (149), α \overline{O} \overline{O} \overline{O} \overline{O} \overline{O} \mathbf{D} which grouped to group with example a set of the set of the four couples with Eq. (98) provide a set of the Transformal eq. (98) μ and μ \mathcal{R} in a matrix and a matrix \mathcal{R}

$$
\left(\begin{array}{ccc}T-\mu+\Lambda&\tilde{h}&\mathcal{C}&-\mathcal{D}^{\dagger}\\ \tilde{h}^{\dagger}&-T+\mu-\Lambda&-\mathcal{D}^{\dagger}&\mathcal{C}\\ \mathcal{C}^{\dagger}&-\mathcal{D}&E&0\\ -\mathcal{D}&\mathcal{C}^{\dagger}&0&-E\end{array}\right)\left(\begin{array}{c}\mathcal{U}^{k}\\ \mathcal{V}^{k}\\ \mathcal{W}_{k}\\ \mathcal{Z}_{k}\end{array}\right)=\omega_{k}\left(\begin{array}{c}\mathcal{U}^{k}\\ \mathcal{V}^{k}\\ \mathcal{W}_{k}\\ \mathcal{Z}_{k}\end{array}\right)
$$

k
1920 - Paul Barnett, politik eta poli
1921 - Paul Barnett, politik eta poli

Tame the dimension growth Defining quantities W and Z through $\text{H}\mathbf{e}$ the difficient \mathbf{e} giowui

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(wk + Ekikaa) za ekikaalan za eki
Lihat di batan za ekikaalan za Ê $\frac{1}{2}$ \overline{a} \mathbf{G} $(1 + \frac{1}{2})^2$ We do not... How do we select the poles?

Instead, Lanczos projection of Gorkov matrix

$$
\left(\begin{array}{ccc}T-\mu+\Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^{\dagger} \\ \tilde{h}^{\dagger} & -T+\mu-\Lambda & -\mathcal{D}^{\dagger} & \mathcal{C} \\ \mathcal{C}^{\dagger} & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^{\dagger} & 0 & -E\end{array}\right)\left(\begin{array}{c} \mathcal{U}^{k} \\ \mathcal{V}^{k} \\ \mathcal{W}_{k} \\ \mathcal{Z}_{k}\end{array}\right)=\omega_{k}\left(\begin{array}{c} \mathcal{U}^{k} \\ \mathcal{V}^{k} \\ \mathcal{W}_{k} \\ \mathcal{Z}_{k}\end{array}\right)
$$

whose eigenvalues and eigenvalues \mathcal{C} of poles of poles of \mathcal{C} • Conserves moments of spectral functions

₩ Equivalent to exact diagonalization for $N_L \rightarrow$ $\mathbf{1}$ ¦ $\mathbf{1}$ ∂ω * * * for $N_L \rightarrow dim(E)$

Test Lanczos projection

➟ Good convergence towards exact digonalization

Results

Benchmark with coupled cluster method

- **GGF and CC quantitatively similar**
- \rightarrow GGF(3) expected to reach Λ -CCSD(T) accuracy

Shell structure evolution

V¯*k*

 $*\!\!$ **ESPE collect fragmentation of "single-particle" strengths from both N±1**

^a ⇥ ⇥⇥ ⇥*^Mkm^a ^V*¯*ⁿ^k*

$$
\epsilon_a^{cent} \equiv h_{ab}^{cent} \, \delta_{ab} = t_{aa} + \sum_{cd} \bar{V}_{acad}^{NN} \rho_{dc}^{[1]} + \sum_{cdef} \bar{V}_{acdaef}^{NNN} \rho_{efcd}^{[2]} \equiv \sum_k \mathcal{S}_k^{+a} E_k^+ + \sum_k \mathcal{S}_k^{-a} E_k^-
$$

[Baranger 1970, Duguet and Hagen. 2011] *^k* are the generalized separation energies introduced in Eq. (26) and *^S[±]^a ^k* the generalized spectroscopic

ⁿ^a [] *.* (31)

Towards medium/heavy open-shell

✺ Case of 74Ni

- ➟ Very good convergence
- \rightarrow From N=13 to N=11 \rightarrow 200 keV

$$
E (N=13) = -1269.6 \text{ MeV}
$$

$$
E (N=\infty) = -1269.7(2) \text{ MeV}
$$

(Extrapolation to infinite model space from [Coon *et al*., 2012; Furnstahl *et al*. 2012])

74Ni - spectral information

- ➟ Second order compresses spectrum
- ➟ Many-body correlations screened out from ESPEs

✺ 3NF in the Gorkov formalism: work in progress

✺ Already implemented in Dyson GF

[Cipollone, Barbieri, Navrátil, *in preparation*]

Conclusions and outlook

- ✺ Gorkov-Green's functions: first ab-initio open-shell calculations V¯ae¯ cf¯ V¯ $\mathbb Z$ guindy-uitting μ is functions.
- $\mathbf{u} = \mathbf{u} \cdot \mathbf{v}$ ^V^k2[∗] * Good convergence, reasonable scaling, α g $\frac{1}{2}$ $\prod_{i=1}^N E_i$ with $C C$ \mathcal{D} $\frac{1}{2}$ e $\frac{1}{2}$ agreement with CC benchmarks
	- _{**[■] * Provide a manageable way to address**} (near) degenerate systems

✺ Formulation of particle-number restored Gorkov theory ✺ Improvement of the self-energy expansion ✺ Implementation of three-body forces σ coupling to the ✺ Proper coupling to the continuum