#### Gorkov-Green's function approach to open-shell systems  $\mathbf{f}$ n to ope **11** i<br>T uk l-snell s<sub>.</sub>  $+ 4$   $+ 2$ ems





cdef gh,k1k2k<sup>3</sup> **Vittorio Somà** (TU Darmstadt & EMMI)

#### *Based on*:

- ! Somà, Duguet, Barbieri, PRC 84 064317 (2011)
- ! Somà, Barbieri, Duguet, PRC 87 011303(R) (2013)
- $1011$ ! Barbieri, Cipollone, Somà, Duguet, Navrátil, arXiv:1211.3315
- ! Somà, Barbieri, Duguet, arXiv:1304.xxxx
- ! Somà, Cipollone, Barbieri, Duguet, Navrátil, *in preparation*



INT Workshop

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Limited to to doubly-closed-shell  $\pm$  1 and  $\pm$  2 nuclei

## Error estimates in *ab initio* calculations



✪ Long-term goal: predictive nuclear structure calculations

- **→ With quantified theoretical errors**
- **Consistent description of structure and reaction**

✪ Estimation of theoretical errors in *ab initio* methods



## Paths to open-shell systems



✪ Two ways to address (near)-degenerate systems

- (a) Multi-reference approaches
	- ➟ e.g. IMSRG + CI, MR-CC, microscopic VS-SM
- (b) Single-reference approaches **■ explicit account of pairing mandatory**

Self-consistent Gorkov-Green's functions:

- $\odot$  Bogoliubov algebra + Green's function theory
- ➟ Formulate the expansion scheme around a Bogoliubov vacuum ✪ Address explicitly the non-perturbative physics of Cooper pairs
	- **■→ Breaking of particle-number conservation (eventually restored)**

#### Gorkov's framework **G**<br>Gramework <sup>h</sup> *<sup>A</sup>* The present work also relates to the long-term developer to the long-term developer to the long-term developer<br>The long-term developer to the long-term developer to the long-term developer to the long-term developer to th Corkov's framework tials based on the field theory (EFT) control to the set of the set particles are degenerated as  $\rho$  such that the intervals of  $\Gamma$ Gorkov's framework Gorkov's framework<br>
Corkov's framework



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#### ✪ Auxiliary many-body state  $\mathbf{1}$  and  $\mathbf{1}$  starting from underlying nuclear EDFs starting nuclear  $\mathbf{1}$ ially-body state momentum potentials obtained through the further application of renormalization of renormalization  $\mathcal{C}$ .  $\mathcal{L}$  between the long-term developed-term developed-term developed  $\mathcal{L}$  $\overline{\phantom{a}}$ <sup>0</sup> <sup>−</sup> <sup>E</sup><sup>N</sup> <sup>0</sup> <sup>≈</sup> <sup>E</sup><sup>N</sup> 0 − EN−2<br>0 − EN−2<br>2 − EN−2 − E 0 <u>≈ 2µ , (24) , (24) , (24) , (24) , (24) , (24)</u> WAUAHIAI y Hidriy-DOUY State  $\Omega$  Auviliary many-hody state  $\Theta$  Auxiliary many-body state particle number is said to respect the (even) number-is said to respect the (even) number-is said to respect t<br>The first the contract the first the first the first theory is said to respect the first theory is said to res  $\bullet$  reading constants.  $dv$  state  $\overline{27}$

- $\rightarrow$  Mixes various particle numbers  $|\Psi_0\rangle \equiv$  $\sum$  $c_A \, |\psi_0^A\>$  $\begin{pmatrix} A \\ 0 \end{pmatrix}$ even<br>even<br>about the method and method away from the method and method away from the method away from the method is various particle numbers  $\|\Psi_0\rangle \equiv \sum_{i} c_A \|\psi_0\|$  $\overline{A}$  $\sigma_{\text{noise}}$  particle numbers  $|\Psi_{0}\rangle = \sum c_{\text{a}} |q|$  $\frac{\partial}{\partial t} \mathbf{V}$  which can also the exist of  $\mathbf{V} = \sum_i \mathbf{V} \mathbf{A} \mathbf{V}$  $\mathcal{A}$  $\ket{\psi_0^{\prime\,1}}$  $\partial_{\alpha}A\setminus$  $\varphi_0$  /  $\blacksquare$   $\blacksquare$  Mixes various particle numb  $\blacksquare$   $\blacksquare$  Mixes various particle numbers problem problem problem provides the energy of the initial problem as  $\mathbf{r}_i$ nucleonic pairs.  $\frac{1}{A}$  $f \mapsto$  Mixes various particle num  $W$ ives verious portials pumbors  $|W_{\epsilon}| = \sum_{\ell=1}^{\text{even}} c_{\ell} |q|\ell}$ • Mixes various particle numbers  $|\Psi_0\rangle = \sum c_A |\psi_0\rangle$  $\longrightarrow$  Mixes
- **The unity of the automal of the set of the set of**  $\Omega = H \mu A$  (D)  $\theta = H \mu A$ *A A* = h <sup>0</sup>*|A|* <sup>0</sup>i (20) the dependent manipulation of  $\mathcal{D}^{\text{total}}$  $r_{\rm H}$  and  $\sim$ construction from underlying from underlying from underlying  $A$ luce a "grand-canonical" potential  $\Delta t = 1$  $\overline{H}$  matrix  $\overline{H}$  $\frac{1}{2}$  and  $\frac{1}{2}$  many-body per turbation theory, which theor  $\mu = H - \mu A$  $\overline{\phantom{a}}$  Intro  $\overline{a}$ duce a "grand-canonical" → Introduce a "grand-canonical" p the system of the system of the system of the system of the state  $\mu$  $\rightarrow$  introduce a grand-canoince In order to access all one-body information contained all one-body information contained  $\mathcal{L}(\mathcal{L})$ and Introduce a "grand-canonic  $\rightarrow$  muoduce a grand-canonic  $\Gamma$  Introduce a "grand-canonical" potential  $\Gamma$   $\Gamma$   $\Gamma$   $\Gamma$   $\Gamma$   $\Gamma$ w→ Introduce a "gran  $\begin{array}{ccc} \n\frac{1}{1} & \frac{1}{1} & \frac{$  $A$ <br>(apopical" potential  $\overline{O} = H - \mu A$
- allow for the construction of schemes that can be system-system-system-system-system-system-system-system-system $minimize \Omega = \sqrt{\frac{1}{2}}$ connection  $\mathcal{L}_0 = \langle \mathcal{L}_0 | \mathcal{L}_1 | \mathcal{L}_0 \rangle$  and the constraints  $A = \sqrt{\mathbf{L}} \mathbf{L} + \mathbf{L} \mathbf{L}$ in  $A - \langle \Psi_0 | A | \Psi_0 \rangle$  $\epsilon$  ratio for existing phenomenological  $\epsilon$   $\sqrt{\pi}$ . The  $\sqrt{2}$ condition  $A = \langle \Psi_0 | A | \Psi_0 \rangle$ are irreducible by definition. An example at second or- $\mathfrak{b}_\alpha|0|\mathfrak{b}_\alpha|$  under the constr  $\left[\begin{array}{cc} \text{C} & \text{C} & \text{C} \end{array}\right]$  is a second second set of  $\left[\begin{array}{cc} \text{C} & \text{C} & \text{C} \end{array}\right]$  $\cdot \mid$  $\mathbb{E}[\mathbf{V}_e]$  minimizes. which follows from Eqs. (21) and (24). even  $\mathcal{L}^{\mathcal{L}}(\mathcal{L}^{\mathcal{L}}) = \mathcal{L}^{\mathcal{L}}(\mathcal{L}^{\mathcal{L}})$  . particle systems, i.e., ... particle systems, i.e., ... particle systems, i.e., ... particle systems, i.e., ...  $\mathcal{L}^{\mathcal{L}}(\mathcal{L}^{\mathcal{L}})$  $\frac{1}{\sqrt{2}}$  undor the constraint  $\frac{1}{\sqrt{2}}$  or  $\frac{1}{\sqrt{2}}$ **tor**  $|\Psi_0\rangle$  minimizes  $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$  under the constraint  $A = \langle \Psi_0 | A | \Psi_0 \rangle$ In order to access all one-body information contained  $\langle \Psi_0 \rangle$  under the constraint  $A = \langle \Psi_0 | A | \Psi_0 \rangle$  $\langle \Psi_{\rm eff}|\Omega\rangle$  in dor the condition of  $c \times \mathcal{L}[G]$  (24  $\mathcal{L}[G]$ ) can be generated by two substantial bundle  $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$  under the constraint  $A = \langle \Psi_0 | A |$  $\mathcal{L} \left( \left| \mathcal{L} \right| \mathcal{L} \right)$  $\frac{1}{\sqrt{2}}$  $\Rightarrow |\Psi_0\rangle$  minimizes  $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$  under the constraint  $A = \langle \Psi_0 | A | \Psi_0 \rangle$  $\Rightarrow |\Psi_0\rangle$  minimizes  $\Omega_0 = \langle \Psi_0|\Omega|\Psi_0\rangle$  under the constraint  $A = \langle \Psi_0|A|\Psi_0\rangle$

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basis are as defined in Eq. (1) and where the modified in Eq. (1) and where the modified in Eq. (1) and where

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**••** 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  $\Omega_0 = \sum |c_{A^\prime}|^2 \,\Omega_0^{A^\prime} \approx E_0^A - \mu A$  $\overline{0}$  $A<sup>′</sup>$  $\frac{1}{A'}$  |  $\frac{1}{A'}$  $u_0^2 \approx E_0^2 - \mu A$ obtained by means of density matrix expansion  $\mathbb{R}^n$ vables of the N system  $\Omega_0 = \sum |c_{A'}|^2 \Omega_0^A$  and  $\frac{d\mathcal{L}}{dt}$ respectively. The corresponding Hamiltonian can be  $\mu^A_0 - \mu A$  $\mu$ <sub>2</sub>  $\pm$  $\approx E_0^A - \mu A$  $\sigma$  the construction of schemes that can be set system-syst insertions of the first-order term (C13b).  $\overline{A}$  $\overline{\phantom{a}}$  $e_1 = \sum c$ The ervables of the N system  $\Omega = \sum_{\alpha} |a_{\alpha}|^2 Q^{A'} \sim F^{A} - \mu A$ |Ψ0! ≡ N <sup>c</sup><sup>N</sup> <sup>|</sup>ψ<sup>N</sup> <sup>0</sup> !, (20)  $\sum_{\alpha}$  is  $\sum_{\alpha}$   $\alpha A' \sim F^A$  $a_0 = \sum |A'|^{3} a_0$ + Obsery rables of the N system  $\Omega_0 = \sum |c_{A'}|^2 \Omega_0^{A'} \approx E_0^A - \mu A$  $\sum_{i=1}^{\lfloor c}$   $\binom{c}{i}$   $\binom{c}{i}$   $\binom{c}{i}$   $\binom{c}{i}$  $A'$  $A'$  $\sim$   $\sim$   $\sim$   $\sim$  $\Omega$ Observables of the N = WORLD + WO<br>N = WORLD + WO  $\overline{a}$  $\frac{1}{\sqrt{2}}$  $^{\prime}$ a<br>ati  $\overline{a}$ ||<sub>|</sub><br>|-<br>|-

Equation (14) ensures that cent

#### $r_{\rm c}$  and the wave function behaves asymptotically behaves asymptotically support of the wave function behaves asymptotically support of the wave function behaves asymptotically support of the support of the support of  $\overline{J}$ **O** Set of 4 Green's functions [Gorkov 1958] H ≡ T + V NN ± V NNN ≡ T + V NNN ≡ T +<br>H → V NNN ≡ T + V NNN ≡ T  $\bullet$  defined in  $\bullet$  introducing additional objects that  $\bullet$  $\bigcup$  bet of 4 Green s functions. **O** Set of 4 Green's functions  $\bullet$  bet of  $\ddagger$  diterminal objects that  $\ddot{\phantom{a}}$ **O** Set of 4 Green's functions consistent in the sense that the asymptotic behaviour of the former is definition by the latter is defined by the latter, e.g. for  $e^{i\theta}$

where c<sup>N</sup> denote complex coefficients. The sum over even

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

Equation (14) ensures that cent

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take into account the formation and destruction of pairs.

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i.e. it is not an eigenstate of the particle number of the p

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 $\begin{bmatrix} \text{C} \\ \text{C} \end{bmatrix}$  $[600 \text{keV} \, 1200]$ [Gorkov 1958]  $\int$  $\int$  $\alpha t$   $\cos 1050$  $[Gorkov 1958]$ *lated* A-body ground-state, respectively. The static field *h*1, already introduced in Sec. II A, contains both the

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basis are as defined in Eq. (1) and where the modified

denote one- and two-body density matrices of the *corre-*

*h*1, already introduced in Sec. II A, contains both the

<sup>a</sup> (aa) is the creation (annihilation) operator of a

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

$$
i G_{ab}^{12}(t, t') \equiv \langle \Psi_0 | T \left\{ a_a(t) \bar{a}_b(t') \right\} | \Psi_0 \rangle = \begin{pmatrix} a \\ b \end{pmatrix} \qquad i G_{ab}^{22}(t, t') \equiv \langle \Psi_0 | T \left\{ \bar{a}_a^{\dagger}(t) \bar{a}_b(t') \right\} | \Psi_0 \rangle = \begin{pmatrix} \bar{a} \\ b \\ \bar{b} \end{pmatrix}
$$

self-consistency characterizing the method.

<sup>a</sup> (t)

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 $\mathcal{L}_{\mathcal{B}}$  as the targeted state the initial probability  $\mathcal{L}_{\mathcal{B}}$  as the initial problem initial prob-

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a (aa) is the creation (annihilation) operator  $\alpha$  is the creation (annihilation) operator of annihilation) operator of a

#### Spectrum and spectroscopic factors  $\sim$ d spectroscopic factors ) + iθ(t =<br>|-<br>| <del>+</del> ! #Ψ0|a† b|<u>|</u><br>|<u>|Ψk" = international population</u><br>| ) .  $\overline{C}$  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



#### ✪ Separation energy spectrum Generation anowever encorrection  $\bullet$  deparation energy  $k$ **From Separation energy spectrum** *n*<sub>2</sub> *a*<sub>1</sub> *energy* spectrum *µ*2*HA*+1  $\sigma$ <sub>V</sub> spectrum ⌫2*HA*<sup>1</sup>

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

Lehmann representation <sup>a</sup> <sup>V</sup>k<sup>∗</sup> V¯k∗ <sup>a</sup> <sup>U</sup>¯<sup>k</sup> <u>Labmann</u> representation *i* Lehmann representation respondence with states of a single-particle basis of *H*<sup>1</sup> ing) a nucleon to the single-particle state center states in the single-particle state center state center states  $\Gamma$ 

where

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 $\left\{ \begin{array}{c} {} \\ {} \\ {} \end{array} \right.$  $k^* = \langle \Psi_k | a^\dagger | \Psi_k \rangle$ **\** Vktara Uk∗<br>a Uk∗  ${\cal U}_a^{k*} \equiv \langle \Psi_k | a_a^\dagger | \Psi_0 \rangle$  ${\cal V}_a^{k*} \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle$  $\int {\cal U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle$  $\bar{k}^* \equiv \langle \Psi_k | \bar{a} \rangle$ correlated on  $\mathcal{U}_a^{\kappa *} \equiv \langle \Psi_k | a_a^\dagger | \Psi_0 \rangle$ where  $\sum_{k} k^* = \langle \Psi_k \rangle$  $\int \mathcal{U}^{k*}_{\alpha} \equiv \langle \Psi_k | a_{\alpha}^{\dagger} | \Psi_0 \rangle$   $\ddot{\alpha}$ where  $\left\{\begin{array}{c} \n\alpha_a - \frac{1}{2} E | \omega_a | + 0 \end{array}\right\}$  $V_a^{\prime\prime\prime} \equiv \langle \Psi_k | a_a | \Psi_0 \rangle$ 

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  $\bigcap_{\alpha=1}^{\infty} C_{\alpha}$  $\Gamma$ **O** Spectroscopic factors **A1** troscopic *factors*  $\bullet$  Spectroscopic factors Engelroconic factore  $\bullet$  opernoscopic incrois

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

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



[figure from J. Sadoudi]

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expression now evaluated at  $\sim$  which can be rewritten at  $\sim$ 



 $T$  diagrammatic rules for computing the irreducible interaction  $\mathcal{L}$ −<br>− i *nt* eigenva *'ependent* eigenvalue p  $\sigma$  Gorkov equations  $\longrightarrow$ self-energies are then the same of the reducible case, with C↓  $\mathbf{1}$  $|C|$  $u$ t eige س<br>سادت  $\mathbf{H} \mathbf{V}$  alue **©** Gorkov equations  $\overline{a}$  and  $\overline{a}$ convention introduced in Rule 6. Inserting the Lehmann and are written respectively as  $\overline{\phantom{a}}$  $\overline{a}$  $\sum_{i=1}^{n} a_i$  $\overline{\phantom{a}}$ ! <sup>−</sup> <sup>ω</sup> ✪ Gorkov equations energy *dependent* eigenvalue problem  $\overline{a}$  $\frac{1}{2}$ 

 $\overline{L}$ 

$$
\left[\sum_{b}\left(\frac{t_{ab}-\mu_{ab}+\Sigma_{ab}^{11}(\omega)}{\Sigma_{ab}^{21}(\omega)}-\frac{\Sigma_{ab}^{12}(\omega)}{-t_{ab}+\mu_{ab}+\Sigma_{ab}^{22}(\omega)}\right)\right|_{\omega_{k}}\left(\frac{\mathcal{U}_{b}^{k}}{\mathcal{V}_{b}^{k}}\right)=\omega_{k}\left(\frac{\mathcal{U}_{a}^{k}}{\mathcal{V}_{a}^{k}}\right)
$$

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 $\bar{g}$   $\int d\bar{d}$ 

 $\omega''$   $\downarrow \omega'''$ 

 $\overline{h}$   $\overline{b}$ 

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 $\sum_{a}^{n} \frac{1}{a}$ 

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 $\blacksquare$ 

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<sup>g</sup> <sup>U</sup>¯k3<sup>∗</sup> <sup>e</sup>  $\frac{b}{1}$ 

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and  $\mathcal{A}$ 

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 $\downarrow \omega'''$  $\bar{h}$   $\bar{b}$ 

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ω − Ek1k2k<sup>3</sup> + iη

 $\bigwedge$   $\omega''$ 

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#### order self-energy diagrams. The first normal contribution contribution  $\epsilon$  $T_{\text{Mott}}$  $Circ 18$ order self-energy diagrams.  $\mathbf{U}$  Ist order  $\mathbf{I}$  energy-independe dard Hartree-Fock self-energy. It is depicted as  $\mathcal{L}$  $\overline{16}$ **۞** 1<sup>st</sup> order <sup>•••</sup> energy-independent self-energy L  $\overline{a}$  $\sim$  $\Omega$  1<sup>st</sup> order  $\rightarrow$  er **O** 1<sup>st</sup> order <del>" •</del> energy-independent self-energy −e:  $\ddot{\bullet}$   $\ddot{\bullet}$  $-1$  $\overline{a}$  $\mathbf{5}$ The above integral, defined on the real axis, is computed by extending the integration to a large semicircle in the  $\mathbf{D}$  1st order  $\mathbf{F}$  energy-independent self-energy  $\tau$  branch do not  $\sigma$  and  $\sigma$  integral between bord the  $\sigma$  $\bullet$  1st and an  $\pm$  as an energy-in dependent potential. The second  $\boxdot$  Ist order  $\blacksquare$  energy-independent self-energy.

self-energies are the same of the reducible case, with the reducible case, with the same of the same o

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

With the same technique we can evaluate all other terms contributing to the second order self-energy. We have

Σ12 (1)

\$ <sup>t</sup>ab <sup>−</sup> <sup>µ</sup>ab <sup>+</sup> <sup>Σ</sup><sup>11</sup>

 $\mathbf{d}$  order  $\mathbf{r}$  er  $\mathbf{I}$ ינ<br>זינ  $k = 3$  $\frac{1}{2}$  dependent colf epoxe <u>HUCHI</u> SCII-**۞** 2<sup>nd</sup> order <sup>11</sup> energy-dependent self-energy order contributions. The first term is the standard contribution of the standard standard standard standard st  $\frac{1}{2}$ **۞** 2<sup>nd</sup> order <del>"→</del> energy-dependent self-en ergy.  $\overline{1}$ 2  $\sim$   $\sim$   $\sim$   $\sim$  $\frac{1}{2}$ <u>ependent</u> sel  $\int$  c vecessors energy  $\frac{1}{2}$ 

$$
\Sigma_{ab}^{11\,(2)}(\omega) = \Upsilon \omega' \left( \begin{matrix} 1 \\ 0 \\ 0 \end{matrix} \right) \left( \begin{matrix} 1 \\ 0 \end{matrix} \right)
$$

b



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

#### $\Omega$  Transformed into an energy *independent* eigenvalue problem nanb + Λ[α] d into an energy *independent* eigenvalue problem  $m_{\rm H}$   $\sim$   $2$   $\mu$   $\$ and using Eqs. (144), (144), (146), (147), (146), (147), (147), (147), (147), (147), (147), (147), (147), (147<br>(147), (147), (147), (147), (147), (147), (147), (147), (147), (147), (147), (147), (147), (147), (147), (147)  $\mathbf n$ which grouped to group groups and the equation of the four controls in the four controls in the C T that control  $\Omega$  Transformed into an energy independent ejections for problem  $\bullet$  mansioning incomplete



k<br>1920 - Paul Barnett, politik eta poli<br>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



k ± Ekikaat in Ekikaat<br>Kabupatèn Panah ing a <sup>−</sup>D<sup>k</sup>1k2k<sup>3</sup> <sup>a</sup> <sup>U</sup><sup>k</sup>  $\overline{a}$  $\mathbf{FAT} = \mathbf{1}$  computed in terms of second-order second-order self-energies can be rewritten as  $\mathbf{FAT} = \mathbf{FAT} + \mathbf{FAT}$ We do not... ✪ How do we select the poles?



a

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

where  $\Xi$  is an energy-independent Hermitian matrix. The diagonalization of  $\Xi$  is equivalent to solving the second-



contributions, is used to recast  $G$  Gorec's equations under the form of an energy-independent eigenvalue problem,  $\mathcal{L}$  and  $\mathcal{L}$ Lanczos

- $\Gamma$  second-order second-order  $\alpha$ **■ Conserves moments of spectral functions** 
	- 11 e<br>aleret te  $\mathbf{P}$ for  $N_1$  - $\overline{\text{d}}$  $\text{for } N_1 \rightarrow \text{dim}(E)$ a Ckinka<br>a Ckinka  $\mathcal{L} = \mathcal{L}$ ➟ Equivalent to exact diagonalization



# Testing Krylov projection





## Self-consistency and scaling



✪ Fully (dashed) vs. partially (solid) SC



- ➟ Scaling does not depend on A
- ➟ Partial self-consistency grasps most of the correlations
- ➟ MBPT(2) inadeguate

## Towards medium/heavy open-shell



#### $Q^{74}$ Ni



➟ NN interaction: chiral N3LO SRG-evolved to 2.0 fm-1

[Entem and Machleidt 2003]

- ➟ Very good convergence
- $\Rightarrow$  From N=13 to N=11 → 200 keV

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

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

(Extrapolation to infinite model space from [Furnstahl, Hagen, Papenbrok 2012] and [Coon et al. 2012])



✪ NN only

- ➟ Systematic along isotopic/isotonic becomes available
- ➟ Overbinding (increasing with A): need for three-body forces





**O** Inclusion of 3NF as effective 2NF

where the normal density matrix  $\rho$  has been defined in Eq. (76) and  $\rho$  and  $\rho$  and  $\rho$ 

where the normal density matrix  $\rho$  has been defined in Eq. (76) and has been defined in Eq. (76) and  $\rho$ 

• Average over the 3<sup>rd</sup> nucleon in each nucleus

=

**■→ Additional term in the Galitskii-Koltun sum rule** [Cipollone *et al.* 2013]

$$
E_0^{\text{A}}=\frac{1}{4\pi i}\int_{C\uparrow}d\omega \operatorname{Tr}_{\mathcal{H}_1}\big[\mathbf{G}^{11}(\omega)\left[\mathbf{T}+(\mu+\omega)\;\mathbf{1}\right]\right]-\frac{1}{2}\langle\Psi_0|W|\Psi_0\rangle
$$

 $\vec{b}$   $\vec{b}$   $\vec{c}$   $\vec{d}$   $\vec{c}$   $\vec{d}$   $\vec{d}$   $\vec{d}$   $\vec{d}$   $\vec{d}$ V <sup>k</sup> **3** 3N interaction: chiral N<sup>2</sup>LO (400 MeV) SRG-evolved to 2.0 fm<sup>-1</sup> [Navrátil 2007] with *µ* being the chemical potential and *N* the particle-

- $\alpha$  and t four-body systems only **Fit to three- and four-body systems only**  $_{\text{c}}$   $_{\text{$
- $\begin{array}{ccccccccccccccccc}\n C & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1\n\end{array}$  $\sim$ zeer, *systems* only<br>duce induced 4N contributions **■ Modified cutoff to reduce induced 4N contributions** [Roth *et al.* 2012] *d* ⌦<sup>0</sup> = h <sup>0</sup>*|*⌦*|* <sup>0</sup>i (27)

## Calcium isotopic chain



✪ First *ab initio* calculation of the whole Ca chain with NN + 3N forces

- ➟ 3NF bring energies close to experiment
- ➟ Induced 3NF and full 3NF investigated



## Calcium isotopic chain



- ➟ Original 3NF correct the energy curvature
- **Good agreement with IM-SRG (quantitative when 3<sup>rd</sup> order included)**



### Potassium isotopic chain



✪ Exploit the odd-even formalism: application to K

- **■→ Trend and agreement similar to calcium**
- ➟ Future: consistent description of medium-mass driplines





✪ Neutron-rich extremes of the nuclear chart

- **Good agreement with measured S2n**
- ➟ Towards a quantitative *ab initio* description of the medium-mass region



## Pairing gaps

![](_page_18_Picture_1.jpeg)

 $\odot$  Three-point mass differences  $\mathbf{C}$  $\mathbf{h} \cdot \mathbf{f}$ 

$$
\Delta_n^{(3)}(A) = \frac{(-1)^A}{2} [E_0^{A+1} - 2 E_0^A + E_0^{A-1}]
$$

![](_page_18_Figure_4.jpeg)

## Pairing gaps

![](_page_19_Picture_1.jpeg)

#### ✪ Inversion of odd-even staggering

![](_page_19_Figure_3.jpeg)

<sup>■→</sup> Second order <u>and</u> 3NF necessary to invert the staggering

## Pairing gaps

![](_page_20_Picture_1.jpeg)

### ✪ Comparison with other microscopic SM and EDFs

![](_page_20_Figure_3.jpeg)

FIG. 2. (Color online) Three-point mass differences ∆(3) <sup>n</sup> from <sup>40</sup>Ca to <sup>60</sup>Ca calculated to third-order ladders in MBPT with [Holt, Menéndez, Schwenk 2013]

3N forces are shown following the legend of Fig. 1, and in comparison with experiment [24, 67]. [Lesinski, Hebeler, Duguet, Schwenk 2012]

- $\ddot{\phantom{0}}$ ⊕ General agreement with other methods
- 1.5 •• Initial 3NF increase the gaps with respect to NN + induced 3NF

#### Benchmarks and chiral EFT interactions strainants and childing in 2011

![](_page_21_Picture_1.jpeg)

- **O** *Ab initio* calculations as a test for chiral EFT interactions
- <sup>3</sup> Different approaches agree in O and Ca chains  $\sum$  merent approaches agree in  $\sum$  and  $\sum$

the inclusion of an extra provides enough extra provides enough extra provides enough extra provides enough extra<br>In the inclusion of an extra provides enough extra binding extra binding extra binding extra binding extra b

➟ Current chiral NN+3N forces overbind medium/heavy-mass nuclei  $\overrightarrow{C}$ ated by the extra proton and the repulsion of the filling of the filling

![](_page_21_Figure_5.jpeg)

![](_page_22_Picture_1.jpeg)

![](_page_22_Figure_2.jpeg)

 $\overline{a}$ 

![](_page_23_Picture_1.jpeg)

✪ One-neutron separation energies

![](_page_23_Figure_3.jpeg)

### *Shell structure evolution*

*V*¯*k*

![](_page_24_Picture_1.jpeg)

*<sup>n</sup><sup>a</sup>* [] *.* (31)

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

*<sup>a</sup>* ⇥ ⇥⇥ ⇥*<sup>M</sup>km<sup>a</sup> <sup>V</sup>*¯*<sup>n</sup><sup>k</sup>*

$$
\epsilon_a^{cent} = h_{ab}^{cent} \delta_{ab} = t_{aa} + \sum_{cd} \bar{V}_{acad}^{NN} \rho_{dc}^{[1]} + \sum_{cdef} \bar{V}_{acdaef}^{NNN} \rho_{efcd}^{[2]} = \sum_{k} S_k^{+a} E_k^+ + \sum_{k} S_k^{-a} E_k^-
$$
\n[Baranger 1970, Duguet and Hagen 2011]\n\n  
\nSeparation energies\n  
\n
$$
\sum_{n=1}^{15} \frac{5/2}{1/2} e^{-6/2} = 0
$$
\n
$$
\sum_{n=1}^{1
$$

### Towards medium/heavy nuclei

![](_page_25_Picture_1.jpeg)

![](_page_25_Figure_2.jpeg)

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

![](_page_25_Figure_5.jpeg)

![](_page_25_Figure_6.jpeg)

## Conclusions and outlook

![](_page_26_Picture_1.jpeg)

### ✪ Gorkov-Green's functions:

- $\frac{1}{\sqrt{2}}$  $f(x) = \frac{1}{2}$  $\frac{1}{2}$   $\frac{1}{2}$   $\frac{1}{2}$  (c21)  $\frac{1}{2}$  (c21)  $\frac{1}{2}$  (c21)  $\frac{1}{2}$  (c21)  $\frac{1}{2}$ ➟ Manageable route to (near) degenerate systems
- $\overrightarrow{ah}$  $\ddot{\phantom{0}}$ *itio* desci .<br>intiere et **→** *Ab initio* description of medium-mass chains
- $\overline{a}$  $\blacksquare$  $\overline{u}$   $\overline{v}$   $\overline{v}$ 3NF: towards f  $\mathbf{r}$ e<br>en van de verwys ™ 2NF + 3NF: towards predictive calculations
- d¯g¯¯bh¯  $\overrightarrow{a}$  Froncisco quanti  $\mathcal{L}$  (we give  $\mathcal{L}$  of  $\mathcal{L}$  )  $\mathcal{L}$  $\mathsf{a}^{\mathsf{A}}$  $\frac{1}{2}$  c  $\frac{1}{2}$   $\frac{1}{2}$  $\mu$  agreement ➟ Energies: quantitative agreement
	- ➟ Spectra: study of shell structure evolution

![](_page_26_Figure_8.jpeg)

![](_page_26_Figure_9.jpeg)

✪ Improvement of the self-energy expansion

- $\epsilon$  coupling to the ✪ Proper coupling to the continuum
- ✪ Formulation of particle-number restored Gorkov theory
- ✪ Towards consistent description of structure and reactions

### *Collaborators*:

Carlo Barbieri (University of Surrey, UK) Andrea Cipollone (University of Surrey, UK)

Thomas Duguet (CEA Saclay, France)

Petr Navrátil (TRIUMF, Canada)

![](_page_27_Picture_5.jpeg)

### *Funding*:

German Research Foundation

*Computing resources*:

Centre de Calcul Recherche et Technologie

![](_page_27_Picture_10.jpeg)

![](_page_27_Picture_11.jpeg)

![](_page_27_Picture_12.jpeg)

![](_page_27_Picture_13.jpeg)

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