INT program on "Nuclear Physics from Lattice QCD" – Spring 2016



### Medium-mass isotopes from chiral and lattice QCD interactions

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## Current Status of low-energy nuclear physics

### **Composite system of interacting fermions**

Binding and limits of stability Coexistence of individual and collective behaviors Self-organization and emerging phenomena EOS of neutron star matter

Extreme neutron-protos

Experimental programs RIKEN, FAIR, FRIB

Extreme mass

**II)** Nuclear correlations Fully known for stable isotopes [C. Barbieri and W. H. Dickhoff, Prog. Part. Nucl. Phys **52**, 377 (2004)]

**Unst** Neutron-rich nuclei; Shell evolution (far from stability)

**I)** Understanding the nuclear force QCD-derived; 3-nucleon forces (3NFs) First principle (ab-initio) predictions

protons

Be

Li He

neutrons

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**III) Interdisciplinary character** Astrophysics Tests of the standard model Other fermionic systems: ultracold gasses; molecules;

## Concept of correlations



[CBuged We H. Dickhoff, Prog. Part. Nucl. Phys **52**, 377 (2004)]

## Concept of correlations



# Ab-Initio SCGF approaches



# The FRPA Method in Two Words

Particle vibration coupling is the main cause driving the distribution of particle strength—on both sides of the Fermi surface...

D(2h1p

= hole

(ph)

(ph)

Oll (pp/hh)

R<sup>(2p1h</sup>

= particle

CB et al., Phys. Rev. C**63**, 034313 (2001) Phys. Rev. A**76**, 052503 (2007) Phys. Rev. C**79**, 064313 (2009)

•A complete expansion requires <u>all</u> <u>types</u> of particle-vibration coupling

"Extended" Hartree Fock

...these modes are all resummed exactly and to all orders in a *ab-initio* many-body expansion.

•The Self-energy  $\Sigma^*(\omega)$  yields both single-particle states and scattering

## The FRPA Method in Two Words

Particle vibration coupling is the main cause driving the distribution of particle strength—a least close to the Fermi surface...





## Self-Consistent Green's Function Approach



Global picture of nuclear dynamics

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- Reciprocal correlations among effective modes
- Guaranties macroscopic conservation laws

## Self-Consistent Green's Function Approach



## <sup>56</sup>Ni neutron spectral function



W. Dickhoff, CB, Prog. Part. Nucl. Phys. 53, 377 (2004) CB, M.Hjorth-Jensen, Pys. Rev. C**79**, 064313 (2009)





Truncation scheme:	Dyson formulation (closed shells)	Gorkov formulation (semi-/doubly-magic)		
1 <sup>st</sup> order:	Hartree-Fock	HF-Bogolioubov		
2 <sup>nd</sup> order:	2 <sup>nd</sup> order	2 <sup>nd</sup> order (w/ pairing)		
 3 <sup>rd</sup> and all-orders sums, P-V coupling:	ADC(3) FRPA etc	G-ADC(3) work in progress		







## Gorkov and symmetry breaking approaches

V. Somà, CB, T. Duguet, , Phys. Rev. C 89, 024323 (2014)
V. Somà, CB, T. Duguet, Phys. Rev. C 87, 011303R (2013)
V. Somà, T. Duguet, CB, Phys. Rev. C 84, 064317 (2011)

> Ansatz 
$$(... \approx E_0^{N+2} - E_0^N \approx E_0^N - E_0^{N-2} \approx ... \approx 2\mu)$$

> Auxiliary many-body state  $|\Psi_0
angle \equiv \sum_N^{\mathrm{even}} c_N |\psi_0^N
angle$ 

Mixes various particle numbers

ightarrow Introduce a "grand-canonical" potential  $\ \ \Omega = H \! - \! \mu N$ 

 $\implies |\Psi_0\rangle$  minimizes  $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$  under the constraint  $N = \langle \Psi_0 | N | \Psi_0 \rangle$ 

This approach leads to the following Feynman diagrams:

 $\Sigma_{ab}^{11\,(1)} = \qquad \stackrel{a}{\overset{o}{b}} - - - \stackrel{c}{\overset{o}{d}} \bigcirc \downarrow \omega'$   $\Sigma_{ab}^{12\,(1)} = \qquad \stackrel{a}{\overset{c}{\phantom{ab}}} - - - \stackrel{\overline{b}}{\overset{d}{\phantom{ab}}} \stackrel{\overline{b}}{\overset{d}{\phantom{ab}}}$ UNIVERSITY OF



Carlo Barbieri – 18/11

## Espressions for 1st & 2nd order diagrams

 $= \sum \sum \sum \eta_a \eta_{k_1} f_{a_k n_k n_k}^{n_k n_k n_k} C_{h_k n_k}^{J_k M_k}$ 



Ab INITIO SELF-CONSISTENT GORKOV-GREEN's ...

#### 5. Block-diagonal structu

a. First or The goal of this subsection is to discuss how the block-diagona reflects in the various self-energy contributions, starting with the fir and (C19) into Eq. (B7), and introducing the factor

$$f_{\alpha\beta\nu\delta}^{n_sn_bn_cn_d} \equiv \sqrt{1 + \delta_{\alpha\beta} \delta_{n_s\delta}}$$

one obtains

where the block-diagonal normal density matrix is introduced throu  $\rho_{n_a n_b}^{[\alpha]} = \sum \mathcal{V}_{n_b [\alpha]}^{n_b}$ 

and properties of Clebsch-Gordan coefficients has been used. The  $\delta_{\pi_a \pi_b}$  and  $\delta_{q_a q_b}$ , leading to  $\delta_{\alpha \beta} = \delta_{j_a j_b} \delta_{\pi_a \pi_b} \delta_{q_a q_b}$ . Similarly, for  $\Sigma^{22(1)}$ 

$$\begin{split} \Sigma_{ab}^{22(1)} &= -\sum_{cd,k} \tilde{V}_{bcdd} \tilde{V}_{c}^{k} \tilde{V}_{d}^{k*} \\ &= \sum_{m|M_{c}} \sum_{n,n,n,n} \sum_{q_{c}} \sqrt{2}_{i} \\ &= -\delta_{a\beta} \delta_{m,m_{c}} \sum_{n,n,n} \sum_{q_{c}} \sum_{j} \int_{\sigma_{j}}^{\pi_{i}} \int_{\sigma_{j}}^{\pi_{i}} \\ &= -\delta_{j} \delta_{m,m_{c}} \sum_{n,n,n} \sum_{q_{c}} \pi_{k} \int_{\sigma_{c}}^{\pi_{i}} \\ &= -\delta_{j} \delta_{m,m_{c}} \sum_{n,n,n} \sum_{q_{c}} \pi_{k} \int_{\sigma_{c}}^{\pi_{i}} \\ &= -\delta_{j} \delta_{m,m_{c}} \sum_{n,n,n} \sum_{q_{c}} \pi_{k} \int_{\sigma_{c}}^{\pi_{i}} \\ &= -\delta_{a\beta} \delta_{m,m_{c}} \sum_{n,n,n} \sum_{q_{c}} \pi_{k} \int_{\sigma_{c}}^{\pi_{i}} \\ &= \delta_{a\beta} \delta_{m,m_{c}} \sum_{n,n,n} \pi_{k} \int_{\sigma_{i}}^{\pi_{i}} \\ &= \delta_{a\beta} \delta_{m,m_{c}} \sum_{n,n} \pi_{k} \int_{\sigma_{i}}^{\pi_{i}} \\ &= \delta_{a\beta} \delta_{m,m_{c}} \sum_{n,n} \pi_{k} \int_{\sigma_{i}}^{\pi_{i}} \\ &= \delta_{a\beta} \delta_{m,m_{c}} \sum_{n,n} \pi_{i} \int_{\sigma_{i}}^{\pi_{i}} \\ &= \delta_{a\beta} \delta_{m,m_{c}} \sum_{n} \sum_{n,n} \sum_{n} \sum_{n,n} \sum_{n} \sum_{n}$$

where general properties of Clebsch-Gord

Let us consider the anomalous contributions to the first-order self-er derives  $\Sigma_{ab}^{12\,(1)} = \frac{1}{2} \sum \overline{V}_{abcd} \overline{V}_c^{k*} \overline{U}_d^k$ 

$$\mathcal{N}_{a}^{*(n,n)} = \delta_{J_{10}j_a} \delta_{M_{10}m_a} \sum_{n,n}$$

4.1.1.1

$$= -\frac{1}{2} \sum_{n_i,n_i,n_i} \sum_{\gamma} \sum_{m_i} \sum_{J_M} f_{\alpha\beta\gamma\gamma}^{n_i,n_i,n_i,n_i} \eta_b \eta_c C_j$$
One can show that the same result is obtain

$$\begin{split} & \int_{a_{n,a_{d}}}^{a_{n,a_{d}}} y \sum_{m_{s}} \sum_{j} \sum_{n,a_{d}} \sum_{\gamma} \sum_{m_{s}} \int_{a_{d}}^{a_{s},a_{s},a_{s},a_{s}} \int_{J} f_{d}^{a_{d},a_{s},a_{s},a_{s}} f_{d}^{a_{d},a_{s},a_{s}} f_{d}^{a_{d},a_{s},a_{s}} f_{d}^{a_{d},a_{s},a_{s}}} \int_{a_{d}} f_{d}^{a_{d},a_{s},a_{s}} f_{d}^{a_{d},a_{s},a_{s}} f_{d}^{a_{d},a_{s},a_{s}}} \int_{a_{d}} f_{d}^{a_{d},a_{s},a_{s}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s},a_{s}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s},a_{s}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s},a_{s}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s},a_{s},a_{s}}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s}}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s},a_{s}}} f_{d}^{a_{d},a_{s}}} f_{d}^{a_{d},a_{s}}} f_{d}^{a_{d},a_{s}}} f_{d}^{a_{d},a_{s}}} f_{d}^{a_{d},a_{s}}} f_{d}^{a_{d},a_{s}}} f_{d}^{a_{d},a_{s}}} f_{d}^{a_{d},a_{s}}} f_{d}^{a_{d},a_{s}}} f_{d}^{a_{d},a$$

 $\equiv \delta_{J_{uv} j_{s}} \delta_{M_{uv} m_{s}} N_{s}$ 

.

 $\equiv \delta_{\alpha\beta} \delta_{m_a m_b} \Sigma_n^{21}$ 

 $= \delta_{\alpha\beta} \delta_{\alpha} m$ 

 $\sum_{m_1m_2m_3M_r}\sum_{rst} C_{j_{k_1}m_{k_1}j_{k_2}m_{k_2}}^{J_rM_r} \zeta$ 

 $\times C_{j_1,m_1,j_2,m_3}^{J_{00}M_i} C_{J_{00}M_{10}}^{J_{00}M_{10}} C$  $=\sum_{m_1m_2m_3}\sum_{M_i}\sum_{n_in_in_j}\sum_{J_iM_i}\eta_{k_3}f_{\alpha\kappa_3}^{n_in_j}$ 

Block-diagonal forms of second-order s

where the block-diagonal anomalous density matrix is introduced th

$$\tilde{\rho}_{n_{a}\bar{n}_{b}}^{[\alpha]} = \sum_{n_{b}} U_{n_{b}[\alpha]}^{n_{b}} V_{n_{a}[\alpha]}^{n_{b}}$$

momenta, one has

$$\mathcal{C}_{n_{\alpha}[ax_{1}\kappa_{1},n_{\alpha}]}^{\kappa_{1},\kappa_{2},\kappa_{3}} \equiv \frac{1}{\sqrt{6}} \left[ \mathcal{M}_{n_{\alpha}[ax_{1}\kappa_{1},\alpha_{2},\alpha_{3}]}^{\kappa_{1},\kappa_{1},\alpha_{2},\kappa_{3}} - \mathcal{P}_{n_{\alpha}[ax_{1}\kappa_{1},\alpha_{2}]J_{c}}^{\kappa_{1},\kappa_{2},\kappa_{3}} - \mathcal{R}_{n_{\alpha}[ax_{1},\kappa_{1},\alpha_{3}]}^{\kappa_{1},\kappa_{2},\kappa_{3}} \right] = 0$$

 $\Sigma_{n_{0}n_{0}}^{22(\alpha)(2)} = \sum_{n_{0},n_{0},n_{0}} \sum_{k} \sum_{e,s\in s} \left\{ \frac{\mathcal{D}_{n_{e}}^{e_{1},n_{0},n_{0},n_{0}}}{\omega - (\omega_{k} + \omega_{k} + \omega_{k}) + in)} + \frac{\left(\mathcal{C}_{n_{e}}^{e_{1},n_{0},n_{0}}, \frac{e_{1}}{\omega}, \frac{e_{1}}{\omega}$ 

6. Block-diagonal structure of Gorkov's equations

In the previous subsections it has been proven that all single-particle Green's functions and all self-energy contributions entering

(C43a)

(C44a)

(C44b)

(C44c)

(C44d)

### [V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011) $|_{J_{\epsilon}} \left( \mathcal{C}_{n_{\delta} [\alpha\kappa_{1}\kappa_{1}, n_{\delta}]}^{\kappa_{1}, n_{\delta}, n_{\delta}} \right)^{*} + \frac{\left( \mathcal{D}_{n_{\delta} [\alpha\kappa_{1}, \kappa_{1}, n_{\delta}]}^{\kappa_{1}, n_{\delta}, n_{\delta}} \right)^{*} \mathcal{D}_{n_{\delta} [\alpha\kappa_{1}, \kappa_{1}, n_{\delta}]}^{\kappa_{1}, n_{\delta}, n_{\delta}} + \frac{\left( \mathcal{D}_{n_{\delta} [\alpha\kappa_{1}, \kappa_{1}, n_{\delta}]}^{\kappa_{1}, n_{\delta}, n_{\delta}} \right)^{*} \mathcal{D}_{n_{\delta} [\alpha\kappa_{1}, \kappa_{1}, n_{\delta}]}^{\kappa_{1}, n_{\delta}, n_{\delta}} I_{\epsilon} - \frac{1}{\omega} + \left( \omega_{k_{1}} + \omega_{k_{1}} + \omega_{k_{2}} \right) - i \eta$

which recovers relation (72a). The remaining quan  $\{k_1, k_2, k_3\}$  indices and can be obtained from Eqs. (C  $j_{k_1}$  to  $J_{10t}$  and  $J_c$  as follows:

 $= -\delta_{A_{\alpha}i_{\alpha}}\delta_{M_{\alpha}-m_{\alpha}}\eta_{\alpha}\Lambda$ 

$$\mathcal{P}_{a(J_{c}J_{us})}^{k_{1}k_{2}k_{3}} = \sum_{I_{c}} (-1)^{J_{c}+J_{d}+j_{k_{2}}+j_{k_{3}}} \sqrt{2J_{c}}$$

$$= -\delta_{J_{ab}j_{a}}\delta_{M_{ab}m_{a}}\sum_{n,n,n_{c}}\sum_{J_{d}}\pi_{J}$$

$$\times \overline{V}^{J_{d}[\alpha\kappa_{2}\kappa_{1}\kappa_{3}]}\mathcal{U}^{n_{1}} - \mathcal{U}^{n_{2}}$$

$$\times \overline{V}_{n_a n_i n_i n_i}^{J_a (a \kappa_1 \kappa_1 \kappa_1)} U_{n_i \kappa_1 n_i}^{n_{i_1}} U_{n_i \kappa_1 n_i}^{n_{i_1}} [J_{n_i \kappa_1 n_i}^{n_{i_1}}]$$

$$\equiv \delta_{J_{a \kappa_1 J_a}} \delta_{M_{a \kappa_1} m_a} \mathcal{P}_{n_a (a \kappa_1 \kappa_1 \kappa_2) I_a}^{n_{i_1} n_{i_2} n_{i_3}}$$

$$Q_{\alpha(J_{i},J_{ac})}^{k_{i}k_{jk}} = \sum_{J_{d}} (-1)^{J_{i}+J_{d}+j_{k_{2}}+j_{k_{2}}} \sqrt{2J}$$
  
=  $\delta_{J_{ac},j_{a}} \delta_{M_{ac}m_{a}} \sum \sum \pi_{k_{2}}$ 

$$\times \overline{V}_{n_{c}n_{c}n_{c}n_{c}}^{J_{d}(ax_{2}x_{1}x_{1})} \overline{V}_{n_{c}(x_{1})}^{n_{d}} \overline{V}_{n_{c}(x_{1})}^{n_{d}} \\ = \delta_{J_{ac},l_{c}n_{c}} \mathcal{Q}_{n_{c}}^{n_{d}} \mathcal{Q}_{n_{c}(n_{d}),n_{c}}^{n_{d}} \mathcal{Q}_{n_{c}(n_{d}),n_{c}}^{n_{d}} J_{c}$$

$$\mathcal{R}_{a(J_cJ_{ut})}^{k_1k_2k_3} = \sum_{J_d} (-1)^{2j_1+2J_d} \sqrt{2J_c+1}$$

$$= -\delta_{J_{ac}j_{c}}\delta_{M_{ac}m_{c}}\sum_{n,n,n_{c}}\sum_{l_{d}}\pi_{l}$$

$$\times \tilde{V}_{n_{a}n,n,n_{c}}^{l_{d}(ax)+cc,2} [J_{n_{c}}^{n_{l_{d}}}] U_{n_{c}}^{n_{d_{d}}}|_{l_{c}}^{n_{d_{d}}}$$

$$\equiv \delta_{J_{ac}j_{c}}\delta_{M_{ac}m_{c}} \mathcal{R}_{n_{c}(ax)+cc_{d}}^{n_{d}(ax)+cc_{d}}] I_{c}$$

$$= \delta_{J_{uv}, j_u} \delta_{M_{uv} m_u} \sum_{n, n, n_v} \sum_{J_d} \pi_{k_1}$$

$$\times \tilde{V}_{n, l_d(av_1, v_{12})} V_{n_1(k_1)}^{\tilde{n}_{k_1}} V_{n_1(k_1)}^{\tilde{n}_{k_2}}$$

 $\equiv \delta_{J_{uv}J_{u}} \delta_{M_{uv}m_{u}} S^{n_{k_1}n_{k_2}n_{k_3}}_{n_{u}} [ar_{v}r_{v}r_{v}]_{J_{u}}.$ 

These terms are finally put together to form the different contributions to second-order self-energies. Let us consider  $\Sigma_{ab}$  as

an example [see Eq. (75)]. By inserting Eqs. (C35) and (C36) and summing over all possible total and intermediate angular

$$-\frac{1}{2}\sum_{cdefgh} V_{e\bar{f}a\bar{b}}^{l\bar{b}} V_{e\bar{f}a\bar{b}e} \tilde{V}_{g\bar{b}a\bar{b}} \left\{ \frac{\mathcal{V}_{e}^{b} \mathcal{U}_{e}^{b} \mathcal{V}_{e}^{b} \mathcal{U}_{e}^{b} \mathcal{U}_{e}^{b}$$

064317-23

(C45)

326)

(27)

(B31)

$$T_{ab} - \mu \, \delta_{ab} \equiv \delta_{a\beta} \, \delta_{m,m_b} \left[ T_{n,n_b}^{[a]} - \mu^{[q_c]} \, \delta_{n_b n_b} \right],$$
oducing block-diagonal forms for amplitudes  $\mathcal{W}$  and  $\mathcal{Z}$  through

Gorkov's equations display the same block-diagonal structure if the systems is in a 0+ state. Defining

$$W_{k(I_{n},I_{n})}^{k(I_{n},I_{n})} \equiv \delta_{I_{n}I_{1}}\delta_{M_{nl}m_{1}}W_{n_{k}[k(\mathbf{x}),\mathbf{x}_{1}],I}, \qquad (C46a)$$

$$Z_{k(I_{n},I_{n})}^{k(I_{n},I_{n})} \equiv -\delta_{I_{n}I_{1}}\delta_{M_{nl}m_{1}}W_{I_{n}}Z_{I_{n}I_{n}}^{n_{I_{n}}n_{1}} \dots \qquad (C46b)$$

 $[a\kappa_1\kappa_1\kappa_2] J_c$ ],

$$\omega_k - E_{k,k,k} W_{a_1(a_2,a_3)}^{a_1,a_1,a_3} \equiv \sum \left[ \left( C_{a_1(a_2,a_3)}^{a_1,a_2,a_3} \right)^* U_{a_1(a_2)}^{a_1} + \left( D_{a_1(a_2,a_3)}^{a_1,a_1,a_2,a_3} \right)^* V_{a_1(a_3)}^{a_3} \right],$$
 (C47a)

$$(\omega_k + E_{k_1 k_2 k_1}) \mathcal{Z}_{n_k \{n_1, n_1, n_2\}}^{n_{k_1 \{n_1, n_2\}}} \equiv \sum_{s=1}^{n_{s,s}} \left[ \mathcal{D}_{n_s \{n_2, n_1\}}^{n_1, n_1, n_1} \mathcal{U}_{n_s \{n_1\}}^{n_1} + \mathcal{U}_{n_s \{n_1\}}^{n_1, n_1, n_2, n_3} \mathcal{U}_{n_s \{n_1\}}^{n_1} \right], \quad (C47b)$$
(247b)

$$\omega_{k} \mathcal{U}_{n_{c}[\nu]}^{n_{c}} = \sum_{n_{c}} \left[ \left( \mathcal{T}_{n_{c}n_{b}}^{[\nu_{c}]} - \mu^{[q_{c}]} \delta_{n_{c}n_{b}} + \Lambda_{n_{c}}^{[\nu_{c}]} \right) \mathcal{U}_{n_{b}}^{n_{b}} + \frac{1}{h_{c}(n_{c})} \mathcal{U}_{n_{c}[\nu_{c}]}^{n_{b}} \right] \\ + \sum_{n_{c}[n_{c}n_{c}]} \left[ \mathcal{C}_{n_{c}[n_{c}n_{c}n_{c}]}^{n_{c}n_{c}n_{c}} \mathcal{U}_{n_{c}[(n_{c}n_{c}n_{c})]_{c}}^{n_{b}} + \left( \mathcal{D}_{n_{c}[(n_{c}n_{c}n_{c})]_{c}}^{n_{c}n_{c}} \right)^{*} \mathcal{Z}_{n_{c}[(n_{c}n_{c}n_{c})_{c}]_{c}}^{n_{c}n_{c}n_{c}n_{c}} \right],$$

$$(C48a) \qquad ^{129}$$

$$\omega_{k} \mathcal{V}_{n_{c}[a]}^{i_{c}} = \sum_{n_{b}} \left[ - \left[ T_{n_{c}n_{b}}^{[a]} - \mu^{[a_{c}]} \delta_{n_{c}n_{b}} + \Lambda_{(a)}^{[a]} \mathcal{V}_{n_{b}[a]}^{i_{c}} + \tilde{h}_{n_{b}[n_{b}]}^{[a]} \mathcal{I}_{n_{b}[a]}^{i_{c}} \right] \right] \\ + \sum_{n_{c_{1}} n_{c_{2}} n_{c_{3}}} \sum_{e_{i} e_{i} e_{i}} \sum_{J_{c}} \left[ \mathcal{D}_{n_{c}}^{n_{i_{1}} n_{i_{c}} n_{i_{1}}} \mathcal{I}_{n_{e}}^{i_{i_{1}} n_{i_{c}} n_{i_{3}}} \mathcal{I}_{n_{b}[ae_{i}]}^{i_{c}} \mathcal{I}_{n_{c}[ae_{i} e_{i} n_{i_{c}}] J_{c}}^{i_{c}} \right] \mathcal{I}_{n_{c}[ae_{i} e_{i} e_{i}] J_{c}}^{i_{c}} \mathcal{I}_{n_{c}[ae_{i} e_{i} e_{i}] J_{c}}^{i_{c}} + \left( \mathcal{C}_{n_{c}[ae_{i} e_{i} e_{i}] J_{c}}^{i_{c}} \right)^{*} \mathcal{Z}_{n_{c}[e_{i} e_{i} e_{i}] J_{c}}^{i_{i_{1}} n_{i_{c}} n_{i_{3}}}$$
(C48b)
  
130)

### Ab-initio Nuclear Computation & BcDor code



### Ab-initio Nuclear Computation & BcDor code

### http://personal.ph.surrey.ac.uk/~cb0023/bcdor/

### **Computational Many-Body Physics**





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#### Documentation

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#### Welcome

From here you can download a public version of my self-consistent Green's function (SCGF) code for nuclear physics. This is a code in J-coupled scheme that allows the calculation of the single particle propagators (a.k.a. one-body Green's functions) and other many-body properties of spherical nuclei. This version allows to:

- Perform Hartree-Fock calculations.
- Calculate the the correlation energy at second order in perturbation theory (MBPT2).
- Solve the Dyson equation for propagators (self consistently) up to second order in the self-energy.
- Solve coupled cluster CCD (doubles only!) equations.

When using this code you are kindly invited to follow the creative commons license agreement, as detailed at the weblinks below. In particular, we kindly ask you to refer to the publications that led the development of this software.

Relevant references (which can also help in using this code) are: Prog. Part. Nucl. Phys. 52, p. 377 (2004), Phys. Rev. A76, 052503 (2007), Phys. Rev. C79, 064313 (2009), Phys. Rev. C89, 024323 (2014) Medium-mass isotopes from chiral interactions



# Modern realistic nuclear forces



## Oxygen puzzle...



The oxygen dripline is at <sup>24</sup>O, at odds with other neighbor isotope chains.

Phenomenological shell model interaction reflect this in the s.p. energies but no realistic NN interaction alone is capable of reproducing this...

### The fujita-Miyazawa 3NF provides repulsion through Pauli screening of other 2NF terms:





## Chiral Nuclear forces - SRG evolved



## Convergence of s.p. spectra w.r.t. SRG

Cutoff dependence is reduces, indicating good convergence of many-body truncation and many-body forces





# Neutron spectral function of Oxygens



## Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013) *and* Phys. Rev. C **92**, 014306 (2015)



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## Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. 111, 062501 (2013)



 $\rightarrow$  3NF crucial for reproducing binding energies and driplines around oxygen

 $\rightarrow$  d<sub>3/2</sub> raised by genuine 3NF

→ cf. microscopic shell model [Otsuka et al, PRL105, 032501 (2010).]

N3LQV(AST 500 Mev/c) chiral NN interaction evolved to 2N + 3N forces (2.0 fm<sup>-1</sup>) N2 CO (RR400 Mev/c) chiral 3N interaction evolved (2.0 fm<sup>-1</sup>)

## Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013) and Phys. Rev. C **92**, 014306 (2015)



 $\rightarrow$  3NF crucial for reproducing binding energies and driplines around oxygen

→ cf. microscopic shell model [Otsuka et al, PRL105, 032501 (2010).]

UNIVERSITY OF N3LO (Λ = 500Mev/c) chiral NN interaction evolved to 2N + 3N forces (2.0fm<sup>-1</sup>) N2LO (Λ = 400Mev/c) chiral 3N interaction evolved (2.0fm<sup>-1</sup>)

## Results for the oxygen chain

A. Cipollone, CB, P. Navrátil, Phys. Rev. C 92, 014306 (2015)



→ Single particle spectra slightly to spread and

→ systematic underestimation of radii



### Single nucleon transfer in the oxygen chain

[F. Flavigny et al, PRL110, 122503 (2013)]

### $\rightarrow$ Analysis of <sup>14</sup>O(d,t)<sup>13</sup>O and <sup>14</sup>O(d,<sup>3</sup>He)<sup>13</sup>N transfer reactions @ SPIRAL

Reaction	<i>E</i> * (MeV)	$J^{\pi}$	R <sup>HFB</sup> (fm)	<i>r</i> <sub>0</sub> (fm)	$C^2 S_{exp}$ (WS)	$\frac{C^2 S_{\rm th}}{0p+2\hbar\omega}$	R <sub>s</sub> (WS)	$C^2 S_{exp}$ (SCGF)	$C^2 S_{\text{th}}$ (SCGF)	R <sub>s</sub> (SCGF)
$^{14}$ O ( <i>d</i> , <i>t</i> ) $^{13}$ O	0.00	3/2-	2.69	1.40	1.69 (17)(20)	3.15	0.54(5)(6)	1.89(19)(22)	3.17	0.60(6)(7)
$^{14}$ O ( <i>d</i> , $^{3}$ He) $^{13}$ N	0.00	$1/2^{-}$	3.03	1.23	1.14(16)(15)	1.55	0.73(10)(10)	1.58(22)(2)	1.58	1.00(14)(1)
	3.50	$3/2^{-}$	2.77	1.12	0.94(19)(7)	1.90	0.49(10)(4)	1.00(20)(1)	1.90	0.53(10)(1)
$^{16}O(d, t)$ $^{15}O$	0.00	$1/2^{-}$	2.91	1.46	0.91(9)(8)	1.54	0.59(6)(5)	0.96(10)(7)	1.73	0.55(6)(4)
$^{16}$ O ( <i>d</i> , $^{3}$ He) $^{15}$ N [19,20]	0.00	$1/2^{-}$	2.95	1.46	0.93(9)(9)	1.54	0.60(6)(6)	1.25(12)(5)	1.74	0.72(7)(3)
	6.32	$3/2^{-}$	2.80	1.31	1.83(18)(24)	3.07	0.60(6)(8)	2.24(22)(10)	3.45	0.65(6)(3)
$^{18}$ O ( <i>d</i> , $^{3}$ He) $^{17}$ N [21]	0.00	$1/2^{-}$	2.91	1.46	0.92(9)(12)	1.58	0.58(6)(10)			





- Overlap functions and strengths from GF

- Rs independent of asymmetry

### Z/N asymmetry dependence of SFs - Theory

Ab-initio calculations explain (a very weak) the Z/N dependence but the effect is much lower than suggested by direct knockout

Rather the quenchng is high correlated to the gap at the Femi surface.



# Calcium isotopic chain

### Ab-initio calculation of the whole Ca: induced and full 3NF investigated



→ induced and full 3NF investigated

- $\rightarrow$  genuine (N2LO) 3NF needed to reproduce the energy curvature and S<sub>2n</sub>
- $\rightarrow$  N=20 and Z=20 gaps overestimated!

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→ Full 3NF give a correct trend but over bind!

V. Somà, CB et al. Phys. Rev. C89, 061301R (2014)



Two-neutron separation energies predicted by chiral NN+3NF forces:



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→ First ab-initio calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism



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Two-neutron separation energies predicted by chiral NN+3NF forces:



Lack of deformation due to quenched cross-shell quadrupole excitations

→ First ab-initio calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

# The sd-pf shell gap

Neutron spectral distributions for <sup>48</sup>Ca and <sup>56</sup>Ni:



sd-pf separation is overestimated even with leading order N2LO 3NF

Correct increase of  $p_{3/2}$ - $f_{7/2}$  splitting (see Zuker 2003)

		2NF only	2+3NF(ind.)	2+3NF(full)	Experiment
	<sup>16</sup> O:	2.10	2. 41	2.38	2.718±0.210 [19]
CB <i>et al.</i> , arXiv:1211.3315 [nucl-th]	<sup>44</sup> Ca:	2.48	2.93	2.94	3.520±0.005 [20]

### Two-neutron separation energies for neutron rich K isotopes

M. Rosenbusch, et al., PRL114, 202501 (2015)



Measurements @ ISOLTRAP

Theory tend to overestimate the gap at N=34, but overall good

→ <u>Error bar in predictions</u> are from extrapolating the manybody expansion to convergence of the model space.


# Inversion of $d_{3/2}$ — $s_{1/2}$ at N=28



FIG. 1. (color online) Experimental energies for  $1/2^+$  and  $3/2^+$  states in odd-A K isotopes. Inversion of the nuclear spin is obtained in <sup>47,49</sup>K and reinversion back in <sup>51</sup>K. Results are

> J. Papuga, et al., Phys. Rev. Lett. 110, 172503 (2013); Phys. Rev. C 90, 034321 (2014)

> > 51

53

<sup>A</sup>K isotopes Laser spectroscopy @ ISOLDE

#### Change in separation described by chiral NN+3NF:



## NNLO-sat : a global fit up to A≈24

A. Ekström et al. Phys. Rev. C91, 051301(R) (2015)



NNLOsat (V2 + W3) -- Grkv 2nd ord.

From SCGF:

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V2-N3LO(500) + W3-NNLO(400MeV/c) w/ SRG at 2.0 fm<sup>-1</sup>
 A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
 V. Somà, CB *et al.* Phys. Rev. C**89**, 061301R (2014)

## BE and radii for Oxygens

- New fits of chiral interactions (NNLOsat) highly improve comparison to data

- Deficiencies remain for neutron rich isotopes



FIG. 1. Oxygen binding energies. Results from SCGF and IMSRG calculations performed with EM [20-22] and NNLO<sub>sat</sub> [26] interactions are displayed along with available experimental data.

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V. Somà, V. Lapuox, CB, et al., in preparation

## BE and charge radii in <sup>A</sup>Ca



## BE and charge radii in <sup>A</sup>Ca



# charge radii in the pf shell

Size of radii not prefect but remains overall correct throughout the *pf* shell with NNLO-sat.

This suggests that saturation is indeed under control.

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→ Improvements of many-body truncations beyond 2<sup>nd</sup> order Gorkov will also be relevant. (work in progress!)



## Study of nuclear interactions from Lattice QCD

#### Other paths in LQCD, see:



with  $m_{\pi} = 0.51$  GeV and  $m_N = 1.32$  GeV. The bound states are distinguished from the attractive scattering states by investigating the spatial volume dependence of the energy shift  $\Delta E_L$ . In the infinite spatial volume limit we obtain

$$-\Delta E_{\infty} = \begin{cases} 43(12)(8) & \text{MeV for }^{4}\text{He,} \\ 20.3(4.0)(2.0) & \text{MeV for }^{3}\text{He,} \\ 11.5(1.1)(0.6) & \text{MeV for }^{3}\text{S}_{1}, \\ 7.4(1.3)(0.6) & \text{MeV for }^{1}\text{S}_{0}. \end{cases}$$
(17)

PACS-CS PRD 86, 074514 (2012)

## Study of nuclear interactions from Lattice QCD

In collaboration with:





#### Why should we investigate LQCD interactions?

It gives complimentary insight to the EFT approach:

Allows to approach physical interaction from heavy quark masses
(opposite direction than the chiral limit).
Can study implications of SU(3) limit.

No need to fit to experiment. No LEC constants.
Provides consistent interactions in the Hyperon sector.

- It is very fundamental approach (QCD), and an alternative to Chiral-EFT.

#### Challenges and limitations:

- Mostly LO terms of the NN force exploited so far (but being improved).
- Physical pion mass limit requires efforts (but underway).
- NNN only barely addressed.
- Strong short-range repulsion is a challenge to ab-initio approaches.





$$L = -\frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a + \bar{q}\gamma^{\mu}(i\partial_{\mu} - gt^aA^a_{\mu})q - m\bar{q}q$$



а

Vacuum expectation value  $\langle O(\bar{q},q,U) \rangle$ path integral  $= \int dU d\bar{q} dq e^{-S(\bar{q},q,U)} O(\bar{q},q,U)$  $= \int dU \det D(U) e^{-S_U(U)} O(D^{-1}(U))$  $= \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} O(D^{-1}(U_i))$ 

{ U<sub>i</sub> } : ensemble of gauge conf. U generated w/ probability det  $D(U) e^{-S_U(U)}$ 

Well defined (reguralized) \* Fully non-perturvative Manifest gauge invariance

★ Highly predictive

Q

Slide, courtesy of T. Inoue (YITP talk, Oct. 8th 2015)

## The HAL-QCD Method

Define a general potential  $U(\mathbf{r},\mathbf{r}')$  which is and non-local but energy independent up to inelastic threshold, such that:

$$\frac{-\nabla^2}{2\mu}\varphi_{\vec{k}}(\vec{r}) + \int d\vec{r}' U(\vec{r},\vec{r}')\varphi_{\vec{k}}(\vec{r}') = E_{\vec{k}}\varphi_{\vec{k}}(\vec{r})$$

for the Nambu-Bethe-Salpeter (NBS) wave function,

$$\varphi_{\vec{k}}(\vec{r}) = \sum \langle 0|B_i(\vec{x}+\vec{r},t)B_j(\vec{x},t)|B=2,\vec{k}\rangle$$

Operationally, measure the 4-pt function on the QCD Lattice

$$\psi(\vec{r},t) = \sum_{\vec{x}} \langle 0|B_i(\vec{x}+\vec{r},t)B_j(\vec{x},t) J(t_0)|0\rangle = \sum_{\vec{k}} A_{\vec{k}}\varphi_{\vec{k}}(\vec{r})e^{-W_{\vec{k}}(t-t_0)} + \dots$$

and extract U(**r**,**r**') from:

$$\left\{2M_B - \frac{\nabla^2}{2\mu}\right\}\psi(\vec{r},t) + \int d\vec{r}' U(\vec{r},\vec{r}')\psi(\vec{r}',t) = -\frac{\partial}{\partial t}\psi(\vec{r},t)$$

A *local potential*  $V(\mathbf{r})$  is then obtained through a derivative expansion of  $U(\mathbf{r}, \mathbf{r}')$ , which *must give the same observables* of the LQCD simulation:

$$U(\vec{r},\vec{r}') = \delta(\vec{r}-\vec{r}')V(\vec{r},\nabla) = \delta(\vec{r}-\vec{r}')\left\{V(\vec{r}) + \mathcal{O}(\nabla) + \mathcal{O}(\nabla^2) + \dots\right\}$$

$$V(\vec{r}) = \frac{1}{2\mu} \frac{\nabla^2 \psi(\vec{r},t)}{\psi(\vec{r},t)} - \frac{\frac{\partial}{\partial t}\psi(\vec{r},t)}{\psi(\vec{r},t)} - 2M_B$$
Tensor/Yukawa force in S-D
Tensor/Yukawa force in S-D

Prog. Theor. Phys. 123 89 (2010); Phys. Lett. B712 , 437 (2012); Prog. Theor. Exp. Phys. 01A105 (2012)

## The HAL-QCD Method

#### Advantages:

- ✓ No need to separate E eigenstate. Just need to measure  $\psi(\vec{r}, t)$
- $\checkmark$  Then, potential can be extracted.
- ✓ Demand a minimal lattice volume. No need to extrapolate to V=∞.
- ✓ Can output more observables.
- ✓ One can address *large nuclei* too!!





Prog. Theor. Exp. Phys. 01A105 (2012)

## Two-Nucleon HAL potentials



Prog. Theor. Exp. Phys. 01A105 (2012)

# Two-Nucleon HAL potentials



#### Potential in partial waves at the lightest $m_{\pi}$ =469 MeV:

- Repulsive core, attractive pocket, and strong tensor components
- ✓ Similar to phenomenological potentials (e.q. AV18).
- ✓ Central value obtained from least  $\chi^2$  fit to data.

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✓ Higher orders in the velocity expansion will also be available soon...





Symmetric Nuclear Matter 80 → M<sub>PS</sub>=1171 [MeV]  $\longrightarrow$  M<sub>ps</sub>=1015 [MeV]  $\longrightarrow$  M<sub>PS</sub>=837 [MeV] 60 ■ M<sub>PS</sub>=672 [MeV] Energy/Nulceon, E/A [MeV]  $\longrightarrow$  M<sub>PS</sub>=469 [MeV] dashed lines T=5 MeV 20 -20 1.5 2 3.5 0.5 2.5 0 Fermi momentum, p<sub>F</sub> [fm<sup>-1</sup>]

PNM unbound as usual, but less stiff

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SNM saturates at  $m_{\pi}$ = 469 MeV but under bound and at higher densities that physical. T. Inoue et al., Phys. Rev. Lett. 111 112503 (2013).

Finite-T results by A. Carbone, priv. comm.

## Application of microscopic (Ab-Initio) SCGF to potentials with hard cores.

How do we do it??  $\rightarrow$  With a G-matrix!



## Analysis of Brueckner HF

Scattering of two nucleon in free space:



## Analysis of Brueckner HF

Scattering of two nucleons outside the Fermi sea ( $\rightarrow$ BHF):



## Mixed SCGF-Brueckner approach

Solve full many-body dynamics in model space (P+Q') and the Goldstone's ladders outside it (i.e. in Q'' only):



## Different levels of approximation:



### Sensitivity of BHF of the $\varepsilon(k)$ spectrum



#### Treating short-range corr. with a G-matrix

 The short-range core can be treated by summing ladders outside the model space:

Two contributions to the derivative:

- $\Sigma_{\alpha\beta}^{MF}(\omega)$  is due to scattering to (high-k) states in the Q space
- $\Sigma(\mathbf{r},\mathbf{r}';\omega)$  accounts for low-energy (long range) correlations
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### (Galitskii-Migdal-Boffi-) Koltun sumrule

\* Koltun sum rule (with NNN interactions):



Benchmark on <sup>4</sup>He



→ Can expect accuracy on binding energies at about 10%

<sup>1</sup>H. Nemura *et al.*, Int. J. Mod. Phys. E **23**, 1461006 (2014)



## Binding of <sup>16</sup>O and <sup>40</sup>Ca:



Binding energies are ~15 MeV <sup>16</sup>O and 70-75MeV for <sup>40</sup>Ca. Possibly being underestimated by 10%

 $\rightarrow$  16O at m<sub> $\pi$ </sub>= 469 MeV is unstable toward 4- $\alpha$  breakup!

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## Spectral strength in <sup>16</sup>O and <sup>40</sup>Ca:



D SUKKEY

## Matter distribution of <sup>16</sup>O and <sup>40</sup>Ca:



→ Radii discrepancy worsens with increasing A



#### SCGF in infinite SNM @ $m_{\pi}$ =469MeV



## Summary

#### Mid-masses and chiral interactions:

- → Leading order 3NF are crucial to predict many important features that are observed experimentally (drip lines, saturation, orbit evolution, etc...)
- → Experimental binding is predicted accurately up to the lower sd shell (A≈30) but deteriorates for medium mass isotopes (Ca and above) with roughly 1 MeV/A over binding.
- → New fits of chiral interaction are promising for low-energy observables

#### HALQCD Nuclear forces:

→ Strong short range behavior calls for new ideas in ab-initio many-body methods. Diagram resummation through G-matrix is starting point(to be extended)



→ At  $m_{\pi}$ =469MeV, closed shell 4He, 16O and 40Ca are bound. But oxygen is unstable toward 4- $\alpha$  break up, calcium stays bound. Underestimation of radii increases with A do to large saturation density (as for EM(500)+NLO3NF).

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**A. Cipollone, C. McIlroy** A. Rios, A. Idini, F. Raimondi

V. Somà, T. Duguet



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atomique + energies alternati







S. Aoki, **T. Doi, T. Hatsuda**, Y. Ikeda, **T. Inoue**, N. Ishii, K. Murano, **H. Nemura**, K. Sasaki F. Etminan T. Miyamoto, T. Iritani S. Gongyo YITP Kyoto Univ. RIKEN Nishina Nihon Univ. RCNP Osaka Univ Univ. Tsukuba Univ. Birjand Univ. Tsukuba Stony Brook Univ. YITP Kyoto Univ.



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## Optical Potentials Based on the Nuclear Self-energy



## Self-Consistent Green's Function Approach





### Nucleon elastic scattering





### Convergence of Ab-Initio Calculated Optical Potentials



S. Waldecker, CB, W.Dickhoff – Phys. Rev. C84, 034616 (2011)



#### *p*-<sup>16</sup>*O phase shifts* - *positive parity waves*



[C.B., B.Jennings, Phys. Rev. C**72**, 014613 (2005)]

AV18 interaction

•The phase shift are in agreement with the experiment!

BUT does not reproduce phase shifts and bound state energies at the same time → need for improved H / 3NF

•Non-MF resonances "OK"

### Microscopic Optical Potential from FRPA

- absorption away from  $E_F$  is enhanced by the tensor force
- little effects from charge exchange (e.g. p-<sup>48</sup>Ca <-> n-<sup>48</sup>Sc)



J<sub>w</sub>: integral over the imaginary opt. pot (overall absorption)



S. Waldecker, CB, W.Dickhoff – Phys. Rev. C84, 034616 (2011)
# Adding 3-nucleon forces



### Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

\* NNN forces can enter diagrams in three different ways:

→ Define new 1- and 2-body interactions and use <u>only</u> interaction-irreducible diagrams



 Contractions are with <u>fully correlated density matrices</u> (BEYOND a normal ordering...)



### Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

#### - Second order PT diagrams with 3BFs:

(b)

effectively.



three *interaction reducible* ones (b, c and d) that are contained in Fig. 3a.





A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

- Second order PT diagrams with 3BFs:

- Third order PT diagrams with 3BFs:



→ Use if effective interactions

(b)

Need to correct the Koltun sum rule (for energy)

FIG. 5. 1PI, skeleton and interaction irreducible self-energy diagrams appearing at  $3^{rd}$ -order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).



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## Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

- Second order PT diagrams with 3BFs:



- Third order PT diagrams with 3BFs:



- → Use if effective interactions
- Need to correct the Koltun sum rule (for energy)

FIG. 5. 1PI, skeleton and interaction irreducible self-energy diagrams appearing at  $3^{rd}$ -order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).



## 3N forces in FRPA/FTDA formalism

 $\rightarrow$  Ladder contributions to static self-energy are negligible (in oxygen)



CB, arXiv:1405.3002v2 [nucl-th] (2014)

## 3N forces in FRPA/FTDA formalism

 $\rightarrow$  Ladder contributions to static self-energy are negligible (in oxygen)



