Interfaces between structure and reactions for rare isotopes and nuclear astrophysics ---- INT, Seattle, Aug. 8--Sept.2, 2011

Ab-initio Gorkov-Green's function calculations for open shell nuclei



How to predict exotic isotopes?



INT, Aug. 19th, 2011

State-of-the-art ab-initio nuclear structure theory

* Methods for an ab-initio description of *medium-mass* nuclei as of 2011

(1) Coupled-cluster [Dean, Papenbrock, Hagen, ...]

(2) In-medium similarity renormalization group [Tsukiyama, Bogner, Schwenk]

(3) Self-consistent Dyson-Green's function (SCGF) [Barbieri, Dickhoff]

The present status is:

→ Still in need of good nuclear Hamiltonians (3N forces mostly!)

→Only structure calculations and limited to closed-shells or A±1, A±2 (BUT calculations are GOOD!!!)



However, Green's functions can be extended to: Scattering observables Open shell nuclei





- Self-consistent Green's function in closed shells:
 - Faddeev random-phase approximation (FRPA): ⁴He benchmark Scattering (N-A)
- Open shells: Gorkov-GF formalism
 - G-SCGF formalism at 2nd order
 - Preliminary results
- Applications: spectroscopic factors
- Applications: dispersive optical potentials
 - S. Waldecker, CB, W. Dickhoff, arXiv:1105.4257



Concepts of Spectral Funstions and Many-Body Green's Functions



Interfaces between structure and reactions...

Green's functions in many-body theory

One-body Green's function (or propagator) describes the motion of quasiparticles and holes:

$$g_{\alpha\beta}(E) = \sum_{n} \frac{\langle \Psi_{0}^{A} | c_{\alpha} | \Psi_{n}^{A+1} \rangle \langle \Psi_{n}^{A+1} | c_{\beta}^{\dagger} | \Psi_{0}^{A} \rangle}{E - (E_{n}^{A+1} - E_{0}^{A}) + i\eta} + \sum_{k} \frac{\langle \Psi_{0}^{A} | c_{\beta}^{\dagger} | \Psi_{k}^{A-1} \rangle \langle \Psi_{k}^{A-1} | c_{\alpha} | \Psi_{0}^{A} \rangle}{E - (E_{0}^{A} - E_{k}^{A-1}) - i\eta}$$

...this contains all the structure information probed by nucleon transfer (spectral function):



Green's functions in many-body theory

One-body Green's function (or propagator) describes the motion of quasiparticles and holes:

$$g_{\alpha\beta}(E) = \sum_{n} \frac{\langle \Psi_{0}^{A} | c_{\alpha} | \Psi_{n}^{A+1} \rangle \langle \Psi_{n}^{A+1} | c_{\beta}^{\dagger} | \Psi_{0}^{A} \rangle}{E - (E_{n}^{A+1} - E_{0}^{A}) + i\eta} + \sum_{k} \frac{\langle \Psi_{0}^{A} | c_{\beta}^{\dagger} | \Psi_{k}^{A-1} \rangle \langle \Psi_{k}^{A-1} | c_{\alpha} | \Psi_{0}^{A} \rangle}{E - (E_{0}^{A} - E_{k}^{A-1}) - i\eta}$$

...this contains <u>all the structure information</u> probed by nucleon transfer (spectral function):

$$S(r,\omega) = \frac{\mp 1}{\pi} \operatorname{Im} g_{rr}(\omega) = \sum_{n} |\langle \Psi_{n}^{A\pm 1} | c_{r}^{(+)} | \Psi_{0}^{A} \rangle|^{2} \,\delta(\omega \pm (E_{0}^{A} - E_{n}^{A\pm 1}))$$







[CB, M.Hjorth-Jensen, Pys. Rev. C79, 064313 (2009)

CB, Phys. Rev. Lett. 103, 202502 (2009)]





* Perturbative expansion of one-body propagator



* Irreducible self-energy



Solving the Dyson equation

* Different approximations to the self-energy (self-consistent approaches)



INIVERSITY OF

Applications to doubly-magic nuclei



** Successful in medium-mass doubly-magic systems

Expansion breaks down when pairing instabilities appear





Explicit configuration mixing

Single-reference: Bogoliubov (Gorkov)



Interfaces between structure and reactions...

Self-Consistent Green's Function Approach



Faddeev-RPA is a *many-body* method: <

Interfaces between structure and reactions...

INT, Aug. 19th, 2011





Interfaces between structure and reactions...

mean field only

self-consistency in the

INT, Aug. 19th, 2011

estimates from different approx. to

self-consistency

[Nogga et al., Phys. Rev. C70, 061002 (2004)]



Comparison to CC benchmark





Interfaces between structure and reactions...

INT, Aug. 19th, 2011

UNIVERSITY OF



Interfaces between structure and reactions...

Gorkov formalism: open shells

(CB, V. Somà, T. Duguet -- in completion)



Applications to doubly-magic nuclei



** Successful in medium-mass doubly-magic systems

Expansion breaks down when pairing instabilities appear

Explicit configuration mixing

Single-reference: Bogoliubov (Gorkov)

INT, Aug. 19th, 2011

UNIVERSITY OF

Going to open-shells: Gorkov ansatz

***** 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 $|\Psi_0
angle \equiv \sum_N^{\text{even}} c_N |\psi_0^N
angle$

→ Mixes various particle numbers

$$\searrow \quad \text{Introduce a "grand-canonical" potential} \quad \Omega = H - \mu N$$

$$\implies \quad |\Psi_0\rangle \quad \text{minimizes} \quad \Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$$
under the constraint $N = \langle \Psi_0 | N | \Psi_0 \rangle$

$$\implies \qquad \Omega_0 = \sum_{N'} |c_{N'}|^2 \Omega_0^{N'} \approx E_0^N - \mu N$$



Gorkov Green's functions and equations

℁ Set of 4 Green's functions

$$\begin{split} i G_{ab}^{11}(t,t') &\equiv \langle \Psi_0 | T \left\{ a_a(t) a_b^{\dagger}(t') \right\} | \Psi_0 \rangle &\equiv \int_{b}^{a} \\ i G_{ab}^{21}(t,t') &\equiv \langle \Psi_0 | T \left\{ \bar{a}_a^{\dagger}(t) a_b^{\dagger}(t') \right\} | \Psi_0 \rangle &\equiv \int_{b}^{a} \\ i G_{ab}^{12}(t,t') &\equiv \langle \Psi_0 | T \left\{ a_a(t) \bar{a}_b(t') \right\} | \Psi_0 \rangle &\equiv \int_{\bar{b}}^{a} \\ \end{split}$$



$$\boldsymbol{\Sigma}_{ab}^{\star}(\omega) \equiv \begin{pmatrix} \Sigma_{ab}^{\star \, 11}(\omega) \ \Sigma_{ab}^{\star \, 12}(\omega) \\ \\ \Sigma_{ab}^{\star \, 21}(\omega) \ \Sigma_{ab}^{\star \, 22}(\omega) \end{pmatrix}$$

$$\mathbf{\Sigma}^{\star}_{ab}(\omega) \equiv \mathbf{\Sigma}_{ab}(\omega) - \mathbf{U}_{ab}$$



Interfaces between structure and reactions...

 $\mathbf{G}_{ab}(\omega) = \mathbf{G}_{ab}^{(0)}(\omega) + \sum_{cd} \mathbf{G}_{ac}^{(0)}(\omega) \, \boldsymbol{\Sigma}_{cd}^{\star}(\omega) \, \mathbf{G}_{db}(\omega)$

Gorkov equations

1st & 2nd order diagrams and eigenvalue problem

$$\Sigma_{ab}^{11\,(1)} = \qquad \stackrel{a}{\underset{b}{\bullet}} - - - \stackrel{c}{\underset{d}{\bullet}} \bigodot \downarrow \omega' \qquad \qquad \Sigma_{ab}^{12\,(1)} = \qquad \stackrel{a}{\underset{c}{\bullet}} \stackrel{c}{\underset{\omega'}{\bullet}} \stackrel{o}{\underset{\omega'}{\bullet}} \stackrel{d}{\underset{\omega'}{\bullet}}$$

₩ 2nd order → energy-dependent self-energy

$$\Sigma_{ab}^{11\,(2)}(\omega) = \uparrow_{\omega'}^{a} \bigwedge_{b}^{f} \bigvee_{b}^{e} \downarrow_{\omega'''} + \uparrow_{\omega'}^{a} \bigwedge_{b}^{f} \bigvee_{\bar{h}}^{e} \downarrow_{\omega'''} \qquad \Sigma_{ab}^{12\,(2)}(\omega) = \uparrow_{\omega'}^{a} \bigwedge_{\bar{b}}^{f} \bigvee_{g}^{e} \downarrow_{\omega'''} + \uparrow_{\omega'}^{a} \bigvee_{\bar{b}}^{f} \bigvee_{g}^{e} \downarrow_{\omega'''} + \downarrow_{\omega''}^{a} \bigvee_{\bar{b}}^{f} \bigvee_{g}^{f} \bigvee_{g}$$

Gorkov equations

eigenvalue problem

$$\sum_{b} \left(\begin{array}{c} t_{ab} - \mu_{ab} + \Sigma_{ab}^{11}(\omega) & \Sigma_{ab}^{12}(\omega) \\ \Sigma_{ab}^{21}(\omega) & -t_{ab} + \mu_{ab} + \Sigma_{ab}^{22}(\omega) \end{array} \right) \bigg|_{\omega_{k}} \left(\begin{array}{c} \mathcal{U}_{b}^{k} \\ \mathcal{V}_{b}^{k} \end{array} \right) = \omega_{k} \left(\begin{array}{c} \mathcal{U}_{a}^{k} \\ \mathcal{V}_{a}^{k} \end{array} \right)$$

 $\mathcal{U}_{a}^{k*} \equiv \langle \Psi_{k} | \bar{a}_{a}^{\dagger} | \Psi_{0}
angle \ \mathcal{V}_{a}^{k*} \equiv \langle \Psi_{k} | a_{a} | \Psi_{0}
angle$



Interfaces between structure and reactions...

INT, Aug. 19th, 2011

ī

Gorkov equations

$$\sum_{b} \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma_{ab}^{11}(\omega) & \Sigma_{ab}^{12}(\omega) \\ \Sigma_{ab}^{21}(\omega) & -t_{ab} + \mu_{ab} + \Sigma_{ab}^{22}(\omega) \end{pmatrix} \Big|_{\omega_{k}} \begin{pmatrix} \mathcal{U}_{b}^{k} \\ \mathcal{V}_{b}^{k} \end{pmatrix} = \omega_{k} \begin{pmatrix} \mathcal{U}_{a}^{k} \\ \mathcal{V}_{a}^{k} \end{pmatrix}$$



$$egin{aligned} egin{aligned} & T-\mu+\Lambda & ilde{h} & \mathcal{C} & -\mathcal{D}^{\dagger} \ & ilde{h}^{\dagger} & -T+\mu-\Lambda & -\mathcal{D}^{\dagger} & \mathcal{C} \ & \mathcal{C}^{\dagger} & -\mathcal{D} & E & 0 \ & -\mathcal{D} & \mathcal{C}^{\dagger} & 0 & -E \ \end{pmatrix} egin{pmatrix} \mathcal{U}^k \ \mathcal{V}^k \ \mathcal{W}_k \ \mathcal{Z}_k \end{pmatrix} = \omega_k egin{pmatrix} \mathcal{U}^k \ \mathcal{V}^k \ \mathcal{W}_k \ \mathcal{Z}_k \end{pmatrix} \end{aligned}$$

Energy *independent* eigenvalue problem

with the normalization condition

$$\sum_{a} \left[\left| \mathcal{U}_{a}^{k} \right|^{2} + \left| \mathcal{V}_{a}^{k} \right|^{2} \right] + \sum_{k_{1}k_{2}k_{3}} \left[\left| \mathcal{W}_{k}^{k_{1}k_{2}k_{3}} \right|^{2} + \left| \mathcal{Z}_{k}^{k_{1}k_{2}k_{3}} \right|^{2} \right] = 1$$



Interfaces between structure and reactions...

Green's functions: important features

- Self-consistent approach
- Direct connection to observables
- "> Improvability (diagrammatic expansion)
- Control over many-body requirements (conserving approximations)
- *"* Possible connection to nuclear reactions (dispersive optical models)
- # Drawbacks
- Technically and computationally involved



Preliminary Gorgov results



Interfaces between structure and reactions...

Results

* Calculations of ⁴⁰⁻⁴⁸Ca isotopes

- → Spherical HO basis (no-core): 7 shells, ħw = 22 MeV (very preliminary!)
- \rightarrow V_{low-k} from Ch-EFT N³LO potential with cutoff Λ = 2.1 & 2.5 fm⁻¹
- → NN interaction only

* CEA-CCRT massively-parallel high-performance cluster

- → ~ 40 000 cores, ~ 300 Tflops total
- → Parallelized code

Essential for converged self-consistent second-order calculations

[Entem and Machleidt 2003]

Binding energies

* Systematic along isotopic/isotonic chains has become available



---- Correlation energy close to CCSD and FRPA (thorough comparison planed)

- → Overbinding with A: traces need for (at least) NNN forces
- → Effect of self-consistency significant; i.e. less bound than MBPT2



Spectral function



Shell structure evolution

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

$$\epsilon_{a}^{cent} \equiv h_{ab}^{cent} \delta_{ab} = t_{aa} + \sum_{cd} \bar{V}_{acad}^{NN} \rho_{dc}^{[1]} + \sum_{cdef} \bar{V}_{acdaef}^{NNN} \rho_{efcd}^{[2]} \equiv \sum_{k} S_{k}^{+a} E_{k}^{+} + \sum_{k} S_{k}^{-a} E_{k}^{-}$$
[Baranger 1970, Duguet, CB, et al. 2011]

$$\int_{a}^{N-1} \underbrace{E_{ven N} + 1}_{E_{0}^{-(N)}} N = \underbrace{E_{k}^{-(N)} + 1}_{E_{0}^{-(N)}} A = \underbrace{E_{k}^{-(N)} + 1}_{E_{k}^{-(N)}} A = \underbrace{E_{k}^{$$

[pics. J. Sadoudi]

- ESPE not to be confused with guasiparticle peak
- Particularly true for low-lying state in open-shell due to pairing



Shell structure evolution

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

$$\epsilon_{a}^{cent} \equiv h_{ab}^{cent} \delta_{ab} = t_{aa} + \sum_{cd} \bar{V}_{acad}^{NN} \rho_{dc}^{[1]} + \sum_{cdef} \bar{V}_{acdaef}^{NNN} \rho_{efcd}^{[2]} \equiv \sum_{k} S_{k}^{+a} E_{k}^{+} + \sum_{k} S_{k}^{-a} E_{k}^{-}$$
[Baranger 1970, Duguet, CB, et al. 2011]



→ ESPE not to be confused with quasiparticle peak

- Particularly true for low-lying state in open-shell due to pairing



Natural single-particle occupation

* Natural orbit *a*: $\rho_{ab}^{[1]} = n_a^{nat} \delta_{ab}$

* Associated energy: $\varepsilon_a^{nat} = h_{aa}^{cent}$



* Dynamical correlations similar for doubly-magic and semi-magic

* Static pairing essential to open-shells





* Three-point mass differences



- Systematic underestimation of experimental gaps
- \rightarrow Missing NNN in Σ^{11} changes picture qualitatively





• Self-Consistent Green's Functions (SCGF), is a microscopic *ab-initio* method applicable to medium mass nuclei.

•The greatest advantage is the link to experimental information (\rightarrow spectroscopy)



• Three nucleon forces (3NF) are a *MUST* for accurate predictions of exotic isotopes.

Interfaces between structure and reactions...

INT, Aug. 19th, 2011

UNIVERSITY OF





energie atomique • energies alternatives



W.H. Dickhoff, S. Waldecker





A. Rios

A. Polls





T. Otsuka

D. Van Neck, M. Degroote



M. Hjorth-Jensen



C. Giusti, F.D. Pacati



Interfaces between structure and reactions...

Quasiparticle states and spectroscopic factors



Interfaces between structure and reactions...

Dependence of Spect. Fact. from p-h gap

N3LO needs a monopole correction to fix the p-h gap:

$$\Delta V_{fr}^T \to \Delta V_{fr}^T - (-1)^T \kappa_M,$$

$$\Delta V_{ff}^T \to \Delta V_{ff}^T - 1.5(1-T)\kappa_M,$$

 $r \equiv p_{3/2}, p_{1/2}, f_{5/2}$ $f \equiv f_{7/2}$

Experimental Eph is found for $k_{\rm M}$ =0,57



Correlations & model space (RPA and SM)



Particle-vibration coupling dominates the quenching of spectroscopic factors

Relative strength among fragments requires shell-model approach

[see, e.g. Utsuno et al., AIP Conf. Proc. 1120, 81 (2009). Tsang et al., Phys. Rev. Lett. 102, 062501 (2009)]

		10 osc. shells			Exp. [30]	1p0f space		
		FRPA	full	FRPA		FRPA	SM	ΔZ_{lpha}
		(SRC)	FRPA	$+\Delta Z_{\alpha}$				
	⁵⁷ Ni:							
⁵⁷ Ni	$v1p_{1/2}$	0.96	0.63	0.61		0.79	0.77	-0.02
	$v0f_{5/2}$	0.95	0.59	0.55		0.79	0.75	-0.04
	$v1p_{3/2}$	0.95	0.65	0.62	0.58(11)	0.82	0.79	-0.03
	⁵⁵ Ni:							
⁵⁵ Ni	$v0f_{7/2}$	0.95	0.72	0.69		0.89	0.86	-0.03
	⁵⁷ Cu:							
⁵⁷ Cu	$\pi 1 p_{1/2}$	0.96	0.66	0.62		0.80	0.76	-0.04
	$\pi 0 f_{5/2}$	0.96	0.60	0.58		0.80	0.78	-0.02
	$\pi 1 p_{3/2}$	0.96	0.67	0.65		0.81	0.79	-0.02
	⁵⁵ Co:							
⁵⁵ Co	$\pi 0 f_{7/2}$	0.95	0.73	0.71		0.89	0.87	-0.02

[CB, Phys. Rev. Lett. 103, 202502 (2009) ERSITY OF

Interfaces between structure and reactions...

Quenching of absolute spectroscopic factors



Optical Potentials Based on the Nuclear Self-energy

(CB, Jennings, and Waldecker, CB, Dickhoff)

• Proton-¹⁶O scattering [CB, B. Jennings, Phys. Rev. C72, 014613 (2005)]

• Optical model for the ^ACa chain [S. Waldecker, CB, W. Dickhoff, arXiv:1105.4257]



Self-Consistent Green's Function Approach



Interfaces between structure and reactions...

Nucleon elastic scattering



FRPA self-energy is calculated in h.o. basis and re-expressed in k-space:



$$Z_{lj}^{n} = \int_{0}^{\infty} dk \ k^{2} |\psi^{n}(k)|^{2} = \left[1 - \langle \tilde{\psi}^{n} | \frac{d\Sigma_{lj}^{\star}}{d\omega} | \tilde{\psi}^{n} \rangle \Big|_{\omega = E_{\text{c.m.}}^{n}}\right]^{-1}$$

Interfaces between structure and reactions...



Comparison of Calculated Microcopic and DOM Optical Potentials

Comparison to DOM potential, tone through volume integrals:

$$J_W^{\ell}(E) = 4\pi \int dr r^2 \int dr' r'^2 \operatorname{Im} \Sigma_0^{\ell}(r, r'; E)$$
$$J_V^{\ell}(E) = 4\pi \int dr r^2 \int dr' r'^2 \operatorname{Re} \Sigma_0^{\ell}(r, r'; E)$$

N-^ACa scattering calculated with the chiral NN N3LO and AV18 interactions

For the local DOM $U(\boldsymbol{r},\boldsymbol{r'})=U(r)\delta(\boldsymbol{r}-\boldsymbol{r'})$:

$$J_U^{\ell} = 4\pi \int dr \ r^2 \int dr' r'^2 U^{\ell}(r, r') = 4\pi \int U(r) r^2 dr = \int U(r) \ d\mathbf{r} ,$$

for any ℓ

UNIVERSITY OF

[S. Waldecker, CB, W. Dickhoff]

Interfaces between structure and reactions...

Imaginary self-energy/optical pot. for ⁴⁰Ca



J_W gives the overall inelastic absorption

FIG. 6. Imaginary volume integral J_W^l of ⁴⁰Ca self-energy for neutrons with $\ell = 0 - 5$.

[S. Waldecker, CB, W. Dickhoff, arXiv:1105.4257]

Interfaces between structure and reactions...



Dispersive real parts J_V



Volume Integrals of Re Σ_0^{ℓ} for neutrons in ⁴⁰Ca. The horizontal, dashed lines are the volume integrals of $\Sigma_0^{\infty,\ell}(E_F)$.

The OP must dependence on angular momentum! \rightarrow non locality.

Interfaces between structure and reactions...

FRPA



FIG. 8. Angular momentum dependence for the volume Integrals $J_F^{L}=J_V^{\ell}(E_F)$ of $\Sigma^{\infty,\ell}(E_F)$ excluding the contribution of the dynamic part of the self-energy. For each ℓ , results for protons are given by solid diamonds and neutrons by solid circles. Proton potentials are considerably less attractive due to the Coulomb energy. When the Coulomb interaction is suppressed (open diamonds) the proton results are close to the neutron results. The results shown are for $^{40}\mathrm{Ca}$ using the AV18 interaction.





Microscopic Optical Potential from FRPA

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



J_w: integral over the imaginary opt. pot (overall absorption)



[S. Waldecker, CB, W. Dickhoff, arXiv:1105.4257]

Interfaces between structure and reactions...



Interfaces between structure and reactions...

