Proposal for an *ab initio-driven* nuclear EDF method

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FUSTIPEN Topical Meeting
Future directions for nuclear structure and reaction theories: Ab initio approaches for 2020

Outline

I. **Motivations and research proposal**

II. **BMBPT-based off-diagonal EDF kernels**

III. **Resulting EDF scheme and workplan**

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Motivation

✪ **Ab initio many-body approaches**

➟ Considerable progress in mid-mass region over last few years, still limited applicability

➟ New techniques available based on idea borrowed from effective mean-field methods

- Symmetry breaking [Somà *et al.* 2011, Hergert *et al.* 2013, Signoracci *et al.* 2014]
  scgf imsrg cc
- Symmetry restoration [Hergert *et al.* 2013, Duguet 2015, Duguet & Signoracci 2015]
  imsrg cc cc

➟ Down from factorial to «high» polynomial computational scaling

✪ **Nuclear energy density functional method – SR & MR implementations**

➟ Extended reach - codes with fantastic potential ⇔ MR is the real deal today

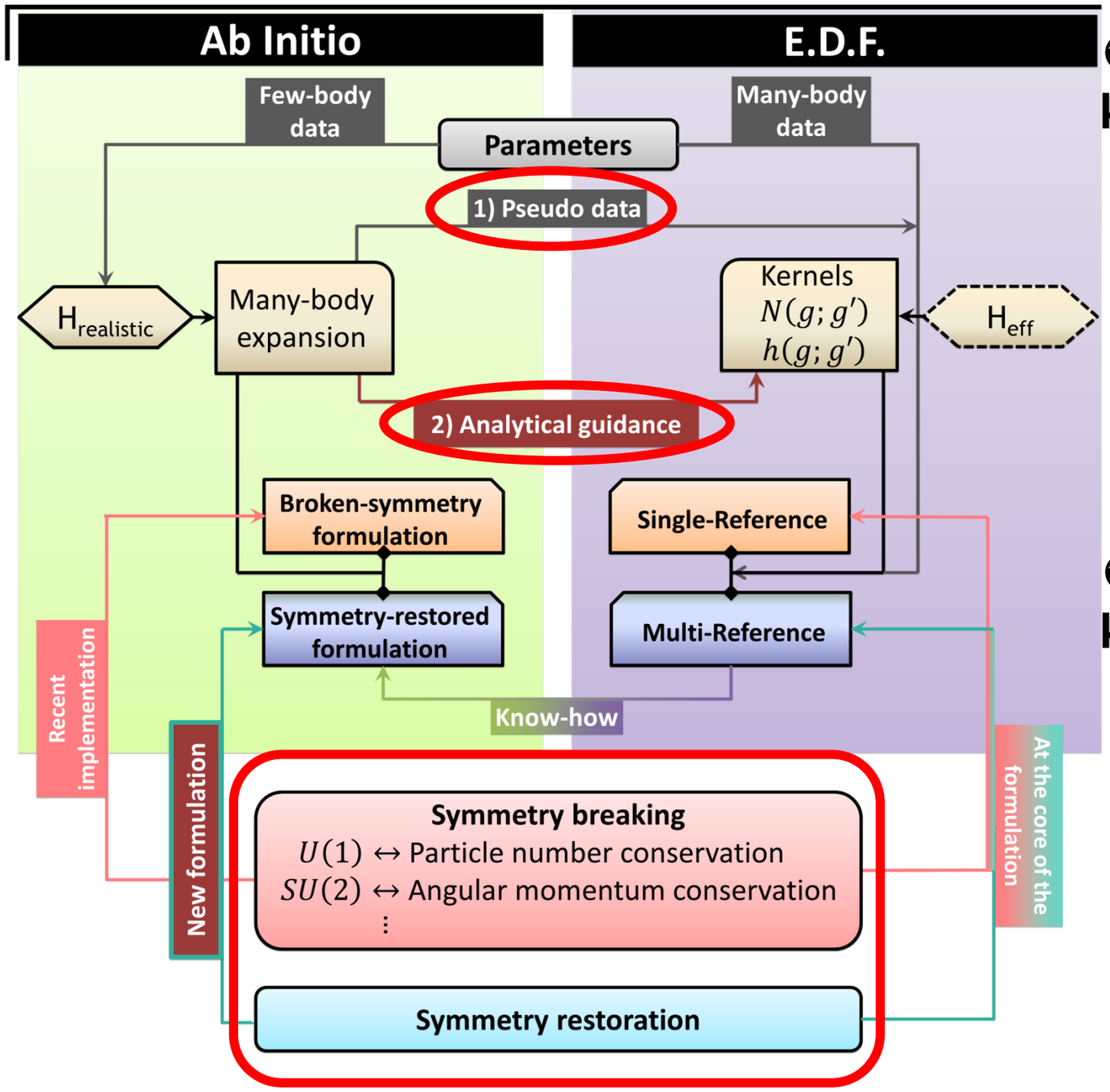
➟ Empirical parameterisations plagued with critical pathologies at MR level

➟ Low polynomial computational scaling for SR but MR is becoming intensive

Can ab initio techniques help in developing safe/correlated/improvable EDFs?

Ab initio vs EDF approaches

In which ways the EDF approach can be rooted into Ab initio many-body methods?



✪ **Pseudo data to fix param. of EDF kernels**

➟ Complement data in unknown regions

➟ H+many-body must be mature enough

Not yet the case for mid-mass nuclei that constitute the natural overlap with EDF method

✪ **Analytical guidance to build EDF kernels**

➟ Must be based on same key principles

➟ Symmetry breaking and restoration

Has made the fortune of the EDF method

Beyond classic SR & MR EDF schemes

✪ Classic SR & MR EDF schemes

➟ Lack of accuracy/predictive power with current form of EDF kernels

➟ MR plagued with pathologies [Dobaczewski *et al.* 2007, Lacroix *et al.* 2009, Duguet *et al.* 2009]

Due to EDF kernels generated from 1) *density-dependent* and/or 2) *different* operators

✪ Possible routes

➟ Regularisation schemes [Bender *et al.* 2009, Satula and Dobaczewski 2014]

➟ Stick to pseudopotentials H_{eff} in mean-field kernels [Dobaczewski *et al.* 2012, Sadoudi *et al.* 2013]

➟ Work at SR level only?

➟ ....

➟ No density-dependence in effective Hamiltonian H_{eff}
➟ Important to do but probable lack of flexibility

✪ This proposal

1) Strict pseudopotential-based method: H_{eff}

2) Use ab initio techniques to build improvable/correlated/safe EDF kernels

3) Symmetry broken&restored BMBPT/BCC techniques allows for guidance

[T. Duguet, J. Phys. G 42 025107 (2015)]
[T. Duguet, A. Signoracci, arXiv:1512.02878]

EDF method in one slide - Focus on U(1) symmetry

Off-diagonal density matrix

$$\mathcal{R}_{ij}(\varphi) \equiv \begin{pmatrix} \dfrac{\langle\Phi|c_j^\dagger c_i|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle} & \dfrac{\langle\Phi|c_j c_i|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle} \\ \dfrac{\langle\Phi|c_j^\dagger c_i^\dagger|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle} & \dfrac{\langle\Phi|c_j c_j^\dagger|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle} \end{pmatrix} \equiv \begin{pmatrix} +\rho_{ij}(\varphi) & +\kappa_{ij}(\varphi) \\ -\bar{\kappa}^*_{ij}(\varphi) & -\sigma^*_{ij}(\varphi) \end{pmatrix}$$

Gauge rotation

$$S(\varphi) \equiv e^{iA\varphi}$$

Bogoliubov state

$$|\Phi\rangle \equiv C\prod_\mu \beta_\mu|0\rangle$$

$$|\Phi(\varphi)\rangle \equiv e^{iA\varphi}|\Phi\rangle$$

Gauge-rotated Bogoliubov state

✪ **Off-diagonal EDF kernels**

All $h(\varphi)$ are functionals of $\mathcal{R}(\varphi)$ — But empirical choices break Pauli principle

Norm kernel
Classic choices
Energy kernel

$$N(\varphi) = \langle\Phi|\Phi(\varphi)\rangle$$

$$h(\varphi) = \frac{\langle\Phi|H_{\rm eff}|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle} \quad \Big| \quad \frac{\langle\Phi|H[\mathcal{R}(\varphi)]|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle} \quad \Big| \quad h[\mathcal{R}(\varphi)]$$

1970s’ 1990s’ 2010s’?

✪ **SR implementation = HFB + particle-number breaking scheme**

✪ **MR implementation = HFB + particle-number restoration scheme**

$$E_{\rm SR} \equiv \mathrm{Min}_{\mathcal{R}(0)}\Big\{H(0) - \lambda\left[\mathrm{A} - A(0)\right]\Big\}$$

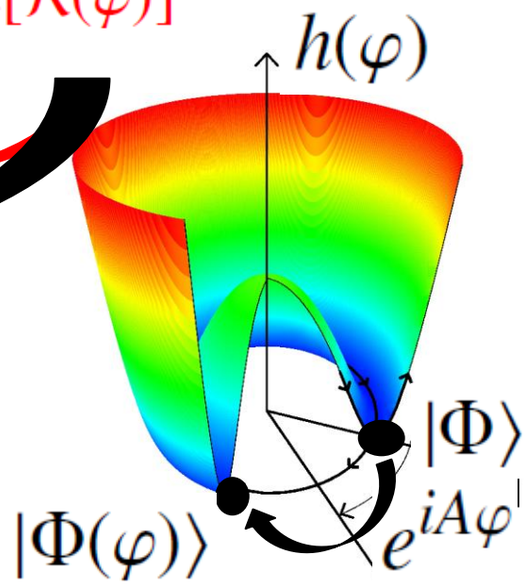
$$E_{\rm MR} = \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{-i\mathrm{A}\varphi}\, N(\varphi)$$

Diagonal kernels

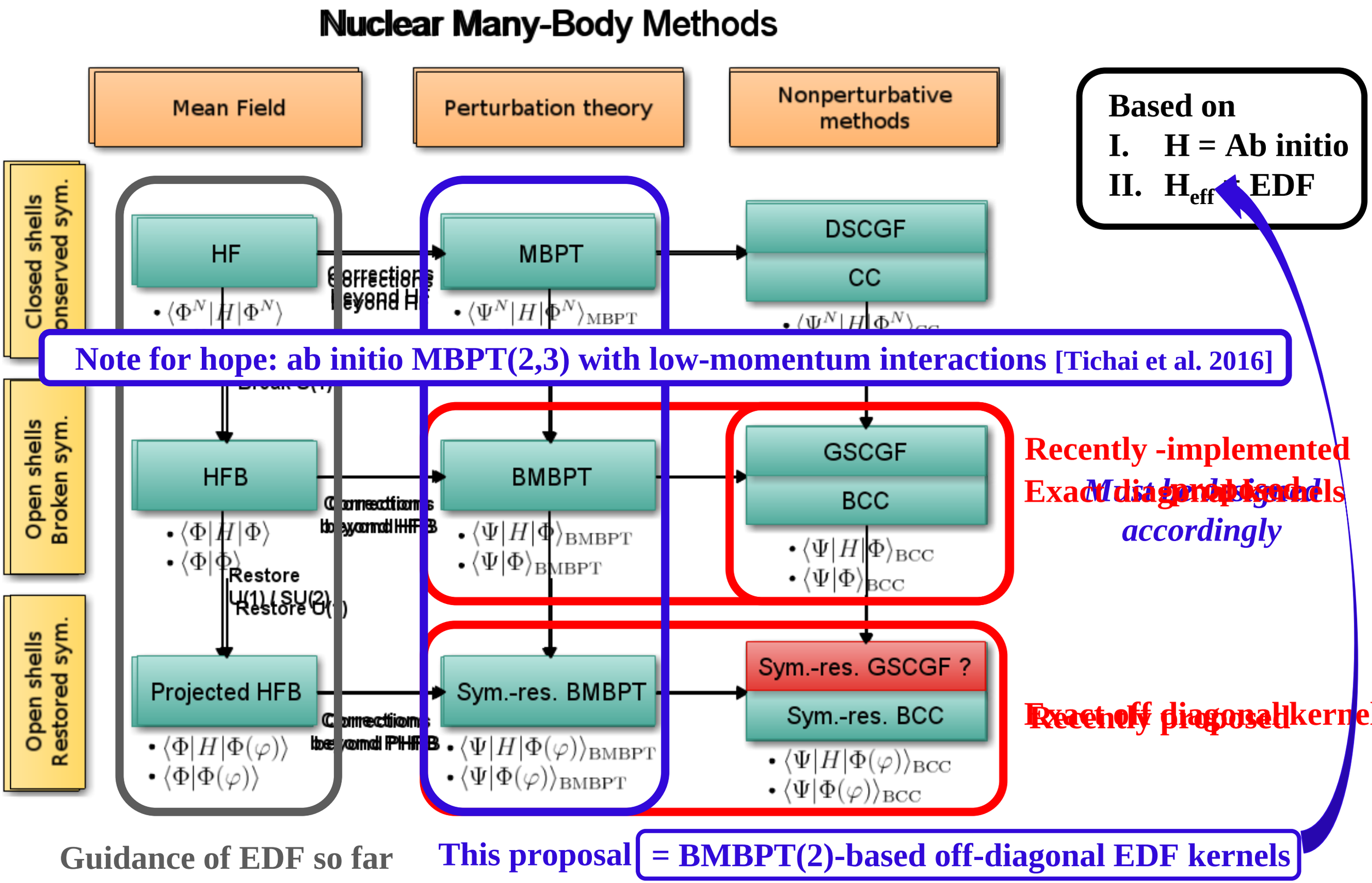
Off-d

H-d

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}\begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$



Correlated/improvable EDF kernels – Focus on U(1) symmetry



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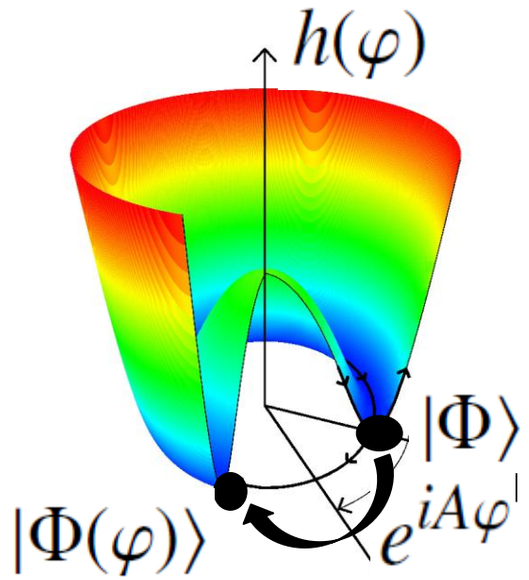
BMBPT of off-diagonal kernels – Focus on U(1) symmetry

✪ **Normal-ordered grand potential (work on Fock space)**



Ω^{ij} ⇔i creation/j annihilation QP operators

$$\begin{aligned}\Omega_{\text{eff}} &\equiv H_{\text{eff}} - \lambda A \\ &= \Omega^{00} + \Omega^{20} + \Omega^{11} + \Omega^{02} + \Omega^{40} + \Omega^{31} + \Omega^{22} + \Omega^{13} + \Omega^{04}\end{aligned}$$

✪ **Exact (fully correlated) off-diagonal kernels**

$$\left.\begin{aligned} N(\varphi) &\equiv \langle\Psi|\Phi(\varphi)\rangle \\ H(\varphi) &\equiv \langle\Psi|H_{\text{eff}}|\Phi(\varphi)\rangle \\ A(\varphi) &\equiv \langle\Psi|A|\Phi(\varphi)\rangle \end{aligned}\right\} \quad \Omega(\varphi) = H(\varphi) - \lambda A(\varphi)$$

Generalized BMBPT

$$\begin{aligned} H(\varphi) &\equiv h(\varphi)N(\varphi) \\ A(\varphi) &\equiv a(\varphi)N(\varphi) \\ \Omega(\varphi) &\equiv \omega(\varphi)N(\varphi) \end{aligned}$$

Linked-connected kernel of the operator
=
Sum of all connected diagrams *linked* to the operator

Technical details, diagrammatic method, full expressions, CC extension etc; see [T. Duguet, A. Signoracci, arXiv:1512.02878]

Off-diagonal kernels at BMBPT(2) – Focus on U(1) symmetry

✪ **Off-diagonal density matrix**

Angle-dependent part

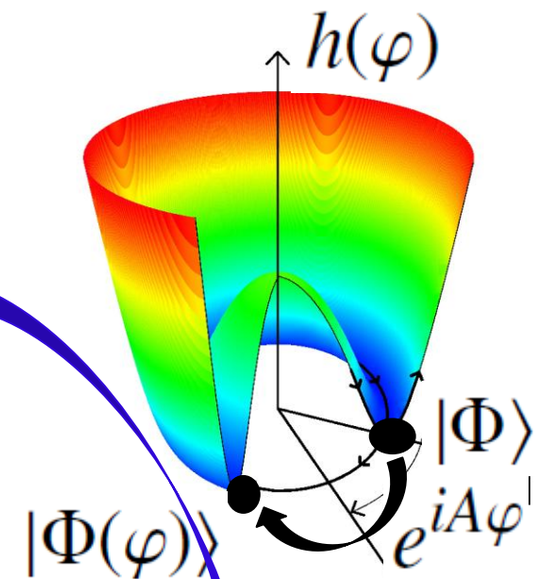
$$R(\varphi) = R(0) + R^{--}(\varphi)$$

Diagonal part

✪ **Non-unitary transformation**

$$\tilde{\Omega}_{\rm eff}(\varphi) \equiv M(\varphi)\Omega_{\rm eff}M^{-1}(\varphi)$$

Polynomial in R(φ)



✪ **Off-diagonal linked/connected grand-potential kernel at BMBPT(2)**

Mean-field

$$\omega^{(2)}(\varphi) = \tilde{\Omega}^{00}(\varphi) - \frac{1}{4}\sum_{k_1k_2k_3k_4}\frac{\Omega^{04}_{k_1k_2k_3k_4}\tilde{\Omega}^{20}_{k_1k_2}(\varphi)}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}R^{--}_{k_4k_3}(\varphi) - \frac{1}{4!}\sum_{k_1k_2k_3k_4}\frac{\Omega^{04}_{k_1k_2k_3k_4}\tilde{\Omega}^{40}_{k_1k_2k_3k_4}(\varphi)}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}$$

$\omega^{(1)}(\varphi)$

Functional of both R(φ) and E_k

✪ **Mean-field kernel ⇔ Standard guidance of EDF**

$\omega^{(2)}(\varphi)$ much richer for given $H_{\rm eff}$

From quartic down to quadratic polynomial in R(φ) + no dep. in E_k

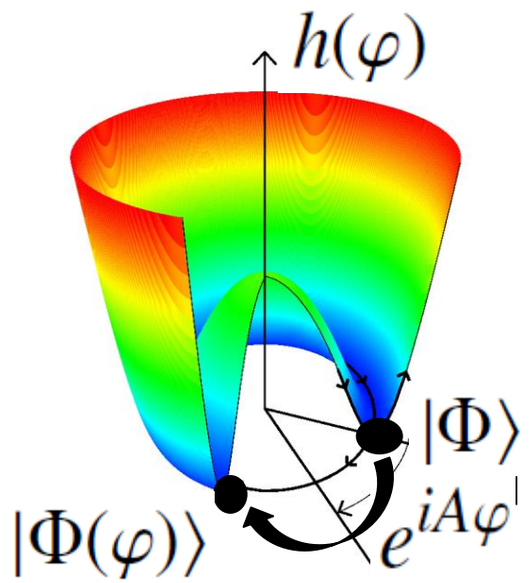
$$\omega^{(1)}(\varphi) \equiv \frac{\langle\Phi|\Omega_{\rm eff}|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle} = \Omega^{00} + \frac{1}{2}\sum_{k_1k_2}\Omega^{02}_{k_1k_2}R^{--}_{k_2k_1}(\varphi) + \frac{1}{8}\sum_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_4}R^{--}_{k_4k_3}(\varphi)R^{--}_{k_2k_1}(\varphi)$$

Off-diagonal kernels at BMBPT(2) – Focus on U(1) symmetry

✪ **Diagonal kernel at φ=0 ⇔ Standard BMBPT(2)**

$$\omega^{(2)}(0) = \frac{\langle\Phi|\Omega_{\text{eff}}|\Phi\rangle}{\langle\Phi|\Phi\rangle} - \frac{1}{4!}\sum_{k_1k_2k_3k_4}\frac{\Omega^{04}_{k_1k_2k_3k_4}\Omega^{40}_{k_1k_2k_3k_4}}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}$$

Recover standard BMBPT(2) at φ=0



✪ **Norm kernel**

$$\frac{d}{d\varphi}\mathcal{N}(\varphi) - i\,a(\varphi)\,\mathcal{N}(\varphi) = 0$$

First order ODE involving linked/connected kernel of A

$$\begin{cases} \mathcal{N}^{(2)}(\varphi) = e^{i\int_0^\varphi d\phi\, a^{(2)}(\phi)} = e^{-\frac{i}{4}\sum_{k_1k_2k_3k_4}\int_0^\varphi d\phi \frac{\Omega^{04}_{k_1k_2k_3k_4}\tilde{A}^{20}_{k_1k_2}(\phi)}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}R^{--}_{k_4k_3}(\phi)}\langle\Phi|\Phi(\varphi)\rangle \\ a^{(2)}(\varphi) = \tilde{A}^{00}(\varphi) - \frac{1}{4}\sum_{k_1k_2k_3k_4}\frac{\Omega^{04}_{k_1k_2k_3k_4}\tilde{A}^{20}_{k_1k_2}(\varphi)}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}R^{--}_{k_4k_3}(\varphi) \end{cases}$$

2nd order correction

Mean field

Consistent correction
Absent from empirical EDF

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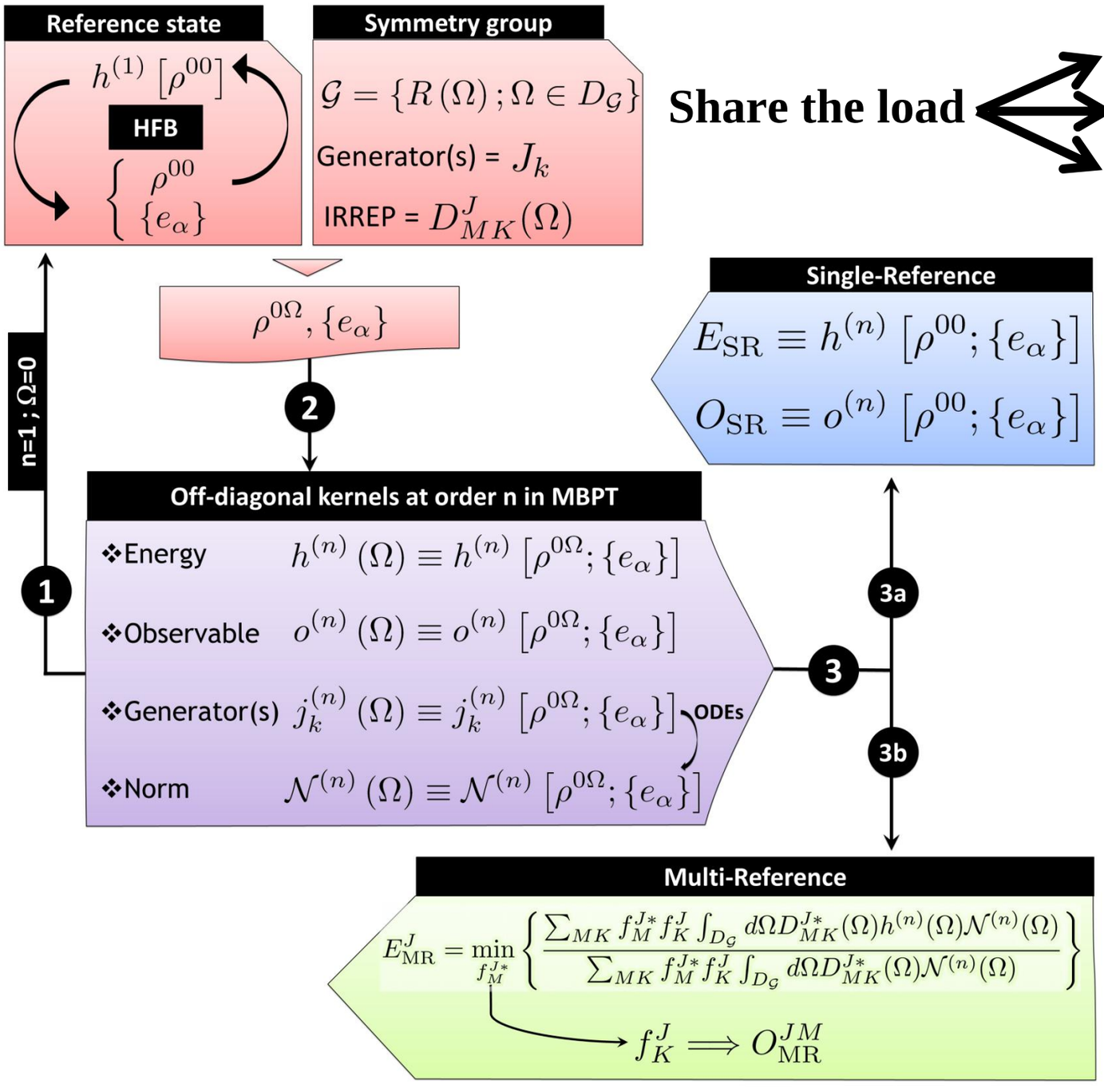
EDF scheme and workplan



✪ Three-fold expansion

Share the load

1. H_{eff}
2. MR mixing = static correlations
3. Kernels expansion = dynamical correlations

Fixed H_{eff} empirically considered here

Need consistent expansion eventually

✪ Short-term plan

1. Deal with U(1) only [SU(2) later]
2. Study safe character vs truncation
3. Validate many-body method for $H_{pairing}$
4. H_{eff} = effective Gaussian vertex

P. Arthuis Ph.D thesis

Sup: J.-P. Ebran, T. Duguet
Collab: V. Somà, M. Bender

Conclusive remarks

- The present formalism consistently treats **non-dynamical** and **dynamical** correlations
  - ➟ Non-dynamical correlations through MR mixing
  - ➟ Dynamical correlations through expansion of kernels in terms of *qp* excitations
  - ➟ In addition, one can enrich H_{eff} with higher-body operators
- Augmenting the content of kernels and/or H_{eff}, parameters of H_{eff} must be **re-optimised**
- Consistent treatment of energy and norm kernels is crucial
- All other operators can be treated on the same footing
- First obvious step is MBPT(2), but other many-body expansions can be envisioned
  - ➟ Optimise balance between complexity of many-body expansions and of Heff
- The formalism allows to perform safe MR calculations, however it does not guarantee it
  - ➟ Incautious many-body truncations might still induce self-interactions/self-pairing
  - ➟ Further study of which are the **safe truncations** is needed