Vertical&horizontal expansions within MR-EDF method

T. Duguet

[1] CEA Saclay, France
[2] KU Leuven, Belgium
[3] MSU, USA

Relevant publications

1) *Symmetry broken and restored coupled-cluster theory: II. Global gauge symmetry and particle number*
T. Duguet, A. Signoracci, J. Phys. G: Nucl. Part. Phys. 44 (2016) 015103
2) *Ab initio-driven nuclear energy density functional method*
T. Duguet, M. Bender, J.-P. Ebran, T. Lesinski, V. Somà, Eur. Phys. J. A51 (2015) 162
3) *Bogoliubov many-body perturbation theory calculations of open-shell nuclei*
P. Arthuis, A. Tichai, H. Hergert, R. Roth, J. P. Ebran, T. Duguet, in preparation
4) *On the norm overlap between many-body states. I. Uncorrelated off-diagonal norm kernels*
B. Bally, T. Duguet, in preparation
5) *On the norm overlap between many-body states. II. Correlated off-diagonal norm kernels*
P. Arthuis, B. Bally, T. Duguet, in preparation

ESNT workshop on *Pertinent ingredients for MR EDF calculations*
February 27 – March 2, 2017, Saclay, France

Outline

I. **Basics and shortcomings of current MR-EDF method**
II. **Many-body expansion of off-diagonal energy&norm kernels**
III. **Norm kernel between arbitrary Bogoliubov product states**
IV. **Conclusions**

Outline

I. **Basics and shortcomings of current MR-EDF method**

II. **Many-body expansion of off-diagonal energy&norm kernels**

III. **Norm kernel between arbitrary Bogoliubov product states**

IV. **Conclusions**

Vertical and horizontal expansions

✪ Vertical expansion

➟ Mix of **orthogonal** product states differing via **non-collective** (quasi-)ph excitations over **one vacuum**

$$|\Phi_1\rangle \equiv \prod_{i=1}^{A} a_i^\dagger |0\rangle \quad , \quad |\Phi_l\rangle \equiv |\Phi_{ij\ldots}^{ab\ldots}\rangle \equiv a_a^\dagger a_i a_b^\dagger a_j \ldots |\Phi\rangle \quad , \quad \forall l = 1, \ldots \dim\mathcal{H}_A$$

➟ Efficienty capture « **dynamical** » correlations (in quantum chemistry language)

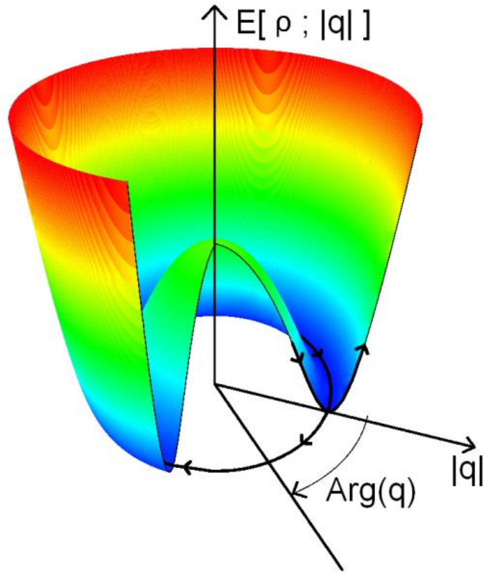
➟ Dominant in **ab initio** philosophy (NCSM, MBPT, CC, IMSRG, D-SCGF…)

➟ Usually implemented on top of **symmetry-conserving** vacuum… but not always (e.g. G-SCGF, BCC)

✪ Horizontal expansion

➟ Mix of **non-orthogonal** vacua differing via **collective** transformations

$$|\Phi_1\rangle \equiv \prod_{k=1}^{\dim\mathcal{H}_1} \beta_k |0\rangle \quad , \quad |\Phi_l\rangle \equiv \mathcal{N}_{(1/l)}\, e^{\frac{1}{2}\sum_{kk'} Z_{kk'}^{20}(1/l)\beta_k^\dagger \beta_{k'}^\dagger} |\Phi_1\rangle \quad , \quad \forall l = 1, \ldots n_{\text{set}}$$



➟ Efficienty capture « **non-dynamical** » correlations associated with **near degeneracies**

➟ Dominant in **EDF** philosophy (i.e. adiabatic GCM + symmetry restoration)

➟ Inherently associated with **symmetry breaking and restoration**

Key concepts and shortcomings of current EDF method

✪ Key concepts

➟ Use of product states essentially following an **horizontal expansion**

➟ Symmetry breaking (SR) = **non-zero order parameter**

➟ Symmetry restoration + GCM (MR) = **fluctuation of phase + norm of order parameter**

➟ Key ingredient = **off-diagonal energy and norm kernels**

Implicitely correlated
-Effective operator
-Density-dependent « operator »
-Density (matrix) functional

Uncorrelated

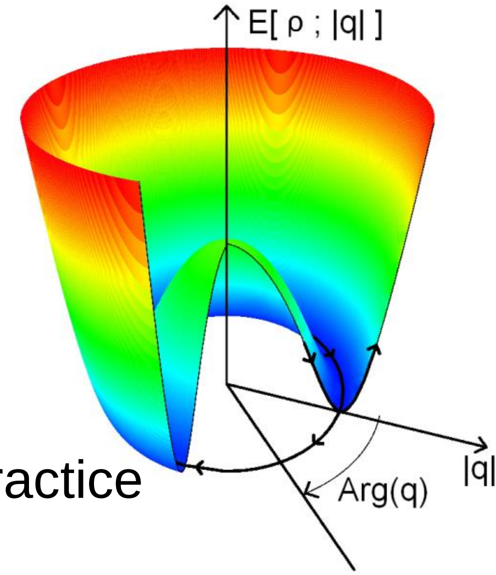
Effective mean-field form

✪ Shortcomings

➟ MR calculations with density-dependent operator/density functional are **ill defined**

➟ Calculations with effective operator + mean-field kernels potentially **lack flexibility**

➟ Lack coupling to **individual excitations/diabatic effects/vertical configurations** in practice



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

Off-diagonal density matrix

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

Gauge rotation

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

Bogoliubov state

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

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

Horizontal set of gauge-rotated Bogoliubov states

✪ Off-diagonal EDF kernels and their parametrisations

Empirical choices break Pauli principle (self interaction/pairing)

[Lacroix et al. 2009, Bender et al. 2009, Duguet et al. 2009]

All $h(\varphi)$ are functionals of $\mathcal{R}(\varphi)$

Pure (effective and phenomenological) **mean-field** kernels

Norm kernel: $N(\varphi) = \langle\Phi|\Phi(\varphi)\rangle$

Classic choices

Energy kernel: $h(\varphi) = \frac{\langle\Phi|H_{\text{eff}}|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle}$ | $\frac{\langle\Phi|H[\mathcal{R}(\varphi)]|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle}$ | $h[\mathcal{R}(\varphi)]$

1970s' 1990s' 2020s'?

✪ SR implementation = particle-number breaking scheme

✪ MR implementation = particle-number restoration scheme

$$E_{\text{SR}} \equiv \text{Min}_{\mathcal{R}(0)}\{H(0) - \lambda[A - A(0)]\}$$

$$E_{\text{MR}} = \frac{1}{2\pi}\int_0^{2\pi} d\varphi\, e^{-iA\varphi}\, N(\varphi) \ldots$$

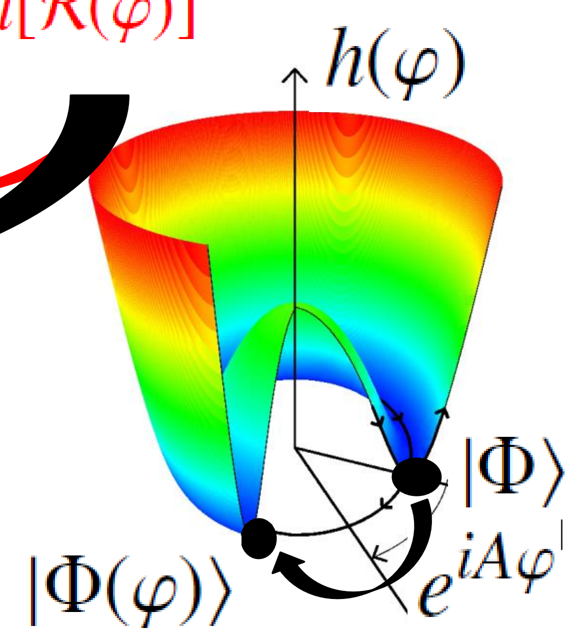
Diagonal kernels

Off-d…

I-de…

[Doba…

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



Outline

I. **Basics and shortcomings of current MR-EDF method**

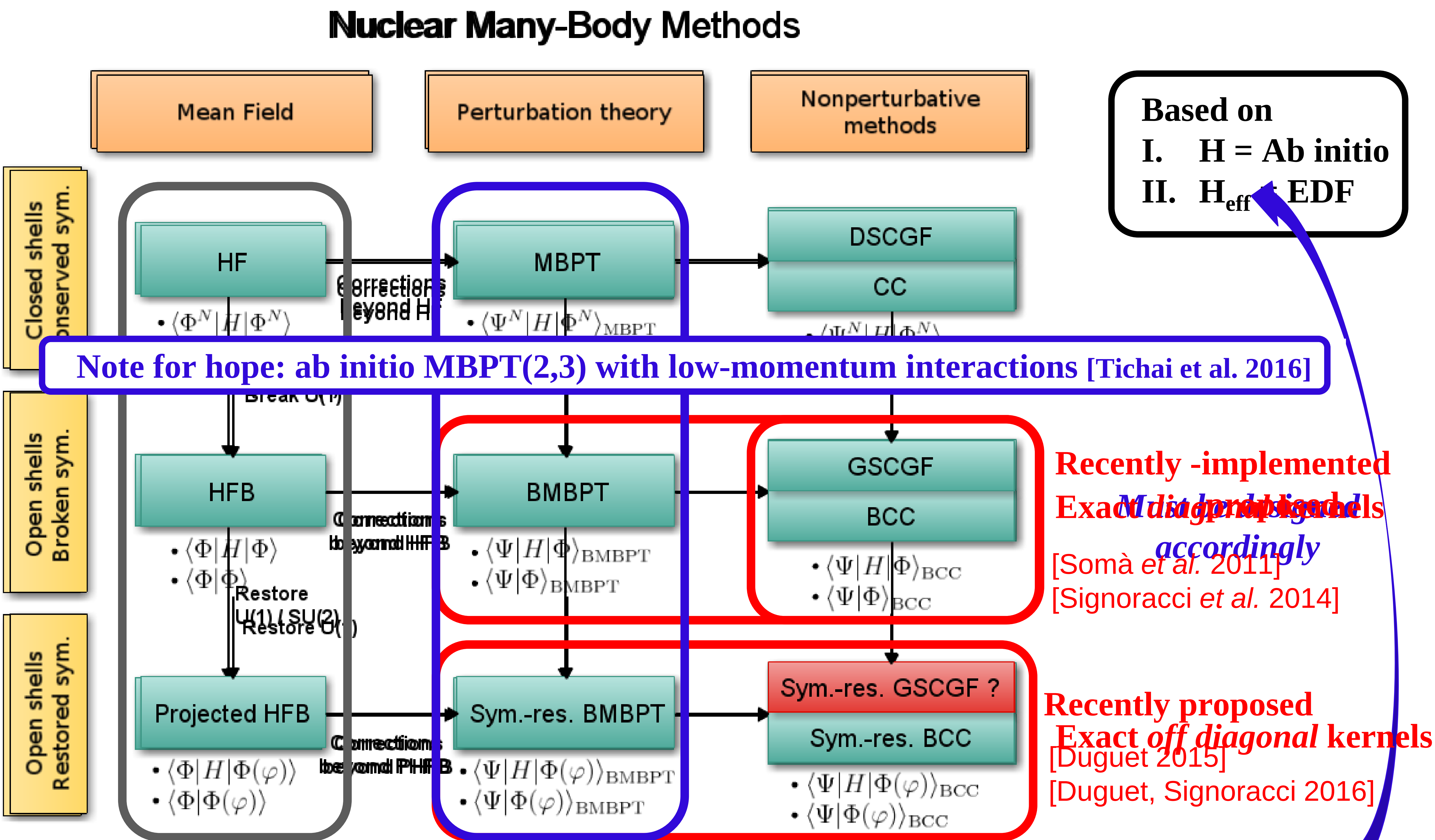
II. **Many-body expansion of off-diagonal energy&norm kernels**

III. **Norm kernel between arbitrary Bogoliubov product states**

IV. **Conclusions**

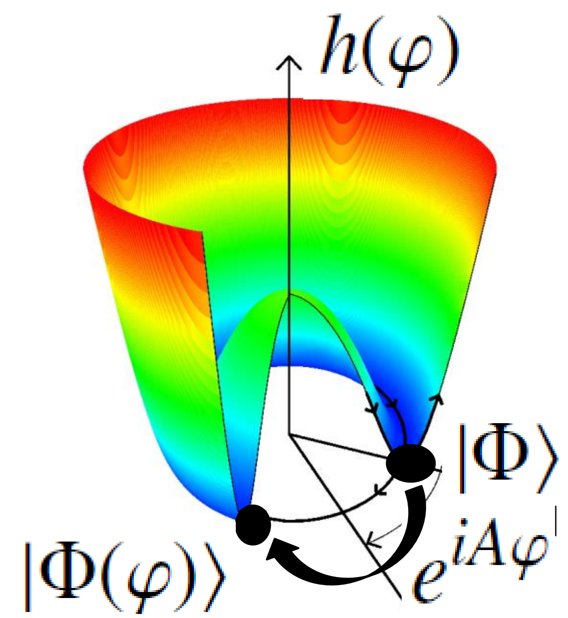
Symmetry broken and restored coupled-cluster theory: II. Global gauge symmetry and particle number
T. Duguet, A. Signoracci, J. Phys. G: Nucl. Part. Phys. 44 (2016) 015103
Ab initio-driven nuclear energy density functional method
T. Duguet, M. Bender, J.-P. Ebran, T. Lesinski, V. Somà, Eur. Phys. J. A51 (2015) 162
Bogoliubov many-body perturbation theory calculations of open-shell nuclei
P. Arthuis, A. Tichai, H. Hergert, R. Roth, J. P. Ebran, T. Duguet, in preparation

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



Guidance of EDF so far — **Our proposal = BMBPT(2,3)-based off-diagonal EDF kernels**

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

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

✪ Correlated off-diagonal kernels

$$|\Psi_0\rangle \equiv U(\infty)|\Phi\rangle$$

Evolution operator

$$\begin{aligned}N(\varphi) &\equiv \langle\Psi_0|\Phi(\varphi)\rangle \\ H(\varphi) &\equiv \langle\Psi_0|H_{\text{eff}}|\Phi(\varphi)\rangle \\ A(\varphi) &\equiv \langle\Psi_0|A|\Phi(\varphi)\rangle\end{aligned}$$

$$\Omega(\varphi) = H(\varphi) - \lambda A(\varphi)$$

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

Diagrammatic, full expressions etc; see [T. Duguet, A. Signoracci, JPG 44 (2016) 015103, P. Arthuis et al., in preparation]

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

✪ **Off-diagonal density matrix**

Angle-dependent part

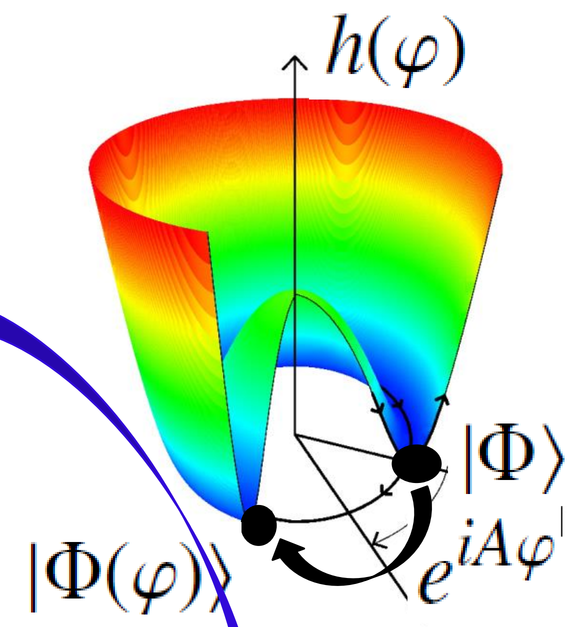
$$R(\varphi) = \underbrace{R(0)}_{\text{Diagonal part}} + \overbrace{R^{--}(\varphi)}^{\text{Angle-dependent part}}$$

Diagonal part

✪ **Non-unitary transformation**

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

Polynomial in $R^{--}(\varphi)$



✪ **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 $R(\varphi)$ and E_k

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

qp/vertical mixing in energy kernel

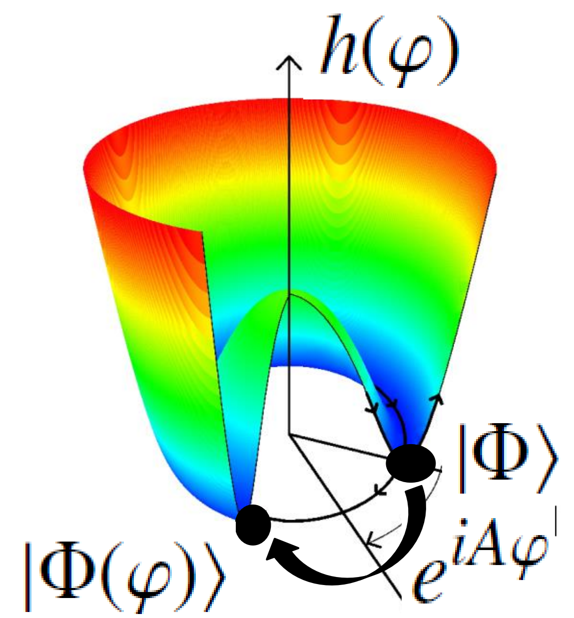
✪ **Mean-field kernel ⇔ Standard guidance of EDF**

$$\omega^{(1)}(\varphi) \equiv \frac{\langle\Phi|\Omega_{\text{eff}}|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle}$$

From quartic down to quadratic polynomial in $R(\varphi)$ + no dep. in E_k

$$= \Omega^{00} + \frac{1}{2}\sum_{k_1k_2}\Omega^{02}_{k_1k_2}R^{--}_{k_2k_1}(\varphi) + \frac{1}{8}\sum_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_4}R^{--}_{k_4k_3}(\varphi)R^{--}_{k_2k_1}(\varphi)$$

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



✪ Diagonal kernel at φ=0 ⬄ Diagonal BMBPT(2)

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

Recover diagonal 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

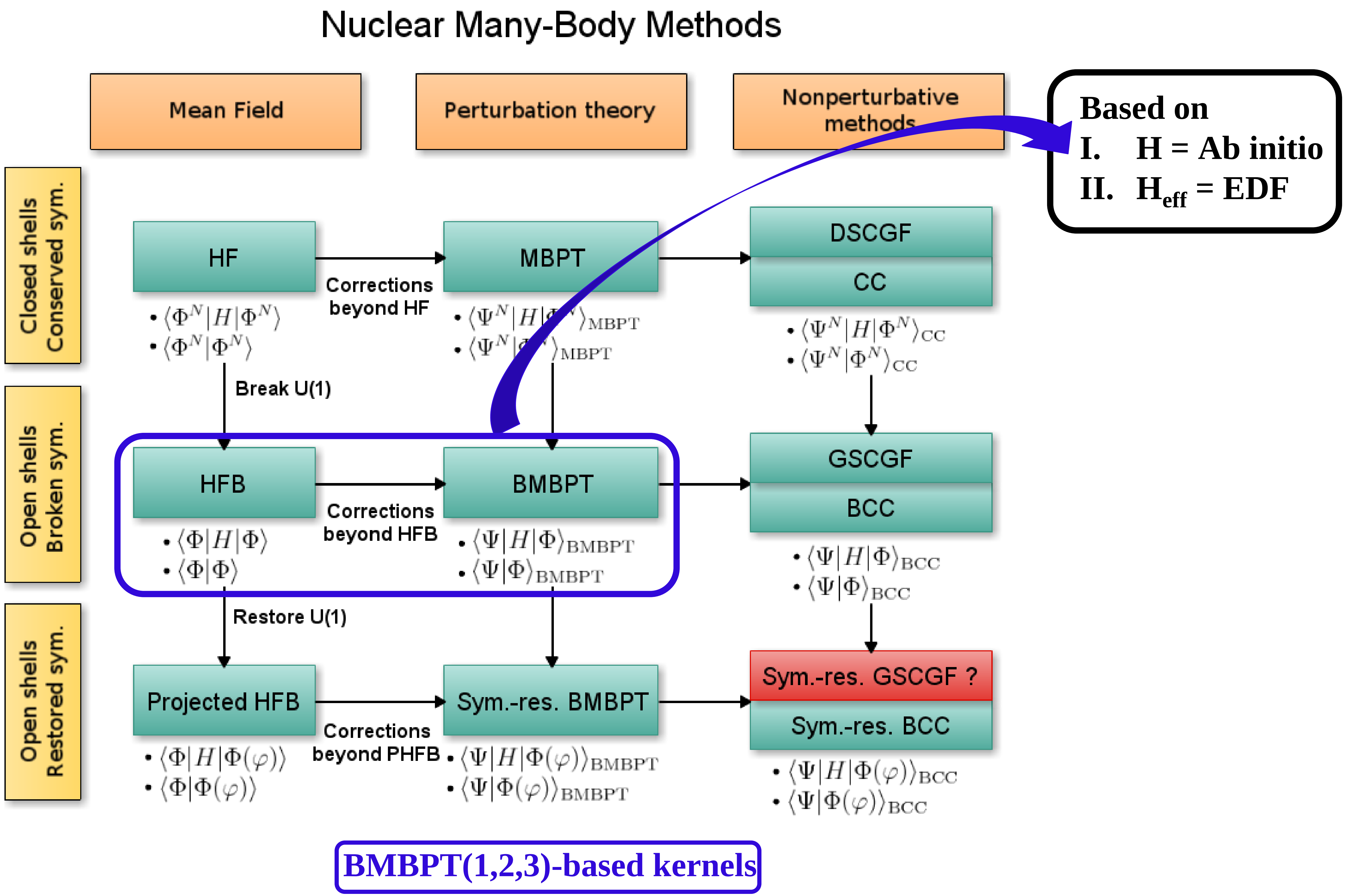
2nd order correction — Mean field

$$\mathcal{N}^{(2)}(\varphi) = e^{i \int_0^{\varphi} d\phi\, a^{(2)}(\phi)}$$ = Closed-form expression at any order $\langle \Phi | \Phi(\varphi) \rangle$

$$a^{(2)}(\varphi) = \tilde{A}^{00}(\varphi) - \frac{1}{4} \sum_{k_1 k_2 k_3 k_4} \frac{\Omega^{04}_{k_1 k_2 k_3 k_4} \tilde{A}^{20}_{k_1 k_2}(\varphi)}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}} R^{--}_{k_4 k_3}(\varphi)$$

Consistent correction
Absent from empirical EDF

First step: diagonal (i.e. SR) BMBPT calculation

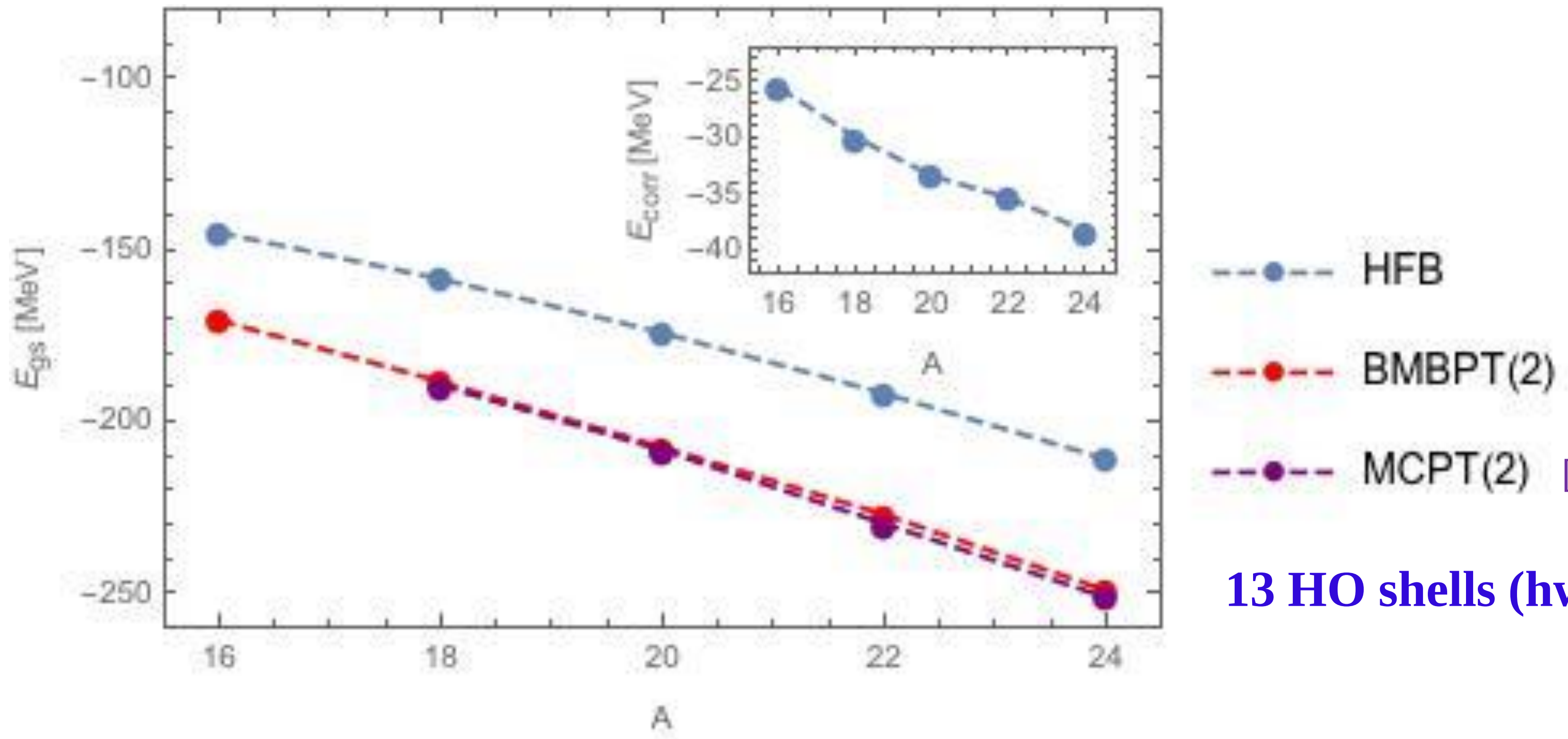


First step: diagonal (i.e. SR) BMBPT calculation

✪ Proof-of-principle BMBPT(1,2) calculations of $^{16-24}O$

➟ SRG-evolved (λ = 1.88 fm^{-1}) E&M 2N χ-EFT interaction (Λ = 500MeV) and **no 3N interaction yet**

➟ **Each order is typically a factor ~10 more CPU intensive** (BMBPT(3) will remain well below BCCSD)



[Tichai, Gebrerufael, Roth, 2017]

13 HO shells (hw = 20 MeV)

➟ Systematic diagonal BMBPT(1,2,3) calculations to come

✪ Next steps

► Implement with **H_{eff}** and proceed to **(re)fit at BMBPT(1,2,3) levels**

« Regularized EDF generator »
K. Bennaceur, J. Dobaczewski et al.
See, e.g., arXiv:1611.09311

► Implement **off-diagonal** kernels and perform **PNR-BMBPT(1,2,3) calculations**

Outline

I. Basics and shortcomings of current MR-EDF method

II. Many-body expansion of off-diagonal energy&norm kernels

III. Norm kernel between arbitrary Bogoliubov product states

IV. Conclusions

On the norm overlap between many-body states. I. Uncorrelated off-diagonal norm kernels
B. Bally, T. Duguet, in preparation

On the norm overlap between many-body states. II. Correlated off-diagonal norm kernels
P. Arthuis, B. Bally, T. Duguet, in preparation

Objectives = General correlated off-diagonal norm kernels

✪ **Given two arbitrary Bogoliubov vacua, i.e. transformations w.r.t known qp set**

$$\left.\begin{array}{l}\begin{pmatrix}\beta\\ \beta^\dagger\end{pmatrix} = \mathcal{W}^\dagger \begin{pmatrix}c\\ c^\dagger\end{pmatrix} \equiv \begin{pmatrix}U^\dagger & V^\dagger\\ V^T & U^T\end{pmatrix}\begin{pmatrix}c\\ c^\dagger\end{pmatrix}\\ \begin{pmatrix}\breve{\beta}\\ \breve{\beta}^\dagger\end{pmatrix} = \breve{\mathcal{W}}^\dagger \begin{pmatrix}c\\ c^\dagger\end{pmatrix} \equiv \begin{pmatrix}\breve{U}^\dagger & \breve{V}^\dagger\\ \breve{V}^T & \breve{U}^T\end{pmatrix}\begin{pmatrix}c\\ c^\dagger\end{pmatrix}\end{array}\right\} \Longleftrightarrow \left\{\begin{array}{l}|\Phi\rangle \;\; \text{such that} \;\; \beta_k^\dagger|\Phi\rangle = 0 \;\forall k\\ |\breve{\Phi}\rangle \;\; \text{such that} \;\; \breve{\beta}_k^\dagger|\breve{\Phi}\rangle = 0 \;\forall k\end{array}\right.$$

✪ **General correlated off-diagonal norm kernel**

$$\boxed{\mathcal{N} = \frac{\langle\Psi_0|\breve{\Phi}\rangle}{\langle\Psi_0|\Phi\rangle}} \qquad \textbf{with} \quad |\Psi_0\rangle \equiv U(\infty)|\Phi\rangle$$

✪ **First order = norm overlap between arbitrary Bogoliubov states**

$$\boxed{\mathcal{N}^{(1)} = \frac{\langle\Phi|\breve{\Phi}\rangle}{\langle\Phi|\Phi\rangle}}$$

Question 1: can we find an alternative to Pfaffians [L.M. Robledo (2009)] to compute $\mathcal{N}^{(1)}$ (including its phase)?

Question 2: can the same method apply to correlated kernels?

Master equations

✪ Auxiliary manifold linking $|\Phi\rangle$ and $|\breve{\Phi}\rangle$

➟ Write unitary transformation $|\breve{\Phi}\rangle = e^{iS}|\Phi\rangle$ with general one-body Hermitian operator S on Fock space

$$S = S^{00} + \sum_{k_1k_2} S^{11}_{k_1k_2}\beta^{+}_{k_1}\beta_{k_2} + \frac{1}{2}\sum_{k_1k_2}\left\{S^{20}_{k_1k_2}\beta^{+}_{k_1}\beta^{+}_{k_2} + S^{02}_{k_1k_2}\beta_{k_2}\beta_{k_1}\right\}$$

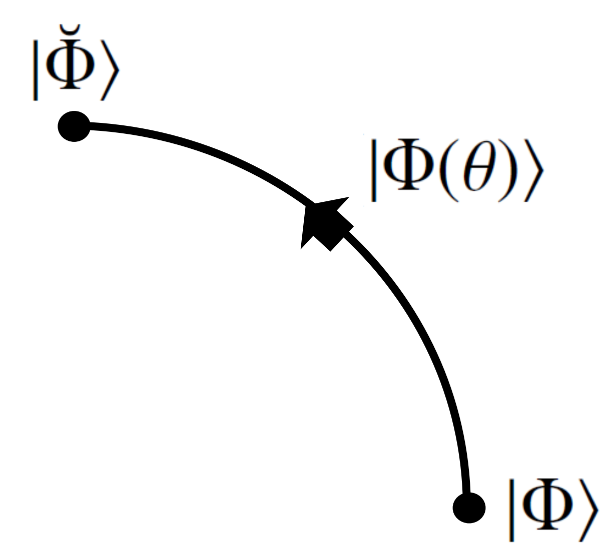
will play a key role

$$= S^{00} + \frac{1}{2}\mathrm{Tr}\left(S^{11}\right) + \frac{1}{2}\begin{pmatrix}\beta^{\dagger} & \beta\end{pmatrix}\underbrace{\begin{pmatrix} S^{11} & S^{20} \\ -S^{02} & -S^{11*}\end{pmatrix}}_{\mathcal{S}}\begin{pmatrix}\beta \\ \beta^{\dagger}\end{pmatrix}$$

$\mathcal{S}$ = Hermitian matrix

To be determined from $\mathcal{W}$ and $\breve{\mathcal{W}}$

Entirely?



➟ Introduce the manifold $\mathcal{M}[|\Phi\rangle, S] \equiv \{|\Phi(\theta)\rangle \equiv e^{i\theta S}|\Phi\rangle, \theta \in [0,1]\}$

✪ Off-diagonal norm kernel along the manifold (arbitrary bra)

$$\mathcal{N}[\langle\Theta|, |\Phi(\theta)\rangle] \equiv \frac{\langle\Theta|\Phi(\theta)\rangle}{\langle\Theta|\Phi\rangle} \Rightarrow \begin{cases} \frac{d}{d\theta}\mathcal{N}[\langle\Theta|, |\Phi(\theta)\rangle] - is[\langle\Theta|, |\Phi(\theta)\rangle]\,\mathcal{N}[\langle\Theta|, |\Phi(\theta)\rangle] = 0 \\ s[\langle\Theta|, |\Phi(\theta)\rangle] \equiv \frac{\langle\Theta|S|\Phi(\theta)\rangle}{\langle\Theta|\Phi(\theta)\rangle} \end{cases}$$

$$\mathcal{N}[\langle\Theta|, |\Phi(\theta)\rangle] = e^{i\int_0^{\theta} d\phi\, s[\langle\Theta|, |\Phi(\phi)\rangle]}$$

Norm kernels

✪ **Correlated off-diagonal kernel for** $\langle\Theta| \equiv \langle\Psi_0|$ and $\theta = 1$

✪ **Uncorrelated off-diagonal kernel for** $\langle\Theta| \equiv \langle\Phi|$ and $\theta = 1$

Closed-form expression

$$\frac{\langle\Phi|\breve{\Phi}\rangle}{\langle\Phi|\Phi\rangle} = e^{i\int_0^1 d\phi\, s[\langle\Phi|,|\Phi(\phi)\rangle]}$$

$$s[\langle\Phi|,|\Phi(\theta)\rangle] \equiv \frac{\langle\Phi|S\,|\Phi(\theta)\rangle}{\langle\Phi|\Phi(\theta)\rangle}$$

✪ **Phase convention**

1) **Calculable without phase ambiguity from GWT**
2) **Involves integration over manifold** $\mathcal{M}[|\Phi\rangle, S]$
3) **Need S and the manifold!**

➟ $\mathcal{W}$ and $\breve{\mathcal{W}}$ are insufficient to fix the relative phase of the associated vacua, i.e. **determine *S* but not S^{00}**

➟ The phase of $\langle\Phi|\breve{\Phi}\rangle$ reflects an implicit or implicit convention fixing the relative phase between both states

➟ Actual problem of interest

$$\{|\Phi\rangle, |\breve{\Phi}\rangle\} \in \mathcal{M}_{\text{set}} \equiv \{|\Phi_1\rangle, \ldots, |\Phi_{N_{\text{set}}}\rangle\} \;\Rightarrow\; N \equiv \begin{pmatrix} \langle\Phi_1|\Phi_1\rangle & \langle\Phi_1|\Phi_2\rangle & \cdots & \langle\Phi_1|\Phi_{N_{\text{set}}}\rangle \\ \langle\Phi_2|\Phi_1\rangle & \langle\Phi_2|\Phi_2\rangle & & \\ \vdots & & \ddots & \\ \langle\Phi_{N_{\text{set}}}|\Phi_1\rangle & & & \langle\Phi_{N_{\text{set}}}|\Phi_{N_{\text{set}}}\rangle \end{pmatrix}$$

Goal = consistent set of norm overlaps for a set of states

➟ Fix their phase relative to given $|\bar{\Phi}\rangle$

Require

$$\text{Arg}(\langle\bar{\Phi}|\Phi_1\rangle) = \text{Arg}(\langle\bar{\Phi}|\Phi_2\rangle) = \ldots = \text{Arg}(\langle\bar{\Phi}|\Phi_{N_{\text{set}}}\rangle)$$

Fix their relative phases
Actual phase relative to $|\bar{\Phi}\rangle$ **unspecified**
Ex: $|\bar{\Phi}\rangle \equiv |0\rangle$ or $|\bar{\Phi}\rangle \equiv |\Phi_1\rangle$

➟ The above phase convention translates into a constrain on S, i.e. it **fixes S^{00}**

$$\langle\Theta| \equiv \langle\bar{\Phi}| \text{ and } \theta = 1 \;\Rightarrow\; \frac{\langle\bar{\Phi}|\breve{\Phi}\rangle}{\langle\bar{\Phi}|\Phi\rangle} = e^{-\Im m\int_0^1 d\phi\, s[\langle\bar{\Phi}|,|\Phi(\phi)\rangle]}\, e^{i\Re e\int_0^1 d\phi\, s[\langle\bar{\Phi}|,|\Phi(\phi)\rangle]}$$

$$\Re e \int_0^1 d\theta\, s[\langle\bar{\Phi}|,|\Phi(\theta)\rangle] = 0$$

Extraction of *S* and of the auxiliary manifold

Key lessons (but not general/practical)
[P. Ring, P. Schuck (1977)]
[K. Hara, S . Iwasaki (1979)]
[K. Takayanagi (2008)]

✪ Bogoliubov transformation linking $|\Phi\rangle$ and $|\Phi(\theta)\rangle$

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \mathcal{X}^\dagger(\theta) \begin{pmatrix} \beta^\theta \\ \beta^{\theta\dagger} \end{pmatrix} \equiv \begin{pmatrix} A^\dagger(\theta) & B^\dagger(\theta) \\ B^T(\theta) & A^T(\theta) \end{pmatrix} \begin{pmatrix} \beta^\theta \\ \beta^{\theta\dagger} \end{pmatrix} \quad \text{with} \quad \begin{cases} \mathcal{X}(0) = 1 \\ \mathcal{X}(1) = \breve{\mathcal{W}}^\dagger \mathcal{W} \end{cases}$$

$$\boxed{\mathcal{X}(\theta) = e^{-i\theta\mathcal{S}}}$$

S^{00} does not appear

✪ Extraction of *S* and χ(θ)

1) Diagonalize unitary matrix

$$\mathcal{X}_{\mathrm{D}}(1) \equiv \mathcal{P}^\dagger \mathcal{X}(1) \mathcal{P}$$

$$\mathrm{Sp}\,\mathcal{X}(1) = \{x_i, |x_i| = 1\}$$

2) Take principal logarithm

$$\mathcal{S} = \mathcal{P} \mathcal{S}_{\mathrm{D}} \mathcal{P}^\dagger$$

$$\mathrm{Sp}\,\mathcal{S} \equiv \{s_i = i \log x_i \in]-\pi, \pi]\}$$

3) Take exponential

$$\mathcal{X}(\theta) = \mathcal{P} \mathcal{X}_{\mathrm{D}}(\theta) \mathcal{P}^\dagger$$

$$\mathrm{Sp}\,\mathcal{X}(\theta) = \{x_i(\theta) = e^{-i\theta s_i}\}$$

✪ Elementary contractions along the auxiliary manifold

$$\mathcal{R}(\theta) \equiv \begin{pmatrix} \frac{\langle\Phi|\beta^\dagger\beta\ |\Phi(\theta)\rangle}{\langle\Phi|\Phi(\theta)\rangle} & \frac{\langle\Phi|\beta\ \beta\ |\Phi(\theta)\rangle}{\langle\Phi|\Phi(\theta)\rangle} \\ \frac{\langle\Phi|\beta^\dagger\beta^\dagger|\Phi(\theta)\rangle}{\langle\Phi|\Phi(\theta)\rangle} & \frac{\langle\Phi|\beta\ \beta^\dagger|\Phi(\theta)\rangle}{\langle\Phi|\Phi(\theta)\rangle} \end{pmatrix} \equiv \begin{pmatrix} R^{+-}(\theta) & R^{--}(\theta) \\ R^{++}(\theta) & R^{-+}(\theta) \end{pmatrix} = \begin{pmatrix} 0 & -B^\dagger(\theta)[A^T(\theta)]^{-1} \\ 0 & 1 \end{pmatrix}$$

Computation of the norm overlap

✪ Final expression

From phase condition (not explicited here) — **Onishi**

$$\frac{\langle\Phi|\breve{\Phi}\rangle}{\langle\Phi|\Phi\rangle} = e^{i\int_0^1 d\phi\, s[\langle\Phi|,|\Phi(\phi)\rangle]} = e^{iS^{00}} e^{\frac{i}{2}\sum_{k_1k_2} S^{02}_{k_1k_2}\int_0^1 d\phi R^{--}_{k_2k_1}(\phi)} \Rightarrow \left|\frac{\langle\Phi|\breve{\Phi}\rangle}{\langle\Phi|\Phi\rangle}\right| = \sqrt{\det A(1)}$$

From $\mathcal{W}$ and $\breve{\mathcal{W}}$

✪ Add arbitrary « third » Bogoliubov transformation (BMZ) to $\mathcal{W}$ and/or $\breve{\mathcal{W}}$

$$\mathcal{W} \Rightarrow \tilde{\mathcal{W}} \equiv \mathcal{W}\mathcal{K} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}\begin{pmatrix} K & 0 \\ 0 & K^* \end{pmatrix} \equiv \begin{pmatrix} \tilde{U} & \tilde{V}^* \\ \tilde{V} & \tilde{U}^* \end{pmatrix} \Rightarrow \tilde{\beta}_k|\Phi\rangle = 0 \Rightarrow |\tilde{\Phi}\rangle \equiv \det K\,|\Phi\rangle$$

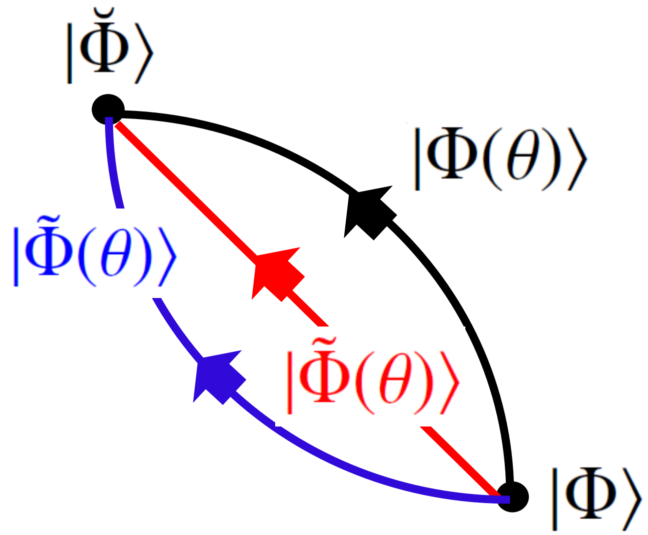
Same vacuum up to a phase

Different manifold ⬇

$$\tilde{\mathcal{S}}, \tilde{\mathcal{X}}(\theta)$$

Constrain on S[00] absorbes extra phase ⬇

$$\boxed{\frac{\langle\Phi|\breve{\Phi}\rangle}{\langle\Phi|\Phi\rangle} = e^{i\tilde{S}^{00}} e^{\frac{i}{2}\sum_{k_1k_2}\tilde{S}^{02}_{k_1k_2}\int_0^1 d\phi\,\tilde{R}^{--}_{k_2k_1}(\phi)}}$$



Same overlap… see next for usefulness in actual applications on the basis of random K

Toy model 1: global gauge rotation for 10-levels BCS model

✪ BCS transformations

▶ $$U(k,\bar{k}) = \begin{pmatrix} u_k & 0 \\ 0 & u_k \end{pmatrix} \qquad V(k,\bar{k}) = \begin{pmatrix} 0 & +v_k \\ -v_k & 0 \end{pmatrix}$$

▶ $$\breve{U}(k,\bar{k}) = e^{+i\varphi}U(k,\bar{k}) \qquad \breve{V}(k,\bar{k}) = e^{-i\varphi}V(k,\bar{k})$$

(u_5, v_5)	$5\ \bar{5}$
(u_4, v_4)	$4\ \bar{4}$
(u_3, v_3)	$3\ \bar{3}$
(u_2, v_2)	$2\ \bar{2}$
(u_1, v_1)	$1\ \bar{1}$

✪ Possible explicit representation

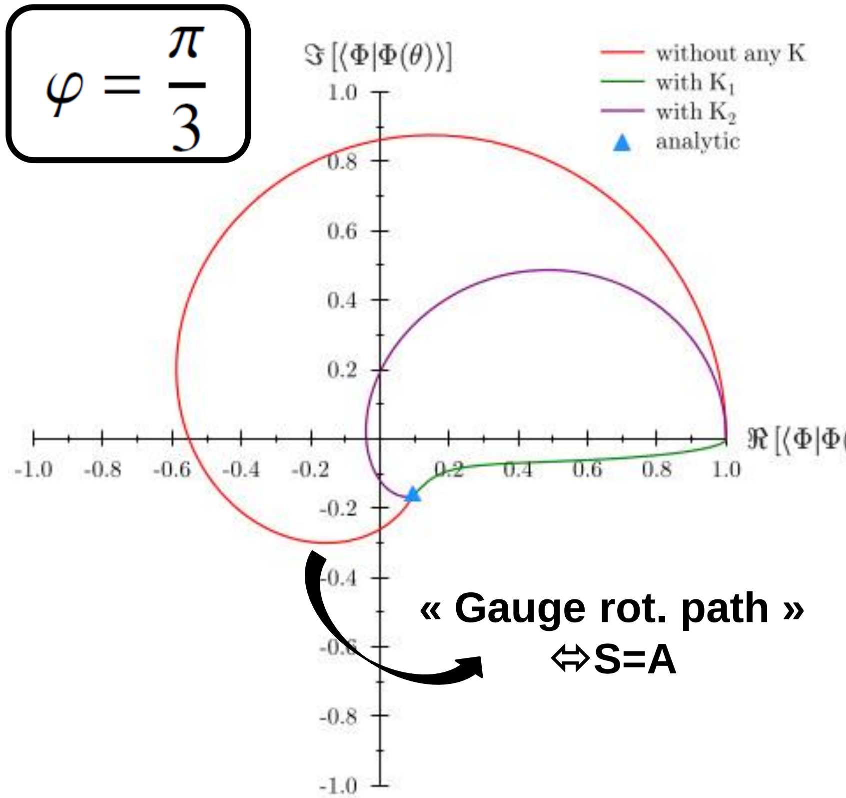
$$|\Phi\rangle \equiv \prod_{k=1}^{5}(u_k + v_k c^\dagger_k c^\dagger_{\bar{k}})|0\rangle$$

$$|\breve{\Phi}\rangle \equiv e^{i\varphi A}|\Phi\rangle$$

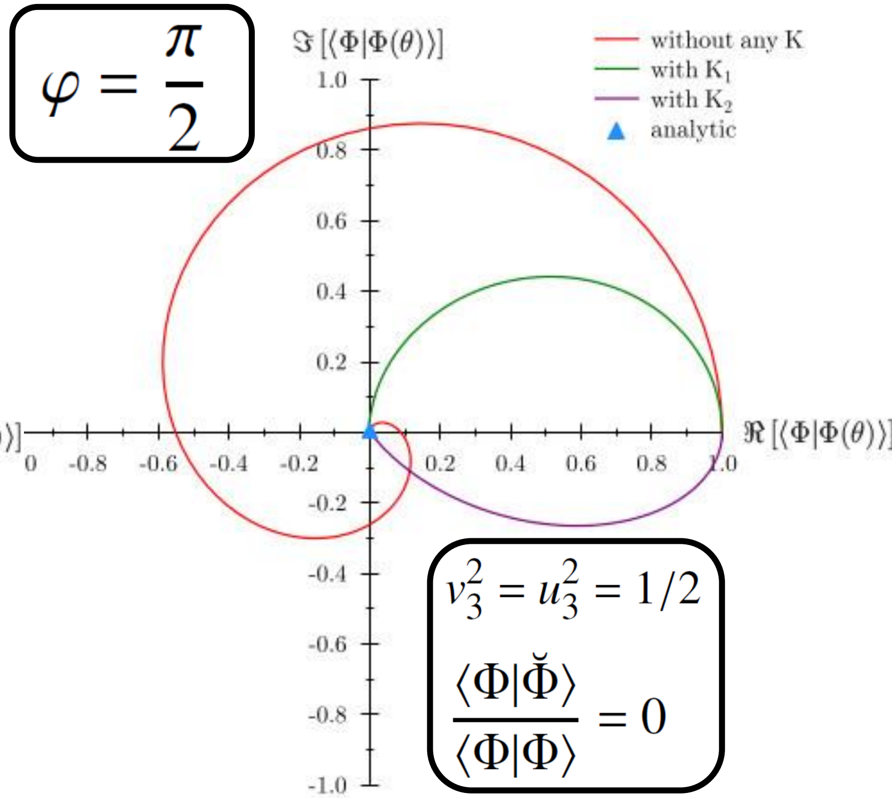
$$\mathrm{Arg}(\langle 0|\Phi\rangle) = \mathrm{Arg}(\langle 0|\breve{\Phi}\rangle)$$

$$\frac{\langle\Phi|\breve{\Phi}\rangle}{\langle\Phi|\Phi\rangle} = \prod_{k=1}^{5}(u_k^2 + e^{2i\varphi}v_k^2)$$

$\varphi = \dfrac{\pi}{3}$



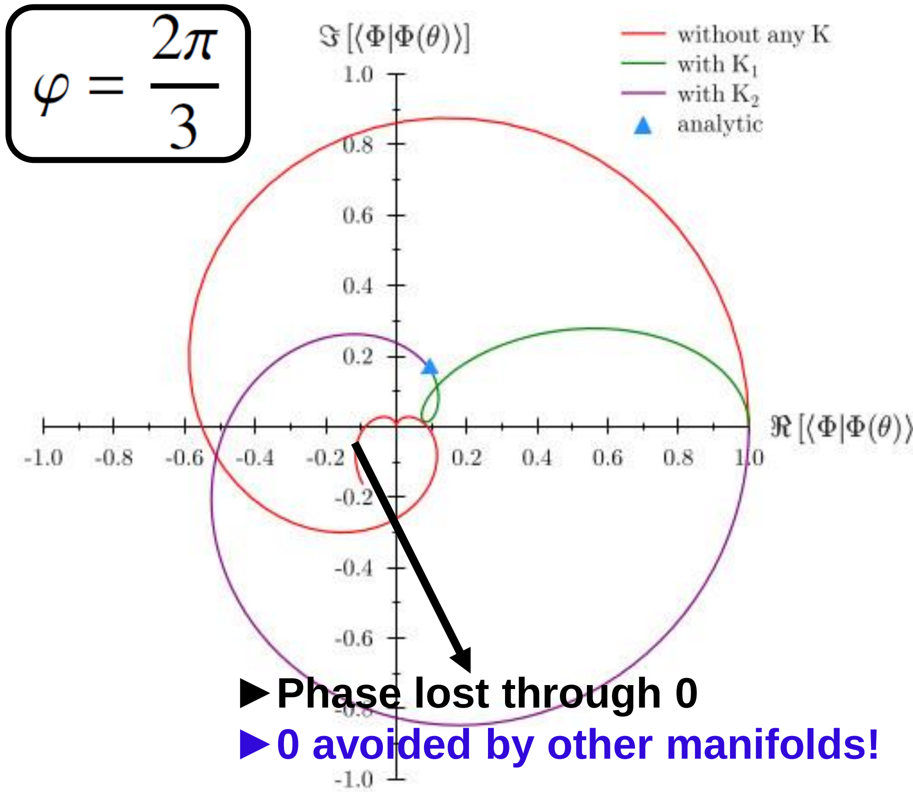
$\varphi = \dfrac{\pi}{2}$



$$v_3^2 = u_3^2 = 1/2$$

$$\frac{\langle\Phi|\breve{\Phi}\rangle}{\langle\Phi|\Phi\rangle} = 0$$

$\varphi = \dfrac{2\pi}{3}$



▶ **Phase lost through 0**

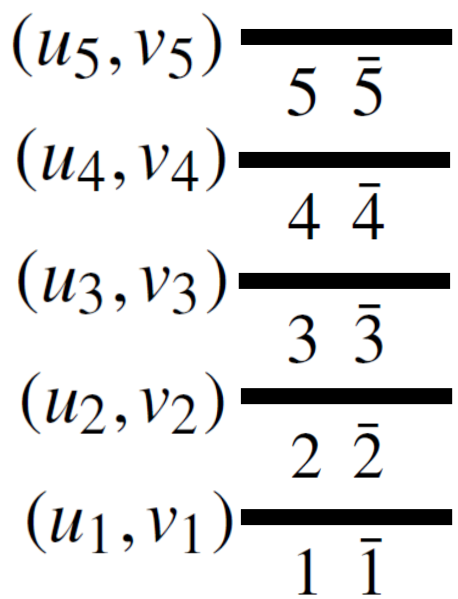
▶ **0 avoided by other manifolds!**

Toy model 2: 10-levels BCS model

✪ BCS transformations

▶
$$U(k,\bar{k}) = \begin{pmatrix} u_k & 0 \\ 0 & u_k \end{pmatrix}$$
$$V(k,\bar{k}) = \begin{pmatrix} 0 & +v_k \\ -v_k & 0 \end{pmatrix}$$

▶
$$\breve{U}(k,\bar{k}) = \begin{pmatrix} \breve{u}_k & 0 \\ 0 & \breve{u}_k \end{pmatrix}$$
$$\breve{V}(k,\bar{k}) = \begin{pmatrix} 0 & +\breve{v}_k \\ -\breve{v}_k & 0 \end{pmatrix}$$



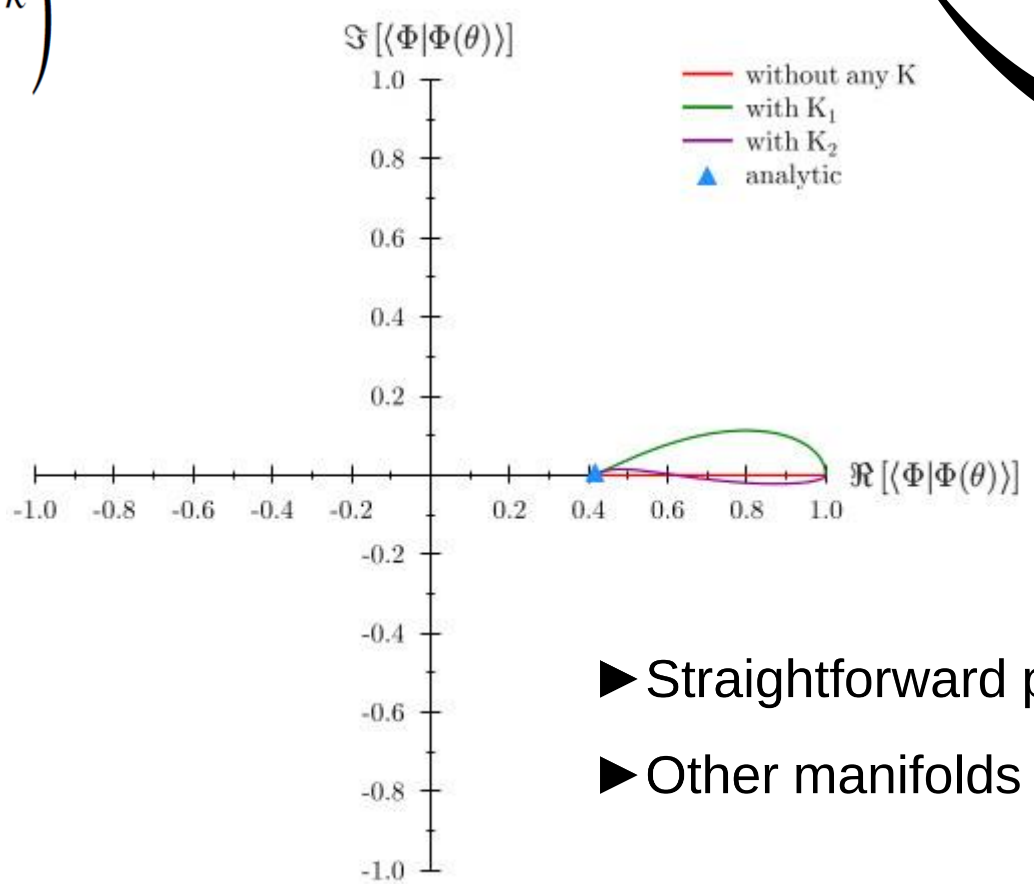
✪ Possible explicit representation

$$|\Phi\rangle \equiv \prod_{k=1}^{5} (u_k + v_k c^\dagger_k c^\dagger_{\bar{k}})|0\rangle$$
$$|\breve{\Phi}\rangle \equiv \prod_{k=1}^{5} (\breve{u}_k + \breve{v}_k c^\dagger_k c^\dagger_{\bar{k}})|0\rangle$$

$$\mathrm{Arg}(\langle 0|\Phi\rangle) = \mathrm{Arg}(\langle 0|\breve{\Phi}\rangle)$$

$$\frac{\langle \Phi|\breve{\Phi}\rangle}{\langle \Phi|\Phi\rangle} = \prod_{k=1}^{5} (u_k \breve{u}_k + v_k \breve{v}_k)$$

Real and positive



▶ Straightforward path goes along the real axis

▶ Other manifolds goes through complex plane

Toy model 3: 4-levels Bogoliubov model

✪ Bogoliubov transformations

▶
$$U(k,\bar{k}) = \begin{pmatrix} u_k & 0 \\ 0 & u_k \end{pmatrix}$$
$$V(k,\bar{k}) = \begin{pmatrix} 0 & +v_k \\ -v_k & 0 \end{pmatrix}$$

(u_2, v_2) — $2 \ \bar{2}$

(u_1, v_1) — $1 \ \bar{1}$

▶
$$\breve{\mathcal{W}} \equiv \underbrace{\begin{pmatrix} L & 0 \\ 0 & L^* \end{pmatrix}}_{\text{Complex s.p. basis transformation}} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$$

Complex s.p. basis transformation

$$Z \equiv V^* [U^*]^{-1}$$
$$\breve{Z} \equiv \breve{V}^* [\breve{U}^*]^{-1}$$

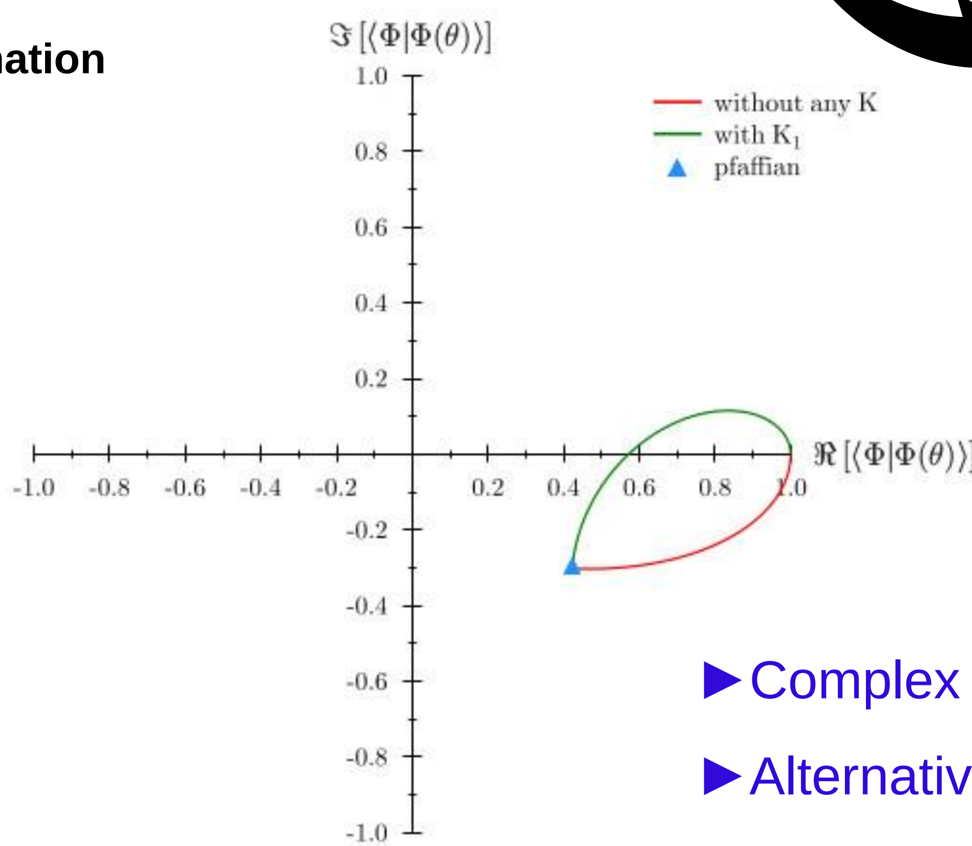
✪ Possible explicit representation

$$|\Phi\rangle \equiv \exp\left(\frac{1}{2} \sum_{kk'=1,\bar{1},2,\bar{2}} Z^{20}_{kk'} c^\dagger_k c^\dagger_{k'} \right) |0\rangle$$
$$|\breve{\Phi}\rangle \equiv \exp\left(\frac{1}{2} \sum_{kk'=1,\bar{1},2,\bar{2}} \breve{Z}^{20}_{kk'} c^\dagger_k c^\dagger_{k'} \right) |0\rangle$$

$$\mathrm{Arg}(\langle 0|\Phi\rangle) = \mathrm{Arg}(\langle 0|\breve{\Phi}\rangle)$$

$$\frac{\langle \Phi|\breve{\Phi}\rangle}{\langle \Phi|\Phi\rangle} = (-1)^{N(N+1)/2} \, \mathrm{pf} \begin{pmatrix} \breve{Z} & -1 \\ 1 & -Z^* \end{pmatrix}$$

[L. M. Robledo (2009)]



▶ Complex norm overlap perfectly captured

▶ Alternative paths/manifolds can be used

Outline

I. **Basics and shortcomings of current MR-EDF method**

II. **Many-body expansion of off-diagonal energy&norm kernels**

III. **Norm kernel between arbitrary Bogoliubov product states**

IV. **Conclusions**

Conclusive remarks

- ✪ **Evolution towards from low-order BMBPT off-diagonal energy and norm kernels**
  - ➟ Dynamical correlations through vertical expansion = qp energy and density matrix functionals
  - ➟ Energy and norm kernels must be treated consistently
- ✪ **Implementions**
  - ➟ Diagonal, S.R., BMBPT(1,2,3) spherical code under completion
  - ➟ To be implemented and fitted with appropriate H_{eff} at BMBPT(1,2,3) levels
    - ► Optimize balance between complexity of many-body expansions and of H_{eff}
  - ➟ To be implemented in PNR calculations
  - ➟ To be generalized to GCM-type horizontal mixing
- ✪ **Norm kernels**
  - ➟ Flexible alternative to Pfaffian for arbitrary Bogoliubov states
  - ➟ Method applicable to norm kernels beyond mean-field level

Background

✪ **Correlated off-diagonal norm kernels within PNR-BCC and PNR-BMBPT theories**

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

$$\mathcal{N}(\varphi) = \frac{\langle\Psi_0|\Phi(\varphi)\rangle}{\langle\Psi_0|\Phi\rangle}$$

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

1st order ODE

$$a(\varphi) \equiv \frac{\langle\Psi_0|A|\Phi(\varphi)\rangle}{\langle\Psi_0|\Phi(\varphi)\rangle}$$

Linked/connected kernel of A

Computable in closed form

$$\mathcal{N}(\varphi) = e^{i\int_0^\varphi d\phi\, a(\phi)}$$

Involves $\{|\Phi(\phi)\rangle \text{ for } \phi \in [0,\varphi]\}$

➟ First order

$$a^{(1)}(\varphi) \equiv \frac{\langle\Phi|A|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle} = A^{00} + \frac{1}{2}\sum_{k_1k_2} A^{02}_{k_1k_2} R^{--}_{k_2k_1}(\varphi)$$

$$\mathcal{N}^{(1)}(\varphi) = \langle\Phi|\Phi(\varphi)\rangle = e^{iA^{00}\varphi + \frac{i}{2}\sum_{k_1k_2}\int_0^\varphi d\phi\, A^{02}_{k_1k_2} R^{--}_{k_2k_1}(\phi)}$$

➟ Second order

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

Depends on the dynamics

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

Analytically scrutinized in
On the norm overlap between many-body states. II. Correlated off-diagonal norm kernel, P. Arthuis, B. Bally, T. Duguet, in preparation