On the norm overlap between many-body states

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B. Bally, T. Duguet, arXiv:1704.05324 and arXiv:1706.04553

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Outline

I. **Background and objectives**

II. **Method for general correlated norm kernels**

III. **Application to arbitrary pair of Bogoliubov product states**

IV. **Numerical tests and validation**

V. **Conclusions**

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I. Background and objectives

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Background 1

✪ A-body Schrödinger equation within a set of non-orthogonal states

➟ Set of *N* non-orthogonal many-body states $\mathcal{M} \equiv \{|\Phi_k\rangle, k = 1\ldots, N\}$

➟ Secular equation = generalized eigenvalue problem

N(N+1)/2 independent elements

$$|\Psi_n\rangle \equiv \sum_{k=1}^{N} f_{nk} |\Phi_k\rangle \iff \mathcal{H}\mathfrak{f}_n = E_n \mathcal{N}\mathfrak{f}_n \iff$$

$(\mathfrak{f}_n)_k \equiv f_{nk}$

$\mathcal{N}_{kl} \equiv \langle\Phi_k|\Phi_l\rangle$ **Hermitian norm matrix**

$\mathcal{H}_{kl} \equiv \langle\Phi_k|H|\Phi_l\rangle$ **Hermitian Hamiltonian matrix**

1) Set of Slater determinants $\mathcal{N}_{kl} \to \det$

2) Set of Bogoliubov states $\mathcal{N}_{kl} \to \text{pf}$ [L. M. Robledo, 2009]

Solved a long-standing problem related to capturing the complex phase

➟ Examples: generator coordinate method and symmetry restoration (proj. only makes use of first line of $\mathcal{N}$)

➟ Complex phases

1) The phase of each state $|\Phi_k\rangle$ can be arbitrarily chosen

2) One must make a choice and compute *all* entries $\mathcal{N}_{kl}$ consistently with it

➟ Practical phase conventions

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

$|\bar{\Phi}\rangle \equiv |\Phi_1\rangle$ Reference state within the set

$|\bar{\Phi}\rangle \equiv |0\rangle$ Reference state outside the set (i.e. Proj.)

Background 2

✪ Particle-number-restored Bogoliubov MBPT and CC theory

[T. Duguet, 2015]
[T. Duguet, A. Signoracci, 2016]

➟ Set of N non-orthogonal **gauge-rotated Bogoliubov states** $\mathcal{M} \equiv \{|\Phi(\varphi)\rangle \equiv e^{iA\varphi}|\Phi\rangle; \varphi \in [0, 2\pi]\}$

$|\Phi\rangle$ such that $\beta_k|\Phi\rangle = 0 \ \forall k$

➟ **Correlated** off-diagonal kernels

Exact ground state

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

Evolution operator in imaginary time

atic expansion

Linked-connected kernel of operator

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

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

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

Sum of connected diagrams *linked* to H/A
Naturally terminating BCC expansion

➟ Lowest order = mean-field kernels

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

$$h^{(1)}(\varphi) = \frac{\langle\Phi|H|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle}$$

$$a^{(1)}(\varphi) = \frac{\langle\Phi|A|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle}$$

➟ Exact ground-state energy

$$E_0^{\mathrm{A}} = \frac{\int_0^{2\pi} d\varphi\, e^{-i\mathrm{A}\varphi}\, \mathcal{H}(\varphi)}{\int_0^{2\pi} d\varphi\, e^{-i\mathrm{A}\varphi}\, \mathcal{N}(\varphi)}$$

Projected HFB theory

Background 2

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

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

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

➡

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

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

1st order ODE

➡ Closed form expression

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

Correlated linked-connected kernel of A

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

➡ First-order diagram

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

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

$$A^{ij} \leftrightarrow \underbrace{\beta^\dagger \ldots \beta^\dagger}_{i \text{ operators}} \underbrace{\beta \ldots \beta}_{j \text{ operators}}$$

$$R^{--}_{k_1k_2}(\varphi) \equiv \frac{\langle\Phi|\beta_{k_1}\beta_{k_2}|\Phi(\varphi)\rangle}{\langle\Phi|\Phi(\varphi)\rangle}$$

$$\Omega \equiv H - \lambda A$$

➡ Second-order diagram

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

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

- ❑ Depends on the dynamics
- ❑ Derived up to 5th order

[P. Arthuis et al., unpublished]

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

Objectives = General correlated off-diagonal norm kernels

✪ **Two *arbitrary* Bogoliubov vacua** $|\Phi\rangle$ **and** $|\breve{\Phi}\rangle$

$$\begin{pmatrix}\beta\\ \beta^\dagger\end{pmatrix} = \mathcal{W}^\dagger \begin{pmatrix}c\\ c^\dagger\end{pmatrix} \equiv \begin{pmatrix}U^\dagger & V^\dagger\\ V^T & U^T\end{pmatrix}\begin{pmatrix}c\\ c^\dagger\end{pmatrix}$$

$$\begin{pmatrix}\breve{\beta}\\ \breve{\beta}^\dagger\end{pmatrix} = \breve{\mathcal{W}}^\dagger \begin{pmatrix}c\\ c^\dagger\end{pmatrix} \equiv \begin{pmatrix}\breve{U}^\dagger & \breve{V}^\dagger\\ \breve{V}^T & \breve{U}^T\end{pmatrix}\begin{pmatrix}c\\ c^\dagger\end{pmatrix}$$

⟷

$|\Phi\rangle$ such that $\beta_k|\Phi\rangle = 0\ \forall k$

$|\breve{\Phi}\rangle$ such that $\breve{\beta}_k|\breve{\Phi}\rangle = 0\ \forall k$

Sole given of the problem → Does *not* specify the phase of the two states

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

$$\mathcal{N} = \frac{\langle\Psi_0|\breve{\Phi}\rangle}{\langle\Psi_0|\Phi\rangle}$$

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

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

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

Question 1: can we find a method to calculate **1) general 2) correlated** norm kernels **without any phase ambiguity**?

Question 2: that provides an alternative to Pfaffians [L.M. Robledo (2009)] at lowest order?

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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

will play a key role

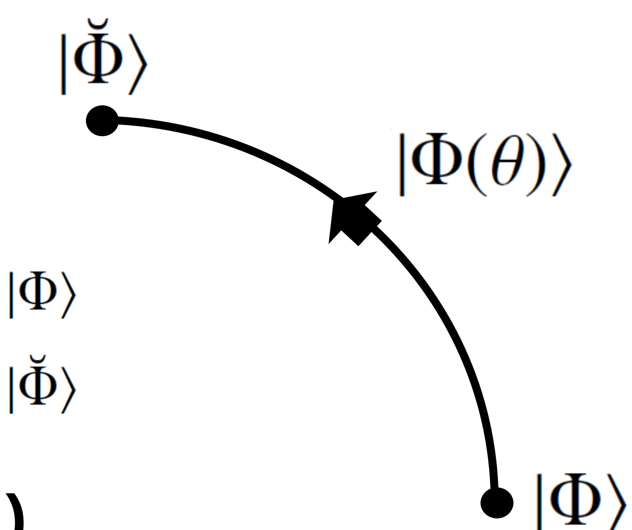
$$S = S^{00} + \sum_{k_1k_2} S^{11}_{k_1k_2}\beta^{+}_{k_1}\beta_{k_2} + \frac{1}{2}\sum_{k_1k_2}\left\{S^{20}_{k_1k_2}\beta^{+}_{k_1}\beta^{+}_{k_2} + S^{02}_{k_1k_2}\beta_{k_2}\beta_{k_1}\right\}$$

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

$\mathcal{S}$ = Hermitian matrix

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

Entirely?



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

$|\Phi(0)\rangle = |\Phi\rangle$

$|\Phi(1)\rangle = |\breve{\Phi}\rangle$

✪ Off-diagonal norm kernel along the manifold (arbitrary bra $\langle\Theta|$)

$$\mathcal{N}[\langle\Theta|, |\Phi(\theta)\rangle] \equiv \frac{\langle\Theta|\Phi(\theta)\rangle}{\langle\Theta|\Phi\rangle}$$

➡

$$\frac{d}{d\theta}\mathcal{N}[\langle\Theta|, |\Phi(\theta)\rangle] - is[\langle\Theta|, |\Phi(\theta)\rangle]\, \mathcal{N}[\langle\Theta|, |\Phi(\theta)\rangle] = 0$$

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

Linked-connected kernel of S

Independent of the relative phase

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

Norm kernels

Closed-form expression

$$\frac{\langle \Psi_0 | \breve{\Phi} \rangle}{\langle \Psi_0 | \Phi \rangle} = e^{i \int_0^1 d\phi \, s[\langle \Psi_0 |, | \Phi(\phi) \rangle]}$$

$$s[\langle \Psi_0 |, | \Phi(\theta) \rangle] = \frac{\langle \Psi_0 | S | \Phi(\theta) \rangle}{\langle \Psi_0 | \Phi(\theta) \rangle}$$

- ✪ **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 $\theta = 1$ ➡
- ✪ **Phase convention**

1) **Calculable without phase ambiguity from generalized diagrammatic (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 S⁰⁰**

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

➟ Actual problem of interest

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

Goal = consistent set of complex phases

➟ 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 S⁰⁰**

$\langle \Theta | \equiv \langle \bar{\Phi} |$ and $\theta = 1$ ➡

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

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

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 $\chi(\theta)$

1) Diagonalize unitary matrix

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

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

2) Take principal logarithm

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

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

3) Take exponential

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

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

✪ Elementary contractions along the auxiliary manifold

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

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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 $\breve{\mathcal{W}}$

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

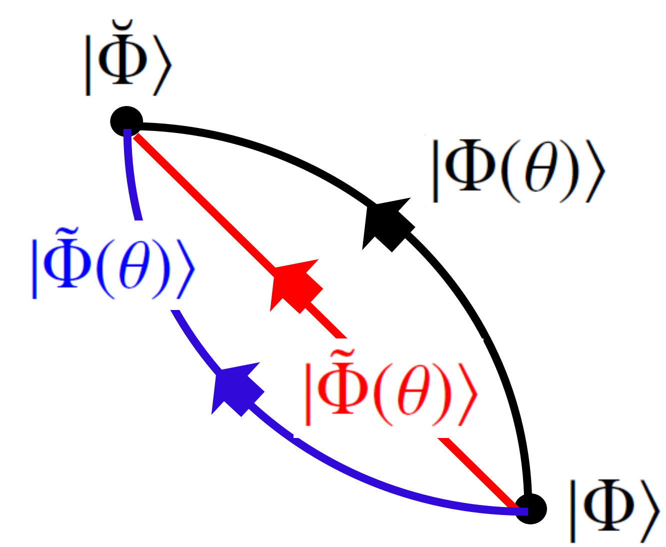
Same vacuum up to a phase

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 following a different unitary paths… see next for usefulness in applications on the basis of random K

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

✪ BCS transformations ($\mathcal{W}$, $\breve{\mathcal{W}}$)

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

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

(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

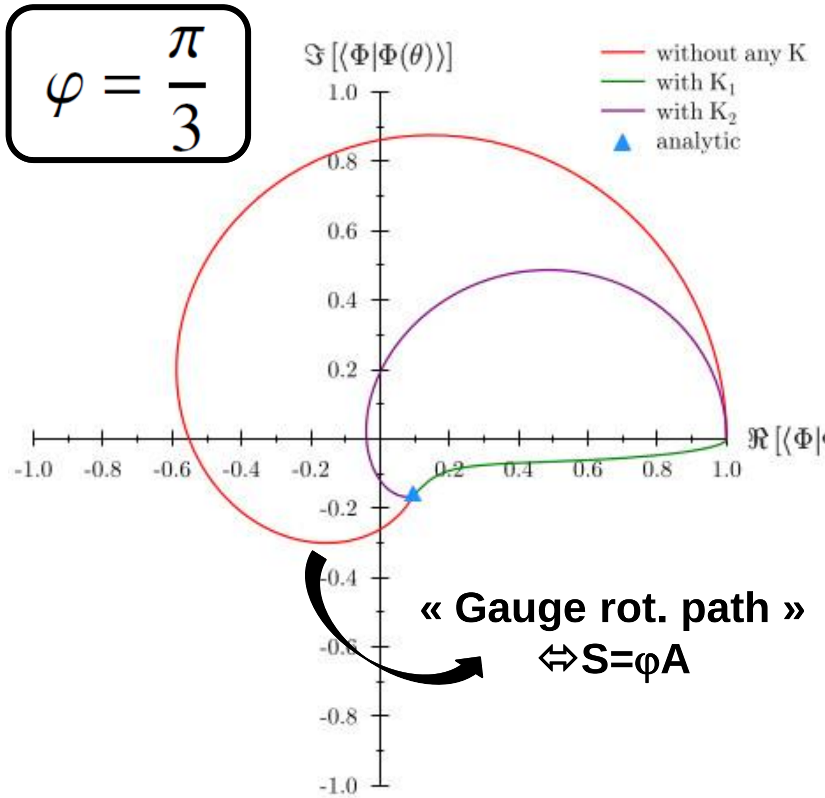
$$|\Phi\rangle \equiv \prod_{k=1}^{5} (u_k + v_k c^\dagger_k c^\dagger_{\bar{k}})|0\rangle$$
$$|\breve{\Phi}\rangle \equiv e^{i\varphi A}|\Phi\rangle$$

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

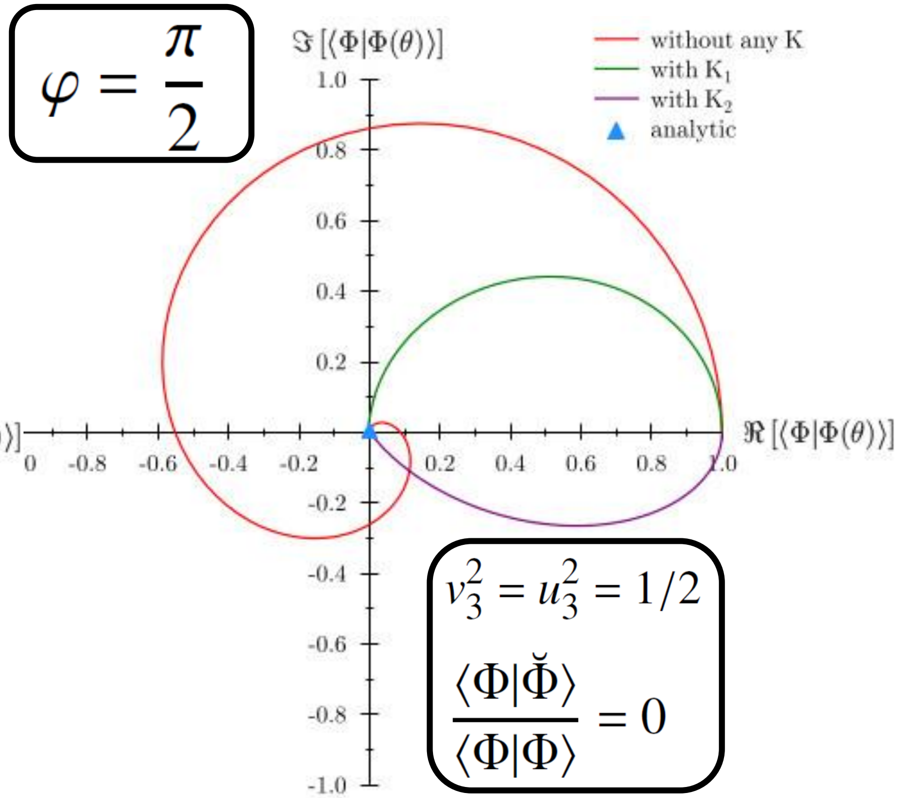
$$\frac{\langle\Phi|\breve{\Phi}\rangle}{\langle\Phi|\Phi\rangle} = \prod_{k=1}^{5}(u_k^2 + e^{2i\varphi} v_k^2)$$

Analytic result

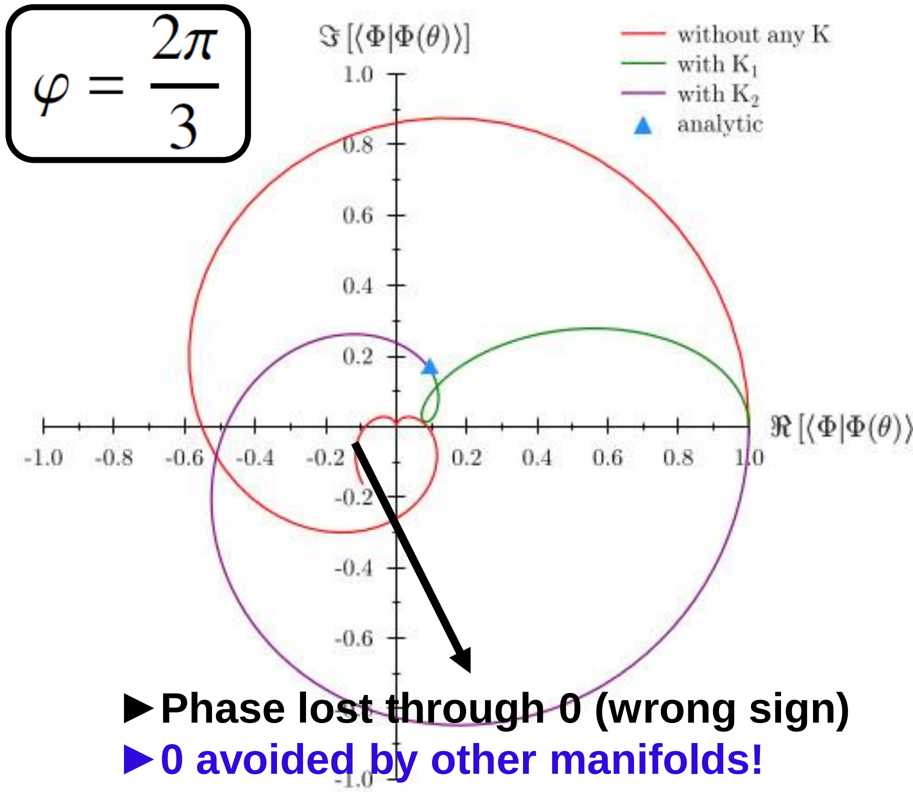
$$\varphi = \frac{\pi}{3}$$



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



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



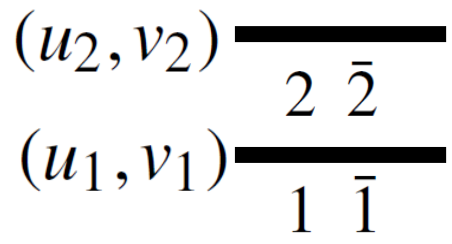
▶ **Phase lost through 0 (wrong sign)**

▶ **0 avoided by other manifolds!**

Toy model 2: 4-levels Bogoliubov model

✪ Bogoliubov transformations

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



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

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

▶ $$\breve{\mathcal{W}} \equiv \underbrace{\begin{pmatrix} L & 0 \\ 0 & L^* \end{pmatrix}} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$$

Complex s.p. basis transformation

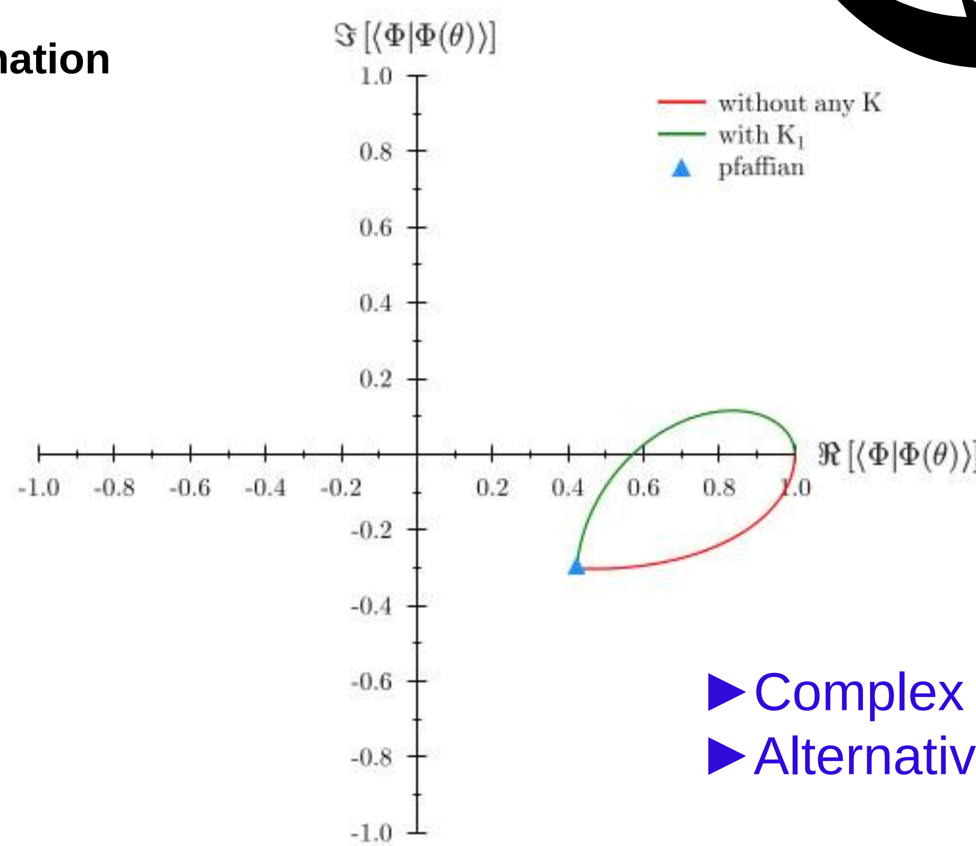
✪ Possible explicit representation

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

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

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

[L. M. Robledo (2009)]



▶Complex norm overlap perfectly captured

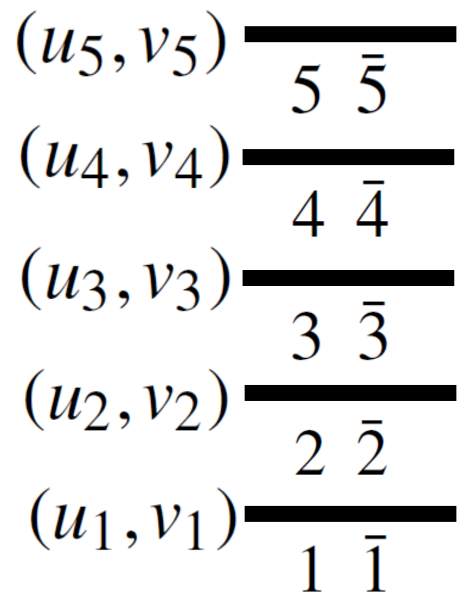
▶Alternative paths/manifolds can be used

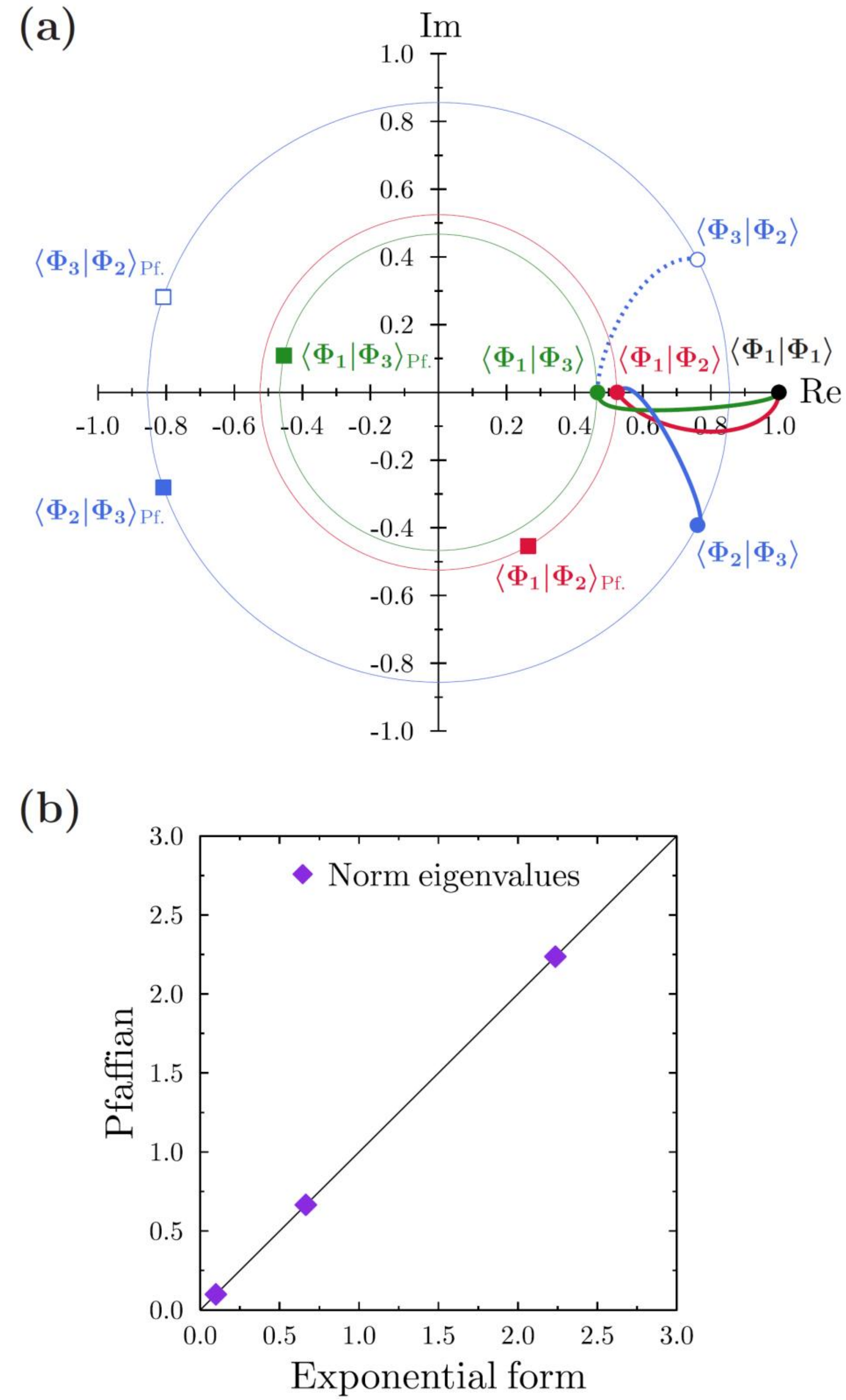
Toy model 3: 10-levels Bogoliubov model

✪ **Set of Bogoliubov vacua** $\mathcal{M} \equiv \{|\Phi_1\rangle, |\Phi_2\rangle, |\Phi_3\rangle\}$

✪ **Norm matrix**

$$\mathcal{N}_{\mathcal{M}} \equiv \begin{pmatrix} \langle\Phi_1|\Phi_1\rangle & \langle\Phi_1|\Phi_2\rangle & \langle\Phi_1|\Phi_3\rangle \\ \langle\Phi_2|\Phi_1\rangle & \langle\Phi_2|\Phi_2\rangle & \langle\Phi_2|\Phi_3\rangle \\ \langle\Phi_3|\Phi_1\rangle & \langle\Phi_3|\Phi_2\rangle & \langle\Phi_3|\Phi_3\rangle \end{pmatrix}$$





✪ **Phase convention**

➟ Pfaffian method

$$\mathrm{Arg}(\langle 0|\Phi_1\rangle) = \mathrm{Arg}(\langle 0|\Phi_2\rangle) = \mathrm{Arg}(\langle 0|\Phi_3\rangle)$$

➟ Present method

$$\mathrm{Arg}(\langle\Phi_1|\Phi_1\rangle) = \mathrm{Arg}(\langle\Phi_1|\Phi_2\rangle) = \mathrm{Arg}(\langle\Phi_1|\Phi_3\rangle)$$

First line/column of norm matrix real

▶Individual overlaps differ by a phase (convention)
▶Eigenvalues of the norm matrix (or any observable) are the same
▶Consistency is what matters!

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Conclusive remarks

✪ **Unambiguous calculation of off-diagonal norm kernels**

➟ Intuitive closed-form expression

➟ Flexible alternative to Pfaffian for arbitrary Bogoliubov states

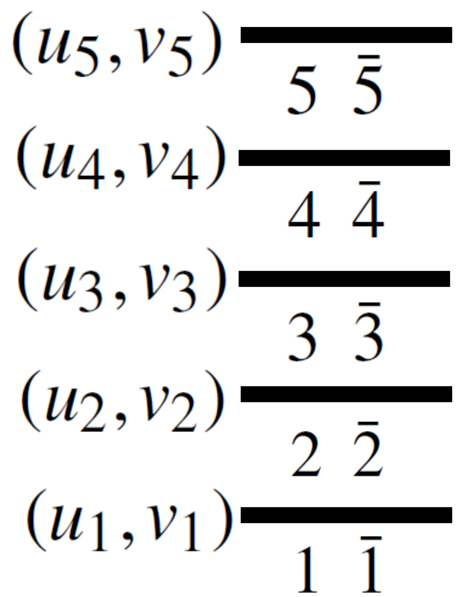
➟ Method applicable to correlated norm kernels

➟ Method potentially applicable to more generic many-body states

Toy model 2: global gauge rotation for 10-levels BCS model

✪ Odd-number parity states for odd systems

$$\begin{cases} |\Phi\rangle = c_2^\dagger \prod_{k=1(\neq 2)}^{5} (u_k + v_k c_k^\dagger c_{\bar{k}}^\dagger)|0\rangle \\ |\breve{\Phi}\rangle \equiv e^{i\varphi A}|\Phi\rangle \end{cases}$$



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

Analytic result

- **Complex overlap reproduced**
- **As versatile as for even systems**

✪ Phase convention

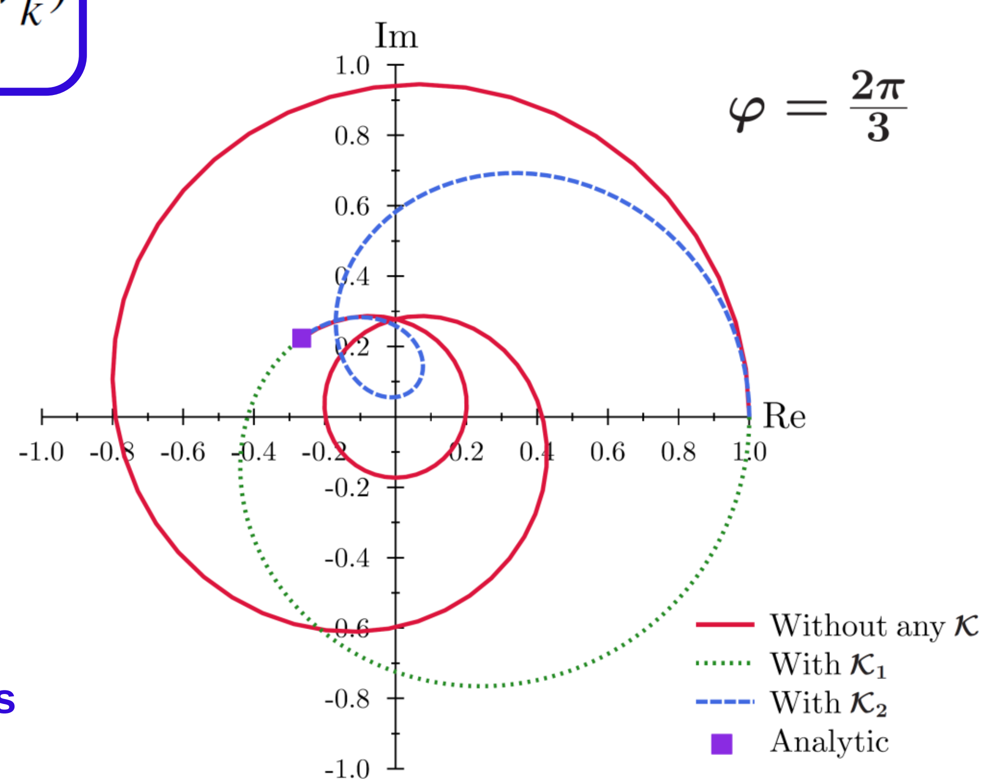
$$\text{Arg}(\langle\bar{\Phi}|\breve{\Phi}\rangle) = \text{Arg}(\langle\bar{\Phi}|\Phi\rangle) + \underbrace{\varphi}$$

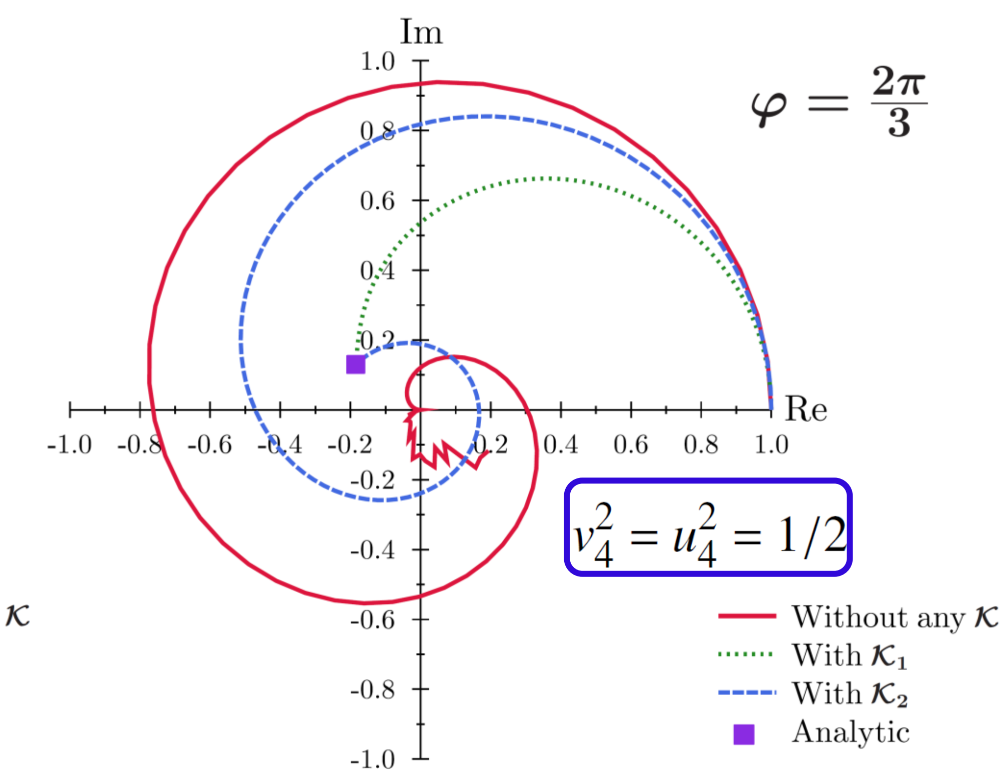
per fully occupied canonical state (1 here)

with $\underbrace{|\bar{\Phi}\rangle = c_2^\dagger|0\rangle}$ **instead of** $|\bar{\Phi}\rangle = |0\rangle$

Slater determinant with fully occupied canonical state(s)

- **Phase lost through 0 (wrong sign)**
- **Imprecise numerics beyond 0**
- **0 avoided by other manifolds!**



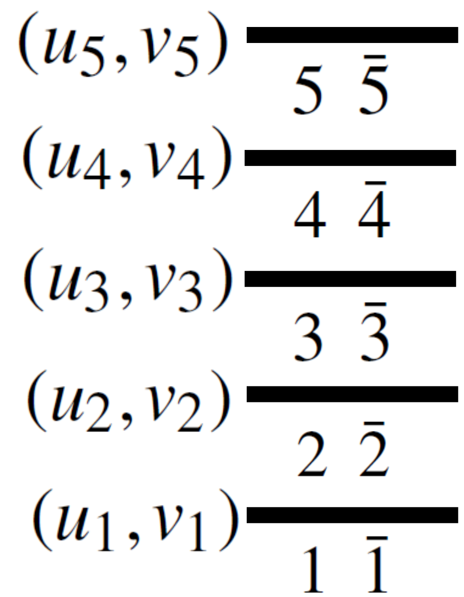


Toy model 2: 10-levels BCS model

✪ BCS transformations ($\mathcal{W}$, $\breve{\mathcal{W}}$)

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

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



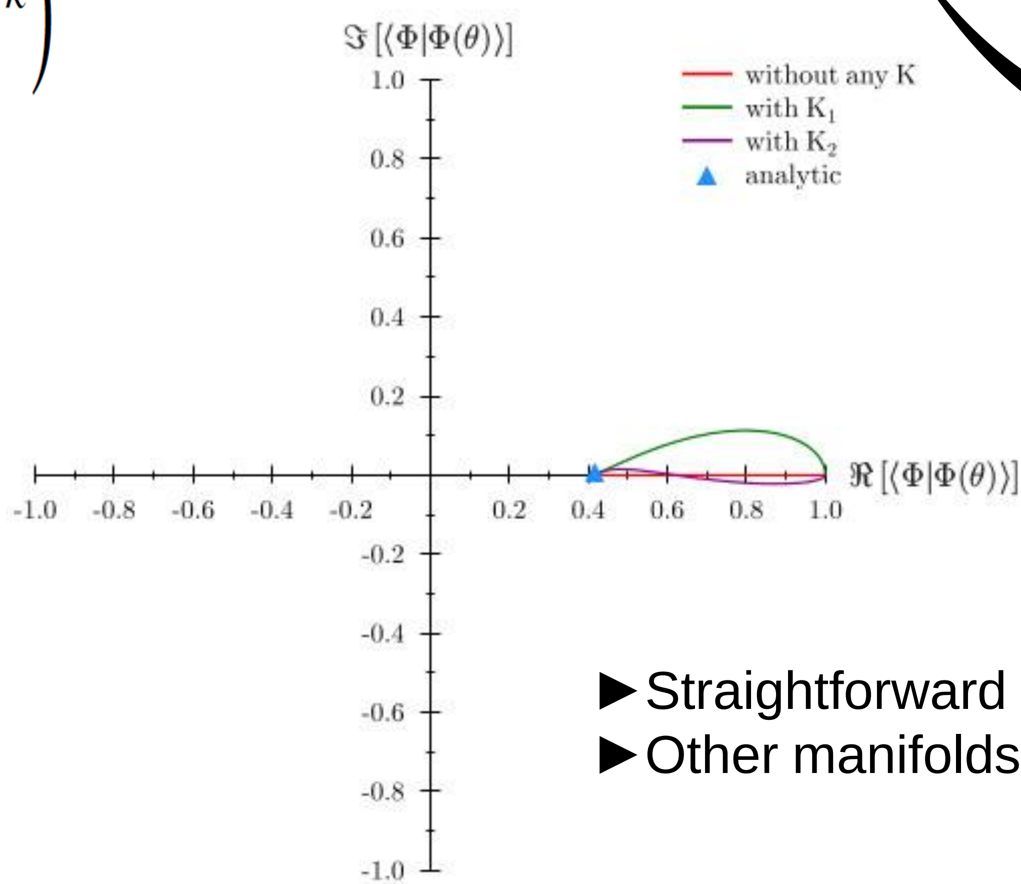
✪ Possible explicit representation

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

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

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

Real and positive



▶ Straightforward path goes along the real axis
▶ Other manifolds goes through complex plane