1-RDMFT for superconductors

Trento (IT), 7.10.22

J Schmidt, **CLBR**, and MAL Marques, PRB **99**, 224502 (2019)

One-Body Reduced Density Matrix

Given a wave function $\left|\Psi\right\rangle$

The one-body reduced density matrix is defined as:

$$\gamma(\vec{x},\vec{y}) = \int \Psi(\vec{x},\vec{x}_2,...,\vec{x}_N)\Psi^*(\vec{y},\vec{x}_2,...,\vec{x}_N)d\vec{x}_2\cdots d\vec{x}_N$$

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Cooper pairs, superconductors

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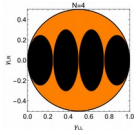
$$E(\hat{h}) = \min[\langle \hat{h}, \gamma \rangle + \mathcal{F}(\gamma)]$$

$\gamma \in$ 

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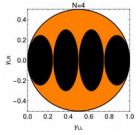

$$\mathcal{F}(\gamma) = \min_{|\Psi\rangle \to \gamma} \langle \Psi | \hat{W} | \Psi \rangle$$

Unified Solution of the Quantum Many-Body Problem

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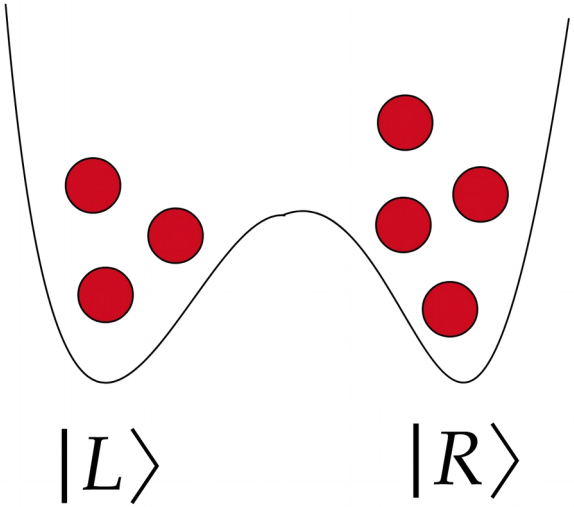
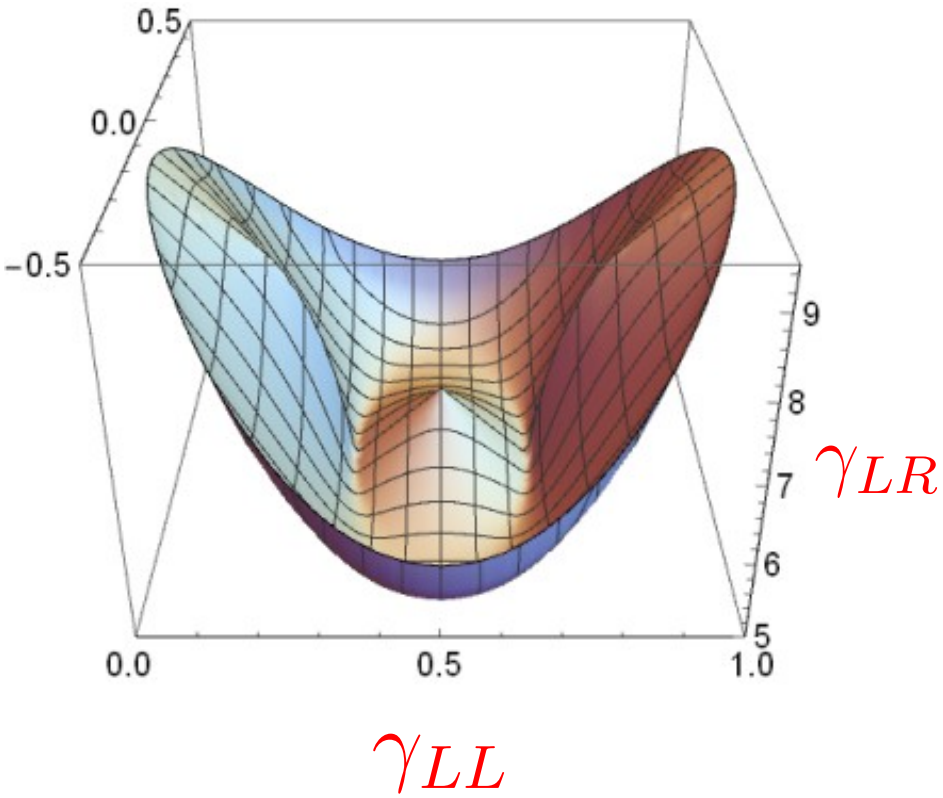
simultaneous (partial) solution
for **all** quantum many-body systems!

1-RDMFT for Bosons



$$\mathcal{F}_{BH}(\gamma) =$$



CLBR et al., PRL (2020).

Spontaneous Breaking of U(1)-Symmetry

$$\hat{H} = \hat{h} + \hat{\Delta} + \hat{W}$$

$$\hat{h} = \sum_i \hat{h}_i \qquad \hat{\Delta} = \sum_i \hat{\delta}_i \qquad \hat{W} = \sum_{i<j} \hat{W}_{ij}$$

1-particle operators

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2-particle operator

$$E(\hat{h}, \hat{\Delta}) = \min_{\gamma, \chi}[\langle \hat{h}, \gamma \rangle + \langle \hat{\Delta}, \chi \rangle + \mathcal{F}(\gamma, \chi)]$$

Spontaneous Breaking of U(1)-Symmetry

$$\mathcal{F}(\gamma, \chi) = \min_{|\Psi\rangle \to \gamma, \chi} \langle \Psi | \hat{W} | \Psi \rangle$$

Generalized 1RDM

Nambu-Gorkov space $\hat{\Psi} = (\psi^\dagger, \psi)$

Generalized 1RDM

$$\Gamma = \langle \hat{\Psi} \otimes \hat{\Psi}^\dagger \rangle = \begin{pmatrix} \gamma & \chi \\ \chi^\dagger & 1 - \gamma \end{pmatrix}$$

$$\gamma(\vec{x}, \vec{x}') = \langle \psi^\dagger(\vec{x}) \psi(\vec{x}') \rangle$$

$$\chi(\vec{x}, \vec{x}') = \langle \psi(\vec{x}) \psi(\vec{x}') \rangle$$

Generalized 1RDM

$$\Gamma = \langle \hat{\Psi} \otimes \hat{\Psi}^\dagger \rangle = \begin{pmatrix} \gamma & \chi \\ \chi^\dagger & 1-\gamma \end{pmatrix}$$

$$\Gamma^2 \leq \Gamma$$

Spontaneous Breaking of U(1)-Symmetry

$$\mathcal{F}(\Gamma) = \min_{|\Psi\rangle \to \Gamma} \langle \Psi | \hat{W} | \Psi \rangle$$

1-RDMFT SC

$$(\hat{h} - \mu, \hat{\Delta}) \Longleftrightarrow (\gamma, \chi) \Longleftrightarrow \rho_{eq} = \frac{e^{-\beta(\hat{H} - \mu \hat{N})}}{Z}$$

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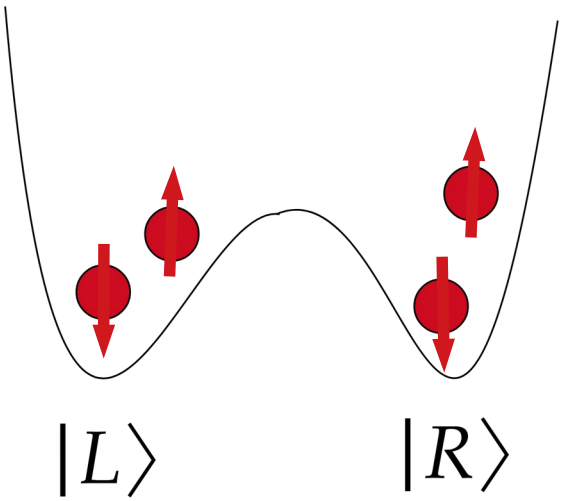
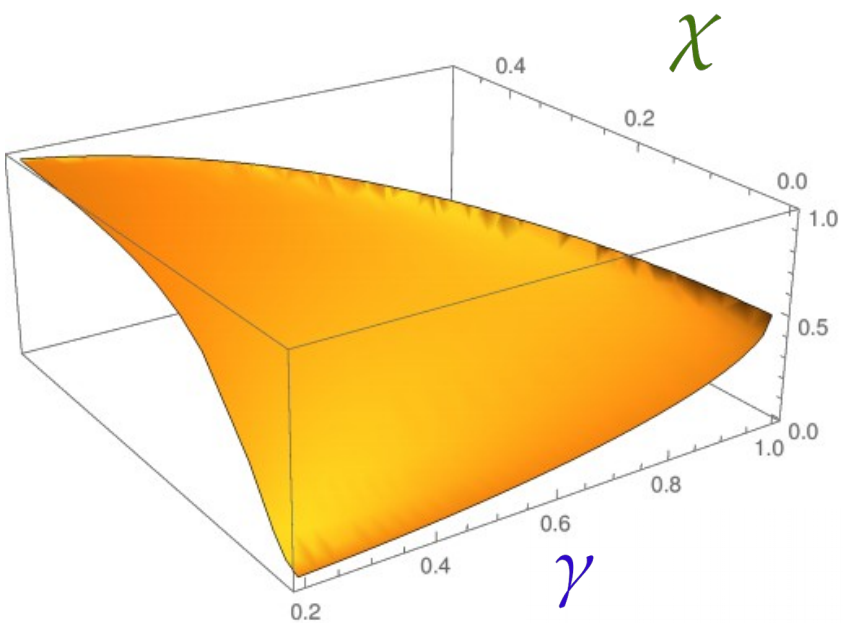
SC theories	Coulomb
BCS-Eliashberg	μ^*
SC-DFT	$E_{xc}[\rho, \chi]$
1RDM theory	$\mathcal{F}_\beta[\gamma, \chi]$

Example of 1-RDMFT for SC

$$H = -\sum_{\sigma}\left(c^{\dagger}_{L\sigma}c_{R\sigma} + c^{\dagger}_{R\sigma}c_{L\sigma}\right) + c^{\dagger}_{L\uparrow}c^{\dagger}_{L\downarrow} + c^{\dagger}_{R\uparrow}c^{\dagger}_{R\downarrow} + h.c. + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$





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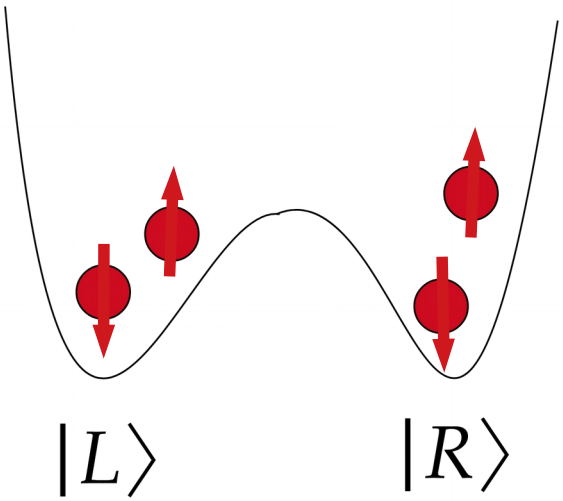
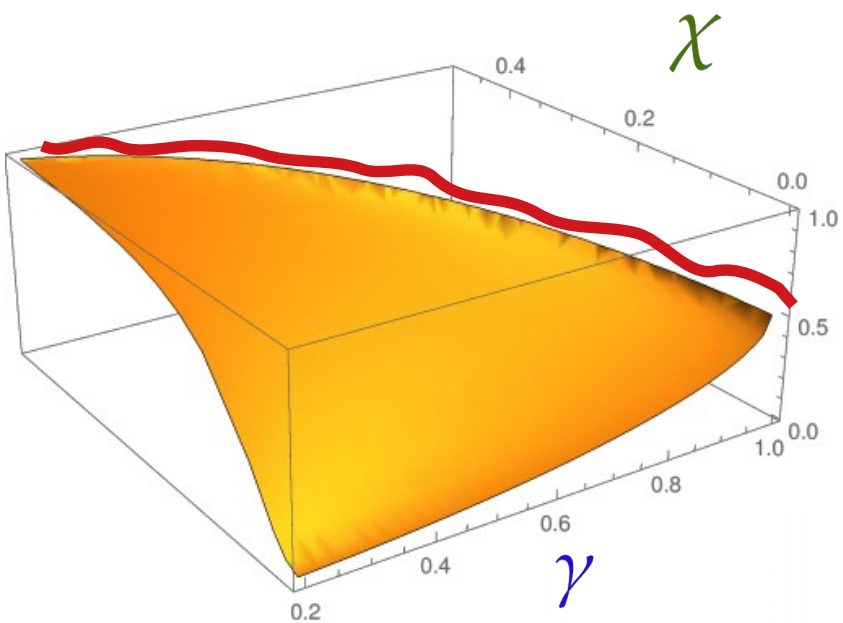
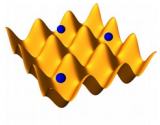


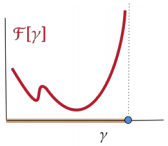


$$\Gamma^2 = \Gamma$$

Outlook



develop a 1-RDMFT for superconductors



physical crossovers of many-body systems

$$\mathcal{F}(\gamma^b) \longleftrightarrow \mathcal{F}(\gamma^f, \chi)$$

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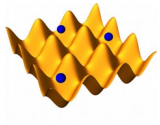

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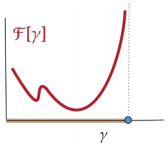

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European Commission