Relating fundamentals of functional theory
An analytic case study

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In collaboration with:

Christian Schilling, Adam Y. Chaou

Motivation

RDMFT variant	**Gilbert**	**Levy**	**Valone**
complexity of domain	very hard ←	hard	trivial
complexity of calculating functional	→		increasing
explanation:	physical intuition + development of numerical ground state methods (fitting of functionals)	mathematical minimization (constrained search)	mathematical intuition + complicated ensembles ($\Gamma \geq 0$)

Reminder: $E(h) = \min_{\gamma} \left[\mathrm{Tr}_1[h\gamma] + \mathcal{F}(\gamma) \right]$

universal functional

[T. Gilbert, Phys. Rev. B **12**, 2111 (1975),
M. Levy, Proc. Natl. Acad. Sci. U.S.A. **76**, 6062 (1979),
S. M. Valone, J. Chem. Phys. **73**, 1344 (1980),
C. Schilling, J. Chem. Phys. **149**, 231102 (2018)]

Outline

1) Foundational aspects of RDMFT

2) Ordinary Hubbard dimer

3) Generalized Hubbard dimer

1) Foundational aspects of RDMFT

1RDM: $\gamma = N\mathrm{Tr}_{N-1}[\Gamma]$

Hamiltonian: $H(h) = h + \boxed{W}$ fixed!

Universal functional:

$$\boxed{\mathcal{F}^{(p/e)}(\gamma) = \min_{\Gamma \mapsto \gamma} \mathrm{Tr}_N[\Gamma W]}$$

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Domain of $\mathcal{F}$:

- $\mathcal{P}^N = \{\Gamma : \mathcal{H}_N \to \mathcal{H}_N \,|\, \Gamma^2 = \Gamma, \mathrm{Tr}[\Gamma] = 1, \Gamma \geq 0\} \xrightarrow{N\mathrm{Tr}_{N-1}[\cdot]} \boxed{\mathcal{P}_N^1}$
- $\mathcal{E}^N = \{\Gamma : \mathcal{H}_N \to \mathcal{H}_N \,|\, \mathrm{Tr}[\Gamma] = 1, \Gamma \geq 0\} \xrightarrow{N\mathrm{Tr}_{N-1}[\cdot]} \boxed{\mathcal{E}_N^1}$

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Real-valued vs. complex-valued wave functions

$$|\Psi\rangle = \sum_I c_I |\Phi_I\rangle$$

Real-valued: $c_I \in \mathbb{R} \Rightarrow \mathcal{F}_{\mathbb{R}}$

Complex-valued: $c_I \in \mathbb{C} \Rightarrow \widetilde{\mathcal{F}}_{\mathbb{C}}$

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$$\boxed{\mathcal{F}_{\mathbb{C}}^{(p)}(\mathfrak{Re}(\gamma)) = \min_{(\gamma-\gamma^*)/2i} \widetilde{\mathcal{F}}_{\mathbb{C}}^{(p)}(\gamma)}$$

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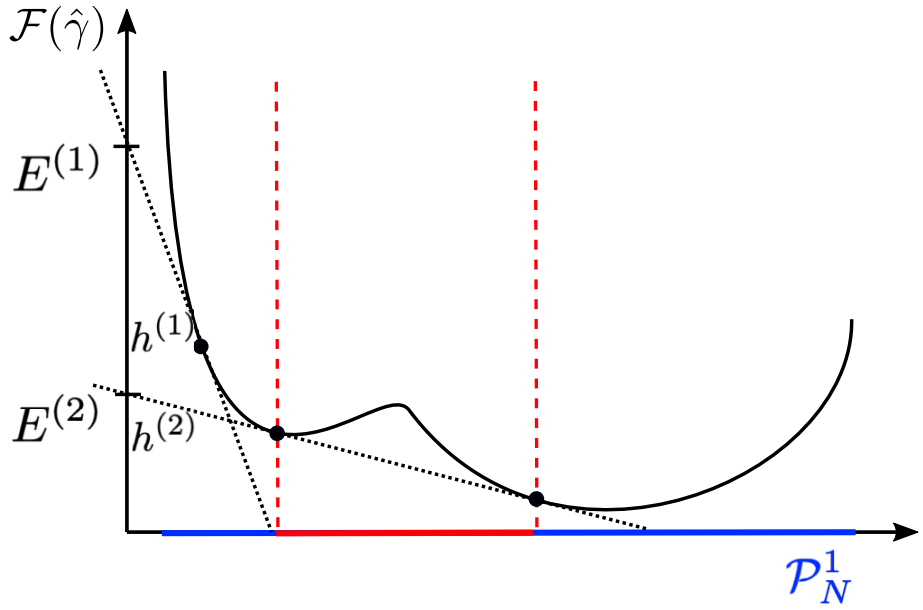
$$\begin{tikzcd}
\widetilde{\mathcal{F}}_{\mathbb{C}}^{(p)} \arrow[r, "\min_{(\gamma-\gamma^*)/2i}"] \arrow[d, "\mathrm{conv}(\cdot)"'] & \boxed{\mathcal{F}_{\mathbb{C}}^{(p)} \quad \leq \quad \mathcal{F}_{\mathbb{R}}^{(p)}} \arrow[d, "\mathrm{conv}(\cdot)"'] \arrow[d, phantom, shift left=6ex, "\mathrm{conv}(\cdot)"] \\
\widetilde{\mathcal{F}}_{\mathbb{C}}^{(e)} \arrow[r, "\min_{(\gamma-\gamma^*)/2i}"] & \mathcal{F}_{\mathbb{C}}^{(e)} \quad = \quad \mathcal{F}_{\mathbb{R}}^{(e)}
\end{tikzcd}$$

v-representability problem

Which 1RDMs are 'physical'?



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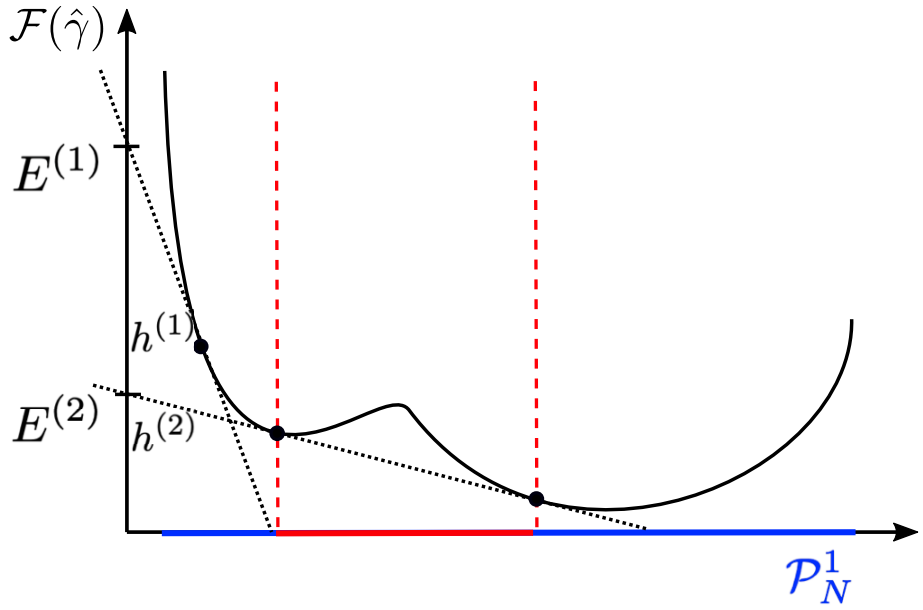

Gilbert: $\mathcal{F}^{(p)}(\gamma_h) = E(\gamma_h) - \mathrm{Tr}_1[h\gamma_h]$

Diverging exchange force: $|\nabla_\gamma \mathcal{F}(\gamma)| \xrightarrow{\mathrm{dist}(\gamma,\partial\mathcal{P}_N^1)\to 0} \infty$

[T. Gilbert, Phys. Rev. B **12**, 2111 (1975),
C. Schilling, R. Schilling, Phys. Rev. Lett. **122**, 013001 (2019)]

2) Ordinary Hubbard dimer

[A.J. Cohen, P. Mori-Sánchez, Phys. Rev. A **93**, 042511 (2016)]

$$H = h + W$$

$$h = \sum_{\sigma=\uparrow,\downarrow} \left[-t \left(c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma} \right) + \varepsilon_1 \hat{n}_{1\sigma} + \varepsilon_2 \hat{n}_{2\sigma} \right]$$

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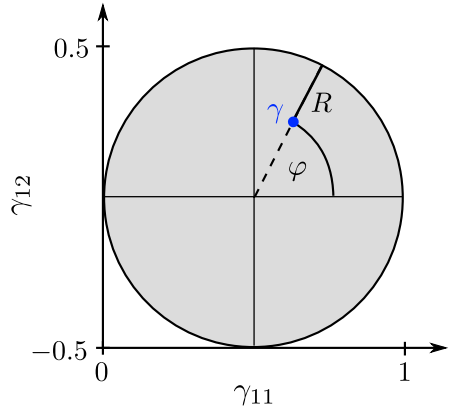

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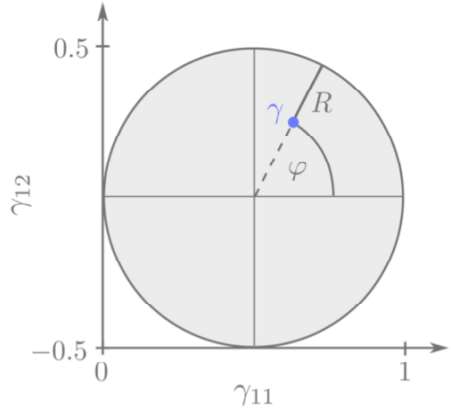
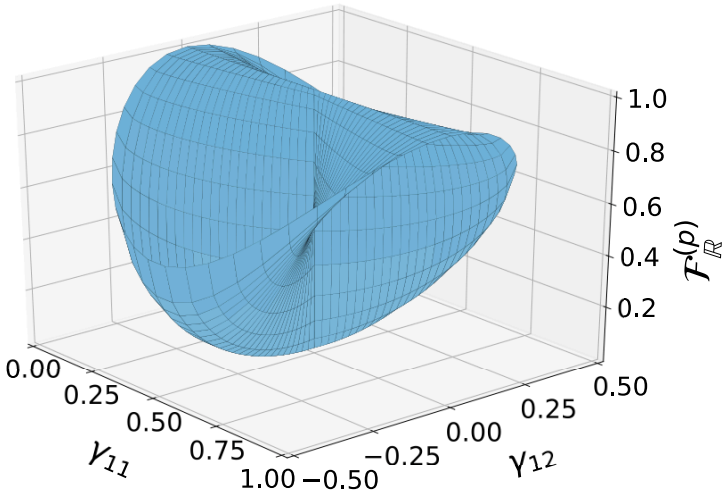
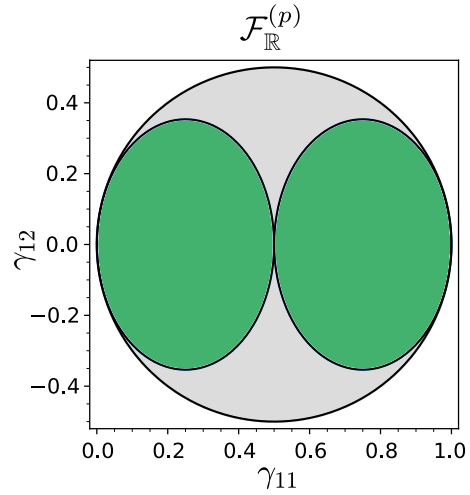


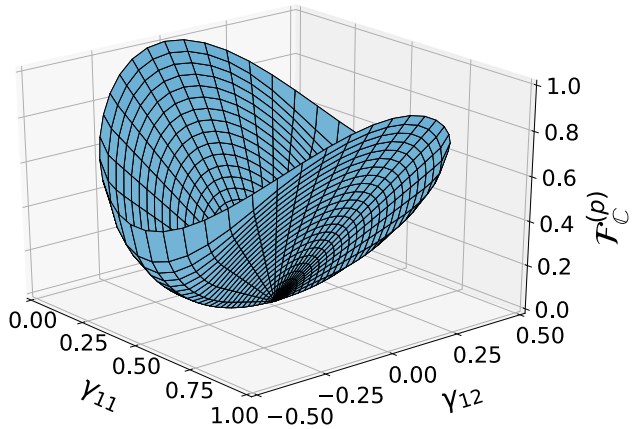
$$\Rightarrow \quad \boxed{\mathcal{F}^{(p)}_{\mathbb{R}}(\gamma) = U \left[1 - \tfrac{1}{2} \sin^2(\varphi) \left(1 + \sqrt{1 - (1 - 2R)^2} \right) \right]}$$

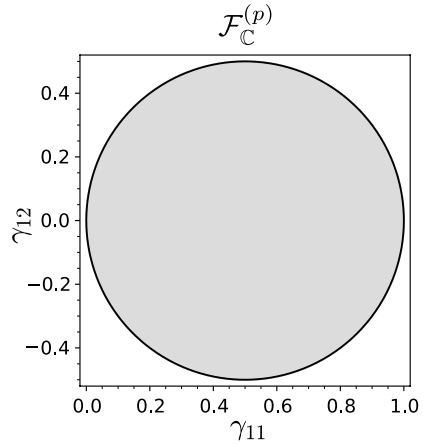




How about $\mathcal{F}_{\mathbb{C}}^{(\mathbf{p})}$?

Numerical result by Cohen and Mori-Sánchez:





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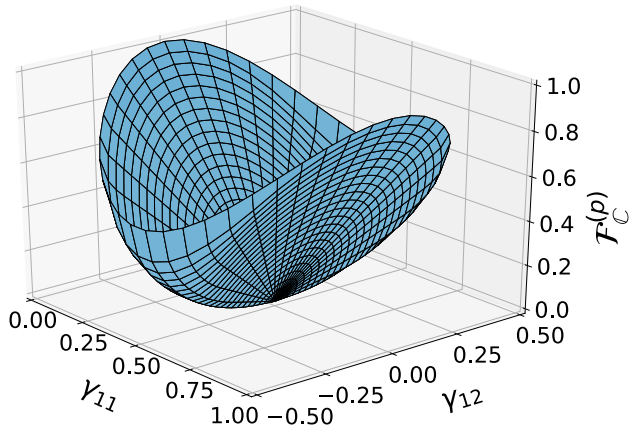

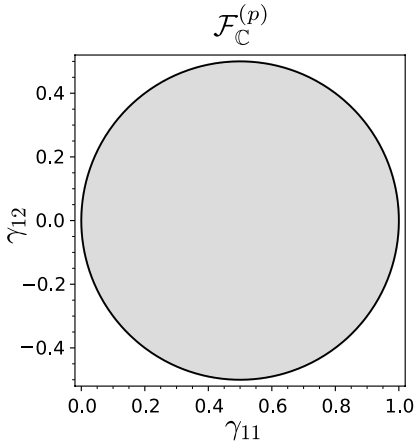

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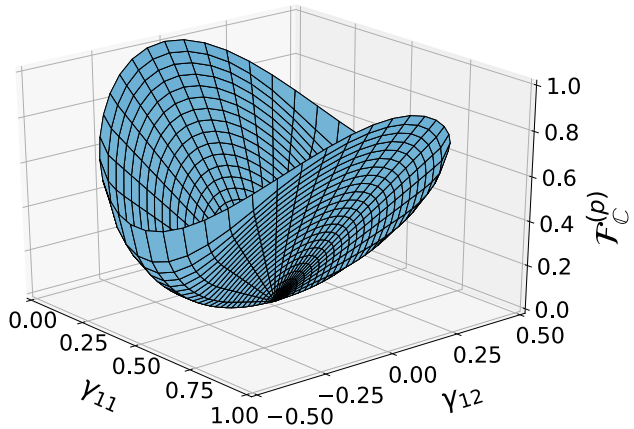

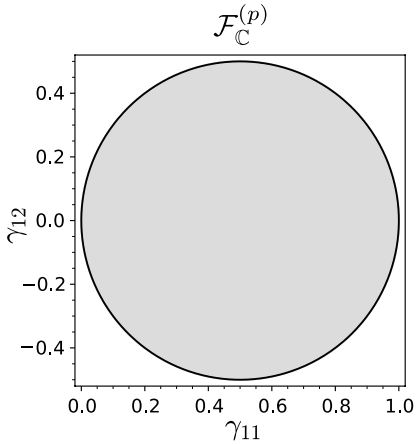

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Can we provide an analytic poof?

$\rightarrow$ **Yes!**

$$|\Psi\rangle = w_r|\Psi_r\rangle + iw_i|\Psi_i\rangle\,, \quad w_r, w_i \in \mathbb{R}$$

$$\Rightarrow \;\; \mathcal{F}_{\mathbb{C}}^{(p)}(\gamma) = \min_{\Gamma^{\mathrm{rank}=2} \mapsto \gamma} \mathrm{Tr}_2[W\Gamma^{\mathrm{rank}=2}]$$

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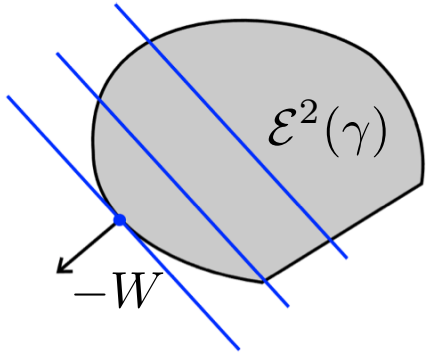

[J. Liebert, A.Y. Chaou, C. Schilling, forthcoming (2022)]

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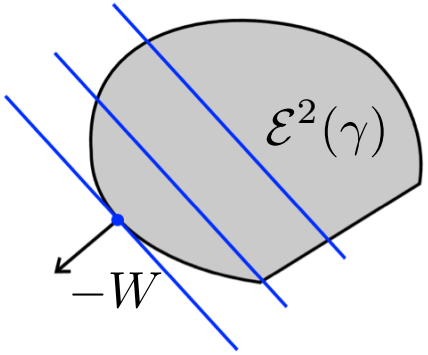

$$\Rightarrow \quad \boxed{\mathcal{F}_{\mathbb{C}}^{(p)} = \mathrm{conv}\left(\mathcal{F}_{\mathbb{R}}^{(p)}\right)}$$

$$\begin{tikzcd}
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\widetilde{\mathcal{F}}_{\mathbb{C}}^{(e)} \arrow[r, "\min_{\mathrm{Im}(\gamma_{12})}"] & \mathcal{F}_{\mathbb{C}}^{(e)} \arrow[r, phantom, "="] & \mathcal{F}_{\mathbb{R}}^{(e)}
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3) Generalized Hubbard dimer

$$W = U\left(|\Phi_1\rangle\langle\Phi_1| + |\Phi_2\rangle\langle\Phi_2|\right) + V\left(|\Phi_1\rangle\langle\Phi_2| + \text{h.c.}\right) + X\left(|\Phi_1\rangle\langle\Phi_3| + |\Phi_2\rangle\langle\Phi_3| + \text{h.c.}\right)$$

Basis states:

$$|\Phi_1\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger|0\rangle, \quad |\Phi_2\rangle = c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger|0\rangle, \quad |\Phi_3\rangle = \frac{1}{\sqrt{2}}\left(c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger - c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger\right)|0\rangle$$

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$$\Downarrow$$

$$\mathcal{F}^{(p)}_{\mathbb{R}}(\gamma) = U + \sqrt{2}X(1-2R)\sin(\varphi) + \frac{1}{2}(V-U)\sin^2(\varphi) - \frac{1}{2}\sqrt{1-(1-2R)^2}\,|(V-U)\sin^2(\varphi) - 2V|$$

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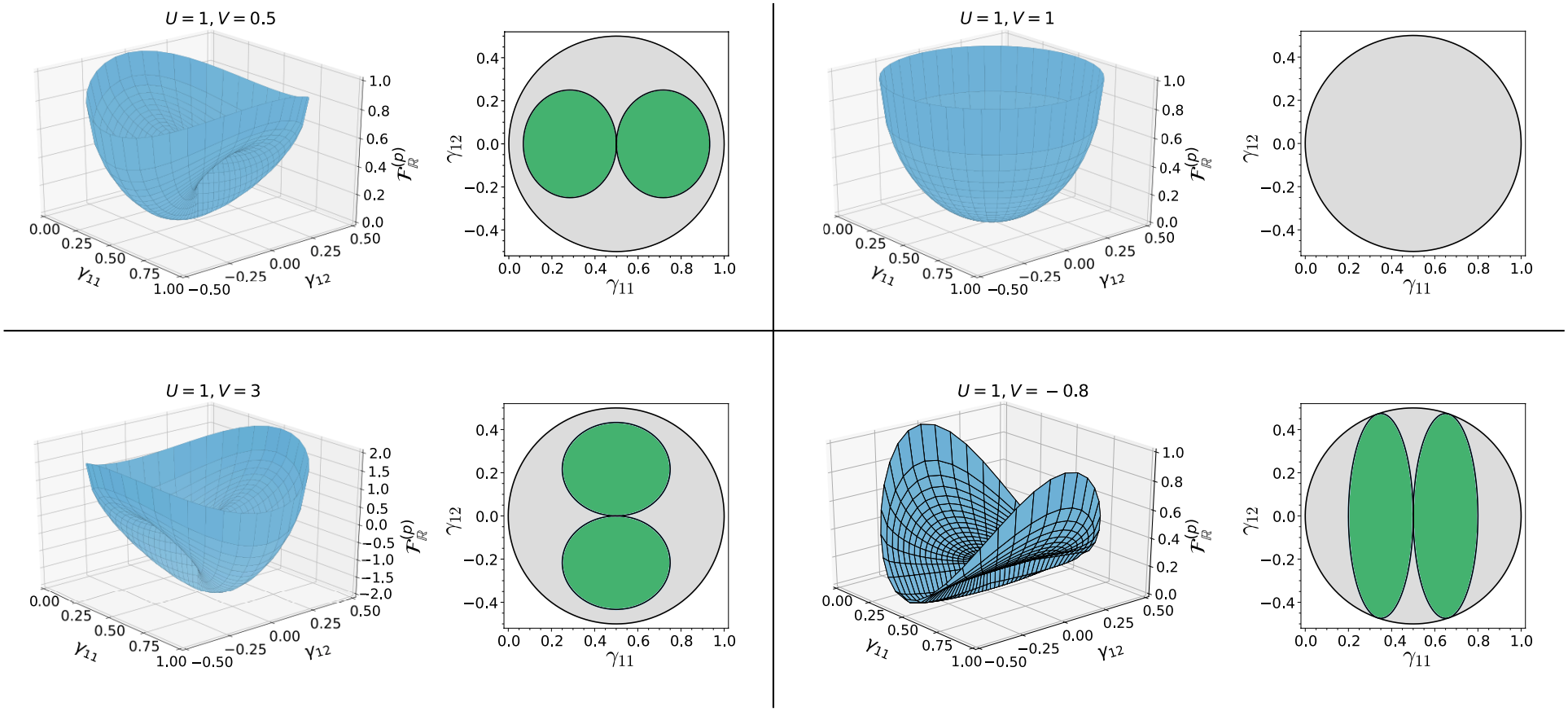

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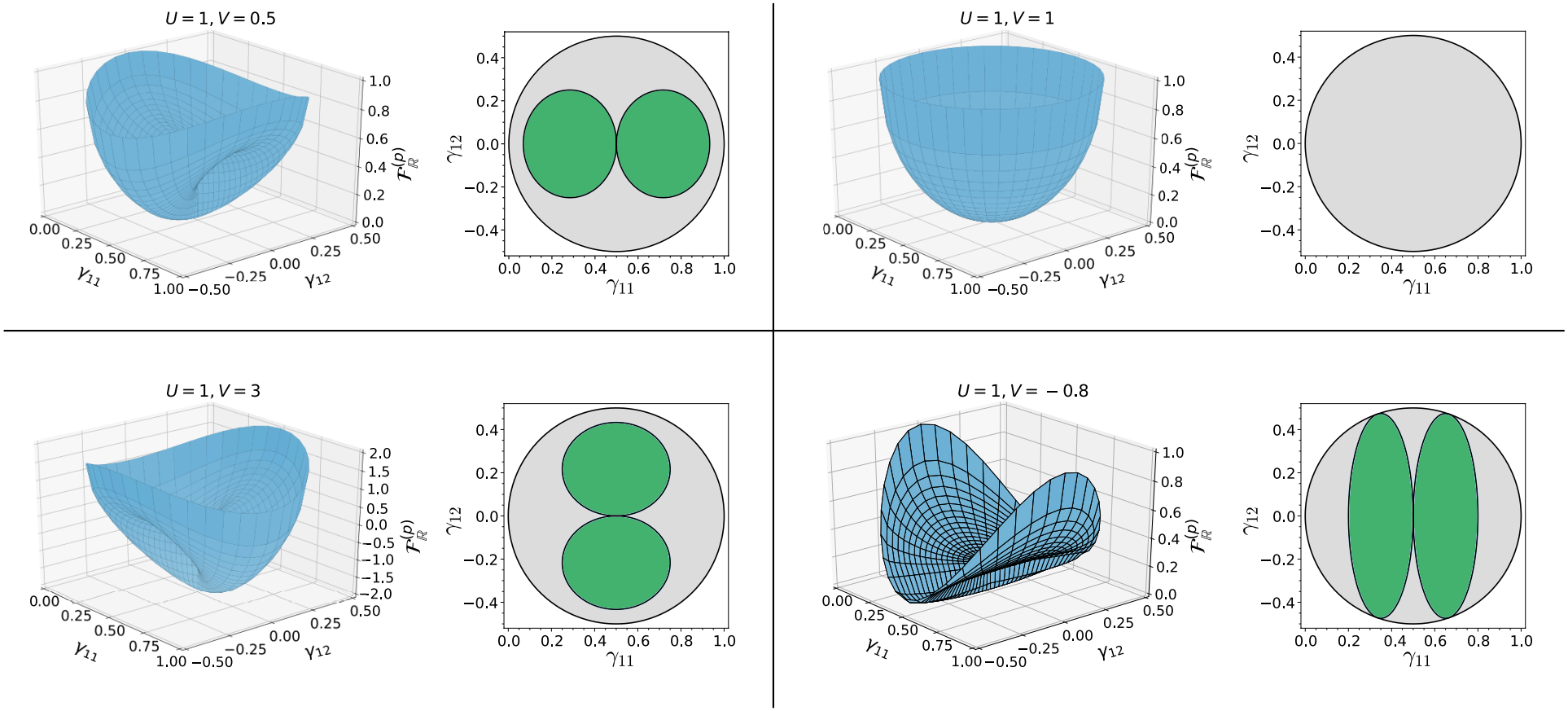

Fermionic exchange force:

$$\frac{\partial \mathcal{F}_{\mathbb{R}}^{(p)}}{\partial R} = -\frac{|\sin^2(\varphi)(V-U) - 2V|}{2}\frac{1}{\sqrt{R}} + \mathcal{O}(R^0)$$

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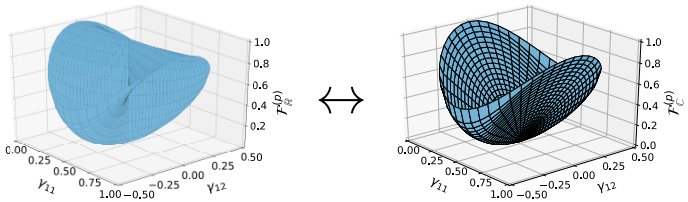
Summary

- Exploiting symmetries vs. complexities of RDMFT



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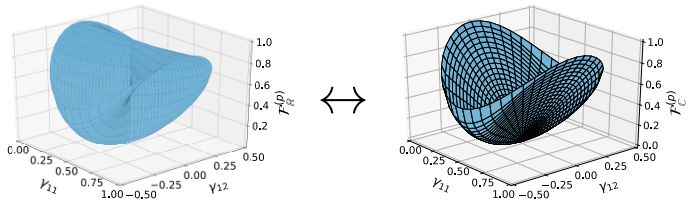

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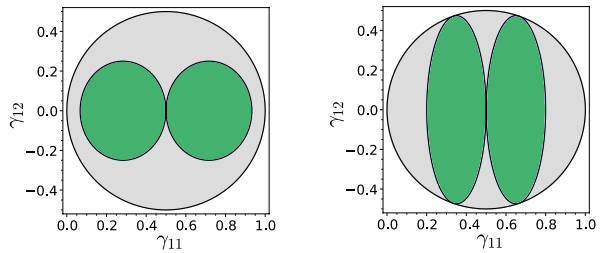
- Role of v-representability in RDMFT



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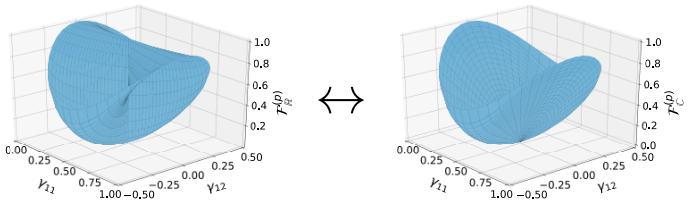

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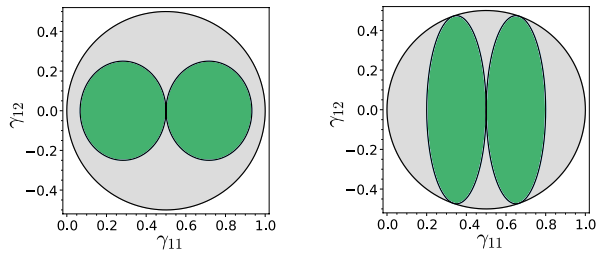

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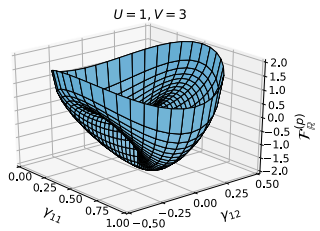

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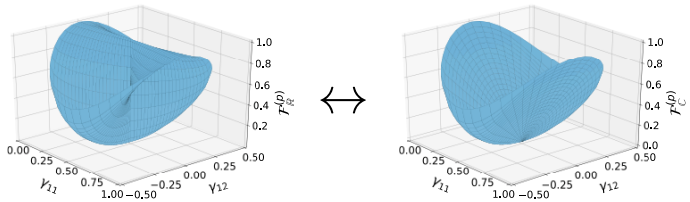

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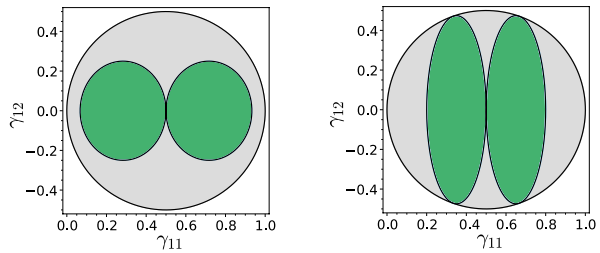

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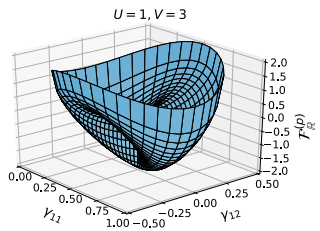

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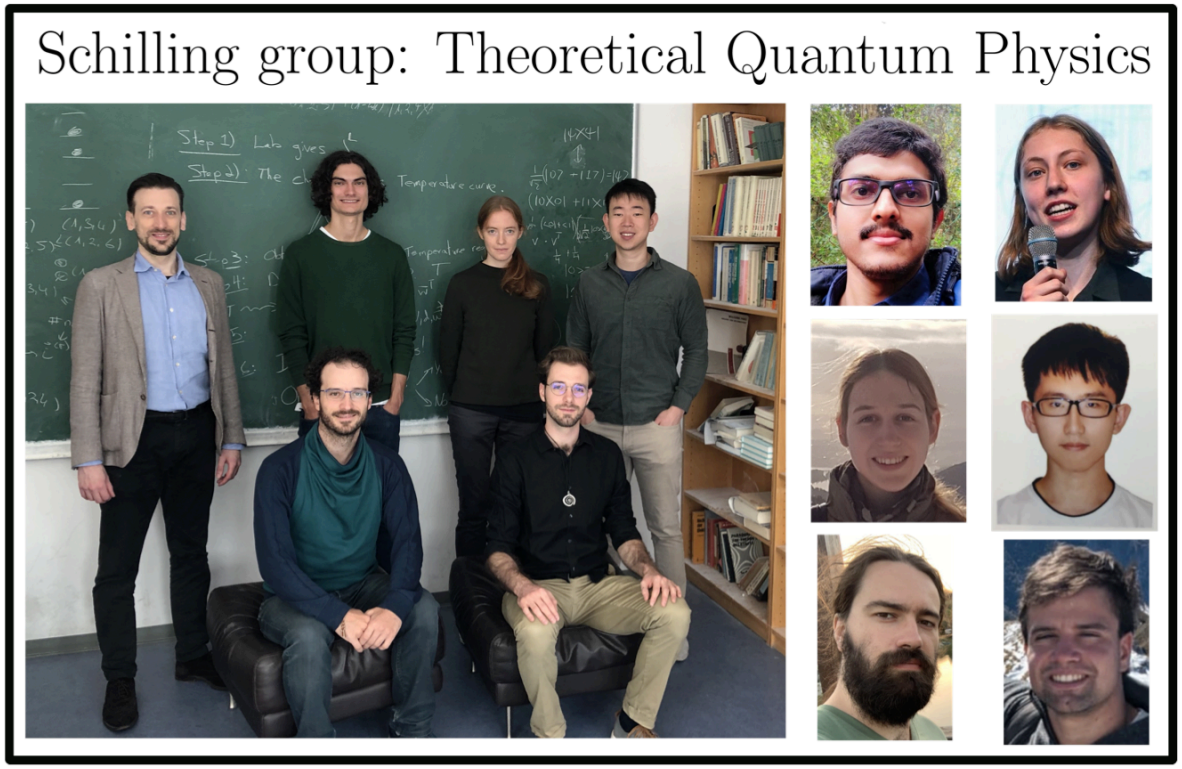

References:

1. A.J. Cohen, P. Mori-Sánchez, Phys. Rev. A **93**, 042511 (2016)
2. J. Liebert, A.Y. Chaou, C. Schilling, forthcoming (2022)