Fundamental aspects of density-functional theory on lattices

Robert van Leeuwen
Department of Physics
University of Jyväskylä

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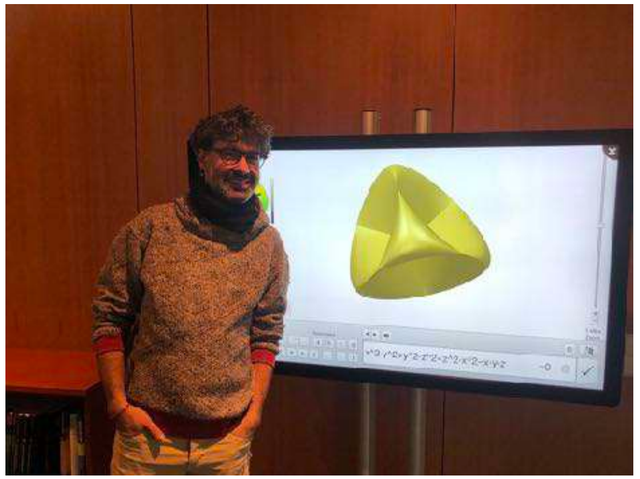
Michael Ruggenthaler

Markus Penz



Overview

- Recent results on v-representability for continuum systems

- Geometrical formulation of the Hohenberg-Kohn theorem on lattices

- Numerical procedure to carry out Levy-Lieb constrained search using imaginary time propagation

v-representability and Hohenberg-Kohn

Continuum case: $\hat{H} = \hat{H}_0 + \hat{V}$ $\quad \hat{H}_0 = \sum_{i=1}^{N} -\frac{1}{2}\nabla_i^2 + \sum_{i>j}^{N} w(\mathbf{r}_i, \mathbf{r}_j)$ $\quad \hat{V} = \sum_{i=1}^{N} v(\mathbf{r}_i)$

We solve: $(\hat{H}_0 + \hat{V})\Psi(x_1, \ldots, x_N) = E\Psi(x_1, \ldots, x_N)$ $\quad x_i = (r_i, \sigma_i)$

space-spin coordinate

$$\rho(r_1) = N \sum_{\sigma_1} \int dx_2 \ldots dx_N |\Psi(r_1\sigma_1, x_2, \ldots, x_N)|^2$$

The v-representability question:
Which densities are ground state densities of some Hamiltonian with a potential v?

If a density is v-representable, is it then uniquely v-representable ?

Hohenberg-Kohn (1964): If two potentials differ more than a constant then they produce two different ground state densities (physicists' proof)

Theorem: HK true for potentials in $L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \quad p > 2$

Louis Garrigue, "Unique continuation for many-body Schrödinger operators and the Hohenberg-Kohn theorem", Math.Phys.Anal.Geom.21, 27 (2018)

Recent result (2024) on v-representability for a one-dimensional periodic domain

Theorem 1. *Define the following set of v-representable densities on the one-dimensional torus* $\mathbb{T}$ *and the dual space of (distributional) one-body potentials,*

$$\mathscr{X}_{>0} = \left\{\rho \in L^2(\mathbb{T}) \mid \nabla\rho \in L^2(\mathbb{T}), \int \rho = N, \forall x \in \mathbb{T} : \rho(x) > 0\right\} \tag{3}$$

$$\mathscr{X}^* = \left\{[v] = \{v + c \mid c \in \mathbb{R}\} \mid v = f + \nabla g \text{ with } f, g \in L^2(\mathbb{T})\right\}. \tag{4}$$

Then for every $\rho \in \mathscr{X}_{>0}$ *there is an equivalence class* $[v] \in \mathscr{X}^*$ *with corresponding potential* $V = \sum_{j=1}^{N} v(x_j)$ *acting on wave functions, such that* ρ *is the density of an (ensemble) ground state of the self-adjoint Hamiltonian* $H = H_0 + V = -\frac{1}{2}\Delta + W + V$.

Sarina Sutter, Markus Penz, Michael Ruggenthaler, RvL, Klaas Giesbertz,
"Solution of the v-representability problem on a one-dimensional torus"
J.Phys.A: Math.Theor. 57, 475202 (2024)

Important consequence: A Kohn-Sham system exists

This is complemented by two important recent works of Thiago Carvalho Corso

"v-representability and Hohenberg-Kohn theorem for non-interacting Schrödinger operators with distributional potentials in the one-dimensional torus" J.Phys.A Math Theor. 58,125203 (2025)

"A rigorous formulation of density functional theory for spinless electrons in one dimension" arXiv:2504.05501 (2025)

Theorem: For the distributional potentials on the one-dimensional torus the ground density is positive and the HK theorem is true. The xc-functional is Gateaux differentiable.

This provides a solid foundation of the Kohn-Sham method for this 1D case.

Our future aim:

The solution of the v-representability problem for the 3D torus

This would be a major result as it would provide a rigorous foundation for Kohn-Sham DFT for periodic solids

Motivation for lattice DFT

- Lattice systems were studied to provide an answer to the v-representability problem but the Hohenberg-Kohn theorem for lattice systems has remained an open issue

- Little is known about the structure of the density domain (pure states, degeneracies); lattice systems provide easy access

- Lattice Hamiltonians are commonly used in the study of strongly correlated systems (Hubbard systems) and are used as benchmarks for (TD)DFT

- The v-representability problem for continuum systems is still not completely solved and further understanding of the proof for lattice systems may be beneficial

Main result: A geometrical formulation of the Hohenberg-Kohn theorem

History of lattice DFT

DFT

W.Kohn, "v-representability and density functional theory", Phys.Rev.Lett.51, 1596 (1983)

v-representable densities on a lattice form an open set

J.Chayes,:.Chayes,M.B.Ruskai, "Density functional approach to quantum lattice systems", J.Stat.Phys.38, 497 (1985)

every normalised density on a lattice such that $0 < \rho_i < 1$ and $\sum_i \rho_i = N$ is v-representable

C.A.Ullrich and W.Kohn, "Degeneracy in density functional theory: topology in v and n spaces", Phys.Rev.Lett.89, 156401, (2002)

degeneracy is common in density space and rare in potential space

TDDFT

R.Baer, "On the mapping of time-dependent densities onto potentials in quantum mechanics", J.Chem.Phys.128, 044103, (2008)

Y.Li and C.A.Ullrich,"Time-dependent v-representability on lattice systems", J.Chem.Phys.129,044105 (2008)

densities that change too fast between adjacent sites are non-v-representable

I.V.Tokatly, "Time-dependent current-density functional theory on a lattice", Phys.Rev.B83, 035127 (2011)

M. Farzahnehpour, I.V.Tokatly, "Time-dependent density-functional theory on a lattice", Phys.Rev.B86,125140 (2012)

proof of 1-1 correspondence for short time scales based on the Picard-Lindelöf theorem

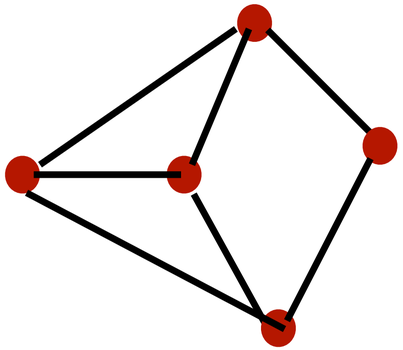
This presentation is based on the following papers

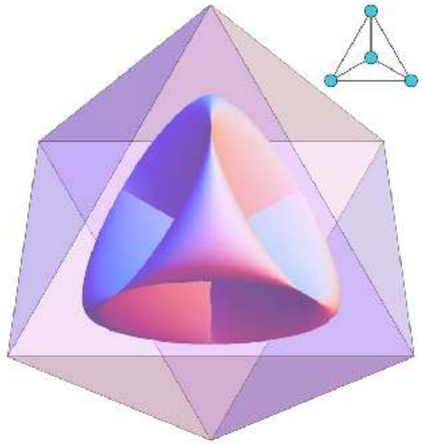
M.Penz and RvL, "Density-functional theory on graphs", J.Chem.Phys. 155, 244111 (2021)

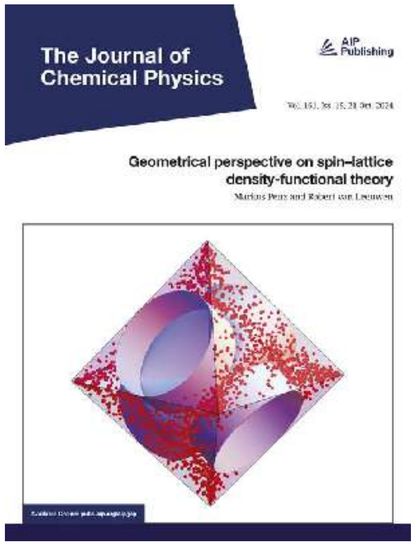
M.Penz and RvL, "Geometry of degeneracy in potential and density space", Quantum 7, 918 (2023)

M.Penz and RvL, "Geometrical perspective on spin-lattice density-functional theory", J.Chem.Phys.161,150901 (2024)

M.Penz and RvL, "Constrained search in imaginary time", arXiv: 2504.05332 (2025)





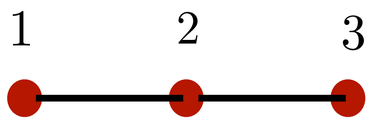


Lattice Hamiltonians

We consider Hamiltonians of the general type

$$\hat{H} = \sum_{i,j}^{M} h_{ij} \hat{a}_i^\dagger \hat{a}_j + \hat{W}$$

two-body interaction



$$h_{12} \neq 0$$

$$h_{23} \neq 0$$

$$h_{13} = 0$$

To each such Hamiltonian we assign a graph or a lattice $\quad i \sim j \quad \Leftrightarrow \quad h_{ij} \neq 0$

The ground state can be expanded in N-particle position kets

$$|\Psi\rangle = \sum_I \Psi_I |I\rangle \qquad |I\rangle = \hat{a}_{i_N}^\dagger \ldots \hat{a}_{i_1}^\dagger |0\rangle \qquad I = (i_1, \ldots, i_N) \quad i_1 < \ldots < i_N$$

and the main object of our interest will be the density

$$\rho_i = \langle \Psi | \hat{\rho}_i | \Psi \rangle \qquad \hat{\rho}_i = \hat{a}_i^\dagger \hat{a}_i \qquad i \in \{1, \ldots, M\} \qquad M \text{ = number of lattice sites}$$

$$\rho_i = \sum_{I \ni i} |\Psi_I|^2$$

$$\sum_I |\Psi_I|^2 = 1 \quad \Rightarrow \quad 0 \leq \rho_i \leq 1$$

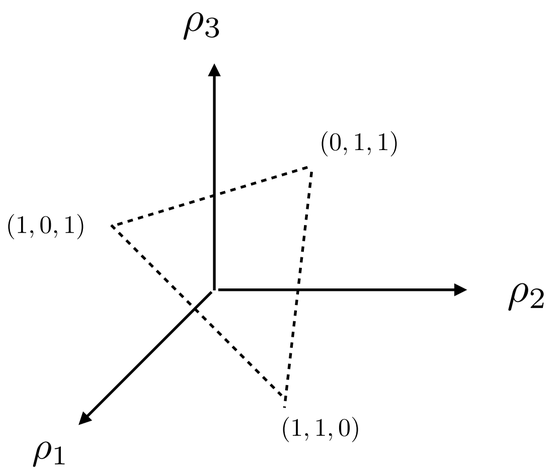
fermionic constraint

Density space

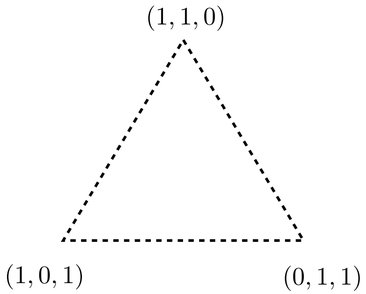
The region of allowed densities satisfies

$$\rho_1 + \ldots + \rho_M = N \qquad 0 \leq \rho_i \leq 1 \qquad \mathcal{P}_{M,N}$$ hypersimplex

For example, M=3, N=2

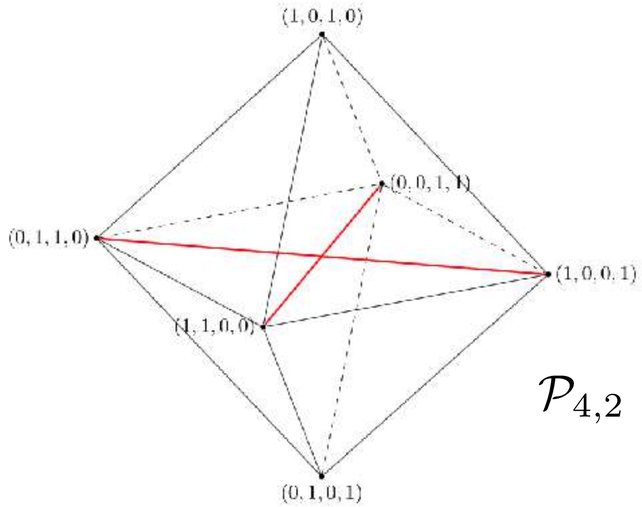


$$\rho_1 + \rho_2 + \rho_3 = 2$$



$\mathcal{P}_{3,2}$

M=4, N=2



$\mathcal{P}_{4,2}$

$$\rho_1 + \rho_2 + \rho_3 + \rho_4 = 2$$

For visualisation reasons most of our examples will have M=4

v-representability

J.Chayes,:.Chayes,M.B.Ruskai, "Density functional approach to quantum lattice systems", J.Stat.Phys.38, 497 (1985)

every normalised density on a lattice such that $0 < \rho_i < 1$ and $\sum_i \rho_i = N$ is ensemble v-representable

The condition that $0 < \rho_i < 1$ implies that we are considering the interior of the density domain

Questions:

What about the validity of the Hohenberg-Kohn theorem?

Which densities are pure-state v-representable?

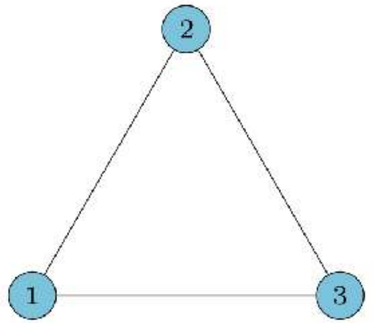
What is the shape of the density regions corresponding to degenerate ground states?

Are the densities on the boundary v-representable?

Example 1

Take a 3-site noninteracting model with one-body hamiltonian

$$h_{ij} = -\Delta_{ij} + v_i \delta_{ij} = \begin{pmatrix} 2+v_1 & -1 & -1 \\ -1 & 2+v_2 & -1 \\ -1 & -1 & 2+v_3 \end{pmatrix}$$



A general 2-particle ground state is of the form

$$|\Psi\rangle = \Psi_{12}|12\rangle + \Psi_{13}|13\rangle + \Psi_{23}|23\rangle = (\Psi_{12}, \Psi_{13}, \Psi_{23})$$

$$\rho_1 = |\Psi_{12}|^2 + |\Psi_{13}|^2 \qquad \rho_2 = |\Psi_{12}|^2 + |\Psi_{23}|^2 \qquad \rho_3 = |\Psi_{13}|^2 + |\Psi_{23}|^2$$

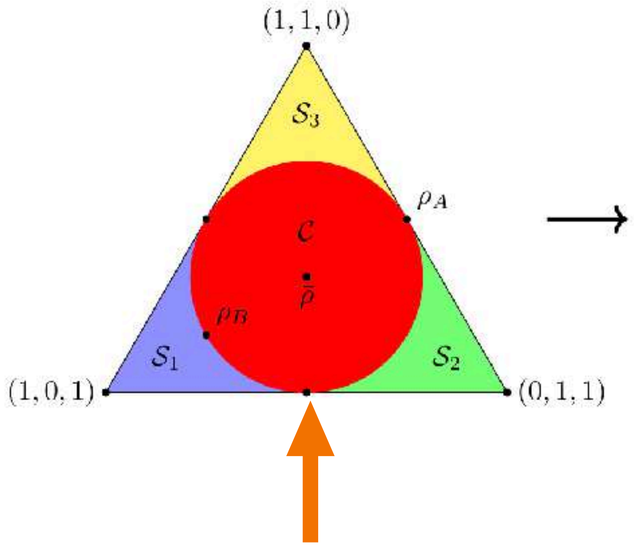
For v=0 we have the two degenerate eigenstates

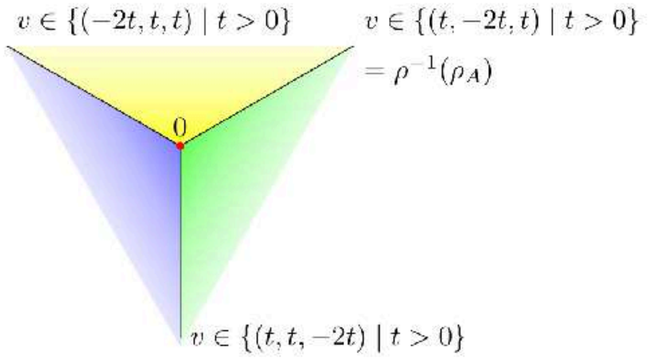
$$\Psi_A = \frac{1}{\sqrt{2}}(1, 0, -1) \qquad \rho_A = (\frac{1}{2}, 1, \frac{1}{2})$$

non-uv density

$$\Psi_B = \frac{1}{\sqrt{6}}(1, 2, 1) \qquad \rho_B = (\frac{5}{6}, \frac{1}{3}, \frac{5}{6})$$

Situation depicted in the density domain $\mathcal{P}_{3,2}$





attractive potential at site 2

$$(0, -x, 0) + \frac{1}{3}(x, x, x) = \frac{1}{3}(x, -2x, x) = (t, -2t, t)$$

Potential space for the gauge $v_1 + v_2 + v_3 = 0$

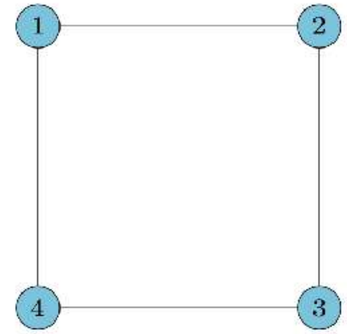
Non-uv density when degeneracy region for v=0 touches the boundary of the density domain

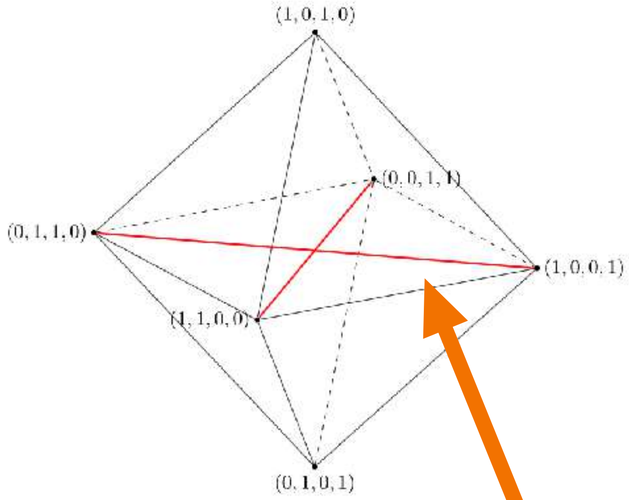
Other densities on the edge are non-v-representable

Example 11

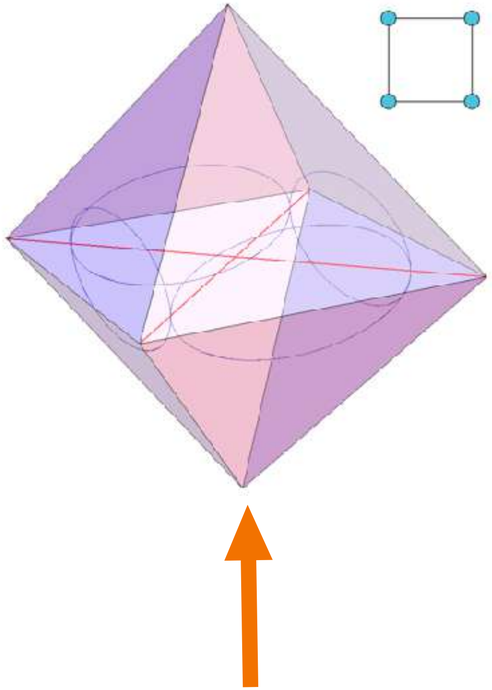
Take a 4-site noninteracting model with hamiltonian

$$h_{ij} = -\Delta_{ij} + v_i \delta_{ij} = \begin{pmatrix} 2+v_1 & -1 & 0 & -1 \\ -1 & 2+v_2 & -1 & 0 \\ 0 & -1 & 2+v_3 & -1 \\ -1 & 0 & -1 & 2+v_4 \end{pmatrix}$$

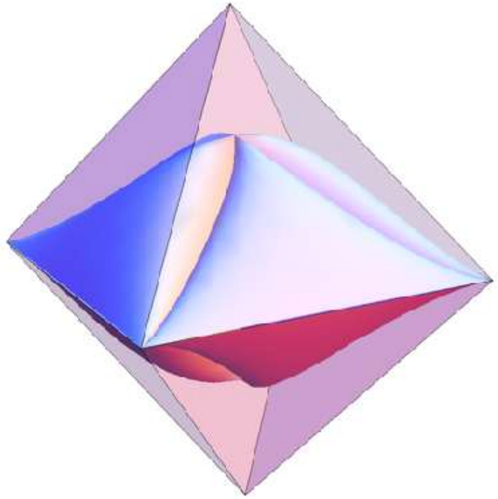




cross of non-uv densities

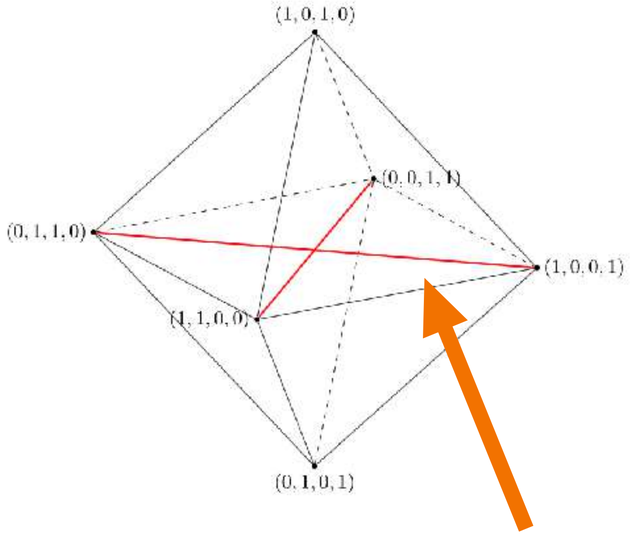


The non-uv densities appear at touching degeneracy regions



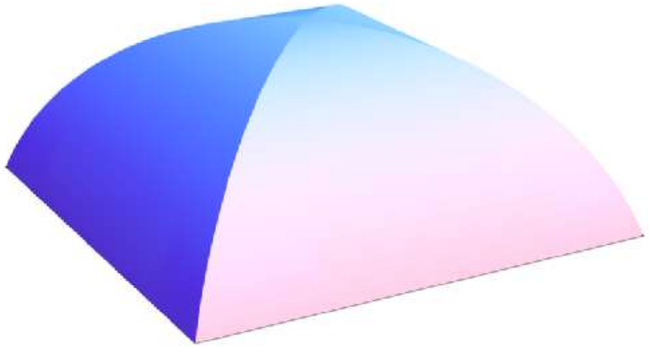
"Bundles" of degeneracy regions

Unique v-representability and subdifferentials



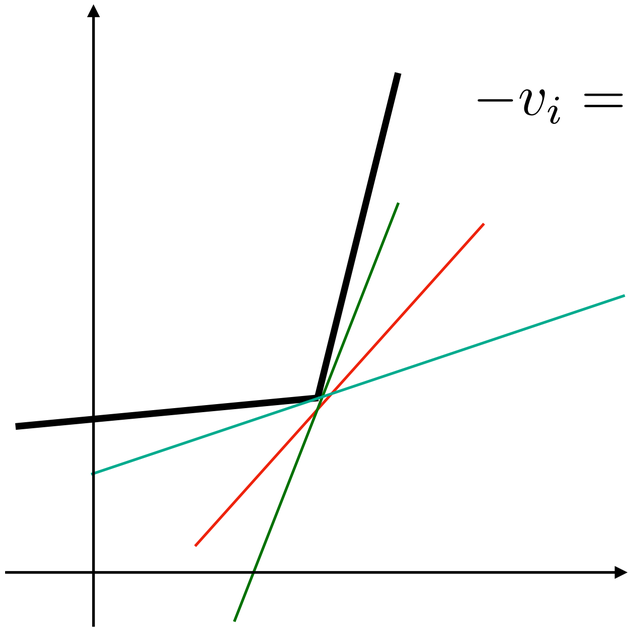
cross of non-uv densities

$-F(\rho)$



at the cross of non-uv densities F has a sharp edge and the subdifferential contains many potentials

$$F(\rho) = \inf_{\Gamma \mapsto \rho} \mathrm{Tr}\, \hat{H}_0 \Gamma.$$



$$-v_i = \frac{\partial F}{\partial \rho_i}$$

at a non-differentiable point the subdifferential contains many tangents

In our setting: many potentials leading to a given density

Degeneracy regions I : pure state densities

(discussion also valid in the continuum case)

If the Hamiltonian is real and symmetric and has a g-dimensional eigenspace $\mathcal{U}$ then this eigenspace is spanned by real orthonormal vectors Φ_i with complex coefficients

$$\mathcal{U} = \mathrm{span}_{\mathbb{C}}\{\Phi_1, \ldots, \Phi_g\} = \{c_1\Phi_1 + \ldots + c_g\Phi_g | c_i \in \mathbb{C}\}$$

This follows simply because

$$\hat{H}\Psi = E\Psi \qquad \Psi = \Psi_1 + i\Psi_2 \quad \Rightarrow \quad \hat{H}\Psi_1 = E\Psi_1 \qquad \hat{H}\Psi_2 = E\Psi_2$$

The set of all possible pure-state densities that can be obtained from states in this degenerate manifold will be denoted by $D_{\mathbb{C}}$

$$\rho \in D_{\mathbb{C}} \quad \Leftrightarrow \quad \rho = \langle\Psi|\hat{\rho}|\Psi\rangle \quad \Psi \in \mathcal{U}$$

We will construct these densities first out of densities from a smaller set

The eigenspace $\mathcal{U}$ contains a subspace that is the span of real combinations of the Φ_i

$$\mathcal{U}_{\mathbb{R}} = \mathrm{span}_{\mathbb{R}}\{\Phi_1, \ldots, \Phi_g\} = \{c_1\Phi_1 + \ldots + c_g\Phi_g | c_i \in \mathbb{R}\}$$

The pure state densities that we can construct out of states in this subspace will be denoted by $D_{\mathbb{R}}$

$$\rho \in D_{\mathbb{R}} \quad \Longleftrightarrow \quad \rho = \langle\Psi|\hat{\rho}|\Psi\rangle \quad \Psi \in \mathcal{U}_{\mathbb{R}}$$

Definition: If X is a subset in a vectorspace then the segment set seg X is defined as

$$\mathrm{seg}X = \{\lambda x + (1-\lambda)y \,|\, x, y \in X, 0 \leq \lambda \leq 1\}$$

Theorem:

$$D_{\mathbb{C}} = \mathrm{seg}\, D_{\mathbb{R}}$$

In other words, every pure-state density in the degenerate manifold is a convex combination of two densities from $D_{\mathbb{R}}$. This simplifies the construction of $D_{\mathbb{C}}$

Proof: $\rho \in D_{\mathbb{C}}$ → $\rho(\Psi) = \langle\Psi|\hat{\rho}|\Psi\rangle$ $\Psi = \Psi_1 + i\Psi_2$ $\|\Psi_1\|^2 + \|\Psi_2\|^2 = 1$

Define

$$\Phi_1 = \frac{\Psi_1}{\|\Psi_1\|} \quad \Phi_2 = \frac{\Psi_2}{\|\Psi_2\|} \quad \lambda = \|\Psi_1\|^2 \quad 1 - \lambda = \|\Psi_2\|^2$$

such that

$$\Psi = \sqrt{\lambda}\,\Phi_1 + i\sqrt{1-\lambda}\,\Phi_2$$

and therefore

$$\rho(\Psi) = \langle\Psi|\hat{\rho}|\Psi\rangle = \lambda\langle\Phi_1|\hat{\rho}|\Phi_1\rangle + (1-\lambda)\langle\Phi_2|\hat{\rho}|\Phi_2\rangle$$

$$= \lambda\rho(\Phi_1) + (1-\lambda)\rho(\Phi_2) \quad \in \mathrm{seg}D_{\mathbb{R}}$$

Degeneracy regions II : ensemble densities

The most general class of densities is that obtained from ensembles of states in $\mathcal{U}$

$$\rho \in D \quad \Longleftrightarrow \quad \rho = \mathrm{Tr}\{\hat{\Gamma}\hat{\rho}\} \qquad \hat{\Gamma} = w_1|\Psi_1\rangle\langle\Psi_1| + \ldots + w_g|\Psi_g\rangle\langle\Psi_g| \quad \Psi_i \in \mathcal{U}$$

In other words it contains the g-fold convex combinations of densities in $D_{\mathbb{C}}$

$$\rho = \sum_{i=1}^{g} w_i \langle\Psi_i|\hat{\rho}|\Psi_i\rangle = \sum_{i=1}^{g} w_i \rho(\Psi_i)$$

This is also called the convex hull of $D_{\mathbb{C}}$ and thus

$$D = \mathrm{ch}\, D_{\mathbb{C}} = \mathrm{ch}\, D_{\mathbb{R}}$$

In the following we take $\mathcal{U}$ to be the ground state manifold

Consequence of the above:

If a density is ensemble v-representable but not pure-state v-representable then $g \geq 3$

Shape of degeneracy regions

We start by constructing the geometric shape of the degeneracy regions from $D_{\mathbb{R}}$

$$\Psi(x) = \sum_{i=1}^{g} x_i \, \Phi_i \qquad\qquad x_1^2 + \ldots + x_g^2 = 1$$

The corresponding densities are given by

$$\rho(x) = \sum_{k,l}^{g} x_k x_l \langle \Psi_k | \hat{\rho} | \Psi_l \rangle = \sum_{k}^{g} x_k^2 \rho_{\bar{k}} + \sum_{k<l}^{g} x_k x_k \rho_{\bar{k}\bar{l}}$$

$$\rho_{\bar{k}} = \langle \Psi_k | \hat{\rho} | \Psi_k \rangle \qquad\qquad \rho_{\bar{k}\bar{l}} = 2 \langle \Psi_k | \hat{\rho} | \Psi_l \rangle$$

Let us take the example of two-fold degeneracy g=2

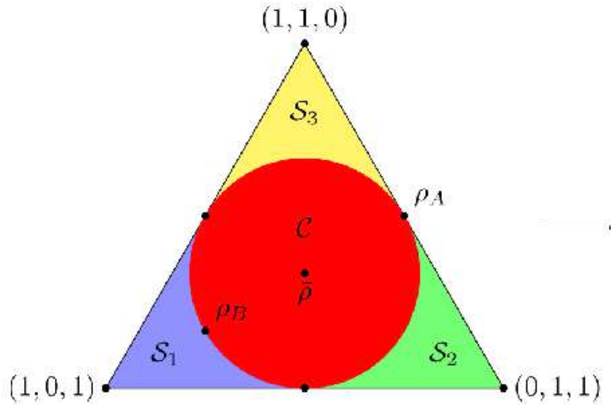
$$\rho(x) = x_1^2\langle\Psi_1|\hat{\rho}|\Psi_1\rangle + x_2^2\langle\Psi_2|\hat{\rho}|\Psi_2\rangle + 2x_1x_2\langle\Psi_1|\hat{\rho}|\Psi_2\rangle = x_1^2\,\rho_{\bar{1}} + x_2^2\,\rho_{\bar{2}} + x_1x_2\,\rho_{\bar{1}\bar{2}}$$

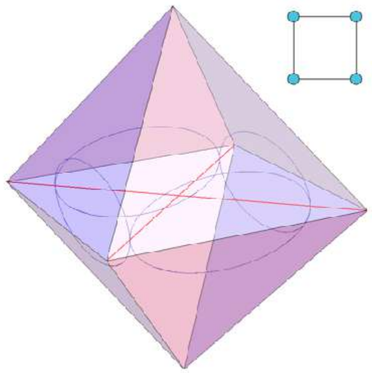
$$x_1^2 + x_2^2 = 1$$

with $(x_1, x_2) = (\cos\varphi, \sin\varphi)$ we can rewrite this as

$$\rho(x) = \frac{1}{2}(\rho_{\bar{1}} + \rho_{\bar{2}}) + \frac{1}{2}(\rho_{\bar{1}} - \rho_{\bar{2}})\cos(2\varphi) + \frac{1}{2}\rho_{\bar{1}\bar{2}}\,\sin(2\varphi)$$

which is the equation of an ellipse with centre $\frac{1}{2}(\rho_{\bar{1}} + \rho_{\bar{2}})$ and semi-axes $\frac{1}{2}(\rho_{\bar{1}} - \rho_{\bar{2}})$ and $\frac{1}{2}\rho_{\bar{1}\bar{2}}$





The density map can be viewed as the composition of two maps

$$\nu(x) = (x_1^2, \ldots, x_g^2, x_1x_2, \ldots, x_{g-1}x_g) \in \mathbb{R}^{g(g+1)/2}$$

Veronese variety

$$\rho(x) = P \circ \nu(x)$$

For example $g = 3$

$$\nu(x) = (x_1^2, x_2^2, x_3^2, x_1x_2, x_1x_3, x_2x_3) \in \mathbb{R}^6$$

Veronese surface

$$x_1^2 + x_2^2 + x_3^2 = 1$$

$$\rho(x) = \begin{pmatrix} \rho_{\bar{1},1} & \rho_{\bar{2},1} & \rho_{\bar{3},1} & \rho_{\bar{1}\bar{2},1} & \rho_{\bar{1}\bar{3},1} & \rho_{\bar{2}\bar{3},1} \\ \vdots & & & & & \vdots \\ \rho_{\bar{1},M} & \rho_{\bar{2},M} & \rho_{\bar{3},M} & \rho_{\bar{1}\bar{2},M} & \rho_{\bar{1}\bar{3},M} & \rho_{\bar{2}\bar{3},M} \end{pmatrix} \begin{pmatrix} x_1^2 \\ x_2^2 \\ x_3^2 \\ x_1x_2 \\ x_1x_3 \\ x_2x_3 \end{pmatrix}$$

$$P$$

What is the dimensionality of $\rho(x)$?

Guiseppe Veronese

La superficie omaloide normale a due dimensioni e del quarto ordine dello spazio a cinque dimensioni e le sue projezioni nel piano e nello spazio ordinario

Atti della Reale Accademia dei Lincei. Memorie della Classe di scienze fisiche, matematiche e naturali (1883 - 1884, Serie 3, Annata 281, Volume 19)

If the matrix P has null space or kernel of dimension κ then the dimensionality of the degeneracy region is

$$\dim(D) = \frac{1}{2}g(g+1) - \kappa - 1 \qquad \kappa = \dim(\ker P)$$

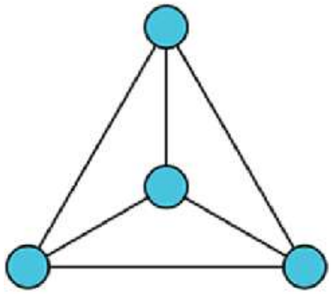
The case $g = 3 \quad \kappa = 2$ has $\dim(D) = 3$ which is nice for visualisation

These are projections of the Veronese surface into three-dimensional space that are known in the mathematics literature as Steiner surfaces and have been classified

W.L.F. Degen, "The types of triangular Bézier surfaces", Proc.6th IMA Conference on the Mathematics of Surfaces, 153, (1994)

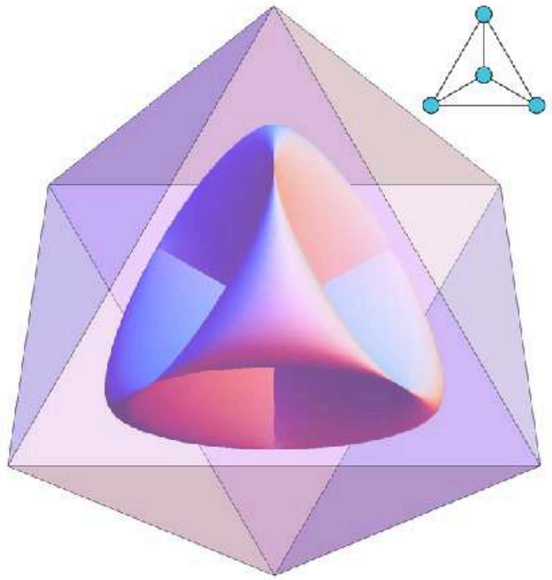
Example: Tetrahedron graph M=4,N=2

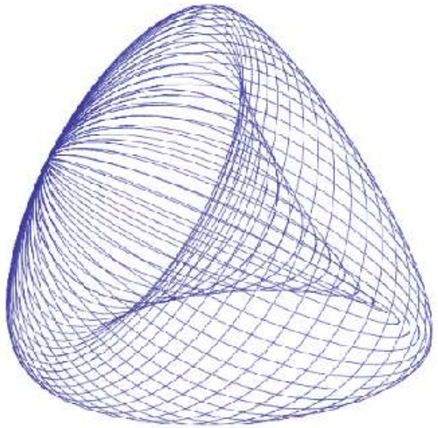
$$\begin{aligned}
\rho_{\overline{k}} &= \overline{\rho} = \tfrac{1}{2}(1,1,1,1) \\
\rho_{\overline{12}} &= \tfrac{1}{2}(1,-1,-1,1) \\
\rho_{\overline{13}} &= \tfrac{1}{2}(-1,1,-1,1) \\
\rho_{\overline{23}} &= \tfrac{1}{2}(-1,-1,1,1).
\end{aligned}$$

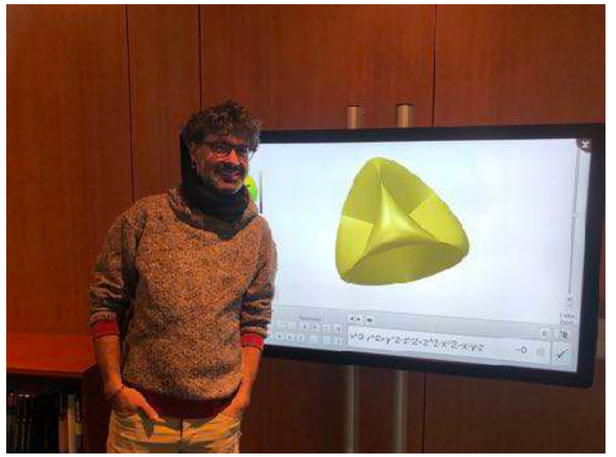


$$\rho(x) = \overline{\rho}\underbrace{\sum_{k=1}^{3} x_k^2}_{1} + \frac{1}{2}\begin{pmatrix} 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} x_1x_2 \\ x_1x_3 \\ x_2x_3 \\ 0 \end{pmatrix}$$

$$x_1^2 + x_2^2 + x_3^2 = 1$$





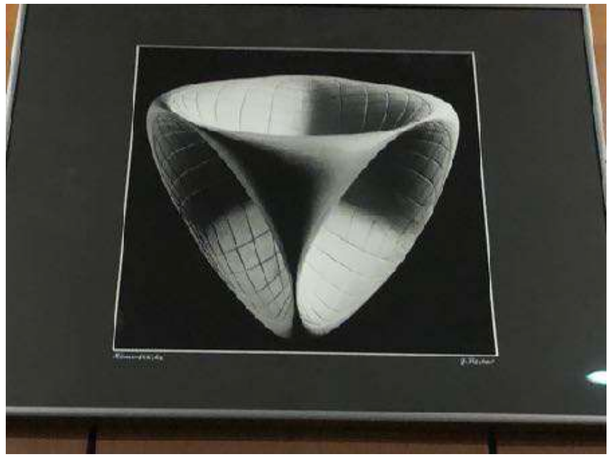


MFO Library

Steiner's Roman surface is degeneracy region $D_{\mathbb{R}}$

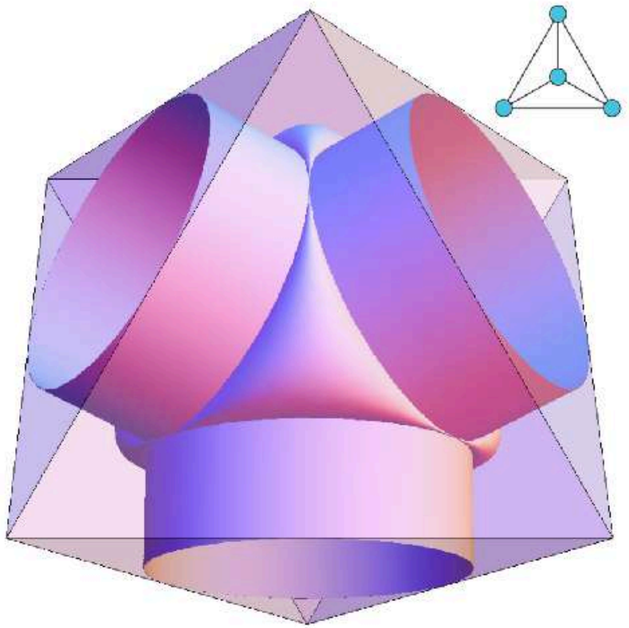
Its segment set builds $D_{\mathbb{C}}$

Since the degenerate eigenspace $\mathcal{U}$ can be decomposed into 2-dimensional subspaces the Roman surface is built out of ellipses



(studied by Cayley, Clebsch, Weierstrass, Lie,…)

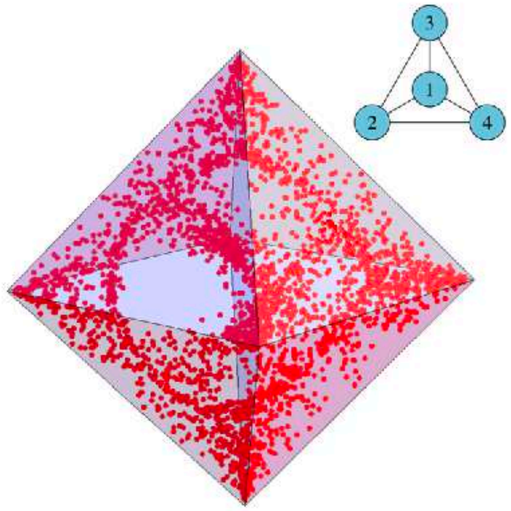
If we add the g=2 degeneracy regions we get a complete picture of all the degeneracy regions of the tetrahedron graph



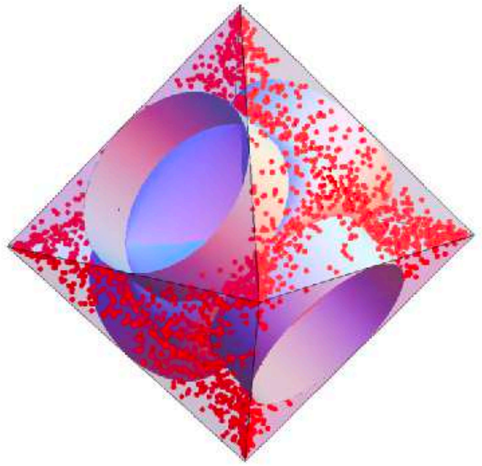
The g=2 bundles of degeneracy regions are added on top of the Roman surface

About 60% of density space corresponds to degenerate densities

Ullrich-Kohn: "Degeneracy is common in density space"



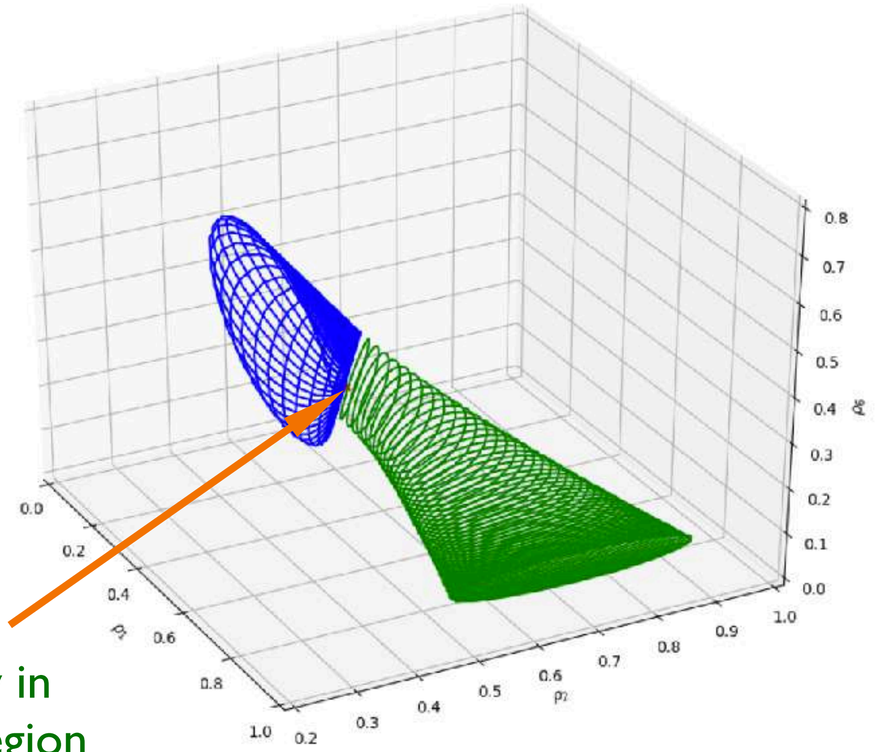
Densities from randomly chosen potentials



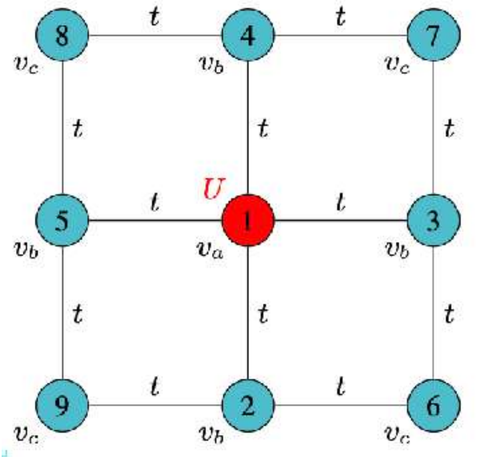
Application: Anderson impurity model

T.Rössler, C. Verdozzi, C.-O. Almbladh, "A v-representability issue in lattice ensemble DFT and its signature in lattice TDDFT" Eur. Phys. J. B91, 219 (2018)

$$\hat{H} = t \sum_{i\sim j,\sigma} \hat{a}^{\dagger}_{i\sigma}\hat{a}_{j\sigma} + \sum_{i,\sigma} v_i \hat{a}^{\dagger}_{i\sigma}\hat{a}_{i\sigma} + U\hat{a}^{\dagger}_{1\uparrow}\hat{a}^{\dagger}_{1\downarrow}\hat{a}_{1\downarrow}\hat{a}_{1\uparrow}$$



Target density in degeneracy region



The claimed v-representability issue is a numerical one caused by the vicinity of the target density to another degeneracy region

The surfaces fit the Degen classification as projections of the Veronese surface

Results

Proofs: Markus Penz, RvL, "Geometry of degeneracy in potential and energy space" Quantum 7, 918 (2023)

Location and measure of non-uv densities

Non-uv densities occur when

a) Two degeneracy regions intersect in a single density or in a degeneracy region of strictly lower dimensionality
b) Or when a density region touches the boundary of the density domain

Non-uv densities are of measure zero in the set of all densities and the uv-densities form an open set

The geometrical Hohenberg-Kohn theorem:

All ground state densities that are not on the boundary of the density domain and that are not at the intersection of degeneracy regions are uniquely given by a potential

Constrained search in imaginary time

In ground state DFT we define $$F(\rho) = \min_{\Psi \to \rho} \langle \Psi | \hat{T} + \hat{W} | \Psi \rangle$$

We describe a procedure to find the Levy-Lieb functional by imaginary time propagation.

We consider the Hamiltonian

$$\hat{H}(\tau) = \hat{H}_0 + \sum_{i=1}^{M} v_i(\tau)\hat{\rho}_i$$

and define

$$\hat{G}(\tau) = \hat{H}(\tau) + v_0(\tau)\hat{\rho}_0 \qquad\qquad \hat{\rho}_0 = \hat{I}$$

where the last terms acts similarly to a time-dependent chemical potential to preserve the norm and then we propagate a Schrödinger type equation in imaginary time

$$-\partial_\tau \Psi(\tau) = \hat{G}(\tau)\Psi(\tau) \qquad\qquad \rho_i = \langle \Psi(0) | \hat{\rho}_i | \Psi(0) \rangle$$

starting from an initial state with the right density

We determine the external potential and "chemical potential" by requiring that the density and norm do not change

$$\partial_\tau \langle \Psi | \hat{\rho}_i | \Psi \rangle = -\langle \Psi | \hat{G}(\tau)\hat{\rho}_i + \hat{\rho}_i \hat{G}(\tau) | \Psi \rangle = \langle \Psi | \{\hat{\rho}_i, \hat{G}(\tau)\} | \Psi \rangle$$

$$\langle \Psi | \{\hat{\rho}_i, \hat{G}(\tau)\} | \Psi \rangle = 0 \quad \Leftrightarrow \quad \sum_{j=0}^{m} \langle \Psi | \{\hat{\rho}_i, \hat{\rho}_j\} | \Psi \rangle v_j(\tau) = -\langle \Psi | \{\hat{\rho}_i, \hat{H}_0\} | \Psi \rangle$$

By taking i=0 we can explicitly solve

$$-v_0(\tau) = \langle \Psi | \hat{H}_0 | \Psi \rangle + \sum_{i=1}^{m} v_i(\tau)\rho_i(\tau) = \langle \Psi | \hat{H}(\tau) | \Psi \rangle = E(\tau)$$

So that

$$\hat{G}(\tau) = \hat{H}(\tau) - E(\tau)\hat{I} \qquad \hat{H}(\tau) = \hat{H}_0 + \sum_{i=1}^{M} v_i(\tau)\hat{\rho}_i$$

$$-\partial_\tau \Psi(\tau) = (\hat{H}(\tau) - E(\tau)\hat{I})\Psi(\tau)$$

We can further calculate that

$$\partial_\tau \langle \Psi | \hat{H}_0 | \Psi \rangle = -\langle \Psi | \{ \hat{H}_0, \hat{G}(\tau) \} | \Psi \rangle = -\langle \Psi | \{ \hat{H}_0, \hat{H}_0 \} | \Psi \rangle - \sum_{i=0}^{m} v_i(\tau) \langle \Psi | \{ \hat{H}_0, \hat{\rho}_i \} | \Psi \rangle$$

and using the constraint equation for the potential it follows that

$$\partial_\tau \langle \Psi | \hat{H}_0 | \Psi \rangle = -2 \langle \Psi | \hat{G}^2(\tau) | \Psi \rangle = -2 \langle \Psi | (\hat{H}(\tau) - E(\tau)\hat{I})^2 | \Psi \rangle \leq 0$$

So the expectation value of the internal part of the Hamiltonian decreases monotonically while the density remains the same!

So the procedure converges to $F(\rho)$ from above!

How to choose the initial state?

$$|\Psi(\tau)\rangle = \sum_I c_I(\tau) |I\rangle \qquad \rho_i = \sum_{I \ni i} |c_I(\tau)|^2$$

Choosing the initial state

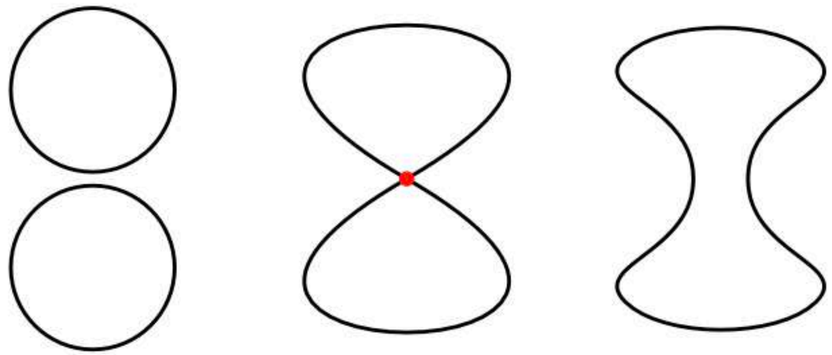
$$|\Psi(0)\rangle = \sum_I c_I(0)|I\rangle \qquad \rho_i = \sum_{I \ni i} |c_I(0)|^2$$

make a choice for $|c_I(0)|$

If we restrict ourselves to real wave functions then we can further take $c_I(0) = \pm|c_I(0)|$

while for complex wave functions we can take $c_I(0) = e^{i\alpha_I}|c_I(0)| \quad \alpha_I \in [0, 2\pi[$

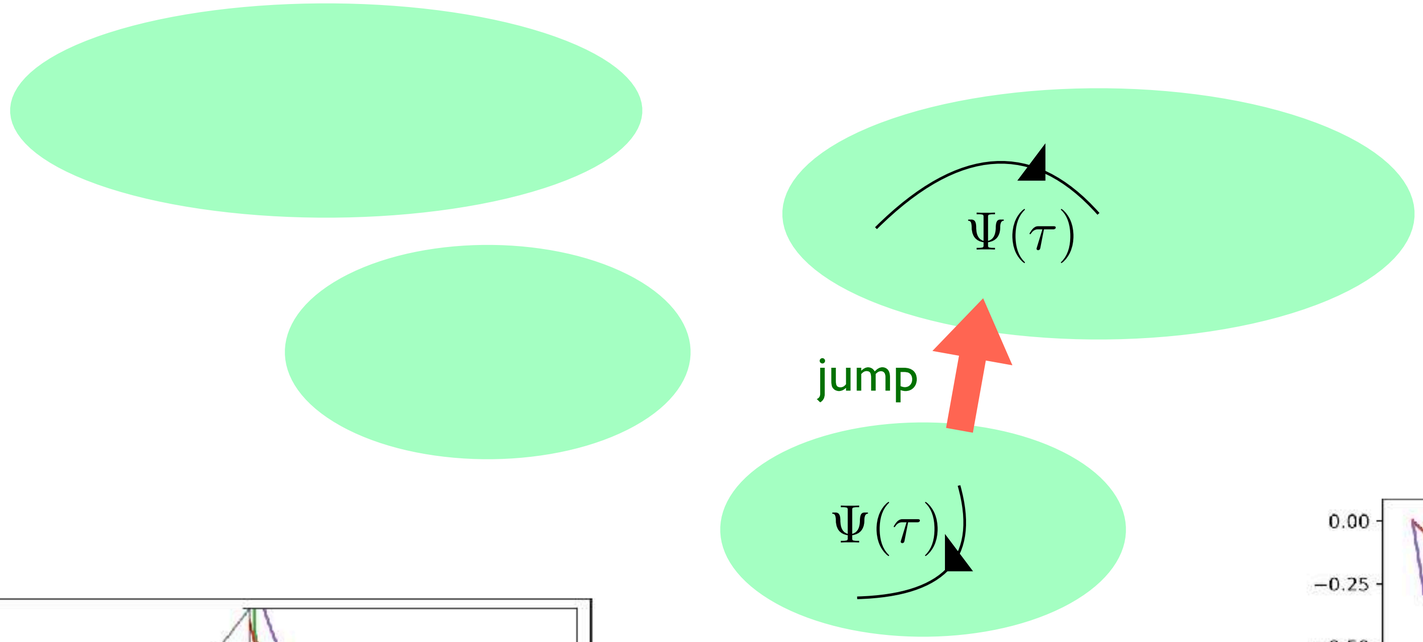
In practice we can make sign flips or random phase choice to see if the internal energy is lower



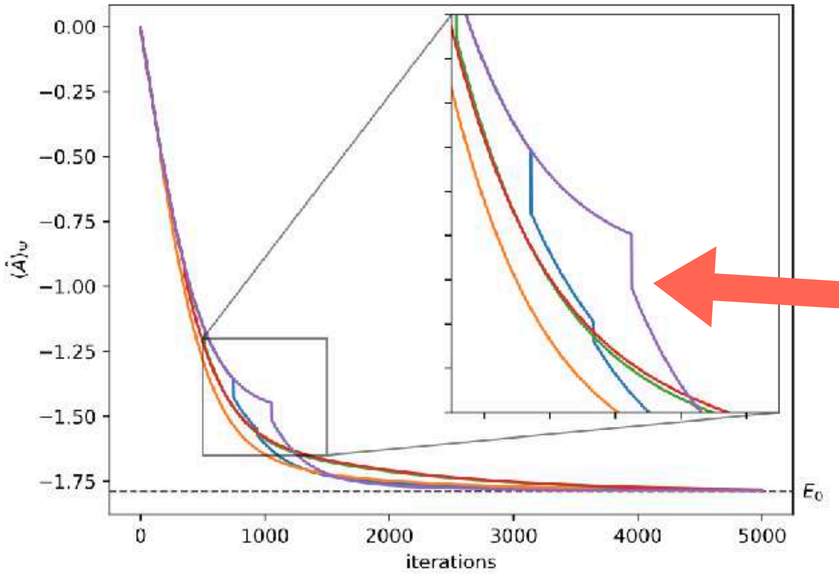
ρ_A ρ_B ρ_C

The density patches in Hilbert space may be disconnected as they represent different nodal structures of the wavefunction. By sign flips we may jump between them

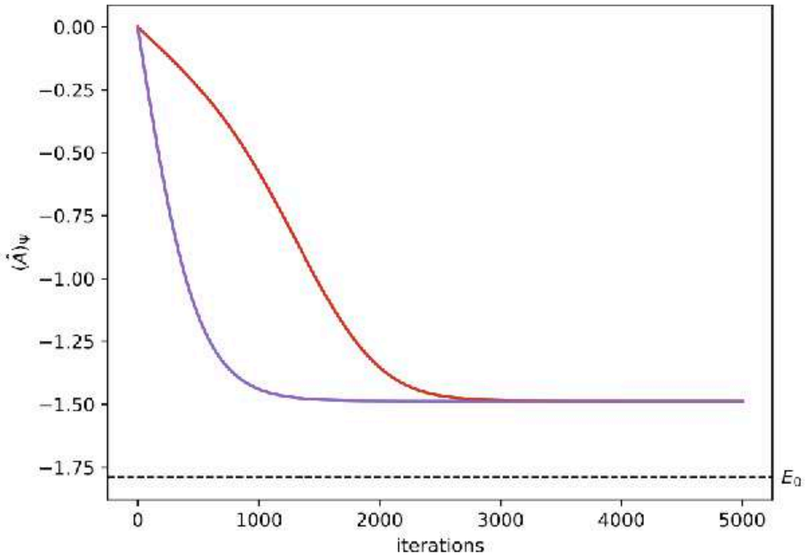
By random phase choices we can jump between "density patches" on the unit sphere in Hilbert space.
We jump during time propagation whenever a phase change lowers the energy



$$\{\Psi|\,\|\Psi\| = 1,\, \langle\Psi|\hat{\rho}_i|\Psi\rangle = \rho_i\}$$



Random phase jump

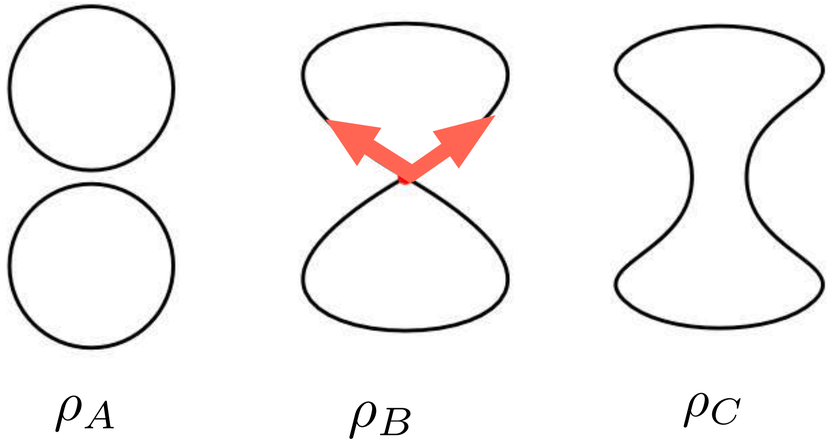


Target density is a complex state in a degeneracy region,
but the initial state real; ends up in an excited state

Some results regarding the imaginary time propagation:

- It can be proven that the constraint equation for the constraining potential always has a solution and that the solution is at least once differentiable with respect to time (Picard-Lindelöf theorem)

- In case the solution passes an irregular point (a point on the constraint manifold with a non-unique normal vector) a solution for the time evolution exists, but is not unique (Peano theorem)



The procedure can be generalised to to minimising an arbitrary self-adjoint operator where we constrain a number of expectation values of a set of commuting operators

$$\hat{T} + \hat{W} \to \hat{A} \qquad \hat{\rho}_i \to \hat{B}_i \qquad b_i = \langle \Psi | \hat{B}_i | \Psi \rangle \qquad [\hat{B}_i, \hat{B}_j] = 0$$

$$F(b) = \min_{\Psi \to b} \langle \Psi | \hat{A} | \Psi \rangle$$

M.Penz and RvL, "Constrained search in imaginary time", arXiv: 2504.05332 (2025)

For example, we can take system with lattice spins, for example a spin glass

$$\hat{A} = \sum_{i,j} J_{ij} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \qquad \hat{B}_i = \boldsymbol{\sigma}_i \qquad \boldsymbol{m}_i = \langle \Psi | \boldsymbol{\sigma}_i | \Psi \rangle$$

$$F(\boldsymbol{m}) = \min_{\Psi \to \boldsymbol{m}} \langle \Psi | \hat{A} | \Psi \rangle$$

The minimiser is the ground state of the Hamiltonian $\hat{H} = \sum_{i,j} J_{ij} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + \sum_i \boldsymbol{\sigma}_i \cdot \boldsymbol{B}_i$

in the presence of a magnetic field given by $\boldsymbol{B}_i = -\frac{\partial F}{\partial \boldsymbol{m}_i}$

Conclusion

The geometrical Hohenberg-Kohn theorem for lattice DFT:

All ground state densities that are not on the boundary of the density domain and that are not at the intersection of degeneracy regions are uniquely given by a potential

Construction of the Levy-Lieb functional using imaginary time-propation

- Can be generalised to minimising general expectation values under constraints
- A quantum algorithm seems to be feasible (work in progress)