Quantum-Electrodynamical Density-Functional Theory

for the Dicke Hamiltonian

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Acknowledgements

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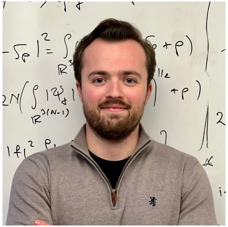
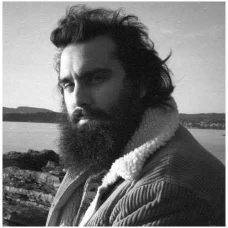
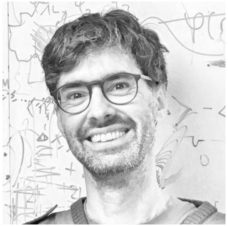

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Outline

Introduction

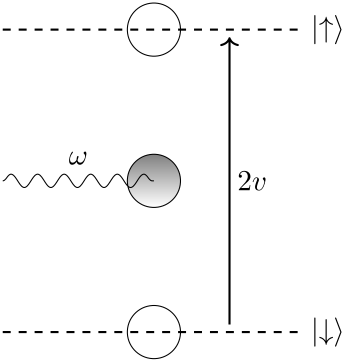
Motivation

- Importance of light-matter interactions $\implies$
  QED = how charged particles interact through coupling to a quantum field
- Simple model (that can be extended)
- Study ground-state effects of coupling photons to electronic systems
- Studying an (almost) explicit form of a DFT functional: QEDFT

- Most of the rigorous considerations in QEDFT are based on the Pauli–Fierz Hamiltonian — various approximations to this Hamiltonian are used as a starting point
- One such quantum-optical model is the Rabi model — physical simplicity, still highly non-trivial and only recently an analytical expression for its spectrum has been found (Bargmann-space reformulation) [1, 2].
- Similar mathematical results have been established for the Dicke model [3, 4]

The Dicke Model

- Two physically different subsystems — matter and light
  - N two-level fermionic systems
  - Individually coupled to M modes of a quantized radiation field, described as quantum harmonic oscillators.
- Susceptible to a “DFT program”.
- We can achieve considerable more mathematically than for standard DFT
  - results concerning v-representability
  - properties of the universal functional



Function spaces

Hilbert space: $\mathcal{H} = \mathcal{H}_{\mathrm{ph}} \otimes \mathcal{H}_{\mathrm{f}}$
$\mathcal{H}_{\mathrm{ph}} = \bigotimes^M L^2(\mathbb{R})$ and $\mathcal{H}_{\mathrm{f}} = \bigotimes^N \mathbb{C}^2 \simeq \mathbb{C}^{2^N}$

$$\mathcal{H} \simeq L^2(\mathbb{R}^M) \otimes \mathbb{C}^{2^N} \simeq L^2(\mathbb{R}^M, \mathbb{C}^{2^N})$$

Inner product $\langle \cdot, \cdot \rangle$ on $L^2(\mathbb{R}^M, \mathbb{C}^{2^N})$,

$$\langle \boldsymbol{\varphi}, \boldsymbol{\psi} \rangle = \sum_{\boldsymbol{\alpha}} \langle \varphi^{\boldsymbol{\alpha}}, \psi^{\boldsymbol{\alpha}} \rangle = \sum_{\alpha_1,\dots,\alpha_N \in \{+,-\}} \int_{\mathbb{R}^M} \overline{\varphi^{\alpha_1,\dots,\alpha_N}(\mathbf{x})} \psi^{\alpha_1,\dots,\alpha_N}(\mathbf{x}) \,\mathrm{d}\mathbf{x},$$

$\psi^{\boldsymbol{\alpha}}$ is the spin projection of ψ corresponding to the eigenvector of the lifted Pauli matrix σ_z^j indexed by the multiindex $\boldsymbol{\alpha} \in \{+,-\}^N$.

Notations

For any $j = 1, \ldots, N$, we have set

$$\sigma_a^j = \mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes \underbrace{\sigma_a}_{j\text{th}} \otimes \mathbb{1} \otimes \ldots \mathbb{1} \in \mathbb{C}^{2^N \times 2^N},$$

where the Pauli matrices are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Vector of lifted Pauli matrices

$$\boldsymbol{\sigma}_a = (\sigma_a^1, \ldots, \sigma_a^N)^\top \in \left(\mathbb{C}^{2^N \times 2^N}\right)^N.$$

Examples

Let $N = 2$, then

$$\boldsymbol{\sigma}_z = \left(\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}, \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} \right)^\top$$

has always diagonal form and

$$\boldsymbol{\sigma}_x = \left(\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \right)^\top$$

Dicke Hamiltonian

"Internal" part of Hamiltonian $\mathbf{H}_0 : \mathcal{H} \to \mathcal{H}$,

$$\mathbf{H}_0 = (-\boldsymbol{\Delta} + |\mathbf{x}|^2)\mathbb{1}_{\mathbb{C}^{2^N}} + \mathbf{x} \cdot \boldsymbol{\Lambda}\boldsymbol{\sigma}_z - \mathbf{t} \cdot \boldsymbol{\sigma}_x \tag{1}$$

$\boldsymbol{\Lambda}\boldsymbol{\sigma}_z$ is to be understood as the M-vector of $2^N \times 2^N$ matrices

$$\boldsymbol{\Lambda}\boldsymbol{\sigma}_z = \left(\sum_{n=1}^{N} \Lambda_{1n}\sigma_z^n, \dots, \sum_{n=1}^{N} \Lambda_{Mn}\sigma_z^n \right)^{\top}.$$

Set $\mathbf{V}(\mathbf{x}) = \left(\mathbf{x} + \frac{1}{2}\boldsymbol{\Lambda}\boldsymbol{\sigma}_z\right)^2$,

$$\mathbf{H}_0 = -\boldsymbol{\Delta} + \mathbf{V} - \mathbf{t} \cdot \boldsymbol{\sigma}_x - \frac{1}{4}\boldsymbol{\sigma}_z \cdot (\boldsymbol{\Lambda}^{\top}\boldsymbol{\Lambda}\boldsymbol{\sigma}_z),$$

$\mathbf{H}_0$ is bounded from below

Dicke Hamiltonian

Full Hamiltonian

$$\mathbf{H}(\mathbf{v},\mathbf{j}) = \mathbf{H}_0 + \mathbf{v}\cdot\boldsymbol{\sigma}_z + \mathbf{j}\cdot\mathbf{x} \qquad (2)$$

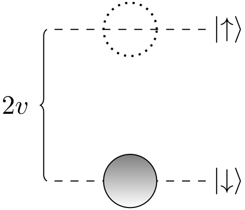
Where the external potentials are

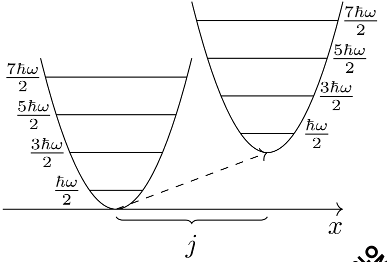
$$\mathbf{v}\in\mathbb{R}^N, \qquad \mathbf{j}\in\mathbb{R}^M$$

Ground-state energy

$$E(\mathbf{v},\mathbf{j}) = \inf_{\substack{\boldsymbol{\psi}\in Q_0\\ \|\boldsymbol{\psi}\|=1}} \langle\boldsymbol{\psi},\mathbf{H}(\mathbf{v},\mathbf{j})\boldsymbol{\psi}\rangle \qquad (3)$$

$Q_0 := Q(\mathbf{H}_0) = Q(-\boldsymbol{\Delta}+\mathbf{V})$ form domain of $\mathbf{H}_0$





Internal "density" variables

Definition (Magnetization vector and photon coordinate)

For $\psi \in \mathcal{H}$, we define

$$\boldsymbol{\sigma}_{\boldsymbol{\psi}} = \langle \boldsymbol{\psi}, \boldsymbol{\sigma}_z \boldsymbol{\psi} \rangle := \begin{pmatrix} \langle \boldsymbol{\psi}, \sigma_z^1 \boldsymbol{\psi} \rangle \\ \vdots \\ \langle \boldsymbol{\psi}, \sigma_z^N \boldsymbol{\psi} \rangle \end{pmatrix} \in [-1,1]^N \subset \mathbb{R}^N$$

$$\boldsymbol{\xi}_{\boldsymbol{\psi}} = \langle \boldsymbol{\psi}, \mathbf{x} \boldsymbol{\psi} \rangle = \int_{\mathbb{R}^M} \mathbf{x} |\boldsymbol{\psi}(\mathbf{x})|^2 \, \mathrm{d}\mathbf{x} \in \mathbb{R}^M .$$

Constraints

For $N = 1, 2, \dots$

- The constraint manifold $\mathcal{M}$ collects all $\psi \mapsto (\boldsymbol{\sigma}, \boldsymbol{\xi}) \in [-1,1]^N \times \mathbb{R}^M$

$$\mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}} = \{\psi \in Q_0 : \|\psi\| = 1,\ \boldsymbol{\sigma}_\psi = \boldsymbol{\sigma},\ \boldsymbol{\xi}_\psi = \boldsymbol{\xi}\}\,. \tag{4}$$

- Recall that $Q_0 := Q(\mathbf{H}_0) = Q(-\boldsymbol{\Delta} + \mathbf{V})$ is the form domain of $\mathbf{H}_0$

Constraints: Example

For $N = 1$, we simply have

$$\left.\begin{aligned} 1 &= \|\psi^+\|^2 + \|\psi^-\|^2 \\ \sigma &= \|\psi^+\|^2 - \|\psi^-\|^2 \end{aligned}\right\} \quad \Longrightarrow \quad \begin{cases} \|\psi^+\|^2 = \dfrac{1+\sigma}{2} \\ \|\psi^-\|^2 = \dfrac{1-\sigma}{2} \end{cases}$$

- $\sigma = +1 \Rightarrow \psi^- \equiv 0$ and $\sigma = -1 \Rightarrow \psi^+ \equiv 0$
- Reverse implication $\psi^+ \not\equiv 0$ and $\psi^- \not\equiv 0$ precisely if $\sigma \in (-1, 1)$.

Unfortunately, this is no longer true for $N \geq 2$.

Constraints: Example

For $N = 2$,

$$\left.\begin{aligned} \frac{1+\sigma_1}{2} &= \|\psi^{++}\|^2 + \|\psi^{+-}\|^2 \\ \frac{1-\sigma_1}{2} &= \|\psi^{-+}\|^2 + \|\psi^{--}\|^2 \end{aligned}\right\} \quad \left.\begin{aligned} \frac{1+\sigma_2}{2} &= \|\psi^{++}\|^2 + \|\psi^{-+}\|^2 \\ \frac{1-\sigma_2}{2} &= \|\psi^{+-}\|^2 + \|\psi^{--}\|^2 \end{aligned}\right\} \Longrightarrow$$

- Whenever $\sigma_1 = \pm 1$ or $\sigma_2 = \pm 1$ (or both), certain spinor components of ψ must vanish.
- Contrary to the $N = 1$ case, it is possible that one (or more) spinor components of ψ vanishes even though $\boldsymbol{\sigma} \in (-1, 1)^2$.

Main Results

Definition

Regular $\boldsymbol{\sigma} \in [-1,1]^N$:

- Let the $N \times 2^N$ matrix $\boldsymbol{\Omega}$ be given by $\Omega_{n,\boldsymbol{\alpha}} = (\boldsymbol{\sigma}_z^n)_{\boldsymbol{\alpha}\boldsymbol{\alpha}}$, i.e., the matrix with the diagonal of σ_z^n as the n-th row vector.
- $\boldsymbol{\sigma}$ is *regular* if for every $\boldsymbol{\omega} \in \mathbb{R}^{2^N}$ with $\omega_{\boldsymbol{\alpha}} \geq 0$ and $\sum_{\boldsymbol{\alpha}} \omega_{\boldsymbol{\alpha}} = 1$ that verifies $\boldsymbol{\Omega}\boldsymbol{\omega} = \boldsymbol{\sigma}$, we have $\mathrm{Aff}\{\boldsymbol{\Omega}\mathbf{e}_{\boldsymbol{\alpha}} : \omega_{\boldsymbol{\alpha}} \neq 0\} = \mathbb{R}^N$.

We denote the set of regular $\boldsymbol{\sigma}$'s by $\mathcal{R}_N$.

Theorem (Hohenberg–Kohn)

Suppose that $\psi^{(1)}, \psi^{(2)} \in Q_0$ are ground states of $\mathbf{H}(\mathbf{v}^{(1)}, \mathbf{j}^{(1)})$ and $\mathbf{H}(\mathbf{v}^{(2)}, \mathbf{j}^{(2)})$ respectively.
If $\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\psi^{(1)}} = \boldsymbol{\sigma}_{\psi^{(2)}}$ and $\boldsymbol{\xi} = \boldsymbol{\xi}_{\psi^{(1)}} = \boldsymbol{\xi}_{\psi^{(2)}}$, then $\psi^{(1)}$ is also a ground state of $\mathbf{H}(\mathbf{v}^{(2)}, \mathbf{j}^{(2)})$ and $\psi^{(2)}$ is also a ground state of $\mathbf{H}(\mathbf{v}^{(1)}, \mathbf{j}^{(1)})$.
Furthermore, $\mathbf{j} = \mathbf{j}^{(1)} = \mathbf{j}^{(2)}$ and

- *(Regular case) If $\boldsymbol{\sigma}$ is regular, then $\mathbf{v}^{(1)} = \mathbf{v}^{(2)}$.*
- *(Irregular case) Otherwise, for all $\boldsymbol{\alpha} \in I^{(1)} \cup I^{(2)}$ there holds*

$$\sum_{n=1}^{N} (\boldsymbol{\sigma}_z^n)_{\boldsymbol{\alpha}\boldsymbol{\alpha}} (v_n^{(1)} - v_n^{(2)}) = E(\mathbf{v}^{(1)}, \mathbf{j}) - E(\mathbf{v}^{(2)}, \mathbf{j}), \tag{5}$$

where $I^{(i)}$ denotes the set of spinor indices $\boldsymbol{\alpha}$ for which $(\psi^{(i)})^{\boldsymbol{\alpha}} \not\equiv 0$.

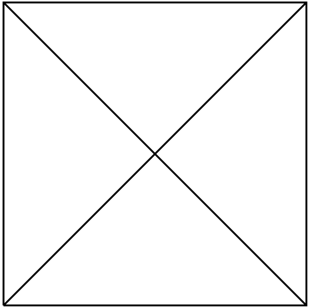
Regular case: Example

$N = 1$. $\mathcal{R}_1 = (-1, 1)$:

- $\sigma \in [-1, 1]$ is regular if and only if $\sigma \in (-1, 1)$.
- $S = \{\boldsymbol{\Omega}\mathbf{e}_{\boldsymbol{\alpha}} : \omega_{\boldsymbol{\alpha}} \neq 0\} \subset \{-1, 1\}$
- So $\mathrm{Aff}(S) = \mathbb{R}$ iff $|S| = 2$.
- But $\boldsymbol{\Omega}\boldsymbol{\omega} = \sigma$ simply reads $\omega_+ - \omega_- = \sigma$, and $\omega_+ \neq 0, \omega_- \neq 0$ if and only if $\sigma \neq \pm 1$.

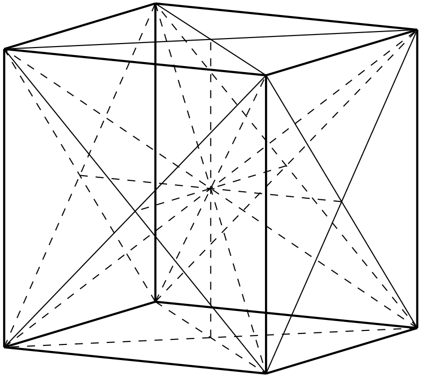
Regular case: Example

$N = 2$. $\mathcal{R}_2 \subset (-1,1)^2$ is the union of 4 congruent open triangles.



Example, $N = 3$

The set $\mathcal{R}_3 \subset (-1,1)^3$ is the union of 24 congruent open tetrahedra.



- The regularity property of $\boldsymbol{\sigma}$ can be seen in analogy to finite-lattice DFT [5, Cor. 10].
- Unlike the HK theorem for the electronic Hamiltonian, the potentials are completely determined in the regular case, i.e., not only up to an additive constant.
- The HK itself is nonconstructive, more precisely, it only states the injectivity of the "potential to ground-state density map" $(\mathbf{v}, \mathbf{j}) \mapsto (\boldsymbol{\sigma}, \boldsymbol{\xi})$ and *not* its surjectivity.
- Whenever $(\boldsymbol{\sigma}, \boldsymbol{\xi}) \in [-1,1]^N \times \mathbb{R}^M$ is the ground-state density of $\mathbf{H}(\mathbf{v}, \mathbf{j})$ for some $(\mathbf{v}, \mathbf{j}) \in \mathbb{R}^N \times \mathbb{R}^M$, we say $(\boldsymbol{\sigma}, \boldsymbol{\xi})$ is v*-representable*.

Levy–Lieb functional

- HK theorem $\implies$ we can formulate the ground-state problem

$$E(\mathbf{v},\mathbf{j}) = \inf_{\substack{\boldsymbol{\psi}\in Q_0\\ \|\boldsymbol{\psi}\|=1}} \langle \boldsymbol{\psi}, \mathbf{H}(\mathbf{v},\mathbf{j})\boldsymbol{\psi}\rangle \tag{6}$$

  in terms of the density pair $(\boldsymbol{\sigma},\boldsymbol{\xi})$.
- We introduce the constraint manifold that collects all states that map to a given $(\boldsymbol{\sigma},\boldsymbol{\xi}) \in [-1,1]^N \times \mathbb{R}^M$,

$$\mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}} = \{\psi \in Q_0 : \|\psi\| = 1,\ \boldsymbol{\sigma}_{\boldsymbol{\psi}} = \boldsymbol{\sigma},\ \boldsymbol{\xi}_{\psi} = \boldsymbol{\xi}\}\,. \tag{7}$$

$$
\begin{aligned}
E(\mathbf{v},\mathbf{j}) &= \inf_{\substack{\boldsymbol{\psi}\in Q_0\\ \|\boldsymbol{\psi}\|=1}} \langle \boldsymbol{\psi}, \mathbf{H}(\mathbf{v},\mathbf{j})\boldsymbol{\psi}\rangle \\
&= \inf_{(\boldsymbol{\sigma},\boldsymbol{\xi})\in[-1,1]^N\times\mathbb{R}^M} \left[\inf_{\boldsymbol{\psi}\in\mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}}} \langle \boldsymbol{\psi}, \mathbf{H}(\mathbf{v},\mathbf{j})\boldsymbol{\psi}\rangle \right] \\
&= \inf_{(\boldsymbol{\sigma},\boldsymbol{\xi})\in[-1,1]^N\times\mathbb{R}^M} \left[\inf_{\boldsymbol{\psi}\in\mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}}} \langle \boldsymbol{\psi}, \mathbf{H}_0\boldsymbol{\psi}\rangle + \langle \boldsymbol{\psi}, \mathbf{v}\cdot\boldsymbol{\sigma}_z\boldsymbol{\psi}\rangle + \langle \boldsymbol{\psi}, \mathbf{j}\cdot\mathbf{x}\boldsymbol{\psi}\rangle \right] \\
&= \inf_{(\boldsymbol{\sigma},\boldsymbol{\xi})\in[-1,1]^N\times\mathbb{R}^M} \left[F_{\mathrm{LL}}(\boldsymbol{\sigma},\boldsymbol{\xi}) + \mathbf{v}\cdot\boldsymbol{\sigma} + \mathbf{j}\cdot\boldsymbol{\xi} \right]
\end{aligned}
\tag{8}
$$

Levy–Lieb (universal density) functional

Definition

For every $(\boldsymbol{\sigma}, \boldsymbol{\xi}) \in [-1,1]^N \times \mathbb{R}^M$ the *Levy–Lieb* (universal density) *functional* $F_{\mathrm{LL}} : [-1,1]^N \times \mathbb{R}^M \to \mathbb{R}$ is

$$F_{\mathrm{LL}}(\boldsymbol{\sigma}, \boldsymbol{\xi}) = \inf_{\boldsymbol{\psi} \in \mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}}} \langle \boldsymbol{\psi}, \mathbf{H}_0 \boldsymbol{\psi} \rangle \tag{9}$$

Immediate question: Is the "$\inf$" in the definition of F_{LL} attained?

Theorem (Existence of an optimizer for F_{LL})

For every $(\boldsymbol{\sigma}, \boldsymbol{\xi}) \in [-1,1]^N \times \mathbb{R}^M$ *there exists a* $\psi \in \mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}}$ *such that*

$$F_{\mathrm{LL}}(\boldsymbol{\sigma}, \boldsymbol{\xi}) = \langle \psi, \mathbf{H}_0 \psi \rangle.$$

- Proof is somewhat different from the analogous one in standard DFT [6] and, e.g., generalization to paramagnetic current-DFT [7, 8]:

  there, one exploits the density constraint on the wavefunction to obtain the tightness of the optimizing sequence.
- In our case, the trapping nature of $\mathbf{H}_0$ provides compactness.

Property of F_{LL}

Trial state constructions to derive useful properties of F_{LL}.

Theorem (Displacement rule)

For every $(\boldsymbol{\sigma}, \boldsymbol{\xi}) \in [-1,1]^N \times \mathbb{R}^M$ *the following hold true:*

$$F_{\mathrm{LL}}(\boldsymbol{\sigma}, \boldsymbol{\xi}) = F_{\mathrm{LL}}(\boldsymbol{\sigma}, 0) + \boldsymbol{\xi} \cdot \boldsymbol{\Lambda}\boldsymbol{\sigma} + |\boldsymbol{\xi}|^2.$$

Or more generaly, for any $\boldsymbol{\zeta} \in \mathbb{R}^M$*,*

$$F_{\mathrm{LL}}(\boldsymbol{\sigma}, \boldsymbol{\xi} + \boldsymbol{\zeta}) = F_{\mathrm{LL}}(\boldsymbol{\sigma}, \boldsymbol{\xi}) + 2\boldsymbol{\zeta} \cdot \boldsymbol{\xi} + \boldsymbol{\zeta} \cdot \boldsymbol{\Lambda}\boldsymbol{\sigma} + |\boldsymbol{\zeta}|^2$$

Displacement rule $\implies$ $\boldsymbol{\xi} \mapsto F_{\mathrm{LL}}(\boldsymbol{\sigma}, \boldsymbol{\xi})$ is smooth and convex for every fixed $\boldsymbol{\sigma} \in [-1,1]^N$.

Optimizers

Constrained opt: Minimize

$$\langle \boldsymbol{\psi}, \mathbf{H}_0 \boldsymbol{\psi} \rangle \quad \text{s.t.} \quad \psi \in \mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}} = \{\boldsymbol{\psi} \in Q_0 : \|\boldsymbol{\psi}\| = 1,\ \boldsymbol{\sigma}_{\boldsymbol{\psi}} = \boldsymbol{\sigma},\ \boldsymbol{\xi}_{\psi} = \boldsymbol{\xi}\}\,. \tag{10}$$

The tangent space of $\mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}}$ at $\boldsymbol{\psi} \in \mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}}$ is given by

$$\mathcal{T}_{\boldsymbol{\psi}}(\mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}}) = \Big\{\boldsymbol{\chi} \in Q_0 : \langle \boldsymbol{\psi}, \boldsymbol{\chi} \rangle = 0,\ \langle \boldsymbol{\sigma}_z \boldsymbol{\psi}, \boldsymbol{\chi} \rangle = 0,\ \langle \mathbf{x}\boldsymbol{\psi}, \boldsymbol{\chi} \rangle = 0\Big\}.$$

Theorem (Optimality)

Let $(\boldsymbol{\sigma}, \boldsymbol{\xi}) \in \mathcal{R}_N \times \mathbb{R}^M$ *and suppose that* $\psi \in \mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}}$ *is an optimizer of* $F_{\mathrm{LL}}(\boldsymbol{\sigma}, \boldsymbol{\xi})$*. Then there exist Lagrange multipliers* $E \in \mathbb{R}$*,* $\mathbf{v} \in \mathbb{R}^N$ *and* $\mathbf{j} \in \mathbb{R}^M$*, such that* ψ *satisfies the strong Schrödinger equation*

$$\mathbf{H}(\mathbf{v}, \mathbf{j})\psi = E\psi \tag{11}$$

and the second-order condition

$$\langle \boldsymbol{\chi}, \mathbf{H}(\mathbf{v}, \mathbf{j})\boldsymbol{\chi} \rangle \geq E\|\boldsymbol{\chi}\|^2, \tag{12}$$

for all $\boldsymbol{\chi} \in \mathcal{T}_\psi(\mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}})$*. Moreover,*

$$F_{\mathrm{LL}}(\boldsymbol{\sigma}, \boldsymbol{\xi}) = \langle \psi, \mathbf{H}_0 \psi \rangle = E - \mathbf{v} \cdot \boldsymbol{\sigma} - \mathbf{j} \cdot \boldsymbol{\xi}. \tag{13}$$

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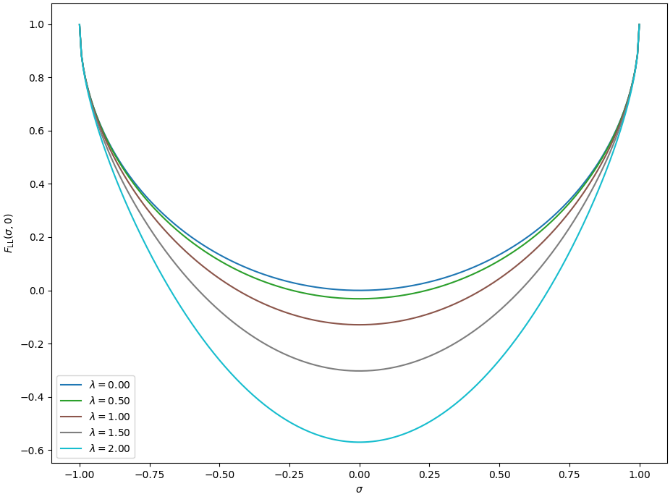
The second-order information (12) about a minimizer gives a result which is analogous to the Aufbau principle in Hartree–Fock theory.

Theorem (Optimizers are low-lying eigenstates)

Let $(\boldsymbol{\sigma},\boldsymbol{\xi}) \in \mathcal{R}_N \times \mathbb{R}^M$*, and suppose that* $\psi \in \mathcal{M}_{\boldsymbol{\sigma},\boldsymbol{\xi}}$ *is an optimizer of* $F_{\mathrm{LL}}(\boldsymbol{\sigma},\boldsymbol{\xi})$*, with Lagrange multipliers* $E \in \mathbb{R}$*,* $\mathbf{v} \in \mathbb{R}^N$ *and* $\mathbf{j} \in \mathbb{R}^M$*, so that* (11) *and* (12) *holds true. Then* ψ *is at most the* $(N+M)$*th excited eigenstate of* $\mathbf{H}(\mathbf{v},\mathbf{j})$*.*

Any $(\boldsymbol{\sigma},\boldsymbol{\xi}) \in \mathcal{R}_N \times \mathbb{R}^M$, while not proven to be pure-state v-representable in the usual sense, can be called “low-lying excited-pure-state v-representable”.

The Universal Density-Functional $M = N = 1$



Sumary

Summary

- Study of an (almost) explicit form of a DFT functional: QEDFT
- Sharper results on Hohenberg–Kohn and v-rep
- More direct properties of the functional (to be used in future work)

Coming to arXiv

Submitted 18th (hopefully not in arXiv prison too long)

Thank you for your attention!

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