Dual Formulation of the RDM Minimization Problem

Reduction to a one-dimensional optimization problem

The polar cone \( C^\circ \) of a cone \( C \) in any Hilbert space is defined as \( C^\circ = \{ x \in \mathbb{X}, \langle x, y \rangle \geq 0 \} \) (where \( \langle \cdot, \cdot \rangle \) is the scalar product). Formulating (2) in terms of \( C(\Gamma)^\circ \) instead of \( C(\Gamma) \)

\[
E = \inf_{\Omega \in \mathcal{P}(\mathbb{X})^N} \{ \mathfrak{h}(\Omega) \} = \inf_{\Gamma \in C(\mathbb{X})^N} \{ \mathfrak{h}(\Gamma) \}
\]

Easily derived from (2) using the Legendre inf-sup formulation

\[
\mathfrak{h}(\Gamma, B, \mu) = \mathfrak{h}(\Gamma) - \mathfrak{h}(B) - \mu(\mathfrak{h}(\Gamma) - N(N - 1))
\]

Optimization problem in dimension 1 over \( \mu \in \mathbb{R} \) which is the variable dual to the constraint \( \mathfrak{h}(\Gamma) = N(N - 1) \).

Identification of the dual cone: \( N \)-representability problem

Necessary conditions for \( N \)-representability are selected, of the form \( L_\ell(\Gamma) \geq 0 \) where \( L_\ell : S_\ell \rightarrow S(\mathbb{X}) \) is a linear map and \( S_\ell \) is some vector space. Minimization over approximated cone and its dual

\[
\mathcal{C}_{\text{app}} = \{ \Gamma \in \mathcal{G} \mid \mathfrak{h}(\Gamma) = N(N - 1) \}
\]

The associated approximate energy is then a lower bound to the true energy

\[
E_{\text{app}} = \inf_{\mathcal{C}_{\text{app}}} \{ \mathfrak{h}(\Gamma) \}
\]

We denote by \( E_{\text{app}} = E_{\text{app}}(N(N - 1)) \).

Usual necessary \( N \)-representability conditions

We consider the P, Q, G conditions. Additional necessary conditions can be considered, such as Eckhart’s T1 and T2 conditions [6, 16, 18].

\[
L_\ell(\Gamma) = \Gamma_{\ell}, \quad \langle \Gamma_{\ell}(\Omega) \rangle_{\delta_k} = \frac{1}{N(N - 1)} \sum_{i \neq j} \delta_k \Omega_{i,j}^\ell
\]

Example: Minimization for \( N \) in a STO-6G basis set using the P,Q,G conditions

Plot of the distance to the cone: \( d(\mu) = \text{dist} \{ (K_N - \mu, \mathcal{C}_{\text{app}}) \} \). Notice that this function is convex on \( \mu \) increasing on \( [\mu_{\text{app}}, \infty) \), and \( \delta = 0 \) on \( (-\infty, \mu_{\text{app}}) \).

References