Diverging Exchange Force and Form of the Exact Density Matrix Functional

Christian Schilling

Arnold Sommerfeld Centre for Theoretical Physics, LMU Munich

For translationally invariant one-band lattice models, we exploit the *ab initio* knowledge of the natural orbitals to simplify reduced density matrix functional theory (RDMFT). Striking underlying features are discovered: First, within each symmetry sector, the interaction functional $\mathcal{F}$ depends only on the natural occupation numbers $\boldsymbol{n}$. The respective sets $\mathcal{P}_N^1$ and $\mathcal{E}_N^1$ of pure and ensemble N-representable one-matrices coincide. Second, and most importantly, the exact functional is strongly shaped by the geometry of the polytope $\mathcal{E}_N^1 \equiv \mathcal{P}_N^1$, described by linear constraints $D^{(j)}(\boldsymbol{n}) \geq 0$. For smaller systems, it follows as $\mathcal{F}[\boldsymbol{n}] = \sum_{i,i'} \overline{V}_{i,i'} \sqrt{D^{(i)}(\boldsymbol{n}) D^{(i')}(\boldsymbol{n})}$. This generalizes to systems of arbitrary size by replacing each $D^{(i)}$ by a linear combination of $\{D^{(j)}(\boldsymbol{n})\}$ and adding a non-analytical term involving the interaction $\hat{V}$. Third, the gradient $\mathrm{d}\mathcal{F}/\mathrm{d}\boldsymbol{n}$ is shown to diverge on the boundary $\partial\mathcal{E}_N^1$, suggesting that the fermionic exchange symmetry manifests itself within RDMFT in the form of an "exchange force". All findings hold for systems with non-fixed particle number as well and $\hat{V}$ can be *any* p-particle interaction. As an illustration, we derive the *exact* functional for the Hubbard square.