Diverging exchange force and form of the exact density matrix functional

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We first provide an elementary introduction into Reduced Density Matrix Functional Theory (RDMFT) and outline how this generalization of Density Functional Theory (DFT) could overcome the fundamental limitations and shortcomings of DFT. This is then followed by a general study of RDMFT for translationally invariant one-band lattice models. We exploit the *ab initio* knowledge of the natural orbitals for those systems to discover a couple of striking features: First, within each fixed 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". As an illustration, we derive the *exact* functional for the Hubbard square.