

Density-functional theory with additional basic variables: Extended Legendre transform

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In a recent series of papers, Higuchi and Higuchi defined an extended constrained-search procedure by extending the Levy constrained search by adding additional constraints. As shown here, this procedure can be equivalently formulated in terms of Lieb's Legendre transformation functional. The Legendre transform approach has advantages in cases where the additional constraints are restrictive enough to cause problems with N -representability. © 2009 The American Physical Society.