

Abstract Submitted  
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**The exact density functional for two electrons in one dimension**

ARON COHEN, University of Cambridge, PAULA MORI-SANCHEZ, Universidad Autonoma de Madrid — The exact universal density functional  $F[\rho]$  is calculated for real space two-electron densities in one dimension  $\rho(x)$  with a soft-Coulomb interaction. It is calculated by the Levy constrained search  $F[\rho] = \min_{\Psi \rightarrow \rho} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle$  over wavefunctions of a two-dimensional Hilbert space  $\Psi(x_1, x_2) \rightarrow \rho(x_1)$  and can be directly visualized. We do an approximate constrained search via density matrices and a direct approximation to natural orbitals. This allows us to make an accurate approximation to the exact functional that is calculated using a search over potentials. We investigate the exact functional and the performance of many approximations on some of the most challenging electronic structure in two-electron systems, from strongly-correlated electron transfer to the description of a localized-delocalized transition. The exact Kohn-Sham potential,  $v_s(x)$ , and exact Kohn-Sham eigenvalues,  $\epsilon_i$ , are calculated and this allows us to discuss the band-gap problem versus the perspective of the exact density functional  $F[\rho]$  for all numbers of electrons. We calculate the derivative discontinuity of the exact functional in an example of a Mott-Insulator, one-dimensional stretched  $H_2$ .

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