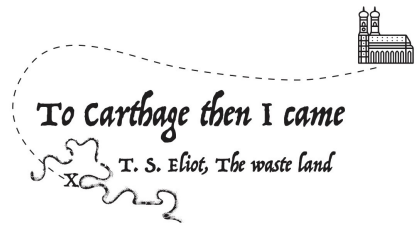


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Tuesday 17th May
12:00 (Tunis time – GMT+1, UTC+1)



The strong-interaction limit of density functional theory

While not reached in nature, the strong-interaction limit of the exact (Hohenberg-Kohn) density functional points the way towards the real physics in strongly correlated many-electron systems missed by the standard approximations used in physics, chemistry and materials science. For example, the strong-interaction limit - unlike the local density approximation, semilocal, or hybrid functionals - gets the dissociation of the H₂ molecule right.

In my talk I cover

- the derivation of the limiting strictly correlated electrons (SCE) functional from the exact functional via Gamma convergence
- equivalent formulations and the mathematical interpretation as optimal transport with Coulomb cost
- rigorous sparsity theorems in the spirit of Brenier's theorem in both the continuous and discretized case
- the recently introduced GenCol (Genetic Column Generation) algorithm which exploits this sparsity and appears to overcome the curse of dimension, allowing for the first time the accurate computation of the strong-interaction limit for general densities.

References:

- GF, Augusto Gerolin and Paola Gori-Giorgi, arXiv:2202.09760, 2022 (recent survey article);
- GF, Andreas Schulz and Daniela Voegler, arXiv:2103.12624, to appear in SIAM JSC, 2022 (algorithm).