POSTER

Exact Maps in Density Functional Theory for a Lattice model

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To understand the failures of approximate functionals, to gain insight into the behavior of the exact functional, and to devise new approximations, we investigate the exact solution of the many-body Schrödinger equation in Fock space for a lattice model with a softened Coulomb interaction term.
Using exact diagonalization, we construct the exact density-to-potential and density-to-wave-function map. We find that the gradient of the density-to-potential map steepens with increasing electron-electron interaction strength and decreasing kinetic hopping probability. We denote this feature of the density-to-potential map, previously also observed for one-dimensional molecules [1] and the two-site Hubbard-model [2], as intrasystem steepening. Similar to the intersystem derivative discontinuity [3] , the intrasystem steepening directly transfers into the density-to-wavefunction and the density-to-observable map. We illustrate how both, the intersystem derivative discontinuity and the intrasystem steepening transfer into the excited-state energy functional, the excited- and transition-state density functional and the von-Neumann entropy functional.

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[2] D. J. Carrascal et al., arXiv:1502.02194 (2015).
[3] J. P. Perdew et al., Phys. Rev. Lett. 49, 1691 (1982).