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Correlation energy of a finite single chain lattice using a Hartree+Exchange approximation, a Jastrow factor and a local density approximation

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We perform a Hartree+Exchange approximation on a finite one dimensional lattice of fractional particle number using the Hubbard Hamiltonian. The resulting approximate Kohn-Sham ground state wavefunction is then acted on by a Jastrow factor operator to retrieve the exact correlation energy and the interacting density that we use for a local density approximation (LDA) of the correlation energy in two different ways. The first approach makes use of the ensemble (fractional) density to get the energies and the second one interpolates the energies between integer particle numbers. An insight into the different results shows that the second approach is more promising and the underlying homogeneous energy density is suitable for applications of LDA.

Apply to be considered for a student award (Yes / No)?

Yes

Level for award (Hons, MSc, PhD, N/A)?

PhD

Main supervisor (name and email) and his / her institution

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Would you like to submit a short paper for the Conference Proceedings (Yes / No)?

Yes

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