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Density Functional Theory on a Lattice: Particle Number Dependence of the Exchange-Correlation Potential.

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Abstract content
   (Max 300 words)
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In Kohn-Sham Density Functional Theory, the interacting system is mapped onto a fictitious independent particle system. In an ensemble continuous particle number formulation the exchange-correlation contribution to the potential of the independent particle system has a discontinuity as a function of particle number at integer particle numbers. This discontinuity is equal to the difference between the fundamental gap of the interacting system and the independent particle system. We numerically investigate the exact exchange-correlation potential as a function of particle number for a finite dimensional Hubbard model and compare the exact results to a local density approximation to the exchange-correlation functional.

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