PHYSICS COLLOQUIUM:

Predictive Power of the Exact Contraints and Appropriate Norms in Density Functional Theory, with Interpretations of Ground-State Symmetry Breaking and Strong Correlation

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Date:
4/9/2021

Time:
10:30 AM-11:50 AM

Link:
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Abstract:

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Kohn-Sham density functional theory is computationally similar to Hartree-Fock theory, but is in principle exact for the ground-state energy and density of a many-electron system. In practice, the density functional for the exchange-correlation energy must be approximated. The SCAN functional[1] satisfies 17 exact constraints plus appropriate norms like the uniform gas, which make it predictive for many atoms, molecules, and solids, including some strongly-correlated ones[2,3]. Strong correlations within a symmetry-unbroken ground-state wavefunction can show up in approximate density functional theory as symmetry-broken spin-densities or total densities. They can arise from soft modes of fluctuations (sometimes collective excitations) such as spin-density or charge density waves at non-zero wavevector. Familiar examples are the unobservable but revealing symmetry breaking in stretched H_2 and the observable symmetry breaking in antiferromagnetic solids. The example discussed here is the static charge-density wave/Wigner crystal phase of a low density ($r_s \approx 69$) jellium. Time-dependent density functional theory is used to show quantitatively that the static charge density wave is a soft plasmon. More precisely, the frequency of a related density fluctuation drops to zero, as found from the frequency moments of the spectral function. Our calculation[4] is based on a recent constraint-based wavevector- and frequency-dependent jellium exchange-correlation kernel.[5] (Supported by NSF DMR & DOE BES.)

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[4] J.P. Perdew, A. Ruzsinszky, J. Sun, N.K.Nepal, and A.D. Kaplan, Proc. Nat. Acad. Sci. USA 118, e201785024 (2021).
[5] A. Ruzsinszky, N.K. Nepal, J.M. Pitarke, and J.P. Perdew, Phys, Rev. B **101**, 245135 (2020).