Physics Colloquium

Thursday, Sept 10th at 3:30PM in SC 234

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Back to the Future: Progress on Primordial Quantum Statistical Mechanics

Can we treat many-electron systems without many-electron wave functions and ensembles? Primordial quantum mechanics gave a provocative but ultimately inadequate affirmative answer: Thomas-Fermi-Dirac theory. Modern density functional theory (DFT) formally confirms that answer but provides no path for construction of the functionals. Even with approximate functionals, the dominant implementation (Kohn-Sham mapping to a non-interacting system and use of it's orbitals to construct the density) introduces computational cost scaling challenges.

Important physical problems motivate the quest for a pure, orbital-free DFT (OFDFT). The warm dense matter pressure-temperature regime ($0{:}1\text{GPa} \le P \le 10^5\text{GPa}$, $10^4\text{K} \le T \le 5 \le 10^5\text{K}$) is relevant to inertial confinement fusion and giant planet interiors. Extremely confined molecular clusters provide another example. For these, *ab initio* molecular dynamics (AIMD) with Born-Oppenheimer forces from Kohn-Sham DFT is the state of the art. But KS-DFT computational cost scales as the cube of the number of occupied orbitals N^3_{occ}. AIMD thus can become prohibitively costly for comparatively small systems.

In principle OFDFT eliminates the bottleneck, because OFDFT cost scales with system size. We are back to the seductive, primordial idea. There are two challenges. We must construct accurate, non-empirical orbital-free approximations for the non-interacting KS free energy functional T_s-TS_s (KE and entropy functionals) and for the exchange-correlation (XC) free-energy F_{xc} functional. After an orientation to DFT basics, I shall discuss the physics of constructing useful, constraint- based T_s, S_s, and F_{xc} approximations. This constraint-based, non-empirical approach has yielded the first effective, fully non-empirical T-dependent generalized gradient approximation functional for the KS free energy, and the first T-dependent local-spin density XC approximation based solely on quantum Monte Carlo data. I will give some examples of consequences in actual calculations, and conclude with a summary of the puzzles which we currently are addressing and the outlook for OFDFT.

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References and software downloads at: http://www.qtp.ufl..edu/ofdft

Refreshments at 3:00PM in SC 103