

## **Peaks and valleys in the search for the "divine functional"**

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### **Abstract:**

One of the most important theoretical formulations of quantum physics is density functional theory (DFT) -- the foundational approach for modern theories for the electronic structure of materials and a linchpin of computational methods in nanoscience and chemistry. DFT is based on a fundamental, universal mapping, or functional, between the electron density of any electronic system and that system's electronic ground-state energy. The proof of existence of this functional has been known for over forty years, and many relatively successful approximations to it have been developed over the years, but the nature of the exact mapping actually used by nature, nicknamed the "divine" functional, has eluded investigators' grasp. I report progress in the search for this "divine" functional based on Monte Carlo simulations of the exchange-correlation (XC) hole -- the change in electron density surrounding the position of an electron due to Pauli exclusion and Coulomb repulsion, and a key theoretical input into DFT. Our data indicate the importance of the Laplacian of the density as a variable in modeling the XC hole and thus improving to our understanding of the universal "divine" density functional.