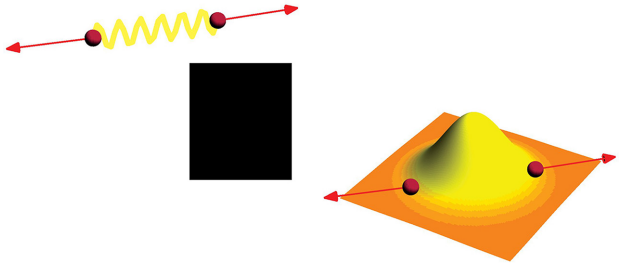
Scilight

16 October 2019

Systematic approach approximates exchange correlation potentials more accurately and applicably

Adam Liebendorfer

Force-balance equations allow determining exchange correlation potentials without using energy or action expressions.



Density functional theory (DFT) offers an alternative, computationally feasible method for calculating key characteristics of electrons, and continues to be one of today's leading approaches for approximating quantum mechanics. One drawback of the theory, however, is the lack of exchange correlation (xc) potentials, a key ingredient of the theory, that are both accurate and generally applicable. A new paper offers one way to consistently construct approximations in different physical settings.

Tchenkoue et al. present a systematic way to determine advanced approximations of xc potentials of density-functional theories. The new approach employs force-balance equations to dynamically obtain approximations, rather than obtaining them from a mathematical formula that expresses the total energy of a system in terms of electronic spatial density.

The result, said author Markus Penz, is an approach that presents the ideas behind DFT in a way that more closely resembles a theory of fluid mechanics.

"The movement of electrons, governing chemical processes, can be described by a current, very similar to a water current that defines the movement of, say, a streamlet," said Penz. "How this current changes in time is given by the force-balance equation that includes different contributions: interactions between the electrons, internal quantum effects and the effect of external fields."

The group's systematic method establishes pointwise determining relations for xc potentials that allow for straightforward orbital-dependent approximations without using energy or action expressions. It is feasible in both a ground-state and time-dependent setting.

The group next looks to explore more ways in which their force-balance approach could be used, such as for systems of electrons coupled to quantized field modes as seen in quantum-electrodynamical DFT.

Source: "Force balance approach for advanced approximations in density functional theories," by Mary-Leena M. Tchenkoue, Markus Penz, Iris Theophilou, Michael Ruggenthaler, and Angel Rubio, *Journal of Chemical Physics* (2019). The article can be accessed at https://doi.org/10.1063/1.5123608.