Commentary
Volume 12:S6, 2021

Journal of Physical Mathematics

ISSN: 2090-0902 Open Access

Illustration on Kinetic Energy Theory

Denmark Sarah*

Department of Physics, University of South Florida, Tampa, USA

Description

The quantum many-body problem has been studied using Density-Functional Theory (DFT) for decades. Its effectiveness originates from the fact that it combines low computational complexity with decent accuracy, making it easier to analyze and forecast experimental results for systems that wave function-based approaches cannot access. By reformulating physical phenomena in terms of density, DFT avoids the exponential computational costs of wave function-based techniques. The main disadvantage of DFT is that it does not provide an accurate energy expression for a quantum system in terms of density, thus approximations must be used in exercise.

There are various different techniques to working with the quantum many-body problem that do not employ the many-body wave function and make modelling the desired physical quantities easier. Higher-order Feynman diagrams can enhance the accuracy of Green's function techniques, but they are significantly more computationally expensive. Functional theories based on Reduced Density Modules (RDM) offer a balance of accuracy and processing expense. Because the kinetic energy is an implicit functional of the RDM through one RDM functional theory only a portion of the interaction energy must be approximated, whereas in two-body RDM (1RDM) functional theory, even the interaction is given by an explicit functional. Although the explicit use of wave functions in these contingencies can be avoided, the RDM still must be described by a wave function.

The so-called N-representability criteria, which guarantee the presence of an underlying wave function is associated with an RDM are far from simple. Moreover, unlike in the DFT example, it is not possible to attach an occurring due of non-interacting particles to every RDM, allowing the N-representability conditions to be substituted by a relatively simpler auxiliary wave function.The feasibility of including the kinetic-energy density as a basic functional variable in DFT alongside density is explored. The idea is to improve density-functional approximation accuracy. This examination is by creating the exact density functionals of traditional DFT and comparing them to the combined kinetic-energy density and density functionals of the Kinetic-Energy Density-Functional Theory (keDFT). We hope to assess the potential benefits of such a strategy when dealing with heavily linked systems in this fashion. For the description of these systems, the so-called kinetic contribution to the exchange correlation potential is crucial. Standard DFT functionals have been proven to fail to capture the consequences of this kinetic contribution such as band narrowing caused by interactions. Its involvement is properly considered directly by integrating the kinetic-energy intensity as a fundamental variable. While the proposed technique was studied in depth primarily for simple few-site applications, it is simple to expand to many sides, arbitrary dimensions, as well as the continuum. With a spatially varying mass term, we can choose a gauge-independent, strictly positive kinetic-energy density formulation.

Conclusion

The key reason why the keKS scheme can be more accurate in the continuum than the traditional KS scheme is that we can explicitly model the kinetic-energy density. The extension to the continuum seems especially compelling because the simple kinetic-energy density estimates we introduced proved to be pretty realistic. Many reference computations exist for homogeneous systems that can be employed to construct a universal local kinetic-energy density approximation that is similar to the uniform approximation described in this article.

How to cite this article: Sarah, Denmark. "Illustration on Kinetic Energy Theory ." *J Phys Math* S6 (2021) : 002

***Address for Correspondence:** Dr. Denmark Sarah, Department of Physics, University of South Florida, Tampa, USA; E-mail: Sarah@gamil.com*

Received date: December 03, 2021**; Accepted date:** December 17, 2021**; Published date:** December 24, 2021