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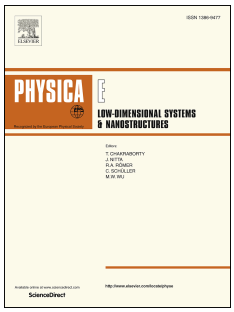

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Gradient Approximated Exchange Energy Functionals With Improved Performances For Two-Dimensional Quantum Dot Systems

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Abstract

Semilocal exchange-correlation functionals are frequently used to accurately describe the complex many-electron effects of two-dimensional quantum systems. Most of these functionals are designed using the reduced density gradient as the main ingredient. A semilocal functional for the exchange and the corresponding enhancement factor is constructed using the inhomogeneity parameter of the generalized gradient approximations by analyzing the small and large-density gradient expansion of the exchange hole. This exchange functional significantly reduces the error compared to the existing gradient approximations. Performance of the proposed semilocal functional is demonstrated by considering parabolic and Gaussian quantum dots with varying particle number and confinement strength. The results are also compared with that of the exact exchange formalism by considering it as the standard.

Keywords: density functional theory, semilocal functional, quantum dot

1. Introduction

The electronic structure calculations of the low-dimensional systems is greatly simplified due to the Hohenberg-Kohn-Sham [1, 2] variant of density-functional theory (DFT). The success of DFT to describe various phenomena is due to the development of the exchange and correlation (XC) functionals [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. The substantial applications of DFT are mainly based on the accuracy of the semilocal density functionals. Despite its grand success, the dimensional crossover is still an open problem in DFT and it has been reported that the three-dimensional (3D) semilocal XC functionals in principle cannot be extended directly to low -dimensional systems due to various limitations [20]. Semilocal exchange energy functionals show divergent nature in the exact 2D limit. However, the 3D exact exchange formalism can be applied directly to the 2D systems without suffering from the dimensional crossover issues. Therefore, the constructions of new semilocal functionals in two dimensions (2D), is an active area of research with promising prospects. Present day studies involving low-dimensional systems [21, 22] e.g. carbenoid, graphene-related materials, silicon nanowire-based biosensors, quantum Hall devices and various types of quantum dots have substantially attracted the attention of researchers. The utility, which two-dimensional electron gas (2DEG) has on the interface region is also studied using DFT [39]. In this regard, many-body effects in low dimensions require to be properly addressed because of its potential impact in solid-state and materials research. But, due to the time lag between the development of the 3D and 2D XC functionals, the latter has not been explored much. It is only during the last decade or so, the developments of 2D XC functionals have been taken up seriously.

Analogous to 3D Jacob's Ladder, the different rungs of 2D XC functionals are also approximated according to the ingredients involved in designing it. On the lowest rung, the 2D local density approximation (2D-LDA) [23] is constructed using the electronic density $\rho(\vec{r})$ as the only ingredient. The 2D-LDA for exchange combined with the 2D correlation has successfully described several systems [24, 25] through its thought-provoking results comparable to those obtained using quantum Monte Carlo simulations [26]. Then, subsequent attempts were made to further reduce the errors present in 2D-LDA [27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37] by introducing more ingredients other than the electronic density. Due to which, the Generalized gradient approximations (2D-GGA) [27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37] became the next effective rungs of the 2D Jacob's Ladder. The first ever 2D-GGA [28] was constructed by extending Becke's formalism [3] to the low-dimensional regime. After that, several semilocal functionals [27, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38] with increasing accuracy has been constructed in recent years.

In DFT, the additional ingredients besides the particle density that are involved in the construction of XC functionals have been introduced so as to take care the degree of inhomogeneity associated with the system as much as possible. Mostly, the construction of XC functionals are based on the reduced density gradient (s), which is the main ingredient of GGA functionals. Unlike GGA, the meta-GGA exchange energy functionals use the non-interacting positive definite Kohn-Sham (KS) kinetic energy (KE) density (τ) and 's' as its ingredients [38]. Thus 's' together with 'τ' forms the higher order rung of the XC functionals. Instead of 's', Becke proposed [40] that a new in-homogeneity parameter which depends on ρ, $\nabla\rho$, $\nabla^2\rho$ and τ

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