Research paper

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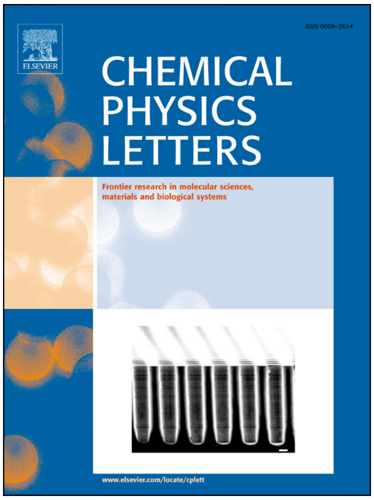

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Shannon information entropy in position space for doubly excited states of helium with finite confinements

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Abstract

Quantifying electron localization in quantum confined systems remains challenging, especially for excited states. A quantum dot (QD) is represented by helium atom in a finite oscillator potential. The effect of dot width variation on the electron localization in QD is systematically examined via Shannon entropy for low-lying doubly excited states ($2s^2\ ^1S^e$, $2p^2\ ^1S^e$, $2s3s\ ^1S^e$) obtained using highly correlated Hylleraas functions. In particular, the most effective dot width where electrons are the most localized is determined successfully and justified by the electron density plot for all three states.

Keywords: Shannon entropy; Helium; Hylleraas functions; quantum confinement; finite oscillator potentials; doubly excited states; electron density; localization; delocalization

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1. Introduction

Quantum confinement [1-3, 10-25] is an active research topic as it is relevant to studies on nanostructures such as quantum dots (QDs), or so-called artificial atoms. For such confined systems, two properties of their electronic structure are of main concerns. One is their energy levels, which have been extensively studied. To be specific, QDs have been synthesized and with energy levels measured by scanning tunneling spectroscopy (STS) [1-3]. The other is the localization or delocalization of the electron density. Although the electron density can be mapped by STS [2], how to properly quantify the extent of electron localization remains as a challenging issue. One attempt finds it roots in quantum information theory, which also plays key roles in the developments on quantum computation, quantum teleportation, and quantum cryptography. There has also been continuous interest in studies on quantum information in atomic and molecular systems [5-16, 26-33], especially the *Shannon entropy* [5-16, 26-31].

Proposed by Shannon in 1948, Shannon information entropy measures the distribution of a random variable [4]. A more *localized* distribution results in a smaller Shannon entropy while a more *delocalized* one leads to a larger Shannon entropy. Later, it is extended to describe the delocalization of electrons [5-6] with calculations for numerous quantum confined systems [7-16]. Simple models such as particle in an infinite well [7], finite well [8], cyclic box [9], quantum corral [10] and infinite circular well [11] have been studied. Furthermore, Corzo *et al.* [10] pointed out that the sum of Shannon entropy in position space and that in momentum space differs for attractive and repulsive potentials. In contrast, standard deviation, as other common index for distribution, does not. Besides, hydrogens subjected to finite and infinite spherical potential are studied as well [12-15]. It should be noted that all works above contain a single electron. As for multi-electron systems, H^-, He and Li^+ atoms within an impenetrable shell have been examined by Sen [12].