

A Geometric Formulation of Quantum Stress Fields in Density Functional Theory

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The quantum stress field allows one to measure a system's energetic response to a spatially localized deformation which can be represented by a strain field. The stress field can therefore provide local energetic information which might not be revealed in other quantities such as the force. Unfortunately, previous formulations of the quantum stress field contain ambiguities, suggesting that it is an ill-defined quantity.

We have derived the stress field for an interacting quantum system via a Riemannian differential geometric approach. The uniqueness of the stress field obtained from this method will be discussed. Also, we will demonstrate applications of this formulation within the local density approximation of density functional theory.