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Geometric Formulation of Quantum Stress Fields in Density Functional Theory

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The quantum−mechanical stress is a fundamentally important quantity which provides insight into the relationship between the electronic structure and the mechanical properties of condensed−matter systems. Nielsen and Martin have provided a tractable and well−defined expression of the macroscopic or total stress for periodic solid−state systems within the framework of density functional theory (DFT), allowing the study and prediction of a large class of structural properties from first principles.

The quantum stress field provides significantly more information than the total stress, allowing one to study the spatial dependence of the stress and its relationship with local electronic and structural phenomena. However, previous derivations of the quantum stress field are not unique since they are determined only up to a gauge term.

We will present a unique expression for the quantum stress field within the local density approximation (LDA). Our formulation exploits a known relationship between the strain tensor field and the Riemann metric tensor, giving rise to a quantity which is gauge invariant with respect to choice of energy density. Stress field results from DFT−LDA calculations of solid molecular hydrogen will be reported. Extensions of the formalism to pseudopotentials and gradient corrected exchange−correlation functionals will be discussed.
