

Geometric Formulation of Quantum Stress Fields

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The variation in energy with respect to strain plays a vital role in many solid systems by linking microscopic structure on the atomic scale with coarser macroscopic properties and phenomena. Mesoscale studies of materials fruitfully treat strain, stress, and higher strain derivatives as spatially varying fields. This approach permits the correlation of stress-induced structural modifications in a particular region of the system with the microscopic stress field in the surrounding area. Formulations of quantum stress fields have been developed. Unfortunately, these formulations have several shortcomings (e.g. gauge variance or non-uniqueness, inability to access stress fields which correspond to aperiodic displacements) or rely on drastic approximations of the system (e.g. 2-body interactions only). Here we present a geometric formulation of the stress field which is based on the relationship between the strain tensor field and the metric tensor field on a generalized Riemannian manifold. Furthermore, we show that this formulation preserves gauge invariance when implemented in Kohn-Sham density functional theory. As a demonstration of this method, we present stress fields obtained from LDA calculations on solid hydrogen.