
The numerical instability in non-collinear DFT

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Spin density function theory (DFT) is a widely used method. In the traditional collinear approach, spin magnetization is defined as the z-component of spin density while in non-collinear approach as the norm of spin density. The non-collinear approach preserves correct spatial symmetry but suffers from numerical instability at points with vanishing spin. The instability can be treated perfectly for local density approximation (LDA) [1], but less satisfactorily for generalized gradient approximation (GGA) [2,3]. In this work, some efforts are made to deal with the numerical instability in non-collinear GGA .

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