

Can effective magnetic fields have monopoles? (and why you should care)

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Using three examples, we show how we take *ab-initio* theory from concept, through mathematical development and coding[1] to final comparison with experiment. The first arises from the question of whether the exchange-correlation magnetic field of density functional theory should contain monopoles. A simple procedure is used to remove the source-term from existing functionals. This greatly improves the predictions of the theory, particularly the local moments in high- T_c pnictides[2], and indicates that the exact functional should have this property.

The second example is a follow-on from our work on femtosecond spin dynamics where we predicted a new phenomena called OISTR (optical inter-site spin transfer) that dominates[3,4,5,6,7] the physics of demagnetization in early times ($\lesssim 10$ fs) in multi-component magnets. In order to extend this to ultra long length scales we have developed a new ansatz for calculations which effectively contain millions of atoms and yet are atomistic and *ab-initio*. With this we can simulate a range of physics from parameter-free micro-magnetics to long-range, dynamic charge fluctuations and light-light interaction.

The last example concerns the destruction and recovery of the superconducting order-parameter by a laser pulse. We have derived a mathematical method for including quantum nuclear motion which will allow for parameter-free calculations of the time-evolution of superconductivity[8].

1 References

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