First-principles theory of spatial dispersion effects

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Density-functional perturbation theory (DFPT) is nowadays the method of choice for the accurate computation of linear and non-linear response properties of materials from first principles. A notable advantage of DFPT over alternative approaches is the possibility of treating incommensurate lattice distortions with an arbitrary wavevector, \( q \), at comparable computational cost as the lattice-periodic case. In this talk I will show that \( q \) can be formally treated as a perturbation parameter, and used in conjunction with established results of perturbation theory (e.g. the “2\( n \)+1” theorem) to perform a long-wave expansion of an arbitrary response function in powers of the wavevector components. This provides a powerful, general framework to accessing a wide range of spatial dispersion effects that were formerly difficult to calculate by means of first-principles electronic-structure methods. In particular, the physical response to the spatial gradient of any external field can now be calculated at essentially no cost, by using the response functions to uniform perturbations (electric, magnetic or strain fields) as the only input. [1] I will also discuss special issues that need to be addressed for the calculation of the flexoelectric tensor, such as the finite-\( q \) generalization of the polarization [2] response and of the strain [3, 4] perturbation.

References