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, $\mathbf{q}$, at comparable computational cost as the lattice-periodic case. In this talk I will show that $\mathbf{q}$ can be formally treated as a perturbation parameter, and used in conjunction with established results of perturbation theory (e.g. the "$2n+1$" 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-$\mathbf{q}$ generalization of the polarization [2] response and of the strain [3, 4] perturbation.

References

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