A Generalized Muffin Tin Augmented (Plane)Wave Method

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Abstract

Since its invention the full potential LAPW method as implemented for example in the Wien2k code[1] has been used to compute the properties of periodic structures, i.e. solids quite successfully. However, this muffin-tin-type method is not very suitable for non-periodic system, i.e. molecules. Although one can make the unit cell larger and larger in order to get results for an isolated molecule this quickly blows up the number of degrees of freedom N_{DOF}.
In this contribution we proceed to replace the *plane waves* in this method by the tensor products of sine functions in three dimensions, viz.

$$F_{ijk} = \sin(iq_{\min}x)\sin(jq_{\min}y)\sin(kq_{\min}z) \text{ where } q_{\min} = \frac{\pi}{L} \text{ and } 1 \leq i,j,k \leq N-1\,,$$

in terms of the linear system dimension L, while making use of the Fast Sine Transform[2] for computational efficiency. These basis functions vanish on the surface of the domain $\Omega = [0,L]^3$ and thus make the method suitable for non-period systems.
The changes to the LAPW formalism are, that the matrices implementing the boundary conditions at the surfaces of the atomic spheres will be calculated via numerical integration instead of using the plane wave expansion formula in terms of spherical harmonics and that the atomic orbitals will not be obtained at a initial energy together with their energy derivatives but rather solved for as part of one eigenvalue problem with coefficients for all domains, i.e. one interstitial domain and N_A atomic spheres. The atomic orbitals will be expanded in terms of real-valued spherical harmonics R_{lm}, and the radial channel functions in terms of finite elements as in [3]. The implementation of the boundary conditions in the eigenvalue problem is discussed in detail and some preliminary results for small molecules will be shown and compared with results of competing methods.

References

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2. http://scipy.org . Fourier Transforms (scipy.fftpack). https://docs.scipy.org/doc/scipy/reference/tutorial/fftpack.html.
3. M Braun and K O Obodo . Multi-domain muffin tin finite element density functional calculations for small molecules. Computers and Mathematics with Applications 74 (2017) 35–44.