The Tilted Plane Condition

Andrew C. Burgess[1], Edward Linscott[2], and David D. O'Regan[1]

[1]*School of Physics, Trinity College Dublin, The University of Dublin, Ireland*
burgesan@tcd.ie
[2]*Laboratory for Materials Simulations, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland*

ABSTRACT

The flat plane condition [1] defines the shape of the ground-state energy surface with respect to variations in electron count N and certain limited variations in magnetisation M. The violation of this exact condition has been directly linked to poor performance in the prediction of band gaps, molecular dissociation, and electronic transport by standard XC approximations. We derived the tilted plane condition [2], a generalisation of the flat plane condition as exemplified in Fig. 1, which rigorously defines the energy surface for all values of N and M. The magnetic analog of the DFT Koopmans' theorem is also derived as a corollary. From this condition we show that energy functionals of occupancies must take different forms depending on symmetry-imposed degeneracies. We will also highlight our recent proof of the long-assumed convexity condition of DFT [3], which lifts a standing assumption in the piecewise linearity condition with respect to electron count.

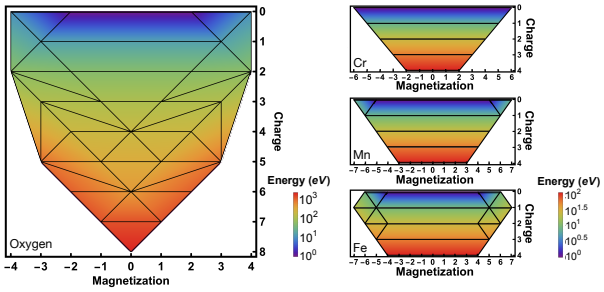

Figure 1: The projection of the $E_v[N, M]$ surface of the oxygen, chromium, manganese and iron atoms onto the $N - M$ plane.

References

[1] Yang, W.; Zhang, Y.; Ayers, P.W. *Phys. Rev. Lett.* **2000**, *84*, 5172.

[2] Burgess, A.C.; Linscott, E.; O'Regan, D.D. *arXiv preprint.* **2023**, 2307.16003.

[3] Burgess, A.C.; Linscott, E.; O'Regan, D.D. *J. Chem. Phys.* **2023**, *159*, 211102.