BODY-ORDERED APPROXIMATIONS OF ATOMIC PROPERTIES

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ABSTRACT

We survey some recent results [1, 2] on the sparsity of the potential energy landscape (PEL) aimed to justify and extend the theory of machine-learning for interatomic potentials. Firstly, we show that the PEL can be decomposed into site contributions which only depend on an exponentially small atomic neighbourhood. The asymptotic behaviour of the pre-factors and exponents in these estimates are characterised with respect to vanishing Fermi-temperature and, in the case of insulators, the band gap.

Moreover, we show that the site contributions may be approximated by a body-ordered approximation of low body-order. Specifically, we prove that the resulting body-ordered approximation for analytic observables has an exponential rate of convergence both at finite Fermi-temperature as well as for insulators at zero Fermi-temperature. We discuss potential consequences of this observation for modelling the PEL, as well as for solving the electronic structure problem.

A particular feature of all our results is that they depend only weakly on the point spectrum which arises from the study of point defects in crystals, for example. This observation extends and strengthens the previous locality results of [3, 4].

References

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