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Extended Dynamical Equations of the Period Vectors of Crystals under Constant External Stress to Many-body Interactions

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Since crystals are made of periodic structures in space, how to determine their three independent period vectors (starting from any values) is a basic physics problem. One choice is to minimize (Gibbs) energy or enthalpy for the situation where crystals are under constant external pressure. For crystals under constant external stress, we derived dynamical equations of the period vectors, for pair potentials recently (Can. J. Phys. 93: 974-978, dx.doi.org/10.1139/cjp-2014-0518). The derived dynamical equations show that the period vectors are driven by the imbalance between the internal and external stresses. The internal stress has both the kinetic energy term and a full virial term. Here we will extend it to many-body potentials.

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