

Dynamical Equations Of Periodic Systems Under Constant External Stress

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Abstract

Periodic boundary conditions are widely used in the simulation of systems with an extremely large number of particles, and the period vectors become a degree of freedom. In this work, dynamical equations for the periods are generated by applying Newtonian Dynamics onto halves of the system while considering constant external stress explicitly. Then statistics over system translations and directions of particle movements are applied to the dynamical equations. This leads to the full interaction and kinetic-energy terms in the internal stress. In the resulting expressions, the periods are driven by the imbalance between the internal and external stresses. (The manuscript has been published as <http://arxiv.org/pdf/cond-mat/0209372v10.pdf>, and submitted to the Canadian Journal of Physics for formal publication on Jan. 08, 2014.)