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Equipartition theorem in glasses and liquids VALENTIN A. LEVASHOV, TAKESHI EGAMI , University of Tennessee, RACHEL S. AGA , JAMES R. MORRIS, Oak Ridge National Laboratory — In glasses and liquids phonons have very short life-time, whereas the total potential energy is not linear with temperature, but follows the T**(3/5) law. Thus it may appear that atomic vibrations in liquids cannot be described by the harmonic oscillator model that follows the equipartition theorem for the kinetic energy and potential energy. We show that the description of the nearest neighbor oscillation in terms of the atomic level stresses indeed provide such a description. The model was tested for various pair-wise potentials, including the Lennard-Jones potential, the Johnson potentials, and only the repulsive part of the Johnson potential. In all cases each of the local elastic energies of the six independent components of the stress tensor is equal to kT/4, thus the total potential energy is equal to (3/2)kT. Thus this model provides the basis for discussing the thermodynamic properties of glasses and liquids based on atomistic excitations. An example of this model leading to the description of the glass transition temperature in metallic glasses is discussed [1].
[1] T. Egami, et al., Phys. Rev. B 76, 024203 (2007).

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