

Abstract Submitted
for the OSS16 Meeting of
The American Physical Society

Dissociation transitions for 1D chains and molecules bound by a general anharmonic interatomic potential DONALD PRIOUR, Youngstown State University — Interatomic potentials provide a phenomenological description of atomic interactions, whether in the case of comparatively weak Van der Waals bonding (Lennard Jones) or relatively strong covalent bonding (Morse potential and variants). We consider a general unimodal anharmonic interatomic potential with a well defined minimum, decaying at large distances, and rising sharply if the atomic pair is in close proximity. Under these assumptions, we derive a perturbative series for the partition function, leading to analytical expressions for the mean bond length, the specific heat, and the coefficient of thermal expansion. In this manner, the dissociation transition at low temperature is accurately described as the pressure term becomes small, allowing thermal fluctuations to dissociate a molecule or induce in a 1D chain a crossover from a condensed state to a loosely bound gaseous state. In particular, using exact results to highlight agreement, we show that for dissociation in the low temperature regime, the mean bond length is given by $\langle l \rangle = R_0(1 + A\eta^{-2}\varepsilon^{-1/2}e^{-\varepsilon})$; with ε and η being the dissociation energy and the characteristic pressure energy scale pR_0 respectively, divided by $k_B T$.

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Date submitted: 19 Mar 2016

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