

Some solvable questions in lattice dynamics: chasing the continuum, handling simple things by complex tools

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ABSTRACT

Studies in lattice dynamics go back to, at least, the times of Lagrange, whereas after an establishment of the prominent role of digital computers in research, the concept of `discretization' led to numerical scheme of similar character for solving `continuum' problems, say, restricting to the problems in mechanics of solids/fluids arising in engineering applications. The complexity of molecular interactions and numerical computations, and some exclusive benefits of exact solutions, still motivates one to simplify, or even solve, the discrete, or discretized problems, with less computation than that needed for a `direct numerical solution'. From an atomistic viewpoint, many features of molecular dynamics framework for crystalline solids rely on lattice dynamics. It is useful to consider `linearized' regime with nearest-neighbors as dominant on the lines of `discretized' linear theory of elasto-dynamics and, therefore, in a sense the continuum limit is still chased. With this backdrop, in the title, the word `simple' can be substituted with the phrase — numerically rather `easy' and linear algebraic, and `complex' can be replaced by — analytically `not simple' while carrying a warning `handle with care'!


Partially motivated by classical results and techniques in solving the problem of scattering of waves by edges such as crack-tips, I will discuss the example of discrete `simple' problem of lattice dynamics in steady state associated with scattering of time harmonic waves due to `sharp' crack-tip. First the case of scalar problem on two-dimensional lattice, associated with an out-of-plane displacement (ref. anti-plane shear in elasticity), and then the vectorial problem associated with in-plane displacement (ref. plane problems in elasticity) with dynamic mode I/II loading. The former prepares the groundwork for the latter, but the two problems differ considerably in the difficulty of treatment. If time permits, I will show some relevance of the results for lattice models to tight-binding models in solid state physics, as well as a glimpse of what transpires in the presence of randomness and from the viewpoint of inverse problems associated with structure identification.

ABOUT THE SPEAKER

Prof. Basant Lal Sharma received Bachelor of Technology in Mechanical Engineering from the Indian Institute of Technology Bombay, Powai, Mumbai, India in 1999. In 2004 he received Ph.D. in Mechanics (P. Rosakis) from the Cornell University, Ithaca, NY, USA. After post-doctoral positions at Cornell University (S.H. Strogatz) and École Polytechnique, Palaiseau, Paris, France (L. Truskinovsky), he joined the Department of Mechanical Engineering, Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh, India in January 2007 as a Faculty member. He is interested in studying physical phenomena that occur due to the presence of small length scales, for example, the structure and dynamics of defects in crystals.



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