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Wave Motions Along Lattices with Nonlinear On-Site and Inter-Site Potentials. Cooperation and/or Competition Leading to Lattice Solitons and/or Discrete Breathers.

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Coupling the Einstein and the Debye wave harmonic models of a crystalline solid offers the opportunity of studying, in fact, the full quantum solid state physics. Just for illustration this includes data on the specific heats and experimentally observed features of electron transport when an excess free electron is added, provided the latter's evolution is guided by the quantum Schödinger equation, e.g., in the tight binding approximation. Not much is known when the above mentioned harmonic potentials are replaced by nonlinear ones, like a cubic or a quartic interaction (so-called FPU models), the popular textbook Lennard-Jones potential or the empirically obtained Morse potential. This is the situation addressed in this communication, save that before we tackle the problem of adding an excess electron we wish to explore the rich wave phenomenology offered by the pure classical lattice dynamics. In a subsequent work we shall explore the dynamics of the mixed classical-quantum (lattice-electron) problem at high enough temperatures so that the classical description of the lattice dynamics is enough and significant for the understanding of, e.g., supersonic lattice soliton-assisted transport. This includes for instance electron or energy storing and transport along some polymers, DNA and other bio-molecules [1-6].
Our problem is defined by the following Hamiltonian:

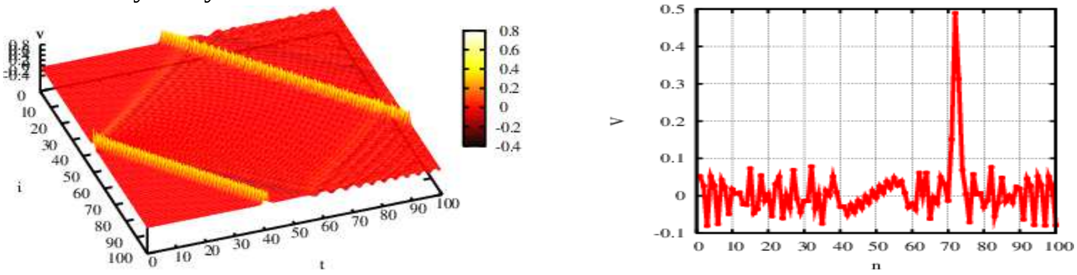
$$H = H_{inter} + H_{onsite} = \sum_i \left(\frac{m v_i^2}{2} + U_{inter}(x_{i+1} - x_i) \right) + \sum_i U_{onsite}(x_i)$$

from where the equations of motion follow with $q_i = b(x_i - i\sigma)$ and σ the inter-unit equilibrium distance:

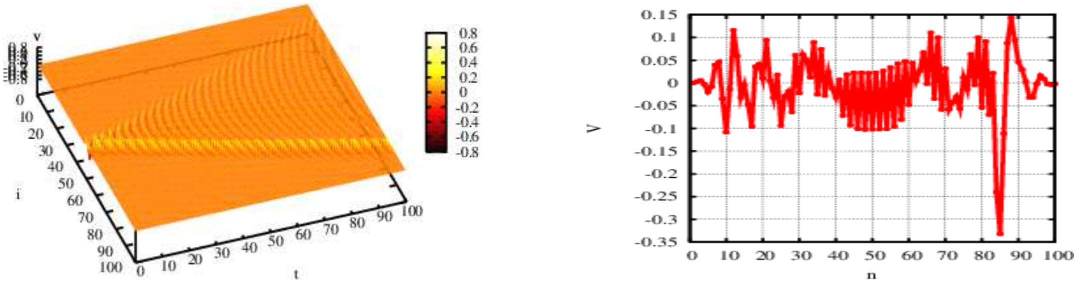
$$\frac{d^2 q_n}{dt^2} + [(\frac{\partial U^M_{inter}}{\partial r})|_{r=|q_{n+1}-q_n|} - (\frac{\partial U^M_{inter}}{\partial r})|_{r=|q_n - q_{n-1}|}] + \frac{\partial}{\partial r} U^M_{onsite}|_{r=q_n} = 0$$

Both potentials are of the Morse type but with different stiffnesses and well depths (aka dissociation energies): $U^M = D\left(e^{-2br} - 2e^{-br}\right)$. The ratios $\eta_b = \frac{b_{onsite}}{b}$ and $\eta_D = \frac{D_{onsite}}{D}$ are the parameters offering the possibility of analyzing the possible cooperation or competition between on-site and inter-site Morse potentials $(b,D)=(b,D)_{inter}$. The characteristic equilibrium distances for both potentials are supposed to be equal for simplicity ($\sigma_{onsite} = \sigma_{inter} = \sigma$). The figures depict some of the results found. On the left panel we show the space-time trajectory of an excited wave lattice disturbance, $v_i(t)$, whereas on the right panel v_i is plotted along the lattice at time 100, in units of the inverse (linear) Morse frequency ω_M^{-1}. The wave is excited by providing an initial momentum (velocity) in one of the sites like $v_{50}(t=0)=1$, in units of the sound velocity. Sequentially we have the following illustrative cases (with periodic boundary conditions and appropriate initial conditions given):

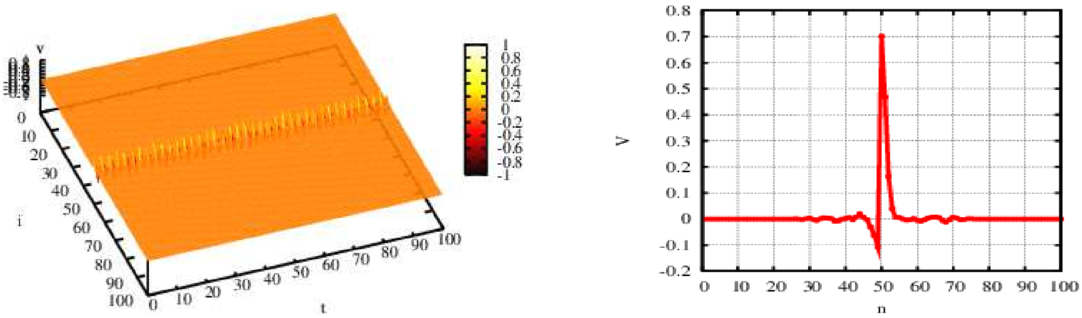
a) η_D=0, η_b=2. The panels depict a *supersonic* lattice soliton-like wave fostered by the action of only Debye inter-site interactions/oscillators:



b) η_D=1, η_b=2. The panels show that the Einstein on-site oscillators perturb the Debye oscillators in such a way that there is tendency to sweeping from a soliton-like wave (still dominating the process as illustrated in the right panel) to discrete breather-type of *subsonic* excitation, not yet exhibiting the time periodicity so characteristic of the latter.



c) η_D=4, η_b=8. The panels show that upon significantly increasing the stiffness ratio the Einstein on-site oscillators tend to suppress the soliton-like excitations fostered by the Debye oscillators thus benefiting pinned, hence immobile discrete breather-like excitations.



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