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DISSIPATIVE SOLITONS AND COMPLEX CURRENTS IN ACTIVE LATTICES

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We first summarize features of free, forced and stochastic harmonic oscillations and, following an idea first proposed by Lord Rayleigh in 1883, we discuss the possibility of maintaining them in the presence of dissipation. We describe how phonons appear in a harmonic (linear) lattice and then use the Toda exponential interaction to illustrate solitonic excitations (cnoidal waves) in a one-dimensional nonlinear lattice. We discuss properties such as specific heat (at constant length/volume) and the dynamic structure factor, both over a broad range of temperature values. By considering the interacting Toda particles to be Brownian units capable of pumping energy from a surrounding heat bath taken as a reservoir we show that solitons can be excited and sustained in the presence of dissipation. Thus the original Toda lattice is converted into an *active* lattice using Lord Rayleigh's method. Finally, by endowing the Toda–Brownian particles with electric charge (i.e. making them positive ions) and adding free electrons to the system we study the electric currents that arise. We show that, following instability of the base linear Ohm(Drude) conduction state, the active electric Toda lattice is able to maintain a form of high-T supercurrent, whose characteristics we then discuss.

Keywords: Dissipative solitons; anharmonicity; lattices; superconductivity.

1. Introduction

The soliton concept, and the coinage of the word soliton, originates from the work of Zabusky and Kruskal [1965]. They dealt with the dynamics of one-dimensional (1D) anharmonic lattices and their (quasi)continuum approximation [Christov *et al.*, 1996], provided by the Boussinesq–Korteweg-de Vries equation [Boussinesq, 1877; Korteweg & de Vries, 1895]. That work was built on research done by Fermi *et al.* [1965] who tried to understand equipartition in a lattice by adding anharmonic forces. They used 1D lattices with 16, 32 and 64 units interacting with springs obeying x^2 and x^3 anharmonic forces and another described by a nonlinear but "piecewise linear" function. The force proportional to displacement or elongation (x) follows Hooke's law and defines the realm of linear oscillations (harmonic in Fourier space), phonons in the corresponding lattice [Kittel, 1995]. Also worth mentioning are the significant achievements of Visscher and collaborators using the Lennard–Jones potential [Payton III *et al.*, 1967] who, while trying to understand heat transfer, explored the role of anharmonicity and of impurities (doping a given lattice with different masses, thus generating isotopically disordered lattices). More recently, Heeger, Schrieffer and collaborators have used solitons to explain the electric conductivity of polymers [Heeger *et al.*, 1988]. We also wish to highlight the work done by Toda on the lattice (he invented) with a peculiar exponential interaction (Fig. 1). It was the first (1967) many-body problem exactly solved [Toda, 1989a, 1989b].

(N.B: We make no claim of completeness in the list of references offered here. For a thorough, albeit now a bit old, review of solitons in condensed matter see [Bishop *et al.*, 1980]; for an in-depth discussion of heat transfer see [Toda, 1979]; see also [Scott *et al.*, 1973; Ben Jacob & Imry, 1978; Brazovskii *et al.*, 1982; Christiansen & Scott, 1983; Lee, 1987; Yu, 1988; Davydov, 1991; Zolotaryuk *et al.*, 1991; Scott, 2003]).

The Toda interaction yields the hard rod/sphere impulsive force in one limit (the perfect gas) while in another limit it becomes a harmonic oscillator (the ideal solid lattice crystal). Through a suitable Taylor expansion it provides the aforementioned x^2 and x^3 anharmonic forces beyond Hooke's law. Figure 1 illustrates Toda's interaction (with its exponential-repulsive and linear-attractive parts) relative to the Lennard–Jones and the Morse

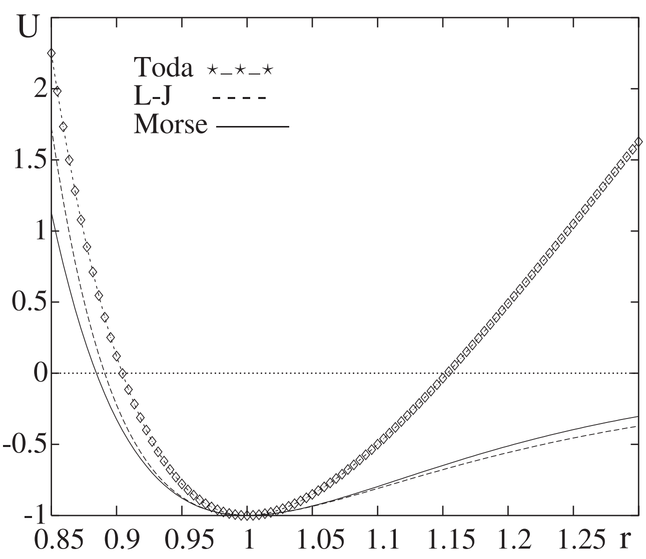

Fig. 1. Toda potential ($U = U^T = (a/b)[e^{-b\sigma(r-1)} - 1 + b\sigma(r-1)]$), Morse potential ($U = U^M = (a/2b)[(e^{-b\sigma(r-1)} - 1)^2 - 1]$) and Lennard–Jones potential ($U = U^{L-J} = U_0[(1/r^{12}) - (1/r^6) - 1]$). In order to have all the three minima of the potential functions at the same location $(1, -1)$ we have suitably adjusted the free parameters with the basic frequency the same; $r = R/\sigma$. It clearly appears that Toda's interaction captures well the repulsive core whereas its attractive part becomes unphysical for large values of the displacement. Due to the use of exponentials both the Toda and the Morse potentials are easily implemented with present-day electronics.

interaction. As the latter is a combination of exponentials, both Toda's and Morse's interactions are easy to implement electronically; a mechanic–electric analogy has also been fruitfully exploited by researchers [Remoissenet, 1999; Toda, 1989b; Makarov *et al.*, 2000; Makarov *et al.*, 2001; del Rio *et al.*, 2003].

The concept of *dissipative* solitons extends the classical theory to nonconservative systems where energy (rather than being conserved) is pumped and dissipated in an appropriate balance, thus exciting and, eventually, maintaining past an instability threshold the localized structure (or a periodic nonlinear wave [Chu & Velarde, 1991; Nekorkin & Velarde, 1994; Christov & Velarde, 1994, 1995; Nepomnyashchy *et al.*, 2002; Nekorkin & Velarde, 2002; Velarde, 2004]). The concept of *dissipative* solitons is also the natural generalization of maintained *dissipative* linear waves with an underlying *dissipative* harmonic oscillator as a dynamical system [Velarde & Chu, 1988; Chu & Velarde, 1989].

We stick in this text entirely to one-dimensional (1D-)systems and study them in classical (not quantum) mechanics. Although we are aware of limitations and peculiarities of 1D systems yet we believe much can be understood about the physics of problems if their 1D caricature is appropriately handled before embarking on more realistic systems. Besides there is a tradition in physics about exploring results with models that can be worked out to a great depth [Bernasconi & Schneider, 1981; Mattis, 1993]. About the interest of the quantum mechanics study of our system we comment in the last section of the text.

In the study of (nonlinear) lattices it is of great interest to elucidate the consequences on the excitation spectra of coupling a finite system to a heat bath, clustering, phase-transition-like diagrams, etc. 1D-lattices with Morse interactions with few particles ($N \leq 4$) have been thoroughly analyzed. As here we are not interested in equilibrium features we refer the reader to a few recent publications on this subject where further references can be found [Chetverikov *et al.*, 2005; Ebeling & Sokolov, 2005].

The (collective) behavior of a (linear, 1D) lattice with springs obeying Hooke's law is best expressed by the Fourier analysis of its dynamics and, hence, by transferring from the "real" space (x, t, say) to Fourier space using harmonic modes/phonons (quantized lattice vibrations). The latter quantities (or new "degrees of freedom" alternative to positions and momenta) allow a more transparent understanding of the evolution (and the physics) of the problem. This was cleverly seen by Einstein, Debye, Born and other great predecessors. We recall the basics of phonons in Sec. 3. Earlier in Sec. 2 we provide a summary of results about (free) harmonic oscillations as well as driven, forced and stochastic harmonic oscillations, to prepare the subsequent study of the evolution of a Toda lattice coupled to a heat bath (noise) with added driving forces. Hence we shall be discussing here the basic elements underlying the evolution of a driven-dissipative generalized Toda lattice. Then in Sec. 4 we recall how solitons (and nonlinear periodic cnoidal waves) appear in a Toda lattice, and a few other results needed in the subsequent sections of this text. Section 5 is devoted to a description of a first generalization of Toda's lattice by adding an energy pumping-dissipation balance. In Sec. 6 we discuss equilibrium properties of our generalized Toda lattice, including its specific heat at constant length/volume and the temperature evolution of the dynamic structure factor of the system. In Secs. 7 and 8 we add electric charges and we discuss the complex currents that our generalized driven-dissipative Toda lattice can exhibit in the presence of an external electric field. In particular, we discuss the recent intriguing discovery [Velarde *et al.*, 2005] about the onset and eventual sustainment of electron–soliton dynamic bound states (solectron), and the "truth and consequences" that follow: a form of (purely classical) "high"-temperature supercurrent in a transition past a well defined threshold from the linear (Ohm–Drude) conduction state. Section 9 provides conclusions and suggestions for future research.

2. A Single Unit/Oscillator-Free Harmonic Oscillations versus Driven, Forced and Stochastic Harmonic Oscillations

The harmonic oscillator described by the equation of motion

$$\frac{d^2}{dt^2}x(t) + \omega_0^2 x(t) = 0, \tag{1}$$

has the solution

$$x(t) = x_0 \cos(\omega_0 t + \delta), \tag{2}$$

whose amplitude, x_0, and phase δ, are determined by the initial conditions. This is a conservative system, as the total (mechanical) energy remains constant in time. Generally, viscous friction and other forms of dissipation, are present in working systems, and hence a term proportional to the velocity is added to Eq. (1). This damping term makes the origin ($x = \dot{x} = 0$) asymptotically stable. There are several ways to compensate dissipation and viscous friction and hence maintain the vibrations of an oscillator (1). To our knowledge the earliest scientist to propose a useful one was Lord Rayleigh [1945]. Back in 1883, he suggested augmenting Eq. (1) with a driving term of the following form

$$\frac{d}{dt}v(t) + \omega_0^2 x(t) = -\gamma(x, v)v, \tag{3}$$

with

$$\gamma(x, v) = -\gamma_1 + \gamma_2 v^2. \tag{4}$$

Three decades later, van der Pol proposed

$$\gamma(x, v) = -\gamma_1 + \gamma_2 \omega_0^2 x^2, \tag{5}$$

for modeling sustained oscillations in electronic devices. In both cases γ_1 and γ_2 are positive. (N.B. Underlying most models used to describe axonal action potential transmission, excitability and other features in neurodynamics, is the Rayleigh or van der Pol *active* friction force. On occasion such an *active* force is called *negative* friction if we denote by *positive* friction, a standard, passive, friction. Such a *negative* friction pumps rather than dissipates energy).

By multiplication of Eqs. (3) and (4) with the velocity v we find for the energy, $\epsilon = mv^2/2 + m\omega_0^2 x^2/2$,

$$\frac{d}{dt}\epsilon = m(\gamma_1 - \gamma_2 v^2)v^2. \tag{6}$$

It follows that the energy is changing unless

$$v^2 = v_0^2 = \frac{\gamma_1}{\gamma_2}, \tag{7}$$

hence, in an average sense, v_d is an attractor in the velocity space. Assuming that on average, equipartition of energy holds, we get for the energy $\epsilon_0 = mv_0^2$, with m denoting the mass of the particle undergoing the harmonic motion. The corresponding (approximate) displacement of a sustained oscillation is

$$x(t) = \frac{v_0}{\omega_0}\cos(\omega_0 t + \delta), \tag{8}$$

which yields an ellipse in the phase space. (N.B. When oscillations are maintained they are generally limit cycles of the corresponding dynamical system. In phase space, depending on parameter values, such a limit cycle may have a regular form, or it may appear as a drastically deformed curve, albeit topologically equivalent to the former.)

We may also maintain an oscillation by applying a periodic external force that balances the linear friction parameterized by γ_0,

$$\frac{d}{dt}v(t) + \omega_0^2 x(t) = \frac{F_0}{m}\cos(\omega t) - \gamma_0 v(t). \tag{9}$$

The displacement due to such forced oscillation is given by

$$x(t) = \frac{\frac{F_0}{m}}{\sqrt{(\omega^2 - \omega_0^2)^2 + 4\omega^2\gamma_0^2}}\cos(\omega_0 t + \delta). \tag{10}$$

Yet another approach to maintain an oscillation in the presence of damping is to couple the oscillator to a suitable heat bath [Gardiner, 2004]. Then Eq. (1) becomes the Langevin equation with linear friction

$$\frac{d}{dt}v(t) + \omega_0^2 x(t) = -\gamma_0 v(t) + \sqrt{2D}\xi(t), \tag{11}$$

where the stochastic forces $\sqrt{2D}\,\xi(t)$, which model the noise generated by the heat bath (Gaussian white noise), are characterized by

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t')\xi(t) \rangle = \delta(t' - t). \tag{12}$$

In Eqs. (9) and (11), the term γ_0 describes the friction between the particles and the heat bath. For a *passive* system the friction obeys Einstein's fluctuation-dissipation theorem

$$D = k_B T \gamma_0 m \tag{13}$$

where T accounts for the temperature of the heat bath (noise) and k_B is Boltzmann's constant.

In thermal equilibrium the system is described by the canonical distribution

$$\rho(x,\, v) = Z^{-1}\exp\left[-\frac{H}{k_B T}\right], \tag{14}$$

where H is the Hamiltonian and Z is the partition function of the system. Correspondingly, the mean energy is $\langle H \rangle = k_B T$. We may excite stochastic (thermal) oscillations by appropriately heating the system. Then, to study these oscillations in detail, we may quench the temperature to zero or some low value and study individual trajectories of the system.

The concepts of *active* Brownian motion, Brownian motors and ratchets are timely and of interest. Although here we use friction in a parameter range where it constitutes an *active* force for Brownian particles we are not interested in a detailed discussion of these issues and refer the reader to some recent publications [Klimontovich, 1986, 1994, 1995; Erdmann *et al.*, 2000; Schweitzer, 2003; Ebeling & Sokolov, 2005].

3. Phonons — Elementary Excitations in Linear Lattices

Let us now consider a collection of coupled harmonic oscillators or better points linked by harmonic forces. In what follows we restrict consideration to nearest-neighbor interactions. In particular, let us assume a one-dimensional (1D) lattice with N units (each of mass m) connected by linear (Hooke) springs, with periodic boundary conditions. The particles are described by coordinates, $x_j(t)$, and velocities, $v_j(t)$, $j = 1, \ldots, N$, with

$$x_j + L = x_j. \tag{15}$$

(For a ring $x_{j+N} = x_j$.) Let σ be the interparticle equilibrium distance and the deviations from it $r_j = x_{j+1} - x_j - \sigma$. The potential energy stored in the ring is

$$U = \sum_{i=1}^{N} U_i(r_i), \tag{16}$$

where

$$U_i(r_i) = \frac{m}{2}\omega_0^2 r_i^2,$$

denotes the harmonic pair interaction potential. The evolution of the lattice follows Newton equations of motion

$$\frac{d}{dt}x_j = v_j, \tag{17}$$

$$m\frac{d}{dt}v_j = -\frac{\partial U}{\partial x_j}, \tag{18}$$

or, in another form, which extends (1) to the lattice case

$$\frac{d^2}{dt^2}x_j - \omega_0^2\,(x_{j+1} + x_{j-1} - 2x_j) = 0. \tag{19}$$

The solution of this system is obtained using Fourier modes

$$x_j^{(n)}(t) = x_j^{(n)}(0) + A^{(n)}\cos(\omega_n t - k_n j\sigma), \tag{20}$$

where $x_j^{(0)}$ denotes the equilibrium positions. We have dropped an arbitrary phase. The corresponding accelerations are

$$a_j^{(n)}(t) = -A^{(n)}\omega_n^2\cos(\omega_n t - k_n j\sigma). \tag{21}$$

There exist N different excitations corresponding to different wave lengths and wave numbers

$$-\frac{N}{2} < n \leq +\frac{N}{2}, \quad \text{for } N \text{ even}, \tag{22}$$

and

$$-\frac{(N-1)}{2} \leq n \leq +\frac{(N-1)}{2}, \quad \text{for } N \text{ odd},$$

or wave "vectors" $k_n = 2\pi n/N\sigma$,

$$-\frac{\pi}{\sigma} < k_n \leq \frac{\pi}{\sigma}, \quad \text{for } N \text{ even}, \tag{23}$$

and

$$-\frac{(N-1)}{N}\frac{\pi}{\sigma} \leq k_n \leq \frac{(N-1)}{N}\frac{\pi}{\sigma}, \quad \text{for } N \text{ odd}.$$

This is the so-called Brillouin zone [Kittel, 1995]. Note that k-values $k \pm 2\pi j/\sigma$ $(j = 1, 2, 3, \ldots)$ are equivalent due to the periodicity of the $\cos(x)$.

The spectrum of eigenfrequencies corresponding to the phonons is

$$\omega_n = 2\omega_0 \left| \sin\left(\frac{\sigma}{2}k_n\right) \right|, \tag{24}$$

for the "acoustical" branch. The frequency increases with the k-value. There might be also an "optical" branch for lattices with different masses or different spring constants. Here we restrict ourselves to the case of masses and spring constants, all equal, hence the simplest case.

4. Solitons and Cnoidal Waves — Excitations in Nonlinear Lattices

Let us consider a 1D lattice but now with Toda interactions between nearest-neighbor units (Fig. 1). Thus we replace Hooke's law by the force corresponding to

$$U_i^T(r_i) = \frac{a}{b}[\exp(-br_i) - 1 + br_i]. \tag{25}$$

The relative mutual displacement between the mass i and the mass $i+1$ is $r_i = x_{i+1} - x_i - \sigma$. Then (in the infinite case) there is an exact solution of the corresponding dynamical system (the system is integrable), as found by Toda [1989a, 1989b]. Note that if we expand (25) in a Taylor series

$$U^T(r) = \frac{ab}{2}\left(r^2 - \frac{b}{3}r^3 + \cdots\right), \tag{26}$$

for low values of the displacements, r_i, from equilibrium positions we recover, at lowest-order, the harmonic oscillator. Subsequent terms in the series (r^3, r^4) reproduce the earlier mentioned interactions used by Fermi, Pasta and Ulam, that, save an external, periodic, forcing term, define the (asymmetric nonlinear) Helmholtz oscillator [del Rio *et al.*, 1992] and the (symmetric nonlinear) Duffing oscillator, respectively. The former is the dynamical system underlying the Boussinesq–Korteweg-de Vries equation analyzed by Zabusky and Kruskal [1965]. The latter is the widely used approximation [Choquard, 1967; Payton III, 1967; Kittel, 1995] to account for thermal expansion and heat transfer in the simplest model of a crystalline lattice solid (recall that phonons in the linear case are "independent" degrees of freedom). We see from the expansion (26) that in the Toda potential the parameter ab controls the basic oscillation frequency and the parameter ab^2 controls the anharmonicity of the forces acting between the particles hence b can be interpreted as the stiffness parameter of the springs. Clearly, in an appropriate limit case the Toda lattice possesses solutions in the form of phonons. However, we are interested in the new (nonlinear) exact solutions found by Toda, i.e. solitons and (periodic) cnoidal waves which are for the Toda lattice the new "degrees of freedom". The uniform infinite Toda lattice possesses soliton-type solutions that represent stable local lattice excitations (compression–expansion). They generate local energy spots which run along the lattice. For a uniform lattice $b_n = b$, $(-\infty < n < \infty)$ the exact solutions found by Toda are the cnoidal waves (Fig. 2)

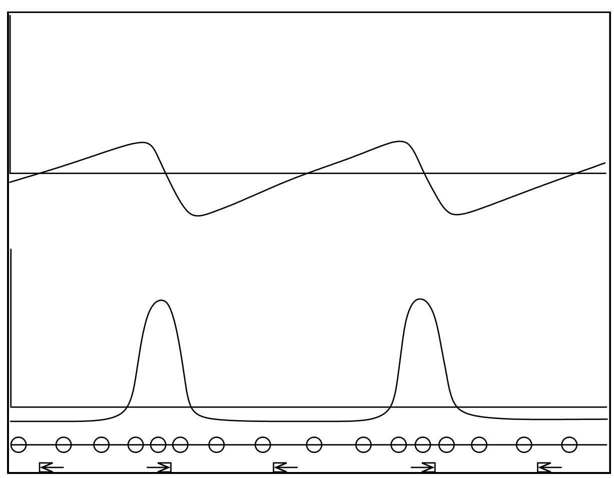

Fig. 2. Toda lattice. Lattice compressions (bottom) create solitons (pulse-like disturbances, solitary waves or periodic cnoidal wave peaks) and momentum distribution along the lattice (top). Note that taking into account the velocity sign (left to right motion) the former is the derivative (with negative sign) of the latter.

$$\exp(-br_n) - 1 = m\frac{(2K\nu)^2}{ab}\left(dn^2\left[2\left(\nu t \pm \frac{n}{\lambda}\right)K\right] - \frac{E(k)}{K(k)}\right), \tag{27}$$

where the wavelength λ and the frequency ν are related by the dispersion relation

$$\nu(\lambda) = \frac{\sqrt{\frac{ab}{m}}}{2K(k)\sqrt{sn^{-2}\left(\frac{2K(k)}{\lambda}\right) - 1 + \frac{E(k)}{K(k)}}}. \tag{28}$$

Here $sn(u)$ and $dn(u)$ are elliptic functions with modulus k ($0 < k \leq 1$) [Abramowitz & Stegun, 1965; Toda, 1989a]. (For simplicity we assume here units with $\sigma = 1$.) The complete elliptic integrals $K(k)$ and $E(k)$ are defined by

$$K(k) = \int_0^{\pi/2} \frac{d\Theta}{\sqrt{1 - k^2 \sin^2 \Theta}}, \tag{29}$$

$$E(k) = \int_0^{\pi/2} d\Theta \sqrt{1 - k^2 \sin^2 \Theta}\,. \tag{30}$$

By adjusting appropriately the periodic boundary conditions for the N particles we find N normal modes, which are the nonlinear generalizations of the phonon modes.

The wave profile and dispersion of cnoidal waves in the Toda lattice are similar to those of harmonic (sinusoidal) waves in a linear lattice when the modulus k is not close to unity. Indeed when the modulus is close to zero (small values of the displacement) we get $E/K \simeq 1 - k^2/2$ and

$$r_n \simeq -\frac{\pi^2\nu^2k^2}{2ab^2}\cos 2\pi\left(\nu t \pm \frac{n}{\lambda}\right). \tag{31}$$

In the limit $k \to 1$, the cnoidal wave approaches a sequence of equally spaced delta-functions. For $\lambda \approx K \to \infty (k \to 1)$ the result is a solitary wave

$$\exp(-b(r_{n+1} - r_n)) = 1 + \sinh^2(\chi)\,\mathrm{sech}^2\left(\chi n - \frac{t}{\tau}\right). \tag{32}$$

These solitonic excitations correspond to local compressions of the lattice with the characteristic compression time

$$\tau_{\mathrm{sol}} = (\omega \sinh \chi)^{-1}, \tag{33}$$

and with the spatial "width" χ^{-1}. This quantity is connected with the energy of the soliton by

$$\epsilon_{\mathrm{sol}} = 2\frac{a}{b}(\sinh\chi\cosh\chi - \chi), \tag{34}$$

with σ taken as the unit of length. The soliton velocity is given by

$$v_{\mathrm{sol}} = \sigma\sqrt{\frac{ab}{m}}\frac{\sinh\chi}{\chi}, \tag{35}$$

which is supersonic as the sound velocity in the corresponding linear lattice is $\sqrt{ab/m}$, both velocities given in common appropriate units [$\omega_0\sigma = \sigma\sqrt{ab/m}$, $\sigma = 1$ and even $\omega_0 = 1$ in most of the text]. Figure 2 illustrates how compressions create the solitonic peaks and the wave motion along the Toda lattice.

Let us emphasize that we have discussed a conservative, Hamiltonian, integrable system and hence the soliton energy is determined only by the initial conditions. In this sense, like for harmonic oscillations obeying Eq. (1), a soliton in such a conservative lattice could live forever. If, however, dissipation appears, then for solitons (solitary waves or periodic cnoidal waves) we are faced with a similar problem to that faced by Lord Rayleigh for harmonic oscillations. Accordingly, in the next section we describe how to maintain solitons (or periodic nonlinear waves) with an appropriate *active* friction force.

(N.B: A few basic facts and warnings are worth recalling. A linear (harmonic) lattice obeying Hooke's law has no thermal expansion. A hard rod/sphere gas has the thermal expansion of Boyle's ideal gas. A (uniform, monoatomic) harmonic lattice cannot maintain a temperature gradient. Hence, heat transfer according to Fourier's law does not apply to a uniform harmonic lattice as such heat transfer is proportional to the temperature difference between the two ends of the lattice. In other words, the thermal conductivity (heat flux divided by the internal temperature gradient) diverges because the gradient vanishes. However, in an isotopically disordered lattice an internal temperature gradient is possible. The Toda lattice (with the full exponential interaction) also has a divergent thermal conductivity since an internal temperature gradient cannot be maintained due to solitons (independent degrees of freedom) which run free in the lattice. However a lattice with truncated exponential interaction, Eq. (26), at e.g. quartic order, or a lattice with Lennard–Jones interaction does have finite thermal conductivity as both interaction models allow an internal temperature gradient to be established.)

5. Active Toda Lattice

The natural extension of the arguments presented in Sec. 2 for harmonic oscillations with the aim of driving, forcing and hence maintaining nonlinear oscillations in a Toda lattice leads to the following Langevin equations

$$\frac{d}{dt}x_i = v_i, \tag{36}$$

$$m\frac{d}{dt}v_i + \frac{\partial U}{\partial x_i} = K_i(t) + F_i(v_i) + m\sqrt{2D}\,\xi_i(t),$$

governing the evolution of the ith particle on the lattice. Here the stochastic forces are characterized by zero mean and delta-correlated

$$\langle \xi_i(t)\rangle = 0$$
$$\langle \xi_i(t)\xi_j(t)\rangle = \delta_{ij}\delta(t'-t).$$

We have added a time-dependent force, $K_i(t)$, whose value is in general zero except at the boundaries. This term could mimick a (mechanical) external forcing acting on the boundary element "1" (and "N") by periodically introducing e.g. a piezoelectric perturbation.

In order to define the "dissipative" force, including its *active* component, following Lord Rayleigh, Eq. (3), for later convenience, we define a velocity-dependent friction function by

$$F(v) = F_0(v) + F_a(v) = -m\,\gamma(v)\,v, \tag{37}$$

with

$$\gamma(v) = \gamma_0 + \gamma_a(v). \tag{38}$$

Here the first term, γ_0, describes the standard friction between the particles and the surrounding heat bath. For this *passive* friction we assume the validity of the Einstein fluctuation-dissipation theorem. However, for simplicity we assume that the *active* (nonequilibrium) part of the friction force, γ_a, does not fluctuate. [N.B. A discussion of nonlinear systems, where the fluctuation-dissipation theorem differs from the simple Einstein relation can be found in [Klimontovich, 1986, 1994, 1995].]

The balance for the total energy is

$$\frac{d\epsilon}{dt} = -m\gamma_0\sum_i v_i^2 - m\sum_i \gamma_a(v_i)v_i^2 + m\sqrt{2D}\sum_i v_i\xi_i. \tag{39}$$

Since $\gamma_0 > 0$, the sign of the active term, $\gamma_a(v)$, is crucial for the energy balance of our lattice. As earlier noted this contribution to the friction function may describe *active* forces which, due to their energy pumping effect, can drive the system away from equilibrium. Sticking to Lord Rayleigh's law, we set

$$F_a(v) = -m\gamma_a(v)v = -m(-\hat{\gamma}_1 + \gamma_2 v^2)v; \quad \hat{\gamma}_1,\ \gamma_2 > 0, \tag{40}$$

and hence, for $\hat{\gamma}_1 > \gamma_0$, we rewrite the complete dissipative force as

$$F(v) = m\gamma_0\left(\mu - \frac{v^2}{v_d^2}\right)v, \tag{41}$$

with

$$\mu = \frac{\hat{\gamma}_1 - \gamma_0}{\gamma_0}, \quad v_d^2 = \frac{\gamma_0}{\gamma_2}. \tag{42}$$

We may use instead of the Rayleigh law a more refined law for the dissipative force by introducing the expression

$$\gamma_1 = -\gamma_0\frac{\delta}{1 + \dfrac{v^2}{\hat{v}_d^2}}. \tag{43}$$

Then the total friction force acting on a particle may be represented as

$$F(v) = -m\gamma_0\left[1 - \frac{\delta}{1 + \dfrac{v^2}{\hat{v}_d^2}}\right]v. \tag{44}$$

Note that (44) yields (41) for low velocity values when we replace $(\delta - 1)$ by μ and $\hat{v}_d^2$ by δv_d^2. For simplicity, in the following we restrict consideration to the parameter values $v_d = 1$ and $\hat{v}_d = 1$.

There is a general setting, of particular interest to problems in bioenergetics, where we could place in context Lord Rayleigh's *active* (friction) force [Schweitzer, 2003; Ebeling & Sokolov, 2005]. Let us consider that the units are capable of extracting energy from the heat bath (in more general terms from the environment) with $q(t)$ being the energy flux into the unit's internal depot. The latter could be assumed to have internal dissipation that in the simplest case can be taken proportional to the instantaneous value of the energy, $e(t)$, with a constant rate of energy loss, c. Then the units can be assumed to be capable of transforming the stored (internal) energy into motion (kinetic energy). Let this process be described by a velocity-dependent rate, $d(v)$. A simple form could be dv^2 with d constant. Consequently, we can write the energy balance for the depot

$$\frac{d}{dt}e(t) = q(t) - ce(t) - d(v)e(t). \tag{45}$$

If $d = 0$, then the solution is

$$e(t) = e(0) + \int_0^t d\tau e^{-c\tau} q(\tau), \tag{46}$$

which shows a depot whose contents depends on history as it is being filled. The simplest case would be a steady depot $de/dt = 0$, which is a case of "fast" adaptation. Assume now that $q(t) = q_0 = \text{const.}$ Then the energy balance at the steady state yields

$$e_0 = \frac{q_0}{c + dv^2}. \tag{47}$$

Then in the spirit of Lord Rayleigh's proposal we can set

$$\gamma(v) = \gamma_0 - de_0 = \gamma_0 - \frac{q_0 d}{c + dv^2}. \tag{48}$$

When the friction, Eq. (48), vanishes

$$v^2 = v_0^2 = \frac{q_0}{\gamma_0} - \frac{c}{d}, \tag{49}$$

and hence we can rewrite the friction force as Eq. (44).

Figure 3 illustrates how Rayleigh's model and the depot model account for the *active* part. Slow particles tend to accelerate while the motion of faster particles is slowed down. Rayleigh's function diverges for large values of the velocity ($v > v_d$) whereas the depot model saturates and remains bounded accounting for the standard friction of the Brownian particle with the heat bath.

The parameters μ and δ control the conversion of the energy taken up from the external field, the reservoir, or the heat bath, into kinetic energy. They are, one or the other, the bifurcation parameters of our model. The values $\mu = -1$ and $\delta = 0$ correspond to equilibrium, the region $-1 < \mu < 0$ or $0 < \delta < 1$ stand for nonlinear *passive* friction and $\mu > 0$ or $\delta > 1$, respectively, correspond to *active* friction force. The bifurcation from one to the other regime occurs at $\mu = 0$ or $\delta = 1$, respectively. For the *passive* regime the friction force vanishes at $v = 0$ which is the only attractor of the deterministic motion, i.e. without noise all particles come to rest at $v = 0$. For the *active* case the point $v = 0$ becomes unstable but we have now two additional zeros at

$$v = \pm v_0, \quad v_0 = \hat{v}_d\sqrt{\delta - 1} = \sqrt{\delta - 1}, \quad \text{as } \hat{v}_d = 1$$
$$\text{or} \quad v_0 = v_d\sqrt{\mu} = \sqrt{\mu}, \quad \text{as } v_d = 1. \tag{50}$$

The two velocities, $\pm v_0$, are the new "attractors" of the free deterministic motion. In Fig. 4 we have plotted the friction force for the *passive* and for the *active* cases. Typical for the active case is the existence of three zeros of the total friction function.

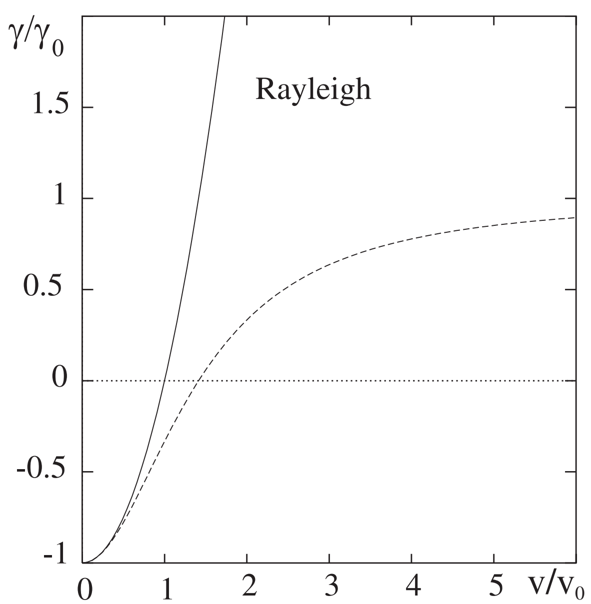

Fig. 3. Friction forces. Rayleigh model $((\gamma(v)/\gamma_0) = -(\mu - (v^2/v_d^2)) = \mu - v^2$, as $v_d = 1)$ and energy depot model $((\gamma(v)/\gamma_0) = 1 - (\delta/(1+v^2/\hat{v}_d^2)) = 1 - (\delta/1+v^2)$, as $\hat{v}_d = 1)$. Parameter values: $\mu = \delta - 1 = 1$. The *active* friction force occurs when γ/γ_0 is negative.

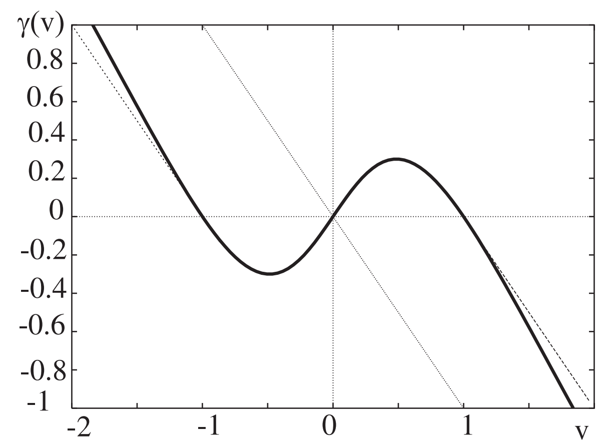

Fig. 4. Force (in ordinate) acting on a particle as a function of its velocity: *passive* case (solid straight line crossing the origin with slope (-1)); *active* case (solid sigmoidal line crossing the origin with positive slope). The curve is reminiscent of a stick-slip law. Units: abcissa, v_0; ordinate, γ_0.

The figure includes the representation of a piecewise linear approximation of the friction force (depot model $\delta = 2$).

We look for a description with universality using dimensionless equations through appropriate choice of scales. A natural choice corresponds to the unit system where $m = 1$, $\sigma = 1$, and $\omega_0 = 1$ holds. The first two assumptions correspond to fixing unit mass and unit length, whereas the third gives a characteristic unit time. In Fig. 5 we show the result of a numerical integration of a lattice without forcing but with *active* friction force. The Toda particles are moving clockwise, the excited soliton is moving counter-clockwise (illustrated by the dotted line). Further, we show in Fig. 6 trajectories for a lattice with purely *passive* (linear) friction $\gamma_0 = 0.0015$ but with external (forced) excitation of the first and the last mass on the chain. We used rectangular pulses. The period was chosen in such a way that the pulse hits the soliton at each trip around. The time delay between the hits on the Nth and the first mass (we could also say the first and the second particles) was chosen as σ/v_{sol}. Figure 6 shows ten trajectories in a reference frame where the lattice is, on average, at rest. We see nonlinear periodic oscillations of the lattice and nicely developed solitons where the tangent (dashed line) gives the soliton velocity.

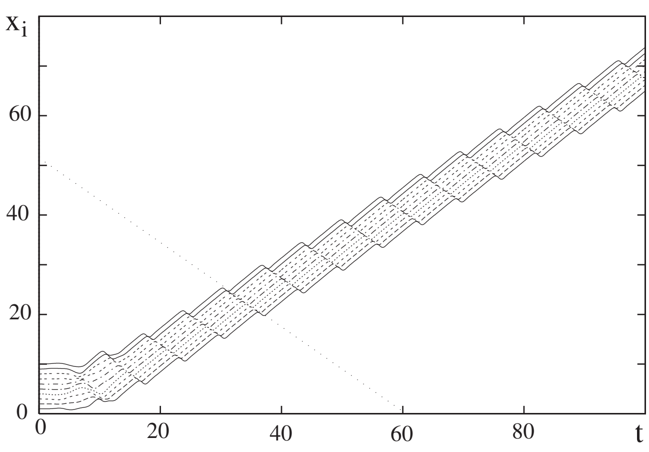

Fig. 5. Active Toda lattice. Trajectories (x, t) of ten particles with added *active* Rayleigh friction force. Solitons (cnoidal waves) appear traveling (dotted line) along the lattice in the opposite direction as the mean motions of the lattice particles. The single soliton appearing in the lattice was obtained by suitably playing with different mean values of randomly distributed initial velocities of the particles. The soliton velocity is given by the slope of the dotted line. Parameter values: $\omega_0 = 1$, $\sigma = 1$, $\gamma_0 = 0.8$, $\mu = 1$, $b = 1$, and $D = 0$.

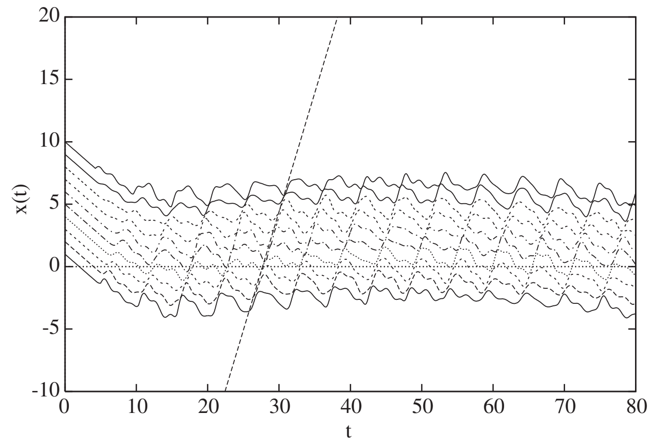

Fig. 6. Forced passive Toda lattice. Trajectories of ten particles (the lattice is at rest and hence vanishing mean velocity) and a soliton (dotted line) as in Fig. 5 excited by periodic pulses externally applied. One after another (with delay $\sigma/v_{\mathrm{sol}} = 2.2t_0$; $t_0 = (2\pi/\omega_0)$) two nearby particles are periodically (period $4t_0$) given an impulse of the same form, with duration $0.1t_0$, and amplitude 30 in units $m\sigma\omega_0^2$. Parameter values: $m = 1$, $\omega_0 = 1$, $\sigma = 1$, $b = 1$, $\gamma_0 = 0.0015$, and $D = 0$; time unit on the abscissa, $2\pi/\omega_0\sqrt{3}$.

6. Nonlinear Toda Lattice in a Heat Bath — Active Toda-Brownian Particles

Once the (nonlinear) Toda lattice is coupled to (or immersed in) a heat bath, let us study a few salient features of the influence of noise and only *passive* (linear) dissipation, both connected by Einstein's fluctuation-dissipation theorem [Toda & Saitoh, 1983]. We have a formally similar mathematical situation as in Sec. 3 with, however, U_i for an individual particle, being now given by (25) and the additional terms provided by (36). In equilibrium the particles are at rest positions separated by $\sigma(L = N\sigma)$. In view of (16) and (26) the angular frequency, ω_0, of oscillations around the equilibrium positions is

$$\omega_0 = \sqrt{\frac{ab}{m}}. \tag{51}$$

The evolution of the system follows the Langevin equations [cf. Eq. (11)]

$$\begin{aligned} \frac{d}{dt}x_i &= v_i, \\ m\frac{d}{dt}v_i + \frac{\partial U}{\partial x_i} &= -m\gamma_0 v_i + m\sqrt{2D}\,\xi_i(t), \end{aligned} \tag{52}$$

governing the ith particle on the lattice ring with

$$D = k_B T \gamma_0 m \tag{53}$$

where, once more, T is the temperature of the heat bath (Gaussian white noise). In thermal equilibrium the system is described by the canonical distribution [cf. Eq. (14)]

$$\rho(x_1, \ldots, x_N; v_1, \ldots, v_N) = Z^{-1} \exp\left[-\frac{H}{k_B T}\right], \tag{54}$$

with the Hamiltonian

$$H = \frac{m}{2} \sum v_i^2 + U(x_1, \ldots, x_N). \tag{55}$$

The partition function Z can be calculated exactly [Toda & Saitoh, 1983; Jenssen & Ebeling, 2000], and hence the free energy

$$F = -k_B T \log Z, \tag{56}$$

and all other thermodynamic functions are exactly known. They may also be determined by computing the internal energy ϵ from numerical simulations (dynamical experiments). The other functions follow from thermodynamic relations.

Figure 7 shows the specific heat at constant length/volume obtained from our simulations. The region where solitons are expected is around the temperature, $T_{\rm tr}$, where the specific heat ($C_v = 0.75 k_B$) shows a transition from $C_v \simeq k_B$ (corresponding to the *classical* phonon region) to $C_v \simeq k_B/2$ (corresponding to the hard sphere gas). Note that at low temperatures Toda's lattice cannot provide other than the classical phonon contribution (i.e. no T^3 power law near zero temperature is possible with the classical Toda lattice).

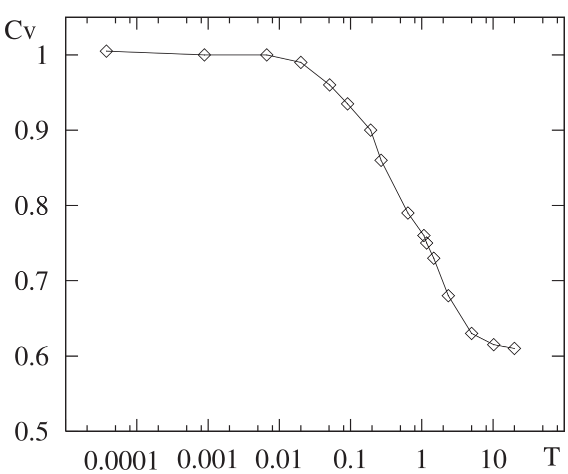

Fig. 7. Toda lattice. Semilogarithmic plot of the specific heat (in units of k_B) at constant volume/length as function of the temperature, T in units $k_{\rm B} T_{\rm tr} = 0.16 m\omega_0^2 \sigma / b$ ($C_v/k_B = 0.75$). For high temperature values the specific heat tends to $k_B/2$, the value for a perfect gas (hard rods). The region around $3k_B/4$, $T = 1$, is the transition region where phonons yield to solitons (cnoidal waves). Simulations were done with ten particles in the lattice. Parameter values: $m = 1$, $\omega_0 = 1$, $\sigma = 1$, $b = 200$, and $\gamma = 10^{-3}$.

Solitons can be observed by suitably heating the Toda lattice. Upon reaching the soliton region we quench the temperature down to zero and follow the evolution of the system. Figure 8 corresponds to such a quenching experiment in a Toda lattice with ten particles. Note that there are two solitons running clockwise and counterclockwise.

There exists another, much finer "microscope" for the observation of phonons and solitons. It is the (Van Hove) *dynamic* structure factor that gives the frequency spectrum of the correlations between density fluctuations of a given wave vector [Egelstaff, 1967; March & Tosi, 1976; Ebeling *et al.*, 2000a]

$$S(k, \omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp(-i\omega t) \langle \rho(k,t) \rho(-k,0) \rangle dt, \tag{57}$$

with

$$\rho(k, t) = \frac{1}{N} \sum_{l,m} \exp[-ik(x_l - x_m)]. \tag{58}$$

Actually, we are in the realm of the fluctuation-dissipation theorem. A measurement of the *dissipation* of energy by an external probe weakly coupled to a many-particle system is directly related

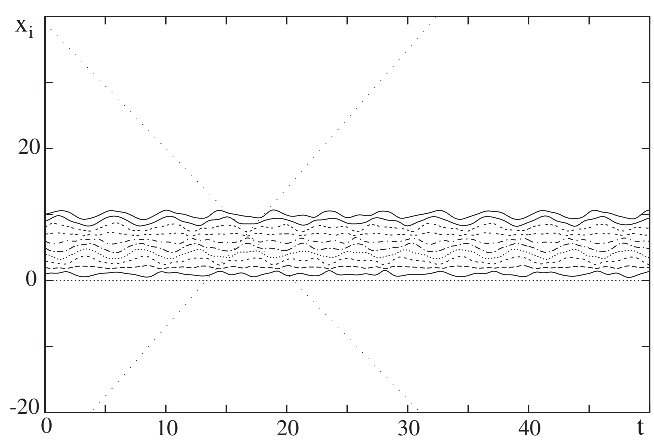

Fig. 8. Toda lattice. After bringing the Toda lattice with ten interacting particles to the transition region (Fig. 7) we quenched it down to zero temperature. We display the trajectories of the ten particles and two solitons (dotted lines) moving with equal velocities (in absolute value) but in opposite directions. Parameter values: $\omega_0 = 1$, $\gamma_0 = 0.0005$, initial temperature: $T_{\rm in} = 0.1 \approx T_{\rm tr}$.

to correlations between *equilibrium* fluctuations in the system. For a real solid the typical experiment is conducted with *thermal* neutrons ($4\,\mathring{A} = 5\,\text{meV} \approx 60\,\text{K}$). Here Fig. 9 illustrates the results. Figures 9(a)–9(d) show the structure factor of a Toda lattice ring for increasing values of the temperature. For simplicity we plot only the mode corresponding to the first phonon ($k_1 = 2\pi/N\sigma$)

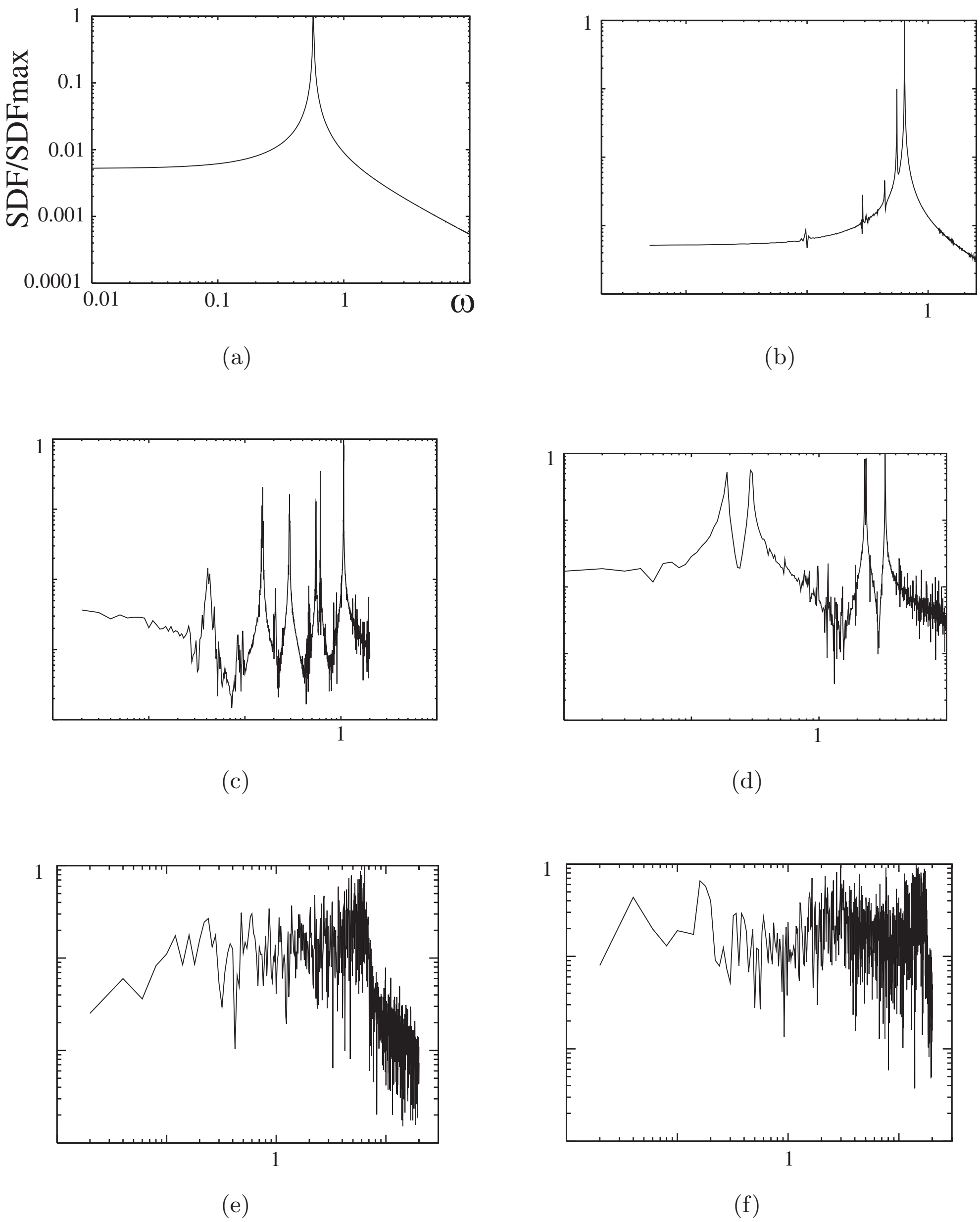

Fig. 9. Toda lattice. Dynamic structure factor of a Toda lattice with ten particles with increasing temperature (log–log plot): (a) ($T = 10^{-2}T_{\rm tr}$) Below the soliton region we have phonons. For simplicity only the *first* phonon in the spectrum ($\omega < 1$) is drawn. (b) ($T = 10^{-1}T_{\rm tr}$) With the increase of temperature the nonlinear phonon interaction leads to lower frequencies being excited. (c) ($T = T_{\rm tr}$) Further increasing the temperature, as the nonlinear interaction dominates the spectrum shows several solitons. The above mentioned *first* phonon evolves into a (supersonic) soliton. (d) ($T = 10T_{\rm tr} > T_{\rm tr}$) When the temperature is in the upper range of the soliton region the spectrum exhibits just solitons. For comparison, we have added (e) ($T = T_{\rm tr}$) and (f) ($T = 10T_{\rm tr} > T_{\rm tr}$) which are the counterparts for a lattice with Lennard–Jones interactions for equivalent temperatures of the cases (c) and (d). The spectrum shows noisy behavior because in that temperature range the solitons are not as stable as in the Toda lattice. For the temperatures in (a) and (b) the Lennard–Jones lattice exhibits identical behavior to the Toda ring. In each case considered, once the heating is done we allow the system to reach a well-defined chosen temperature. Then the structure factor is computed with the noise turned off. Parameter values : $m = 1$, $\sigma = 1$, $b = 100$, and $k_1 = 2\pi/N\sigma$; k_1 identifies the first phonon.

[Fig. 9(a)]. As we see in Fig. 9(b), for higher temperatures new low frequency peaks appear due to nonlinear interaction of deformed phonons. Figure 9(c) shows that when attaining temperatures around the transition (see Fig. 8) the first phonon becomes a soliton-like excitation (highest peak to the right) with velocity twice that of the phonon velocity, hence supersonic as the theory predicts. In Fig. 9(d) we see that beyond the transition temperature two high-frequency peaks appear corresponding to solitons with velocity much larger than the phonon velocity and a decreasing number of low frequency peaks. In Figs. 9(e)–9(f) we show, for comparison, the same situtation as in Figs. 9(c)–9(d) but for a Lennard–Jones interaction in the lattice (Fig. 1). We observe a much broader (noisy) spectrum than for a Toda ring; solitons in a Lennard–Jones ring appear less stable. At the lowest temperatures the dynamical structure factor is identical to that of the Toda lattice [Figs. 9(a) and 9(b)].

7. Electrically Conducting Active Lattices

Phonon excitations play a key role in conductivity phenomena [Kittel, 1995]. In order to estimate the possible role of soliton excitations in our Toda lattice system we shall stay at a purely *classical* level (no quantum effects) and, moreover, we shall disregard the possible feedback of "electrons" (the conducting elements) on the lattice particles (the "ions"). The first theory of conductivity (purely classical) in metals is due to Paul Drude (1900) [Kittel, 1995]. His "ansatz" was that the negative charges, the electrons, as well as the positive charges, the ions, feel a kind of friction that yields in an external field a stationary current. Since then the theory of conductivity has developed to a high level and it has been shown that many types of excitations such as phonons, polarons, excitons, solitons, etc. mediate electric conduction [Kittel, 1995; Heeger *et al.*, 1988; Yu, 1988; Davydov, 1991; Zolotaryuk *et al.*, 1991].

Let us see the role of our *dissipative* solitons in the active Toda lattice endowed with electric charges (ions and electrons) [Velarde *et al.*, 2005]. Hence let us consider now the Toda particles as ions (charge $+e$ and mass m_i; $m_i = m$) interacting with *free* electrons (charge $-e$ and mass $m_e \ll m_i$, $m_i \approx 10^3 m_e$; we expect no confusion concerning, the subscripts "e" and "i" which here refer to electrons and ions, respectively). Since the ions are rather densely packed what really matters is the repulsion if two ions come close together. If we approximate the repulsion of the ions by a simple exponential law (see Fig. 1) then the 1D ion system on a ring is equivalent to a 1D Toda lattice (25),

$$U(r_k) = \frac{m\omega_0^2}{b^2}\exp(-br_k). \tag{59}$$

($a/b = m\omega_0^2/b^2$, $\sigma = 1$). Figure 10 shows the potential acting on an ion in the lattice, if its two nearest neighbors are fixed at their equilibrium positions. For small displacements the ion moves in a harmonic potential and for increasing values of the displacement it feels at either side a stiff (exponential) repulsion. One of the free parameters is the oscillation frequency which might be fitted to some realistic value. The second parameter is the stiffness b which, in principle, is also free. Let us study the influence on the dynamics of the system and its eventual electric conductivity of the apparently minor deviation from the parabolic, harmonic potential shown in Fig. 10. We have checked, albeit not systematically, that adding a Coulomb repulsion between ions does not practically change the situation.

Let us place the N electrons at the positions y_j (thus having electroneutrality), free to move in the nonuniform and in general time-dependent electric field generated by the positive lattice particles (ions) located at lattice positions x_k. For simplicity we decribe the electron-ion interaction by a

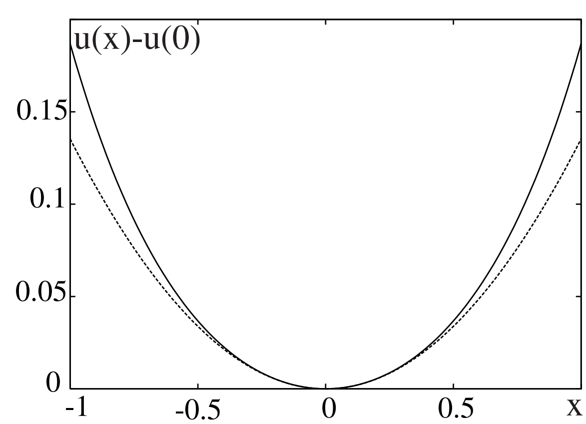

Fig. 10. Effective potential (see also Fig. 1) acting on a lattice ion moving between two other nearest-neighbor ions (hence interacting from either side with exponentially repulsive Toda forces) separated by a distance 2σ (x denotes the elongation or displacement from the minimum; stiffness parameter $b = 2$). The dotted (parabolic) line shows the harmonic approximation.

pseudopotential with an appropriate cut-off

$$U_e(y_j) = \sum_k \frac{(-e)e}{\sqrt{(y_j - x_k)^2 + h^2}}. \tag{60}$$

This potential avoids the pole (Coulomb singularity) by introducing a cut-off at $U_{\min} = -e^2/h$; $h \approx \sigma/2$ is the cut-off distance and σ is the equilibrium inter-ion mean distance. Equation (60) is justified by the fact that in a real solid the ion core is a region of high electronic density, finite size, and hardly penetrable by a *free* electron. Figures 11 and 12 illustrate the role of the cut-off, h, and of the compression of the Toda springs in the lattice. Note that to avoid Coulomb singularities in 1D or 2D geometry in (60) we consider the *free* electrons to be moving along the lattice in 3D. Accordingly, the electrons are able to move from one side of an ion to the other one and may develop electron currents opposite to the ion currents, as we describe below.

For simplicity the interaction between electrons is neglected. We stay on the same classical level as the Drude theory. Thus, with N ions placed at coordinates x_k, with mass m_i and charge $+e$, moving on a lattice of length $L = N\sigma$, the electron dynamics follows the equations

$$\frac{d}{dt} y_j = v_j, \tag{61}$$

$$m_e \frac{dv_j}{dt} + \sum_k \frac{\partial U_e(y_j, x_k)}{\partial y_j} = -eE - m_e \gamma_{e0} v_j + m_e \sqrt{2D_e}\, \xi_j(t).$$

As earlier we assume periodic boundary conditions.

For further simplicity, we may on occasion consider just one electron located at position y rather than N electrons at coordinates y_j. The dynamics of the electrons is assumed to be passive (i.e. standard damping for all velocities), including white noise. The stochastic force models a surrounding heat bath (Gaussian white noise) as earlier discussed. The friction force acting on the electron is small relative to that on the ions, $m_e \gamma_{e0} \ll m_i \gamma_{i0}$.

Let us consider now the ion dynamics. The ions have their own evolution which due to the large difference of the masses, $m_e \ll m_i$, will be largely independent of the electron dynamics. Therefore we may use an "adiabatic" approximation. The potential energy stored in the ring is now [recall Eq. (16)]

$$U = \sum_{k=1}^{N} [U_i^T(r_k) + U_e(r_k)], \tag{62}$$

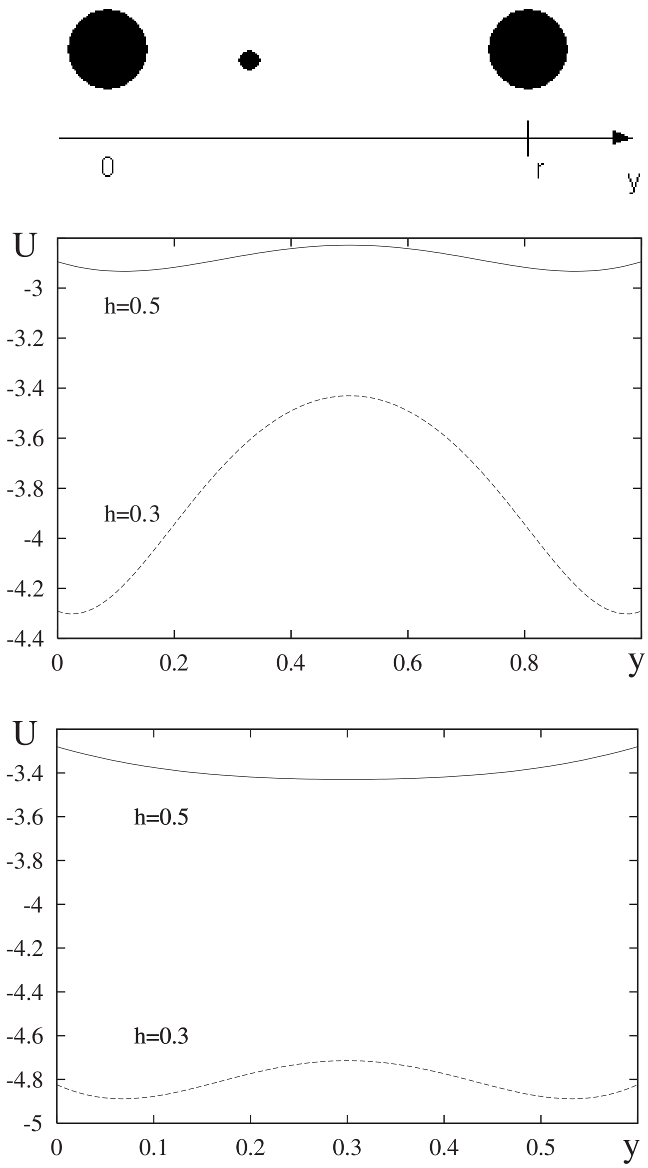

Fig. 11. Pseudopotential felt by an electron placed between (y, $0 < y < r$) two nearby ions ($x_1 = 0$ and $x_2 = r$): $U_e(y)/e^2 = -[(y-x_1)^2+h^2]^{-1/2} - [(y-x_2)^2+h^2]^{-1/2}$. The coordinate r illustrates the absence of compression ($r = 1$, upper figure with the potentials) and a 40% compression ($r = 0.6$) of the "spring" between ions. It is clear (bottom figure) that both compression, r, and cut-off, h, help the electron achieve a minimum midway between the two lattice ions.

with $U_i^T(r_k)$ denoting the Toda pair interaction, exponential potential (25). $U_e(r_k)$ is the electron-ion potential given by (60). The external electric field E also acts on the charge $e_i = +e$ of the Toda particles (ions). Following the discussion presented in Sec. 5 we add a Rayleigh-like dissipative velocity-dependent force, $F_1(v_k)$, to make the lattice *active*. Hence, the evolution of the ion particles is given by

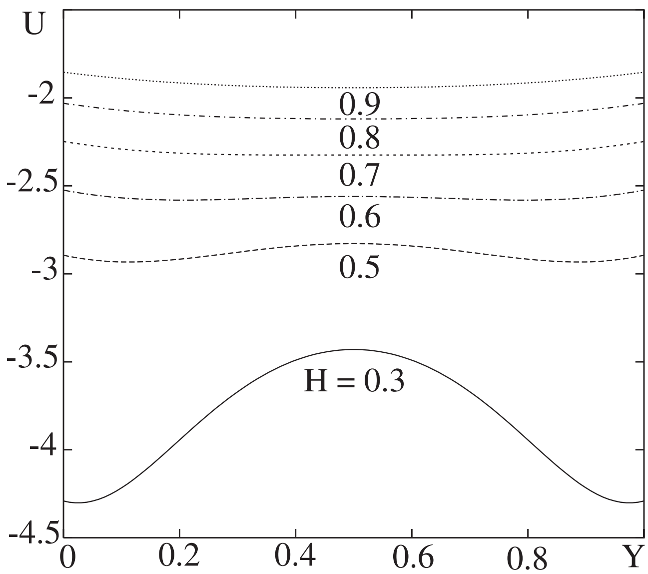

Fig. 12. Pseudopotential felt by an electron placed midway between two nearby ions. The graphs of Fig. 11 are recovered here in universal form by using $H \equiv h/r$, $Y \equiv y/r$, $X \equiv x/r$, hence $x_1 = 0 \rightarrow X = 0$, $x_2 = r \rightarrow X = 1$, and $0 < y < r \rightarrow 0 < Y < 1$. $U(Y)/e^2 = -[Y^2 + H^2]^{-1/2} - [(Y-1)^2 + H^2]^{-1/2}$. As H grows, either because h grows (cut-off length increases) or r decreases (compression increases), the maximum yields to a minimum midway between the two ions.

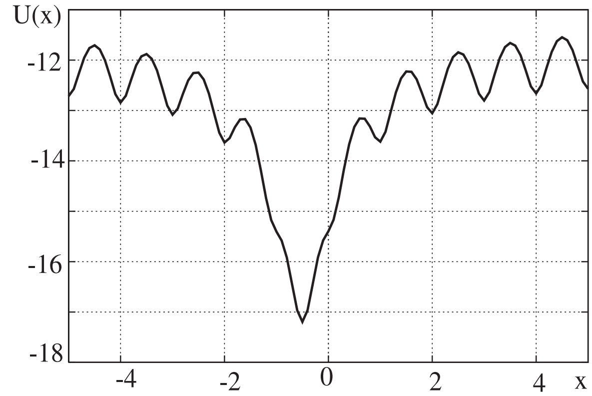

Fig. 13. Snapshot of the effective potential/landscape acting on an electron moving in a lattice with a solitonic excitation which locally creates a deeper potential well. In a long enough lattice the solitonic (negative) peaks (cnoidal waves) define a new periodicity different from the otherwise (quasi) harmonic one. Parameter values: $\sigma = 1$, $b = 1$, $h/\sigma = 0.3$ and $\chi = 1$.

the Langevin equations

$$\frac{d}{dt}x_k = v_k, \tag{63}$$

$$m\frac{d}{dt}v_k + m\gamma_0 v_k + \frac{\partial U}{\partial x_k} = eE + F_a(v_k) + m\sqrt{2D}\,\xi_k(t),$$

governing the stochastic motion of the kth ion on the lattice ring. The stochastic force $\sqrt{2D}\,\xi_k(t)$ has been earlier defined. The dissipative contribution on the l.h.s., γ_0, describes the standard friction force acting on the ions due to the heat bath. Our evolution problem now is the combined set of Eqs. (61) and (63). These equations have been integrated by means of a fourth-order Runge–Kutta algorithm adapted for solving stochastic problems like the Langevin equation [Chetverikov & Dunkel, 2003]. All computer experiments begin with a state of equal distances between ions and their velocities randomly taken from a normal distribution with amplitude v_{in}, $v_k(0) = v_{\text{in}}\xi(k)$. Each electron is placed at rest, $v_j = 0$, midway between two ions. Heavy ions are not affected very much by light electrons and hence (free) electrons move on the background/landscape of the pseudopotential profile created by the ions (Fig. 13). The integration step is chosen to describe correctly the fastest component of the process, oscillations of electrons in a potential well. The equations are written in dimensionless form, with dimensionless variables. In particular, the average distance between Toda-particles, σ, is chosen as the space scale (unit length); the mass of the ions is taken as unity ($m_i = m = 1$); the time scale is associated with the characteristic time of the relaxation of the linear frequency of oscillations of a Toda particle in the potential well, ω_0. To reduce the number of parameters of the problem, the parameters of both Toda and Coulomb potentials, the mass ratio and the particle charges are held fixed. Thus, the damping rates, γ_0 and γ_{e0}, the values of the parameters characterizing the driving forces, $F_a(v_k)$, to be specified below, the initial velocity, v_{in}, chosen to select a solitonic mode, the value of the external field, and the electron temperature, T, are varied in the computer simulations.

8. Bound States (Solectrons) and Complex Currents in Active Lattices

Due to the large difference in the masses of the charged particles, the overwhelming contribution to the current comes from the electrons moving on the nonlinear ion lattice. The current density (per unit length) of the electrons is obtained by taking the average of electron velocities. Hence the electric current density (per unit length) is

$$j_e = -n_e e \sum_j \langle v_j^e \rangle. \quad (64)$$

The average is to be taken over long trajectories. We are interested in the interaction of the electrons with the earlier discussed solitonic excitations in the lattice (Fig. 13). Local compressions of the lattice create the soliton excitations and generate a rather deep local well in the potential landscape.

Before embarking on the study of electric currents we have studied the effect of solitonic excitations generated through quenching by numerically finding the corresponding solutions of the coupled Langevin equations, (61) and (63). Let us first discuss what happens if $E = F = 0$ in (63). Do we have solitons in the lattice? The numerical experiment was conducted by starting with a Gaussian distribution of the ion velocities corresponding to a high-temperature Maxwellian as the initial condition. This temperature is of the order of 200–300 in units of $m\omega_0^2\sigma^2$, the energy of harmonic oscillations with amplitude σ. At this rather high temperature, besides other elementary excitations, solitons are also supposed to be generated. However, they are difficult to identify due to the seemingly chaotic motions of the particles. Then we quench to a temperature near zero in a similar way as done in Sec. 6. The solitons survive since they have a longer life time than other excitations. Figure 14 illustrates the results. Looking at the trajectories we observe the motion of ions (bunch of dotted lines) and an electron (thick solid line) escaping from the ions and traveling bound to the soliton. This only happens for a finite time and so we have a metastable situation. Indeed, the solitons and electron-soliton dynamic bound states (transient solectrons) generated by our quenching experiment decay after a time of order $t_{\rm rel} \simeq 1/\gamma_0$. In principle these excitations also exist under equilibrium conditions yet they are seldom observed [Ebeling *et al.*, 2000b].

In a subsequent set of simulations we combined quenching with active friction ($F \neq 0$) to overcome the dissipation. Again the numerical experiment started with a high-temperature initial condition, then after quenching the solitonic excitations were maintained by feeding energy with Rayleigh's *active* friction force. In this case the system develops driven ionic solitons moving oppositely to the field. The electrons which are

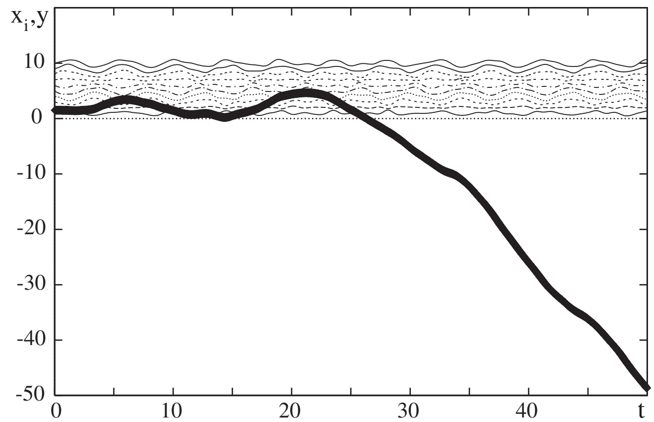

Fig. 14. Passive electric Toda lattice (in the absence of external field) and metastable solectrons. As a result of quenching an initial state with $T(t=0) \approx 0.1$ the trajectories of ten Toda particles (ions, $x_i(t)$) generate solitons. A soliton forms a dynamic bound state with an electron captured by the soliton ("solectron"). During the time of capture the electron trajectory, $y(t)$, is parallel to the sloped trajectories along valleys whose "tangent" provides the soliton (cnoidal wave) velocity. The difference with Fig. 5 is that here a *free* electron has been added to the system and thus we see its transitory trapped by the soliton leading to the dynamic, albeit metastable, bound state. Parameter values: $h = 0.5$, $\mu = -1$, and $\gamma_0 = \gamma_{e0} = 0.00045$. Units: abscissa (time), $t_0/\sqrt{5}$; ordinate (length), σ.

coupled to the charged Toda particles (ions) form rather stable dynamic bound states with the solitons (solectrons). Recall that the dissipative forces are [Eq. (41)]

$$F(v_k) = m\gamma_0(\mu - v_k^2)v_k, \quad \mu = \frac{(\gamma_1 - \gamma_0)}{\gamma_0}, \quad (65)$$

where, as discussed earlier (Sec. 5), μ is a bifurcation parameter. Recall that $v_d = \hat{v}_d = 1$ (hence v_k^2/v_d^2 becomes v_k^2) and also that for $\mu > 0$ the state $v = 0$ becomes unstable and yields to the new attractors of the free deterministic motion if $\mu > 0$, corresponding to the two additional zeros at

$$v = \pm v_0 = \sqrt{\mu}. \quad (66)$$

For illustration we take (unless otherwise specified) $\mu = 1$. Figure 15 illustrates how solitons appear in the ion lattice. They correspond to local compressions of the lattice (see also Fig. 2). The solitons run opposite to the mean ion motion. It is clear in the two snapshots given how the electrons are captured by local concentrations of the ionic charge. Since the electrons search for the deepest nearby minimum of the potential (see Figs. 11 and 12), they will be most of the time located near local ion clusters. Note that we have a dynamic process,

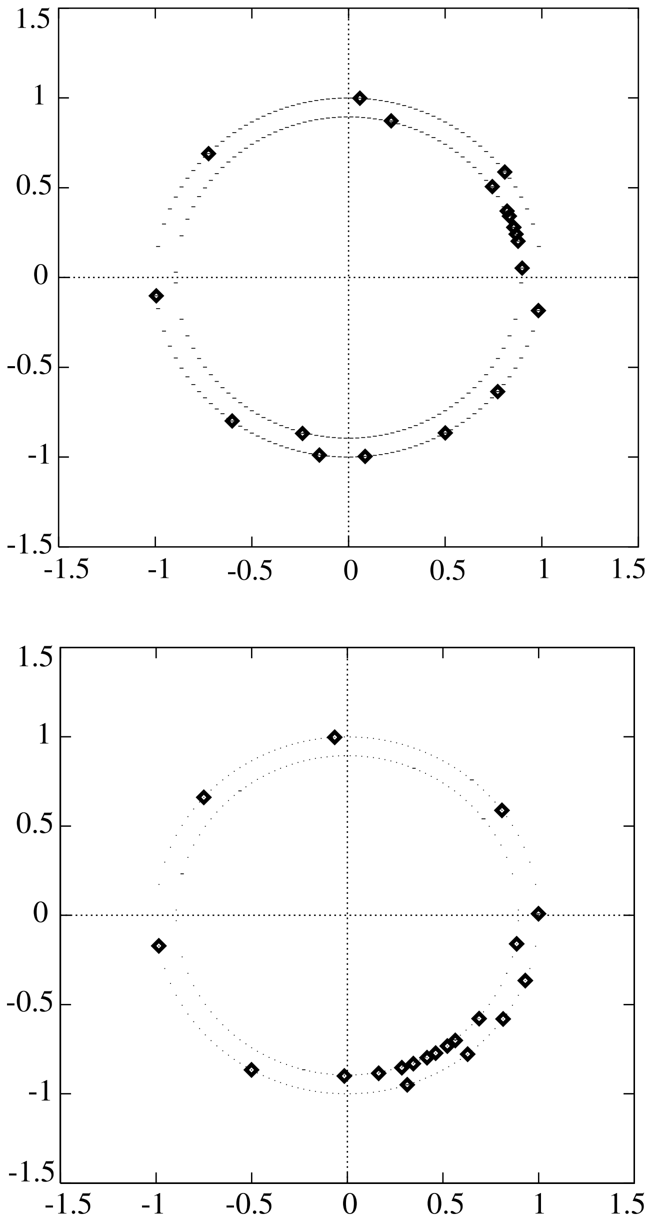

Fig. 15. Active electric Toda lattice in a lattice ring representation to easily visualize motions. Successive snapshots of the configuration of ten electrons (inner ring) and ten ions (outer ring) developing a solitonic excitation of the lattice which is supported by the added (Rayleigh's) *active* friction force. In the left picture the electron cluster (in the right upper quadrant) is still far behind the soliton (bottom of outer ring). The right picture shows that nearly all electrons are captured by the soliton (right lower quadrant). At this moment the electrons appear slightly ahead of the soliton. Parameter values: $h = 0.3$, $\mu = 0.25$, $b = 1$, $\gamma_0 = \gamma_{e0} = 0.5$, $D = D_e = 0$, and $m/m_e = 10^3$.

not a static cluster, the ions participating in the local compression are changing all the time. In other words, the electrons continually have new partners (a kind of promiscuity) in forming short-time bound states. Since we did not take into account electron repulsion and spin effects, we sometimes find many electrons clustering in the same minimum. We expect that adding repulsion and spin effects would make an electron-pairing process more advantageous; the investigation of this and related quantum effects (e.g. treating quantum mechanically the electron-ion interaction, generalizing Bloch's theorem to account for the cnoidal periodicity, Fig. 13, etc.) is left to future studies (see Sec. 9).

(N.B. An active Toda lattice (with Rayleigh's *active* friction force) with N particles possesses $(N + 1)$ basic attractors. $(N - 1)$ are oscillatory and two are nonoscillatory (where, as a whole, the lattice moves right or left or clockwise if a ring). For N even there is also an "optical" mode corresponding to antiphase oscillations. Here we opt not to discuss this wealth of possibilities and hence once more refer the reader to recent publications on the subject [Makarov *et al.*, 2000; Makarov *et al.*, 2001; del Rio *et al.*, 2003].)

In Fig. 16 we show a simulation for the evolution of ten Toda particles (ions) creating one dissipative soliton which moves in the opposite direction and ten *free*, noninteracting electrons. After a sufficient time interval, most electrons,

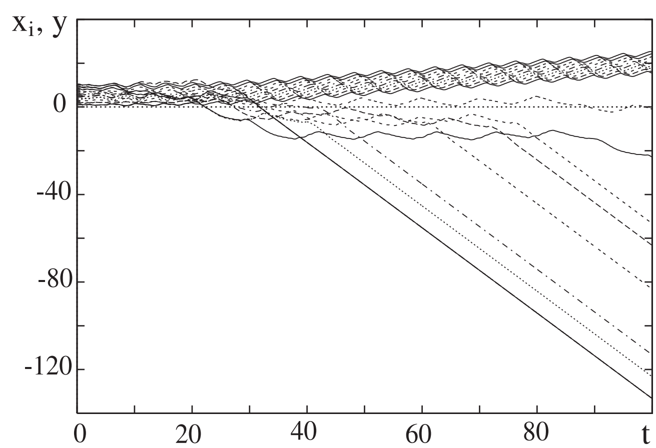

Fig. 16. Active electric Toda lattice. Trajectories are shown for ten particles (ions) moving left to right creating one fast dissipative soliton moving in the opposite direction, and for ten electrons (ending, generally, as slopped lines) captured one after another by the soliton. Three electrons seem to be traveling together (thicker slopped line) while the tenth electron still moves almost free (trajectory around $y = 0$). Parameter values: $h = 0.3$, $\mu = 0.25$, $\gamma_0 = \gamma_{e0} = 0.5$, $D = D_e = 0$, and $m/m_e = 10^3$. Unit time along abscissa: $t/\sqrt{5}$.

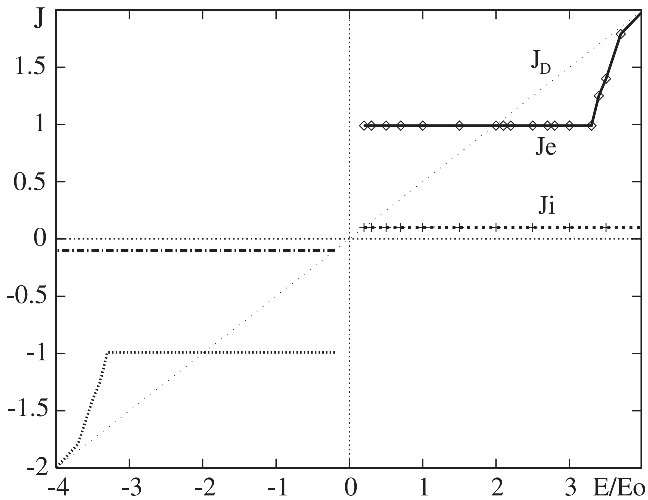

Fig. 17. Active electric Toda lattice. Current-field characteristics displaying the steady current densities (j_D, Ohm-Drude; j_i, ion current, and j_e, electron current). We see nonlinear current-field characteristics with a region of constant current. At very small field values we observe an apparent gap in the values for the current. Parameter values: $h = 0.3$, $\mu = 0.25$, $\gamma_0 = \gamma_{e0} = 0.5$, $D = D_e = 0$, $m/m_e = 10^3$, and $b = 1$.

one after another, bind to the soliton and move approximately with the soliton velocity in a direction opposite to that of the ions.

We have seen in the simulations that in the driven case ($\mu > 0$) the ions execute a slow drift following the direction of the external field. If the field strength is stronger than the decay imposed by the thermal fluctuations, the electrons proceed in opposite direction (counterclockwise, if a ring). After a sufficient time interval, the ion compressions create solitonic excitations moving with soliton velocity, v_{sol}, opposite to the mean drift of the ions. The electrons "like" the potential well formed by the local compression connected with the soliton. After a while the electron is captured by the local compressions and moves with the soliton velocity opposite to the ion drift.

The magnitudes of both the electron and ion currents do not depend very much on the value of the external field over a wide range albeit limited both from below and above. Figure 17 shows both currents versus field strength. The scale E_0 corresponds to the field imparting a velocity v_0 to an electron not interacting with ions. It clearly appears that the stationary currents corresponding to the case of dissipative solitons are stabilized thanks to the *active* friction force (energy pumping). The nonlinear current-field characteristics exhibit a region of constant current (corresponding to zero differential conductivity). We ought to mention that the curves given in Fig. 17 are somewhat idealized. The initial conditions for our computer simulations were generated by a random sampling from a Gaussian distribution. For ten particles the sampling led to a great dispersion and hence we eliminated a rather small part of the initial conditions. Due to this choice the curves in Fig. 17 are an upper limit. At very small values of the field strength we observe an apparent gap in the values for the current. In this narrow region, around zero, we could not obtain reliable data from the computer simulations. However, the existence of a gap may hint at the existence of a very high conductivity [Chaudhari *et al.*, 1988; Mannhart *et al.*, 1988]. For very low electric field strengths we cannot specify the running direction for solitons, they may travel in either direction. On the other hand, intense field values do not allow electrons to be trapped by a potential well as easily. In particular, at the upper boundary of the range there is a very limited domain of initial conditions for ions and electrons from which electrons are captured by the soliton.

Figure 18 illustrates the behavior of the electron current as a function of the temperature

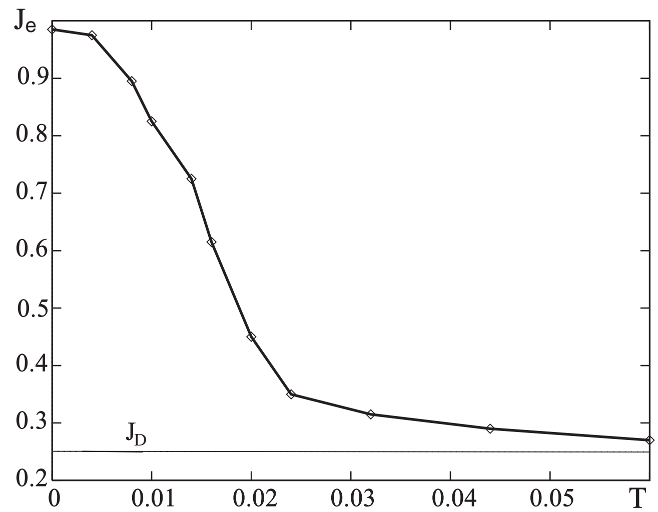

Fig. 18. Active electric Toda lattice. Current-temperature (electron noise) characteristics. The solid line (j_e, electron current) shows a significant increase as the temperature decreases and approaches the soliton range (Fig. 7). The horizontal straight dotted line (ordinate 0.5) corresponds to the Ohm (Drude) current ($j_D = 0.5$). The value at $T = 0$ is the same as the plateau in Fig. 17. Parameter values: $b = 1$, $\mu = 0.25$, $h = 0.3$, $\gamma_0 = \gamma_{e0} = 0.5$, $T = D_e$, $D = 0$, $m/m_e = 10^3$, and $E/E_0 = 0.5$.

(electron noise). We see that upon lowering the temperature the electron current driven by the solectrons grows significantly relative to the Ohm (Drude) current.

9. Conclusions

We have given in this report a survey of phenomena connected with the excitation of *dissipative* solitons in nonlinear lattices. In particular we have studied the dynamics of a Toda lattice with added dissipation and "activity" in the form of an *active* friction force (on occasion called *negative* friction), following an idea put forward by Lord Rayleigh to maintain vibrations. After discussing how (linear) harmonic oscillations of a single particle can be maintained by such an *active* friction force in a system coupled to a heat bath acting as a reservoir where the particle could draw energy, we have recalled basic concepts about phonons in a lattice with many such particles coupled together, yet in a linear system. We have restricted consideration to one-dimensional (1D) lattices. Then we summarized results provided by Toda about 1-D lattices with a particular exponential interaction that in two extreme limits approaches, respectively, the harmonic oscillator and the hard rod/sphere. Subsequently, following the earlier given argument for the harmonic case, we have added an *active* friction force, hence making the Toda particles into *active* Brownian units, and we have shown how solitons can be excited and eventually sustained beyond an instability threshold. We have also discussed a few "equilibrium" features (specific heat at constant length/volume, metastable solitonic excitations, dynamic structure factor as a function of increasing temperature) of Toda lattices. Finally we have studied the electrically charged (with ions and electrons) active Toda lattice and we have shown how the electric field triggers electric currents with intriguing properties. We have shown how in an active Toda lattice a (nonequilibrium) transition occurs from the linear Ohm(Drude) law (that can be considered defining a "disordered" state) to a form of supercurrent (that can be considered characterizing the more "ordered" state). The underlying mechanism to such supercurrent is the formation of electron-soliton dynamic bound states (solectrons) due to the role played by the compressions in the Toda springs. It seems to be a most interesting property of the phenomena studied here that the strength of the external field is nearly without relevance, what matters is its symmetry breaking role.

The study provided here is based on the purely classical dynamics (no quantum mechanics is involved) and evolution of a 1D electrically conducting active Toda lattice model. The results found [Velarde *et al.*, 2005] share common (formal) features with the experimental curves obtained in measurements of characteristics of high-T superconductors [Chaudhari *et al.*, 1988; Mannhart *et al.*, 1988]. We are aware of pictures that look alike yet refer to different objects. Hence, linking the predictions made using the purely classical analysis of a 1D Toda lattice model with data about real systems is beyond the scope of this discussion. However, in view of the results obtained we feel worth generalizing our study by treating quantum mechanically the electron-ion interaction, by adding spin to the electrons, by including the electron-electron coupling, by generalizing the (quantum) Floquet–Bloch's theorem and hence by solving the Schroedinger equation for the cnoidal (nonlinear) periodic landscape (Fig. 13) and, needless to say, by extending the study to 2D and 3D lattices. For recent significant results, see [Velarde *et al.*, 2006; Hennig *et al.*, 2006].

We also feel it is worth exploring the potential of our model system (with its $N + 1$ multiple steady states) endowed with a stick-slip (always positive values, hence *passive* friction force) alternative to Rayleigh's *active* friction force (or to the depot model), as active Brownian motors combining an endogenous ratchet-like potential landscape and thermal motion. The solectron transports electricity but the same dissipative solitons, at the origin of the solectron, could very well transport matter.

Finally, we feel it is of interest to implement electronically the system described in this report. Such an analog computer may prove useful if incorporated as a neural part of a robot.

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