



## ON THE POSSIBILITY OF ELECTRIC CONDUCTION MEDIATED BY DISSIPATIVE SOLITONS

MANUEL G. VELARDE

*Instituto Pluridisciplinar, Universidad Complutense de Madrid,  
Paseo Juan XXIII, 1, 28040-Madrid, Spain  
International Center for Mechanical Sciences (CISM), Palazzo del Torso,  
Piazza Garibaldi, 33100-Udine, Italy  
velarde@fluidos.pluri.ucm.es*

WERNER EBELING

*Institut für Physik, Humboldt-Universität Berlin,  
Newtonstraße 15, 12489-Berlin, Germany  
ebeling@physik.hu-berlin.de*

ALEXANDER P. CHETVERIKOV

*Faculty of Nonlinear Processes, N. G. Chernychevsky State University,  
Astrakhanskaya 83, 410012-Saratov, Russia  
ChetverikovAP@info.sgu.ru*

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Based on the study of the dynamics of a dissipation-modified Toda anharmonic (one-dimensional, circular) lattice ring we predict here a new form of electric conduction mediated by dissipative solitons. The electron-ion-like interaction permits the trapping of the electron by soliton excitations in the lattice, thus leading to a soliton-driven current much higher than the Drude-like (linear, Ohmic) current. Besides, as we lower the values of the externally imposed field this new form of current survives, with a field-independent value.

*Keywords:* Solitons; dissipative solitons; nonlinearity; lattices; superconductivity.

Our understanding of electric conduction in metals owes much to the pioneering work of Drude [Ashcroft & Mermin, 1976]. Present day theory relates conductance to the electron–phonon (lattice) interaction for both normal and superconducting materials. Hints also exist about the possible role played by electron–soliton interactions in accounting for electric conduction but no theory has been developed yet to observe its explicit role in a model problem [Choquard, 1967; Payton III *et al.*, 1967; Krumhansl & Schrieffer, 1975; Lee, 1987; Davydov, 1991]. Note, however, the extensive and fruitful work done on solitons and polarons in conductive polymers [Yu, 1988; Heeger *et al.*, 1988].

Solitons have been extensively studied by many authors [Scott, 2003]. Suffices here to mention the pioneering work on anharmonic lattices done by Fermi *et al.* [1965], which motivated the work by Zabusky and Kruskal [1965], who coined the word, and Toda [1989]. Toda’s lattice with exponential interaction was the first nonlinear, many-body problem exactly solved. This interaction, defined below, has two limit cases, the harmonic (phonon, linear) case and the hard-sphere (gas) interaction.

Toda’s exponential interaction is simpler to implement electronically [Hirota & Suzuki, 1973; Singer & Oppenheim, 1999; Makarov *et al.*, 2001; del Río *et al.*, 2003] than the apparently simpler

cubic or quartic power law potentials used by Fermi *et al.* [1965] and also used in textbooks to account for anharmonic effects in heat diffusion ([Ashcroft & Mermin, 1976]; see also [Payton III *et al.*, 1967]). Accordingly, we consider Toda's lattice as the "simplest" (or most tractable) model of an anharmonic soliton-bearing lattice. Needless to say, quite like the Ising–Lenz model that cannot account for the actual equilibrium properties of a real magnetic material but, however, serves to understand what critical phenomena are about [Bernasconi & Schneider, 1981], the Toda lattice (save the question of dimensionality) is expected to allow understanding basic features of nonequilibrium dynamics, flows and transitions in solids. In the present note we generalize Toda's lattice to include dissipative effects and an energy pumping mechanism in order to study the evolution of a driven-dissipative nonequilibrium model system for an anharmonic solid.

We consider a one-dimensional array of  $N$  identical Brownian point-particles with masses located on a ring of length  $L$ . Hence the coordinates of the particles are  $x_i(t)$  and their velocities  $v_i(t)$ ,  $i = 1, 2, \dots, N$ , with  $x_{i+N} = x_i$ . For the interaction we take

$$U = \sum_{i=1}^N \left[ U_i^T(r_i) + U_e(r_i) \right], \quad (1)$$

with  $U_i^T(r_i) = (a/b)[e^{-b(r_i-\sigma)}]$  denoting Toda's interaction,  $r_i = x_{i+1} - x_i$ ;  $\sigma > 0$  is the mean inter-particle distance. The parameters "a" and "b" refer to the amplitude of the force and the stiffness of the spring constant, respectively.  $U_e$  denotes the interaction with electrons to be made explicit below.

The evolution of the lattice is governed by the following equations

$$\frac{d}{dt}x_k = v_k, \quad (2a)$$

$$m \frac{dv_k}{dt} + \frac{\partial U}{\partial x_k} = e_k E + F(v_k) + \sqrt{2D}\xi_k(t), \quad (2b)$$

where the stochastic component on the r.h.s. mimicks a heat bath as a Gaussian white noise with zero mean and delta-correlated  $\langle \xi_i(t) \rangle = 0$ ,  $\langle \xi_i(t')\xi_j(t) \rangle = \delta_{ij}\delta(t' - t)$ . The quantity  $E$  accounts for an external field acting on charges  $e_i$ . We introduce the dissipative force

$$F(v_k) = -m\gamma(v_k)v_k, \quad (3)$$

such that  $\gamma(v) = \gamma_0 + \gamma_1(v)$ , with  $\gamma_0 > 0$  describing standard friction between particles and the bath. We shall assume Einstein's relation  $D = mk_B T \gamma_0$ , with  $k_B$  and  $T$  denoting Boltzmann's constant and temperature, respectively. The  $\gamma_1$  component of the friction is assumed nonfluctuating [Schweitzer *et al.*, 1998; Erdmann *et al.*, 2000; Dunkel *et al.*, 2001].

Note that without drive and current the ions form an equidistant lattice, with equally spaced unit cells or unit domains. Due to the (nonlinear) interactions the system may develop phonon and soliton excitations. With varying noise/temperature the nonlinearity may be taken to advantage for a disorder–order transition. By adding driving terms,  $\gamma_1$ , the solitons are eventually stabilized. On the other hand, with the nonlinear Toda interaction, each particle is displaced from its equilibrium position to either direction along the lattice ring, making wide excursions within its "domain walls", corresponding to a wandering local compression (more about this below). This is one way to visualize the underlying support of a (nonlinear) wave of *translation* in the lattice (for pioneering work see, e.g. [Takahasi, 1961]). In standard (linear) waves, matter (or charge) transfer is not a first-order effect while it is, indeed, a first-order effect with (nonlinear) waves of translation and hence with solitons or solitonic wave trains (periodic and otherwise). Furthermore, as discussed by Payton III *et al.* [1967] for heat transport, solitons in the nonlinear lattice ring experience little scattering with the "particles" and this seems responsible for the faster transfer relative to a harmonic lattice.

As noted above the lattice is compressed around a soliton (a spike or solitonic peak) and hence in the lattice ring with an exponential repulsion force (akin to the hard-sphere interaction) a soliton is a compression wave. The nonlinear, periodic (e.g. cnoidal) wave causes expansion of the lattice. There is compression around the peaks but the troughs are expanded, hence a nonlinear periodic wave in a Toda lattice consists of sharp spikes and wide troughs. Yet, these two processes in our circular ring are not in conflict with the fact that the length,  $L$ , is held constant.

The total energy balance in the system is

$$\frac{dE}{dt} = - \sum_k m\gamma(v_k)v_k^2 + \sqrt{2D} \sum_k v_k \xi_k(t). \quad (4)$$

Note that the first term in the r.h.s. of Eq. (3) has a sign not yet prescribed. Let us take a simple

Rayleigh-like *active* friction depending on a tunable parameter,  $\mu$ ,

$$F(v) = m\gamma_0 v[\mu - v^2/v_1^2]. \quad (5)$$

This type of *active* friction for mechanical systems with energy input was proposed in the theory of sound developed by Lord Rayleigh. Needless to say, this is not a realistic model for a real material. However, we use it here only as the simplest model for generating dissipative solitons in a lattice [Nekorkin & Velarde, 2002]. It appears that this force model may be considered as a mechanism for *active* Brownian particles that carry refillable energy depots (internal degrees of freedom). More general forms of active friction have been discussed in the literature [Schweitzer *et al.*, 1998; Erdmann *et al.*, 2000; Dunkel *et al.*, 2001]. Due to the restriction to Rayleigh friction we will not be able to discuss in full the role of temperature in the system. It helps, however, seeing in a transparent way the new form and value of the flow currents appearing in the lattice.

The dimensionless parameter,  $\mu$ , in the Rayleigh model controls the conversion of the energy taken from the external energy reservoir into kinetic energy. It plays the role of a bifurcation parameter in our model system. The region  $\mu < 0$  is the region with (nonlinear) *passive* friction, and  $\mu > 0$  is the region of *active* friction. For  $\mu < 0$  the force has a single zero at the velocity  $v = 0$  which is the only attractor of the deterministic system. The critical value is  $\mu = 0$ . For  $\mu > 0$  the motionless state becomes unstable. In the following we shall mostly use a special set of parameters assuming  $\mu = 1$  and  $v_1 = 1$ . Consequently, our dynamical system has the stationary velocity  $v_0 = 1$ .

Let us now add a second kind of charge (electrons) and let us study how stochastics changes the deterministic dynamics. Consider “electrons”,  $-e$ , at positions,  $y_j$ , somewhere along the lattice of “positive” charges (called here ions) located at sites  $x_k$ , and let us assume that the added particles experience a Coulomb interaction with suitable cut-off,

$$U_e(y_j, x_k) = \frac{(-e)e_k}{\sqrt{(y_j - x_k)^2 + h^2}}, \quad (6)$$

with  $h \approx \sigma/2$  as the cut-off distance. Note that we do not treat here proper  $1d$  or  $2d$  charges but rather we are treating particles with  $3d$  interactions (with cut-off) like if we have two separate, parallel rings

near each other (distance  $h$ ). For further simplicity we take

$$\frac{d}{dt}y_j = v_j, \quad (7a)$$

$$m_e \frac{d^2}{dt^2}y_j + \frac{\partial U_e}{\partial y_j} = -eE - m_e\gamma_{e0}v_j + \sqrt{2D_e}\xi_j(t), \quad (7b)$$

hence the electron behaves passively, with friction being small  $m_e\gamma_{e0} \ll m_i\gamma_{i0}$ . The electronic contribution to the current density (current per unit length) can be expressed as

$$j_e = -e\langle v_e \rangle, \quad (8)$$

where  $\langle v_e \rangle$  is the average electron velocity. In the Drude approximation the current density is given as

$$j_D = \left( \frac{e^2}{m_e\gamma_{e0}} \right) E. \quad (9)$$

We will show that the soliton-driven transport of the electron may be much higher. The total current density along the ring, if we take an equal number of electrons and ions (in the simulations we assume  $N = 10$ ), is

$$j = \langle j_i(t) \rangle + \langle j_e(t) \rangle = e_i\langle v_i \rangle - e\langle v_e \rangle, \quad (10)$$

where, accounting for sign of charge and current directions, both terms have equal sign.

Figures 1–4 depict salient findings of our computer simulations. Note that the problem has three parameters, the tuning parameter  $\mu$ , the electric field, and the temperature/noise (in fact two noise-parameters). We restrict consideration here to only a few significant results. Figure 1 illustrates the trajectories of the ten ions moving clockwise which create one dissipative soliton. The trajectory of one of the electrons is also shown. The parameter values used are:  $\sigma = 1$ ,  $a = 13.69$ ,  $b = 1$ ,  $h^2 = 0.08$ ,  $m_i = 10^3 m_e$ ,  $m_e = 1$ ,  $\gamma_{e0} = \gamma_{i0} = 1$ ,  $\mu = 1$ , and  $v_1 = 1$ . In Fig. 2 we show an excitation with four dissipative solitons excited and moving clockwise, and again we show the trajectory of one of the electrons. The two pictures correspond to supercritical (driven) states with  $v_0 = 1$ , arising from different initial conditions and with different values of the  $a/b$  ratio in the Toda potential. For Fig. 2 the ratio  $a/b$  is of lower value than in Fig. 1. The noise is assumed to be very small (practically  $D = D_e = 0$ ). We clearly see that the electron forms dynamic bound states (solelectrons, in short) with the running solitons. The electron is electrostatically bound to the local compression (the soliton spike)

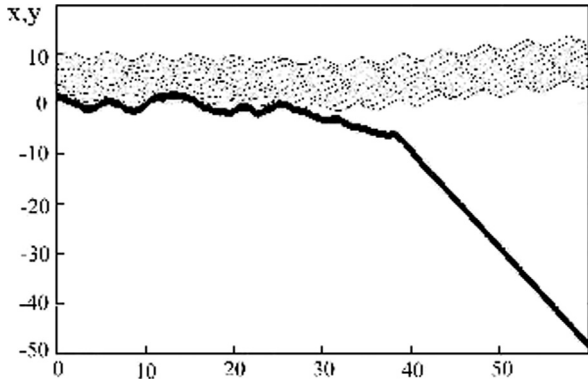


Fig. 1. Trajectories of  $N = 10$  (ten) “ions” (thin lines) and of one of the “electrons” (thick line) in the lattice ring in the case that a cnoidal-like wave with a single solitonic peak is excited. The heat bath temperature is taken very small ( $D = D_e = 0$ ). The weak external field ensures a single direction of ring rotation. The ion is supposed to be a thousand times heavier than the electron. The quantity  $\gamma_{e0}$  is set equal to unity. The initial distance between neighboring ions is unity.

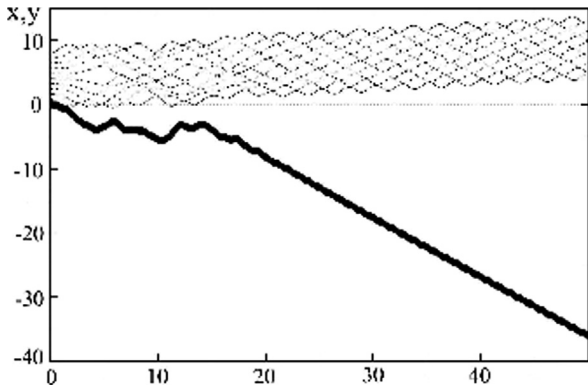


Fig. 2. Trajectories of  $N = 10$  (ten) “ions” (thin lines) and of one of the “electrons” (thick line) in the lattice ring in the case of 4 (four) solitons (like a cnoidal wave) excited. Again the heat bath temperature is taken very small ( $D = D_e = 0$ ). The parameter values are as in Fig. 1, except the ratio  $a/b$  of the Toda potential which is taken here with lower value.

which is running with the soliton velocity counter-clockwise, thus leading to the soliton-driven current. Note that the electron first follows a couple of ions and subsequently jumps on a soliton (negative slopes tangent to the ion trajectories). The electron changes partners all the time and flows with the velocity given by the (absolute) value of the slope.

The actual currents (the electronic current, the Drude current of the electrons and the ionic current) are depicted in Fig. 3 as functions of the strength

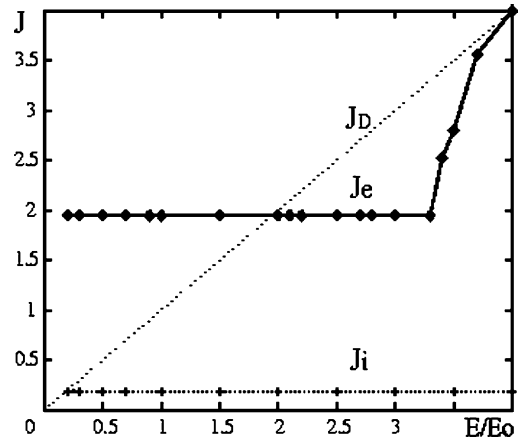


Fig. 3. Different contributions to the electric current as a function of the external electric field. The dotted line shows the Drude-like current,  $j_D$ , of the electrons. The solid line shows the soliton-driven current,  $j_e(t)/|e_e|$ , observed in the simulations with ten ions and ten electrons. The lower broken line gives the ionic current,  $j_i$ . Parameter values are as in Fig. 1.

of the external field. As reference scale or unit we take  $E_0$ , which in the *passive* case would lead to the unit value of velocity,  $v = 1$ .

Let us emphasize the observed effects. Note first that for a wave and, eventually, a current to be observed traveling in one or the other of the two possible directions, the symmetry-breaking bias of an imposed external electric field suffices. Clearly, ions proceed along the direction imposed by the external field while electrons proceed in the opposite direction. Following a transient regime there is self-organization leading to solitonic excitations of the lattice (ions) moving with velocity,  $v_{\text{sol}}$ , opposite to the (mean) drift ion motion. The electron originally placed in the valley between two solitonic peaks drifts a bit towards one of them, being “captured” and moves with the soliton velocity, which is in the opposite direction to the ion drift.

When one soliton is excited with rather high velocity,  $v_{\text{sol}} \approx 2$ , this soliton catches all ten electrons, one after the other. This leads to a rather high electronic current, about ten times lower is the ionic current,

$$j_e \approx 2; \quad j_i \approx 0.2. \quad (11)$$

We see that the currents are independent of the field. The electronic current is much higher than the Drude current. At  $E > 2E_0$ , the Drude current of electrons exceeds the soliton-driven current. Since our main interest is devoted to the soliton-driven

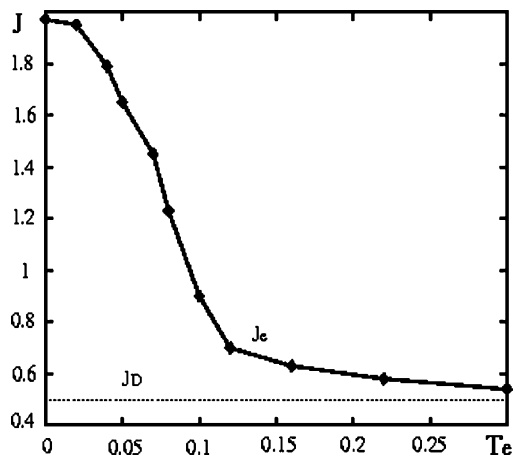


Fig. 4. Different contributions to the electric current,  $j_e$ , as a function of electron temperature,  $T = D_e$ ,  $D \ll 1$  at  $E/E_0 = 0.5$ . The dotted line shows the Drude-like current,  $j_D$ , of the electrons. Parameter values are as in Fig. 1.

current, the region  $E < 2E_0$  is the most interesting in our context. Increasing the temperature ( $D > 0$ ,  $D_e > 0$ ) may destroy the soliton or break loose electrons from the soliton. Because of the difference between the masses of ions and electrons the second effect, generally, prevails. We depict in Fig. 4 the observed temperature dependence of the electronic current for  $D \ll 1$ ,  $E/E_0 = 0.5$ . We see that the cloud of trapped electrons is stable if the electronic temperature  $T = D_e \leq 0.02$ . At  $T \geq 0.02$ , one or more electrons sometimes leave the potential well created by the soliton and form a Drude component of the electronic current during some time intervals. With increasing temperature the solitonic component of the current decreases and the Drude current grows. Accordingly, the total current tends to the Drude value,  $j_D$  (9).

The electronic current is (nearly) independent of the external field (zero differential conductivity) with much higher value than Drude's. Then in the very low range of values of  $E$  the current exhibits a gap (Fig. 3) illustrating a high conductivity near zero field. So far we did not carry out systematic studies of the temperature dependence. However, already from the existing qualitative studies we may say that the soliton-driven (highly conducting, supercritical,  $\mu > 0$ ) current is not destroyed upon increasing the temperature until reaching some higher value of temperature where the soliton-driven current is finally destroyed.

There exist other regimes, where different numbers of solitons are excited as the model-system

possesses more than one attractor. Here, we have illustrated the rich and striking dynamics of the model by considering just the case of some solitons excited in the anharmonic lattice ring where electrons could be captured and transported. Our model with  $N$  units possesses  $(N + 1)$  attractors, two of them are trivial constant rotations [Ebeling *et al.*, 2000; Makarov *et al.*, 2001; del Río *et al.*, 2003]. A special case is that of the “optical” mode which exists with  $N$  even and corresponds to antiphase oscillations of the ions. Worth emphasizing is that the actual value of the external field is of little if any significance while what really matters is its symmetry breaking role as, e.g. done by magnetic fields in the para-ferromagnetic transition in equilibrium.

It is difficult to refrain from speculating about the possible significance of the findings reported here for the understanding of some form of high- $T$  superconductivity. There is ground for serious speculation. On the one hand, evidence (theory, numerics, and experimental) [Nepomnyashchy *et al.*, 2002; Nekorkin & Velarde, 2002] supports the claim that, in the presence of dissipation, solitary waves and, eventually, solitons and solitonic wave trains can be excited and may survive if an appropriate input–output energy balance exists in the system. Solitary waves or solitons, in the moving frame, appear as a kind of dissipative structures [Nicolis & Prigogine, 1977; Velarde, 2004]. Such balance is to be added to, e.g. a (local) nonlinearity–dispersion balance defining the solitary wave, as in the Boussinesq–Korteweg–de Vries (B–KdV) equation [Zabusky & Kruskal, 1965; Nepomnyashchy *et al.*, 2002; Nekorkin & Velarde, 2002]. Another similar case could be the balance between nonlinearity and diffraction leading to the nonlinear (envelope) Schrödinger equation describing optical solitons [Akhmediev & Ankiewicz, 1997]. On the other hand, the B–KdV equation is the continuum limit of the lattice with cubic power law potential used by Fermi *et al.*, [1965]. Real solids ought to exhibit anharmonic excitations like solitons [Payton III *et al.*, 1967; Krumhansl & Schrieffer, 1975; Lee, 1987; Davydov, 1991] and do exhibit dissipation with flow currents. Our Toda–Rayleigh system, or dissipative Toda lattice, exhibits both solitons and dissipation while allowing transition from linear conduction to solitonic conduction. Such a transition bears similarity with those found in other non-equilibrium systems [Nicolis & Prigogine, 1977; Normand *et al.*, 1977].

In view of the results reported here, one can safely say that the following new phenomena are to be expected:

- (i) In many (complex enough) materials, solitonic modes should be observable by suitable excitation of their (nonlinear) lattice dynamics. Solitons, however difficult to find, should not be considered as exotic lattice excitations, void of practical interest. Indeed, the role of solitons is well established in conducting polymers [Yu, 1988; Heeger *et al.*, 1988]. Furthermore, this point is far from abstract when we foresee application to conducting materials as complex as the recently found high-T superconductors.
- (ii) If solitons can be excited in a conducting material, at intermediate temperatures and as the temperature is lowered, the passage from linear to nonlinear lattice excitations ought to be observable in its dynamic structure factor or response using thermal neutrons.
- (iii) Applying an electric field, besides Ohmic linear currents, solectronic currents should be observable in (complex enough) conductors at intermediate (not too high) temperatures, albeit as decaying fluctuations.
- (iv) As the temperature is lowered enough, the above mentioned solectronic currents would be surviving for longer and longer time intervals. Then at a certain (critical) temperature the fluctuations ought to survive as “residual” currents (hence when the field goes to zero).
- (v) As demonstrated in this work, for a system with dissipation capable of experiencing self-organization, and a disorder–order transition leading to solitons, such a soliton-driven current corresponds to a “free ride” on top of the nonlinear waves in addition to the Ohmic linear current. This is very much like the free ride that a surfer experiences when placing him- or herself on top of an (appropriate) wave approaching the sea-shore. Surf-waves like solitary waves in rivers (bore and otherwise; moving downstream or upstream) are waves of translation that travel much faster than the base mean flow.

Finally, it is noteworthy that the known high-T superconducting materials exhibit quite a low electric conductance in the normal state. Measurements have also shown that the conductivity comes with  $1/f$  noise when approaching the transition temperature,  $T_c$  [Maeda *et al.*, 1989]. In terms of

the simple model-problem presented here, does the nonlinear dynamics of the system use white noise to self-organize leading to the solitonic state and then evacuating  $1/f$  noise? [Klimontovich, 1990; Ebeling *et al.*, 2000]. We plan to address this question in a future publication, where we shall provide further results, details of the computer simulations, a discussion of the role of noise/temperature, the fluctuation–dissipation theorem in the general case (and, in particular, with *active* friction), the quantum mechanical description of the electron-ion interaction, the interaction between electrons, and also of the role of the electric field in the case of just *passive* friction. A study of the more complete Morse (including appropriate attraction, and hence akin to the Lennard–Jones) potential model-problem will also be given elsewhere.

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