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Anharmonic Excitations, Time Correlations and Electric Conductivity

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1 Introduction

In a recent letter [1] a soliton-mediated new form of non-Ohmic, relatively fast electric conduction has been proposed. Further details about the dynamics and statistical mechanics of the lattice system and the proposed transport process have been provided in several other publications [2–8]. Besides the general theory [1, 4, 5, 7] we developed the theory in two different lines: (i) applications to the conductivity of gaseous and solid state plasmas [2], (ii) applications to biomolecules [3, 6].

Here we will follow only the first line, having our main attention to quantum effects. The central idea of our model is that the electron carrier is a *supersonic* solitary wave or (periodic) wave train that builds upon the anharmonicity of (positive) ion interactions. In Ref. [1], where a transition from Ohmic to non-Ohmic conductions is predicted, the carrier is a *dissipative* soliton that dynamically binds the electron. The concept of dissipative soliton has been shown of utility in fluid dynamics, in active lattices, nonlinear optics and lasers [9–13]. Although the proposed soliton-mediated transport seems to offer universal features yet the theory above referred suffers from various limitations. On the one hand it comes from the study of one-dimensional (1D) anharmonic lattices. It follows closely the phenomenological Drude - Lorentz approach to electric conduction [14–16]. Further, the original analysis [1] was based on classical mechanics and electromagnetism with no use of quantum mechanics.

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This was overcome in subsequent publications [3,6] without affecting the essence and hence the apparent universality of the finding: solitons in a nonlinear (anharmonic) lattice can be carriers of electricity. To a certain extent this finding should be of no surprise in view of the soliton-mediated Ohmic electric conduction found in polymers like polyacetylene [17, 18]. The supersonic soliton carrier proposed in Ref. [1] comes from anharmonicity in the lattice dynamics before the electron-lattice interaction is introduced. When the latter is added we can foresee a redefinition of the evolution with a new effective anharmonic Hamiltonian incorporating the Toda-Morse like exponential interaction [3, 6].

Fig. 1 taken from Refs. [5, 8] illustrates a snapshot of a portion of the periodic potential landscape (mostly harmonic plus a soliton-induced deeper minimum) offered by positive ions to an electron when compressions in the lattice are strong enough and there is Coulomb interaction between the electron and ion charges (note that each peak of a periodic cnoidal wave found in anharmonic lattices [8] behaves solitonically like an isolated soliton).

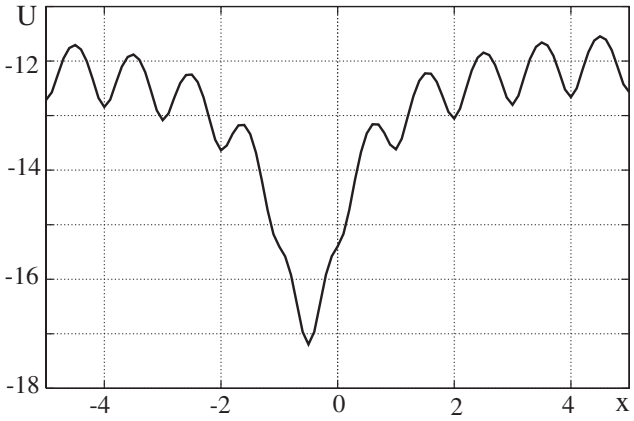

Fig. 1 Snapshot of the typical periodic landscape of the local electric potential created by the solitonic excitation along an ion lattice. The minimum corresponds to a local compression of ions which means an enhanced charge density.

In view of the above in the present work we have taken a more general perspective by looking at the problem from the general approach provided by the linear response transport theory [14, 19, 20], thus connecting transport coefficients like electric conductivity with equilibrium correlation functions. One advantage of this method is that the formulation is independent of the dimension of the sample. From such a perspective we have a theory valid also in two-dimensional or quasi-twodimensional materials in a heat bath without assuming external driving of the excitations, thus overcoming one of the mentioned shortcomings of earlier work [1–6, 8]. Before embarking in such an approach it is worth recalling a few features about electric transport in electron-ion systems.

Present-day theories of thermal and electric transport processes in electron-ion systems like solids or plasmas do take into account different elementary excitations like phonons, polarons, plasmons, and excitons [15, 16, 21, 22]. For a survey of transport theory of dense Coulombic systems including solids and dense plasmas we refer to [23–26].

Here we concentrate on the effects of anharmonicity leading to soliton excitations on electrical transport. As the interference of electron modes with phonon modes is well understood it is thus clear why we shall explore the possibility of interference of electrons with soliton modes. We cannot expect that this will occur under standard conditions. However it seems to be possible in cases where anharmonic excitations play a key role i.e. when we have strong local compressions in the lattice as needed for the prediction made in Ref. [1].

As side remarks let us mention that there are several experimental observations which suggest that in some conducting systems anharmonic effects and solitons may play a key role. For instance, the resistivity anomalies and non-Ohmic behavior observed already in early studies on TTF-TCNQ and $NbSe_3$-samples [27] or in order to explain the observed non-Ohmic effects as well as phenomena found in some high-temperature superconductors, soliton excitation has been proposed [28–30].

Long ago Müller [31] underlined the possible role of "strongly anharmonic phonons due to spin excitations". He proposed a model of anharmonic vibrations of apical oxygen interacting with carriers in CuO_2 planes. Later, Zhao *et al* [32] reported results of magnetization and thermal expansion measurements on samples of copper oxide superconductors advocating "that polaronic charge carriers exist and condensate into Cooper pairs ...". More recently, Gweon *et al* [33] have suggested a dynamical spin-Peierls picture, where the pairing of electrons mutually enhance each other. Further, these authors have proposed to use the term "phonon" loosely to denote quanta of lattice vibrations including spatially localized ones. Clearly, such excitations like so-called anharmonic

phonons or highly deformed phonons are nothing more than solitons in the currently used nonlinear nomenclature [9, 11, 34, 35].
The above comments justify to some extent the interest of our earlier work [1, 2, 4, 5, 8] where we have shown that the dynamics of ion rings with Toda or Morse interactions leads to soliton-like excitations and the already mentioned electron-soliton dynamic bound states (for simplicity denoted by solectrons). The rather deep potential well (Fig. 1) moving (right to left or left to right) along the ion lattice can indeed capture a light electron. Note that when the electron is bound to follow the soliton travel it changes ion partner as the wave moves.

2 Time-correlations and conductivity in simple models

2.1 The Drude-Lorentz model

Since e^2 is a universal constant which is fixed, this corresponds to rather stiff lattices, i.e. large values of ω_0, which, in general, may be reached only in strongly compressed lattices. The dimensionless lattice stiffness constant is $B = b_0 r_0 = 1$. Note that the equivalent stiffness in the Toda lattice would be $b_0 \approx 2 - 3$ [5, 8]. For the friction parameters we took $\gamma_i = 0.02$ and $\gamma_e = 0.002$. The ion lattice temperature is given in $m\omega_0^2 r_0^2$ units. Let us first consider the results for a relatively low temperature $T = 0.005$. Fig. 2 (left part) illustrates the time-dependence of the electron velocities. There is random behavior with spectrum decaying like ω^{-2}. To place later developments in context let us recall the early (classical) theories of conductivity in electron-ion systems taking into account scattering and dissipation [14]. The Drude (1900)-Lorentz (1904) "ansatz" is based on the asumption that the electrons are accelerated in the electric field, thus gaining energy, while in balance they loose it by collisions with the ions thus exciting dissipative modes in the lattice. The final outcome is a stationary current in the external field. In the simplest approximation we may assume that the dissipative dynamics of the electrons is characterized by an *effective* collision frequency. Then we can write

$$v(t) = v(t_0) \exp[-\nu(t - t_0)], \tag{1}$$

where v denotes electron velocity and ν is a collision frequency. The relaxation time is $\tau = \frac{1}{\nu}$. This simple model yields a velocity correlation function of exponential type. Defining the velocity autocorrelation function by

$$A_v(\tau) = \lim \frac{1}{T} \int_0^{T-\tau} dt_0 v(t_0 + \tau) v(t_0), \tag{2}$$

using (1) we get

$$A_v(\tau) = \langle v(\tau) v(0) \rangle = \left\langle v^2 \right\rangle \exp(-\nu|\tau|). \tag{3}$$

The corresponding Fourier transform (power spectrum) reads

$$S_v(\omega) = \langle vv \rangle_\omega = \int_{-\infty}^{\infty} d\tau A(\tau) \exp(i\omega\tau), \tag{4}$$

which for the simple model (1) yields

$$S_v(\omega) = \langle vv \rangle_\omega = \frac{2 \left\langle v^2 \right\rangle \nu}{\omega^2 + \nu^2}. \tag{5}$$

Noteworthy is the characteristic ω^{-2} decay of the spectrum. Then the linear response theory for the static conductivity leads to Drude's formula:

$$\sigma = ne^2 \frac{S_v(\omega = 0)}{2m_e \left\langle v^2 \right\rangle} = \frac{ne^2}{m_e \nu}, \tag{6}$$

where e denotes electric charge (of negative value for electrons), n is the number density ($n = N/L$ with N denoting the number of electrons and L the system length) and m_e electron mass.

2.2 Model conducting nonlinear lattice

Before proceeding to the more general case let us still continue analyzing the problem in 1D in order to assess the influence of nonlinear excitations on the conductivity. We take a quasi-classical electron dynamics and consider a 1D-system consisting of N classical ions and N electrons with periodic boundary conditions (ions are placed on a lattice of length L). For the *light* electrons we assume following Drude's model that they obey classical dynamics. However, instead of a phenomenological damping we include coupling of the electron motion to the nonlinear lattice dynamics with ten heavier ions. In the numerical simulations we consider the lattice units with mass m. The ion particles are described by coordinates $x_j(t)$ and velocities $v_j(t)$, $j = 1, \ldots, N$ ($N = 10$),

$$x_{j+N} = x_j + L. \tag{7}$$

The ions repel each other by Coulomb law and in addition by still stronger repulsive forces induced by the (screened) ion cores $V_{ii}(r)$ with $r = x_{j+1} - x_j$. The subscript "i" denotes ion. Let us assume that the average distance between the ions in the lattice is r_0 ($r_0 = L/N$). We approximate the interaction of ions locally around r_0 by a Toda-like exponential using the Taylor expansion

$$V_{ii}(r - r_0) \simeq V_{ii}(r_0) + V'_{ii}(r_0)(r - r_0) + \frac{m\omega_0^2}{b_0^2}\left\{\exp\left[-b_0(r - r_0)\right] - 1 + b_0(r - r_0)\right\}, \tag{8}$$

with

$$m\omega_0^2 = V''_{ii}(r_0); \qquad b_0 = -\frac{V'''_{ii}(r_0)}{V''_{ii}(r_0)}. \tag{9}$$

Note that here ω_0 refers to the lattice dynamics while ω in Eq. (6) refers to Fourier frequency. This local approximation is correct up to the third order and higher orders are approximated by an exponential series. This approximation works if the lattice forces are strongly repulsive. The great advantage of this method (as shown in [5]) is that the forces have a Toda-like shape which allows some analytical estimates for the excitations. In fact, the constant and the linear contributions to the expansion in Eq. (8) are irrelevant in a system with periodic continuation and what remains is a Toda chain, which allows in part analytical treatment. Cutting the Taylor series after the third or fourth power leads to a Fermi-Pasta-Ulam-type potential. Several authors seem to believe, that a Fermi-Pasta-Ulam-type potential is "better" suited for modelling physical properties than an exponential-type potential. The argument is, that exponential potentials belong to the class of integrable systems and that integrability is a highly nongeneric feature. Our counterargument is that there is no proof that integrable potentials and nonintegrable potentials in their immediate neighbourhood lead to different physical properties. In the opposite, all our simulations have shown that potentials which are close to each other (in functional respect) lead to very similar physical properties.

Let us consider now the "electrons". These are interacting with the lattice units or ions by a potential U_e and, as earlier indicated, obey classical equations of motion as a kind of "Drude-Lorentz-Debye dynamics", with "noise" generated by the collisions with the ions in the lattice,

$$\frac{dv_e}{dt} + \frac{1}{m_e}\frac{\partial U_e}{\partial y_e} = -\gamma_e v_e. \tag{10}$$

The quantity γ_e is the relaxation time due to the electron dissipation $\gamma_e \propto 1/\tau_e$, with τ_e accounting for the decay time scale. Assumption (10) with respect to the electron dynamics is not very realistic. It provides, however, a model which can be easily treated by numerical simulations. It suffices to show, how the dynamical clusters created by soliton excitations act on the electrons. Recall that as earlier noted, a quantum-mechanical treatment of the electron dynamics within the tight-binding approximation has been given elsewhere [3, 6].

In regions where anharmonic, supersonic soliton waves play significant dynamical role as e.g. solectrons, we expect long lasting correlations extending over the solectron lifetime, before the exponential decay starts. Possibly, there might be even maxima at finite times, due to nonlinear effects.

In the numerical simulations we have used a Langevin dynamics for the ions. The electron-ion interaction was modelled by a Coulomb force with appropriate cut-off, h, at small distance. In general, this interaction consists

of a Coulombic tail and short-range pseudopotential modelling the interaction of the electron with the screened hence inpenetrable ion cores. This leads to a finite value of the pseudopotential at zero distance [37,38]. We take

$$V_i(x-x_i) = -\frac{ee_i}{\sqrt{(x-x_i)^2+h^2}}. \tag{11}$$

The potential (11) has a minimum value $V_{min} = -(ee_i/h)$, where $h \simeq r_0/2$ is a free parameter which determines the value of the short-range cut-off. In the presence of random forces (hence non zero temperature) and also external forces the dynamics of lattice units with mass m is described by the Langevin equations ($j = 1, 2, .., N$)

$$\frac{dv_j}{dt} + \frac{1}{m}\frac{\partial(U+U_e)}{\partial x_j} = -\gamma_i v_j + \sqrt{2D_v}\,\xi_j(t), \tag{12}$$

governing the stochastic motion of the jth particle on the lattice (recall that here for illustration, $j = 1, .., 10$). The stochastic forces (with diffusion coefficient D_v) $\sqrt{2D_v}\,\xi_j(t)$ model a surrounding heat bath (Gaussian white noise). The term with γ_i describes the standard friction frequency acting on the ions in the lattice from the side of the surrounding heat bath. The validity of an Einstein relation is assumed

$$D_v = k_B T\gamma_i/m, \tag{13}$$

where T is the temperature of the heat bath and k_B is Boltzmann's constant. Note that due to mass differences $m_e\gamma_e \ll m\gamma_i$. The potential energy stored in the lattice reads

$$U = \sum_{j=1}^{N} U(r_j). \tag{14}$$

In the numerical simulations r_0 is the length unit and ω_0^{-1} is the time unit. The ratio between Coulomb and short range forces on the mean distance r_0 is assumed to be rather small

$$\eta = \frac{e^2/r_0^2}{m\omega_0^2 r_0} \simeq 0.001. \tag{15}$$

Since e^2 is a universal constant which is fixed, this corresponds to rather stiff lattices, i.e. large values of ω_0, which, in general, may be reached only in strongly compressed lattices. The dimensionless lattice stiffness constant is $B = b_0 r_0 = 1$. Note that the equivalent stiffness in the Toda lattice would be $b_0 \approx 2 - 3$ [5,8]. For the friction parameters we took $\gamma_i = 0.02$ and $\gamma_e = 0.002$. The ion lattice temperature is given in $m\omega_0^2 r_0^2$ units. Let us first consider the results for a relatively low temperature $T = 0.005$.

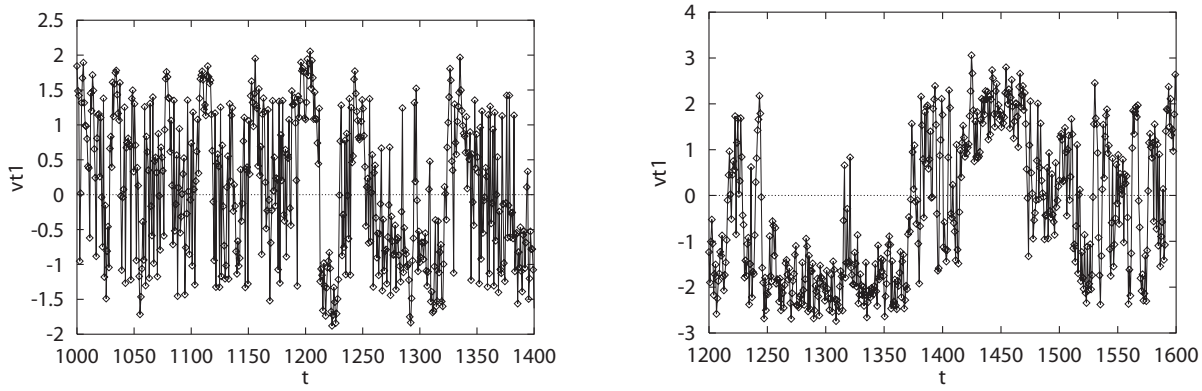

Fig. 2 Typical shapes of the (clsasical) electronic velocity as a function of time. Left figure: trajectory of the electron velocity for a time interval at a low temperature $T = 0.005$; Right figure: electron velocity for a time interval when the temperature is much higher $T = 0.075$ (for the corresponding spectrum see Fig. 4).

Fig. 2 (left part) illustrates the time-dependence of the electron velocities. There is random behavior with spectrum decaying like ω^{-2}. In Fig. 2 (right part) we also show a result for the higher temperature $T \simeq 0.075$, thus allowing further nonlinear excitations. The electron velocities exhibit long lasting coherence with corresponding signature in the low-frequency part of the spectrum. A comparison of the shape of the velocity-velocity correlation function for the two temperatures indicated above is shown in Fig. 3. We clearly see that with increasing temperature also the range of the velocity-velocity correlations increases. However, above $T = 0.075$ the long correlations are destroyed again. Hence such long lasting correlations are specific for a particular temperature range.

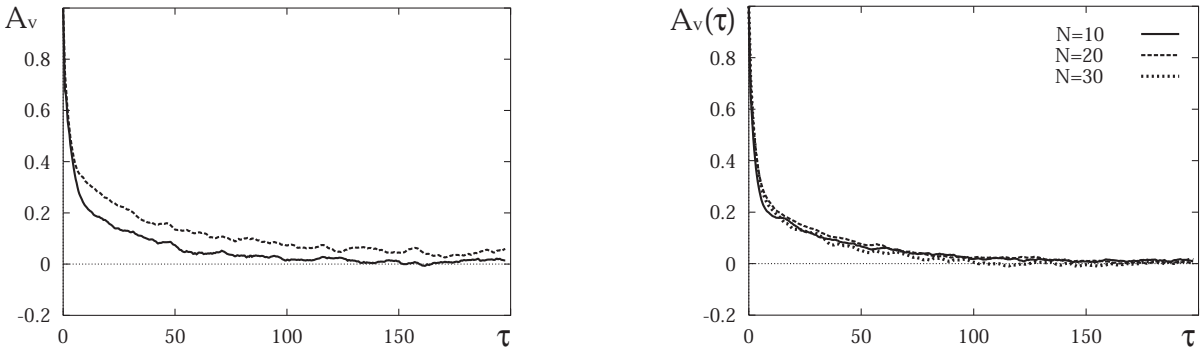

Fig. 3 Velocity-velocity correlation function (3) of the electrons. Left panel: Simulations at $T = 0.005$ (lower curves) and $T = 0.075$ (upper curves). The correlations were calculated by averaging over the ensemble of the ten electrons. Right panel: Comparison of simulations for $N = 10, 20, 30$ ions which show that the stability with respect to N is sufficient.

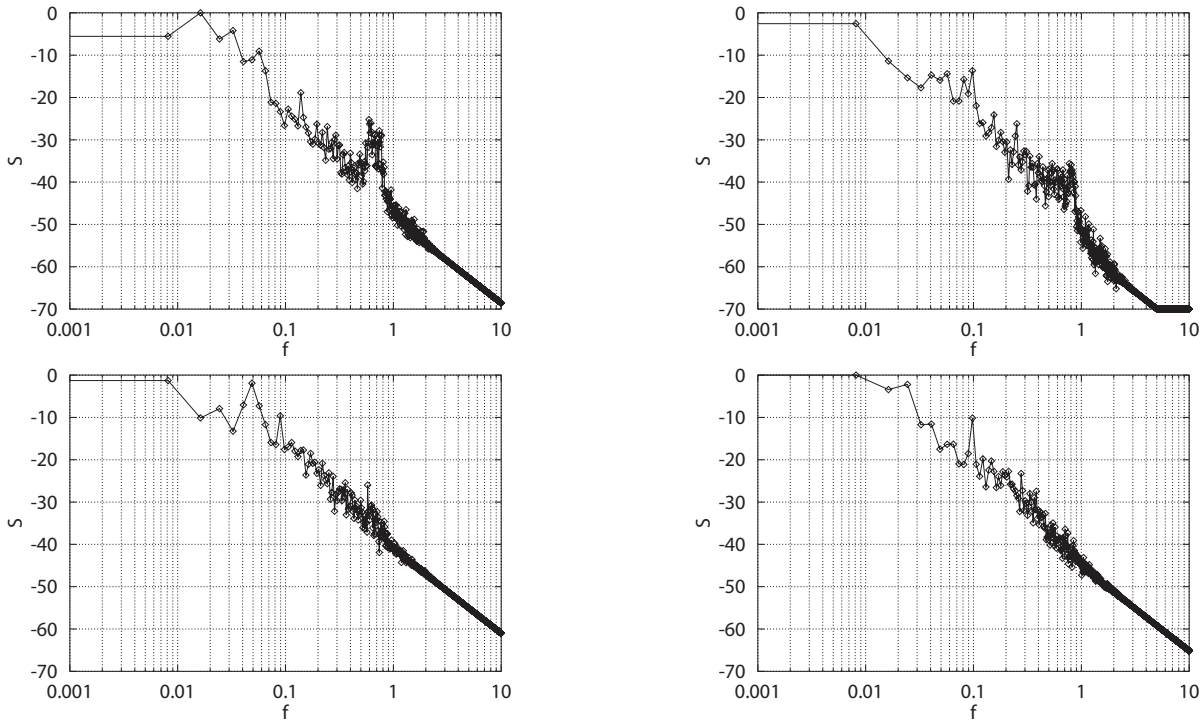

Fig. 4 Spectral power distributions as a function of the frequency ($f = \omega/2\pi$). Upper panels: Simulations at relatively low temperatures of the ion lattice (left: $T = 0.015$; righ:t $T = 0.025$. Lower panels: Simulatons near the critical temperature (left: $T = 0.075$); and at an overcritical temperature (right: $T = 0.100$).

In Fig. 4 where we compare the spectral power densities for several temperatures including the transition temperature $T \simeq 0.075$. These results indicate that $T \simeq 0.075$ is the optimal temperature for the formation of coherent long-range velocity structures. But this same temperature corresponds to the value where the specific heat per unit length of the lattice ($c_v \simeq 3/4$) shows the transition between the ordered (solid-like) and the disordered (gas-like) lattice. Recall that for the Toda lattice [8, 39]

$$k_B T_{tr} \simeq 0.15 \frac{m\omega_0^2 r_0}{b_0}, \tag{16}$$

that for $b_0 \approx 2/r_0$, $\omega_0 = 1$ and $r_0 = 1$, yields $T_{tr} \approx 0.075$.

Let us estimate now the influence of soliton modes on electron transport. Our earlier studies of the current-voltage characteristics, indicate that the low-field conductivity strongly increases [1, 2, 5, 8]. In order to study the influence of long lasting correlations on transport we have to consider long trajectories of the electrons. According to the linear response transport theory the equilibrium velocity-velocity correlations are directly connected to the conductivity [14, 20]. Here the conductivity of the electron system is

$$\sigma = ne^2 \left(\left\langle v^2 \right\rangle / k_B T \right) \int_0^\infty A_v(\tau) d\tau, \tag{17}$$

with

$$A_v(\tau) = \langle v(\tau) v(0) \rangle \, / \left\langle v^2(0) \right\rangle . \tag{18}$$

The averaging refers to a "low-energetic" fraction of the electrons due to the limited length of the computer runs and the rather small number of particles used ($N = 10$). The resistivity is $\rho = \frac{1}{\sigma}$.

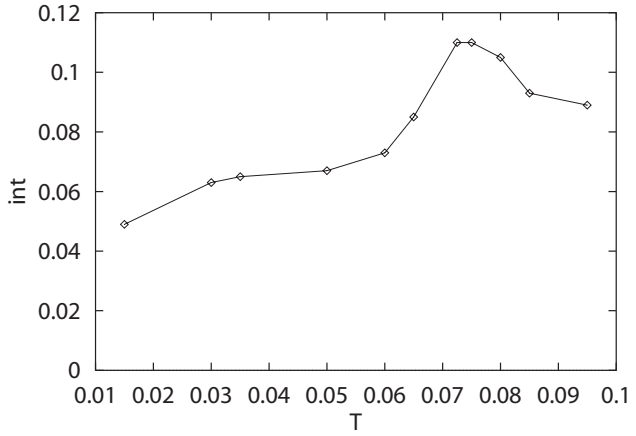

Fig. 5 The integral over the correlation function in eq. (17) as a function of the temperature. This expression corresponds to the static conductivity σ in units $ne^2 \left(\left\langle v^2 \right\rangle / k_B T \right)$.

At the start of a run the electrons were located in the minima of the ion potential landscape (Fig. 1). As time proceeds the electron temperature rises during the run and finally reaches values where the losses are compensated by the energy flow from the ions. However in the numerical simulations the final state corresponds still to rather cold electrons (having about 10 percent of the ion temperature). In order to get complete equilibrium, very long runs are needed.

Let us look at the power spectrum and the time-dependence of the velocity-velocity correlations. One sees from Figs. 2-4 that the time correlation is rather complex and significantly depends on the ion temperature. The character of the power spectrum and the time correlation function $A_v(\tau)$ change with increasing temperature (see the spectra in Fig. 4). At the lowest temperatures (upper parts of Fig. 4) we observe a fast near-exponential decay including a contribution (around $f = 1$) caused by the oscillations around the minima. These oscillations yield a peak in the power spectrum near $f = 0.9$.

With increasing temperature (lower parts of Fig. 4) a non-exponential decay appears. At $T = 0.075$ we are near to the "critical point" where we expect that solitons should play the dominant role. We see small peaks at low frequencies due to the solectronic states. These peaks are located at frequencies which are proportional to $1/N$.

This is remarkable and leads us to foresee that the corresponding conductivity peaks will move with increasing N to lower frequencies. At still higher temperatures we see again exponential decay, which corresponds to the destructions of solectrons, i.e., the electron-soliton bound states dissappear.
So far the results from numerical simulations are still preliminary, since the electrons are not quite fully thermalized, they are too cold. Still we need cold electrons to fulfil the condition that the velocity of the solitons v_{sol} has the same order of magnitude as the thermal electron velocity. In order to overcome this difficulty we have to increase the electron temperature and the soliton velocity at the same time. The latter can be done only by increasing the stiffness of the lattice. In order to estimate the influence of soliton excitations on the conductivity we calculated the integral over the velocity correlations at different temperatures. As shown in Fig. 5, the conductivity shows indeed a peak at the transition temperature, where most (thermally excited) solitons appear in the system. Thus the numerical simulations confirm our expectations: solitons are able to trap electrons, which leads to an enhancement of the conductivity in a narrow temperature region around the soliton transition temperature. In conclusion of this paragraph let us mention that the numerical simulations carried out for our 1D electron-ion model have met several serious numerical difficulties. These problems are connected with the existence of quite significant differences in the characteristic relaxation times of the system. Much longer runs will be required to reach better quantitative results.

3 Quantum transport theory including nonlinear lattice excitations

3.1 General correlation function approach

The model discussed in the previous Section is oversimplified, yet it demonstrates that the expected increase of conductivity by interactions with nonlinear excitations, may exist. In order to switch to more realistic systems we we will study now the electric transport of N electrons interacting with a classical ion system obeying nonlinear dynamics in a rather general framework. We start from the (wind-tree) Lorentz model [14] which assumes that the electrons move in a field of fixed scatterers. However at variance with the standard Lorentz model we admit here that the ions move and experience anharmonic oscillations. The ions are at time t located at the positions R_i ($i = 1, 2, ...N$). There the energy of interaction between an electron at position r and the ion number i is given by

$$V_i(r - R_i). \tag{19}$$

As in earlier discussion, in general, the interactions consists of a Coulomb tail and a short-range pseudopotential modelling the interaction of the electron with the screened ion core (11). For the discussion that follows we do not need a concrete form of the pseudopotential. We have to assume only that its Fourier transform exists

$$V_q = \int dr' V_i(r') \exp(iqr'). \tag{20}$$

Further we assume in the spirit of the Lorentz model, that the electron-electron interaction energy may be neglected. Let us denote the Hamiltonian of the electrons by H, which reads in second quantization

$$H = \sum_p \frac{p^2}{2m} a_p^+ a_p + \sum_{i=1}^{N} \sum_{p,q} V_i(q) a_{p+q}^+ a_p, \tag{21}$$

with

$$V_i(q) = \int dr \exp(iqr) V\left[r - R_i(t)\right] = \exp[iqR_i(t)] V_q, \tag{22}$$

where V_q is the above defined Fourier transform. In the special case of (11) albeit in 3D, we may approximate the potential by a horizontal part at small r and a Coulombic part at larger r. This way we get the following approximation of the Fourier transform

$$V_q \approx -4\pi \frac{e e_i}{q^2} \left[\cos(qh) - \frac{1}{qh} \sin(qh)\right]. \tag{23}$$

We assume that the ions are randomly distributed and obey Newton's classical dynamics. Then the *dynamic* structure factor of the system is

$$S(q,t) = \sum_i \sum_j \exp\left\{iq\left[R_i(t) - R_j(0)\right]\right\}, \tag{24}$$

and its Fourier transform is

$$S(q,\omega) = \int dt \exp(i\omega t) S(q,t). \tag{25}$$

Let us now, still in a first approach, assume that the electrons are also randomly distributed and follow a classical or quasiclassical dynamics. Then the linear transport theory [14] given in the previous Section may be applied. In the quantum-mechanical version we have [24]

$$\sigma = \frac{e^2}{k_B T} \left\langle v; v \right\rangle_0, \tag{26}$$

where the average is defined by ($\eta \to +0$)

$$\left\langle A; B \right\rangle_\omega = \int_{-\infty}^0 d\tau \exp[(\eta + i\omega)\tau] \frac{1}{\beta} \int_0^\beta Tr\left[\rho_0 B(\tau - i\hbar\lambda) A\right]. \tag{27}$$

In the next Section we will discuss some consequences of (26) in more detail.
There exists a different approach originally due to Zubarev [20] which is useful in our context. If the force acting on electrons is defined as

$$F = \frac{i}{\hbar}[H, P] = \sum_{p,q} \sum_i \exp\left[iqR_i(t)\right] qV_q a^+_{p+q} a_p. \tag{28}$$

Then the force-force correlation function can be expressed as

$$\left\langle F; F \right\rangle_\omega = \int_{-\infty}^0 d\tau \exp[(\eta + i\omega)\tau] \frac{1}{\beta} \int_0^\beta d\lambda \left\langle F(\tau - i\hbar\lambda) F \right\rangle. \tag{29}$$

Hence the resistivity of the electron system is [20, 24]

$$\rho = \frac{1}{\sigma} = \frac{\Omega}{3N^2 e^2} \left\langle F(\eta); F \right\rangle. \tag{30}$$

A higher order approximation reads [24]

$$\rho = \frac{1}{\sigma} = \frac{\Omega}{3N^2 e^2} \frac{\left\langle F(\eta); F \right\rangle}{1 + \frac{1}{3Nm} \left\langle P(\eta) F \right\rangle}. \tag{31}$$

The second term in the denominator (relaxation function) is a correction which takes into account the influence of the Debye relaxation effect on the conductivity [24, 40, 41]. We note that such relaxation effect is relevant only in the region of strongly nonideal plasmas. However, this term includes bound state effects. Since dynamics bound states play an important role in nonlinear conducting systems [1, 2] we have to check carefully the effect of this term. We note that positive relaxation contributions decrease the resistivity.

3.2 Frequency effects in the relaxation time approach

For the elementary Drude-Lorentz theory summarized in Section 2.1 we obtained (5) thus leading to the Drude formula for the static conductivity (6). In the same approximation the force-force correlation function reduces to

$$\left\langle F(\tau) F(0) \right\rangle = m^2 \nu^2 \left\langle v^2 \right\rangle \exp(-\nu\tau). \tag{32}$$

This leads to the (static) resistivity

$$\rho = \frac{m\nu}{ne^2}, \tag{33}$$

in accordance with the Drude formula (6).
The frequency-dependent conductivity for the Drude theory reads

$$\sigma(\omega) = \frac{ne^2\nu}{m(\nu^2+\omega^2)}. \tag{34}$$

This corresponds to the fluctuation-dissipation relation

$$\sigma(\omega) \simeq S_v(\omega). \tag{35}$$

Let us consider now the frequency dependendence going beyond the Drude theory. In the general case the frequency-dependent conductivity is the real part of the complex conductivity $\tilde{\sigma}$ which is connected with the complex dielectic function $\tilde{\epsilon}$ by

$$\tilde{\epsilon} = 1 + \frac{i}{\omega}\tilde{\sigma}; \qquad \sigma(\omega) = Re\tilde{\sigma}. \tag{36}$$

We define in the general case the collision frequency $\nu(\omega)$, which is then also a function depending on ω by

$$\sigma(\omega) = \frac{ne^2\nu(\omega)}{m[\nu(\omega)^2+\omega^2]}. \tag{37}$$

So far the discussion is completely general, the quantity $\nu(\omega)$ plays the role of an *effective* collision frequency which models the collisions affecting the electrons. The function $\nu(\omega)$ plays a central role in the relaxation time approach.
Within a perturbation-theoretical approach we get in the static case ($\omega = 0$) [24, 42]

$$\nu(0) = \frac{\pi^2 n_e e^2}{m_e} \sum_p \sum_q q^2 V_q^2 S_i(q) \delta\left[E_p - E(p+q)\right] f_e(p)[1 - f_e(p+q)]. \tag{38}$$

Here $f_e(p)$ is the electron Fermi distribution. Furthermore $S_i(q)$ is the *static* structure factor of the ion subsystem

$$S_i(q) = \int d\omega S(q,\omega). \tag{39}$$

By carrying out the integration over the momenta we get

$$\nu(0) = \frac{\pi^2 n_e e^2}{m_e} \sum_q q^2 V_q^2 S_i(q) f_e(q/2). \tag{40}$$

In a higher approximation we may take into account screening and replace the transform of the potential by an expression which is screened through the dielectric function taken in the static random phase approximation (RPA) [24]

$$V_q^2 \to \frac{V_q^2}{|\epsilon(q,0)|^2}. \tag{41}$$

In most applications, dynamical effects contained in the frequency-dependence of $S(q,\omega)$ and $\epsilon(q,\omega)$ are small and, consequently, give only small corrections. Phonon effects were discussed e.g. by Mahan [22]. Several other dynamical effects including optical response were studied by Reinholz [42]. Building upon these studies we focus on dynamical effects. The reason for this is our assumption that anharmonic dynamic effects may

play a significant role on electric transport. In order to study this we start again from Eq. (16), make the Born approximation and neglect the dynamic structure effects. This gives [23, 42]

$$\nu(\omega) = \frac{\pi n_e e^2}{m_e} \sum_q q^2 \frac{V_q^2}{|\epsilon_{RPA}(q,\omega)|^2} f_e(p+q)\,[1 - f_e(p)]\, S(q,0)\delta\left[\omega - \frac{1}{\hbar}(E_{p+q} - E_p)\right] \frac{\exp(\beta\hbar\omega) - 1}{\beta\hbar\omega}, \quad (42)$$

that for $\omega \to 0$ gives (40). Taking into account now the dynamic effects in the structure factor we find for the frequency-dependent collision frequency

$$\nu(\omega) = \frac{\pi n_e e^2}{m_e} \sum_q q^2 \frac{V_q^2}{|\epsilon_{RPA}(q,\omega)|^2} f_e(p+q)\,[1 - f_e(p)]\, S\left[q, \omega + \frac{1}{\hbar}(E_{p+q} - E_p)\right] \frac{\exp\,[\beta(E_{p+q} - E_p)]}{\beta(E_{p+q} - E_p)}. \quad (43)$$

This is a rather general formula which takes into account (in the Born approximation) the quantum effects (Heisenberg and Pauli effects) as well as all dynamical effects connected with the motion of the ions through the classical *dynamic* structure factor of the ionic subsystem. The frequency-dependent conductivity of the plasma follows from eq. (37).

3.3 The *dynamic* structure factor of nonlinear lattices and an estimate of its influence on conductivity

The function $S(q,\omega)$ for classical systems of particles is known from theoretical estimates [43, 44] and from experimental studies based on investigations of neutron scattering. However at present no experimental data seem to be available which are precise enough, to be used for conductivity calculations including the full q,ω-spectrum.

For 1D systems, features of the dynamic structure factor are available for several models of intermolecular forces [45]. In order to give an example illustrating the general structure we have computed the *dynamic* structure factor for our Toda lattice with $N = 10$ units imposing periodic boundary conditions [46]. The result is shown in Fig. 6 (see also [8] for a detailed discussion of this problem). The effective temperature was chosen such that it corresponds to the transition region from the ordered (solid-like) lattice to (gas-like) disorder. We see a pronounced soliton peak at ω_{sol} near to the frequency corresponding to twice the velocity of the first (longest) phonon and further peaks at several (lower) combination frequencies. Note, however, that the knowledge about dynamic structure factors for two- and three-dimensional conductors is quite limited [44, 47, 48].

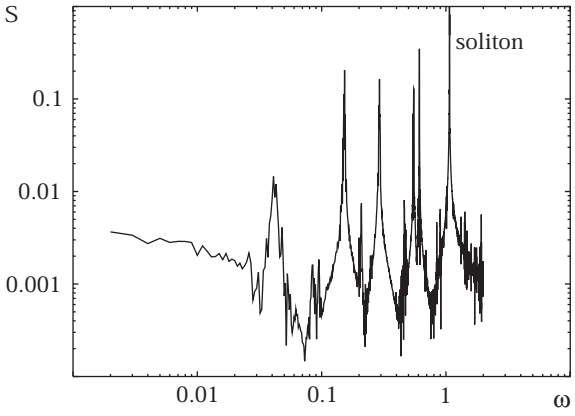

Fig. 6 Dynamic structure factor $S(k,\omega)$ of an anharmonic lattice with exponential repulsion, calculated for $N = 10$ with periodic boundary conditions as a function of ω. The temperature range embraces the transition region from periodic (solid-like) order to (gas-like) disorder. We see a pronounced soliton peak denoted by $(soliton)$ near to the frequency ω_{sol} corresponding to twice the velocity of the first (longest) phonon and further several peaks corresponding to (lower) combination frequencies. For a detailed discussion of the method see Ref. [7, 8, 46].

The functional form of the dynamic structure factor is so difficult that a quantitative integration of the conductivity formula eq. (43) including the full $\omega-$dependence is hopeless with the low accuracy of the available structure factors. We may however estimate at least the direction of the changes due to solitonic effects. As to be seen from the existing investigations (see e.g. [7, 8, 45, 46, 49]), as well as from our Fig. 6, the solitonic contribution to the dynamical structure factor is in some approximation expressed by a δ-like peak at higher frequencies.

$$S(q,\omega) = (1 - \Theta((T))S(q)\delta(\omega) + \Theta(T)S(q)\delta(\omega - \omega_{sol}) \quad (44)$$

As to be seen from eq. (43), the corresponding contributions to the collision frequency yields - beside the normal term - a contribution to the integral at relatively high energy transfer in scattering events. Scattering events which excite or destroy a relative energy-rich soliton are rather seldom, we may omit in a first approximation their contribution to the integral in (43). This way, the solitonic effects may be estimated by a temperature-dependent change of the static structure factor similar as found by Mertens and Büttner [49]. This leads to the following estimate of the quantum-mechanical static collision frequency and the corresponding conductivity

$$\nu(0) = \nu_0(0)(1 - \Theta(T)); \qquad \sigma(0) = \frac{\sigma_0(0)}{1 - \Theta(T)} \tag{45}$$

where $\Theta(T)$ is the fraction of soliton contributions to the static structure factor in dependence on the temperature. This dependence was discussed in [7] and [46] and several values of this function were estimated by Mertens and Büttner [49]. In [7] and [46] was pointed out that the solitonic contribution behaves approximately as the derivatice of the specific heat. The available information on the temperature dependence of the solitonic contributions was used in the estimates presented in Fig. 7a. It should be underlined that this procedure to estimate the conductivity after eq. (43) may give only a rough approximation. It is encouraging however to see the qualitative agreement between the classical calculation of the conductivity given in Fig. 3 and the the quantum-mecahnical estimate presented in Fig. 7b.

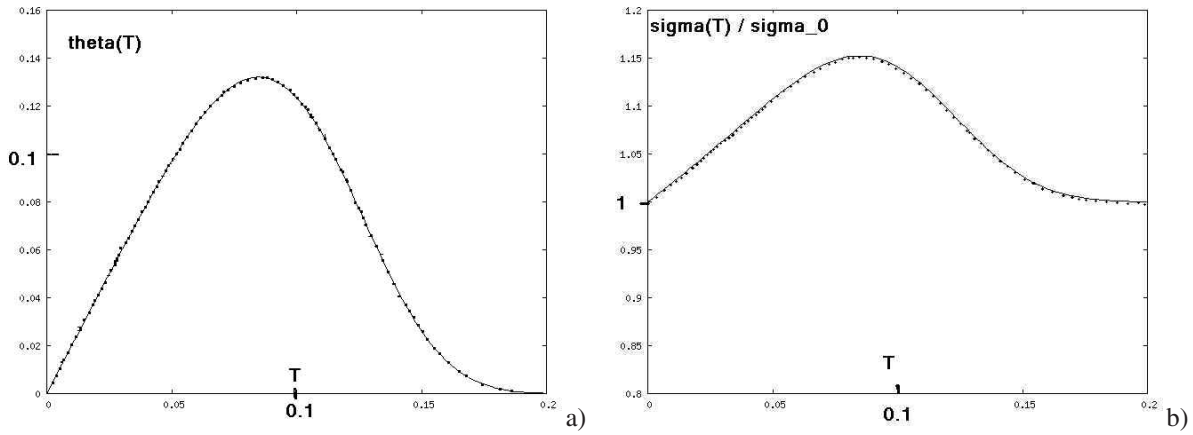

Fig. 7 Left panel: The fraction of solitonic contributions to the static structure factor $S(k)$ in dependence of temperature for a 1D- lattice with exponential repulsion based on the estimates of the relative soliton contributions given in [7, 46, 49]. Right panel: The corresponding estimate of the quantum-mechanical conductivity after eq. (43) in relation to the case without taking into account the dynamic effects.

4 Discussion

We have shown by using time correlations and dynamical structure factors, that the role of nonlinear anharmonic excitations may be significant in conducting lattices. First we have discussed the general dependence of the transport coefficient on the power spectrum of equilibrium correlations and, in particular, on the dynamic structure factor. In principle this connection is known, but so far it has been stated mostly that dynamic effects on conductivity are very small. In spite of the fact that the structure of the ion lattice has a big effect on transport through the static structure factor $S(q)$, the effect of the frequency-dependence gives in general only a small correction. In this respect a remarkable exclusion is the low-temperature superconductivity (BCS) which depends essentially on dynamical effects based on (linear) phonon excitations.

Solitons are hard excitations of the lattice which have a long lasting time correlation and influence a characteristic part of the spectrum. They are local deformations propagating with a *supersonic* soliton velocity v_{sol} which strongly increases with the increase in the stiffness of the lattice. As the soliton velocity is much smaller than the thermal velocity of the electrons, the interaction between soliton-like waves and electrons is weak, since an effective interplay requires that the concentration of electron in the region of the soliton velocity is sufficiently high. In fact electrons captured certain time by solitonic excitations are only weakly affected by scattering processes.

We have used this property for estimating the contribution of solitonic excitations to the collision frequency in Born approximation.
An example of how the interplay between electrons and waves works, is the Landau damping; here wave velocity and thermal velocity should be of same order. In our case we need that the thermal velocity of the electrons be such that $v_{th} \simeq v_{sol}$. This condition is difficult to fulfill and demands strong anharmonic effects.
We have demonstrated here for a simple 1D model with exponential repulsion that an interplay between electron motion and soliton excitations exists which may lead to special electron capturing effects and relatively long correlations. Further we have shown (see in particular Figs. 5 and 7) the existence of a temperature region (near to a characteristic lattice transition temperature T_{tr} which is around $10^2 K$ for typical nonlinear 1D lattices) where relatively many solitons are excited and in which certain increase of the conductivity due to dynamic effects of at least 10-20 percent may be expected.
A study of more realistic 2D and 3D models including quantum effects is possible on the basis of the formulae given in Section 3. However this requires precise data about the dynamic structure factor including the soliton peaks, which are not yet available with the needed accuracy. This remains as a task for future work.

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