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High Conductivity Mediated by Thermal Excitation of Solectrons*

W. Ebeling[1]**, A. P. Chetverikov**[2]***, **G. Röpke**[3]†, and **M. G. Velarde**[4]‡

[1] Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany
[2] Faculty of Physics, State University Saratov, Astrakhanskaya 83, R-410012 Saratov, Russia
[3] Institut für Physik, Universität Rostock, Universitätsplatz 3, D-18055 Rostock, Germany
[4] Instituto Pluridisciplinar, Universidad Complutense, Paseo Juan XXIII, 1, E-28040 Madrid, Spain and Fundacion Universidad Alfonso X El Sabio, Villanueva de la Canada, E-28691 Madrid, Spain

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We study the quantum dynamics and statistics of electrons interacting with nonlinear excitations of a classical thermal lattice of atoms on a semi-phenomenological basis. By theoretical estimates based on tight-binding approximations, Wigner distributions and computer simulations we show the existence of fast and nearly loss-free motions of electrons along crystallographic axes of a nonlinear lattice. Using mass-action relations we estimate the density of moving bound states between electrons and lattice solitons and estimate analytically and by simulations Wigner momentum distributions which are non-Maxwellian. Calculating the currents from these bimodal distributions we show that thermally excited solectrons in nonlinear media may lead to a considerable transport enhancement. Our estimates and simulations demonstrate that in a temperature window, where solectrons are excited and are relatively stable, conductivity and diffusion may be enhanced by up to two orders of magnitude.

1 Introduction

In a previous work we investigated the formation of moving bound states between solitons excited in nonlinear lattices and electrons hopping between the sites [1]. As shown, these so-called solectrons may have supersonic velocity, which is possibly a few $\mathrm{km/s}$. Here we intend to estimate the number density and the momentum distributions of thermally excited solectrons and to show that they may contribute to reach high values of conductivity and other related transport properties. We will show that solectron effects may help to bring thermal electrons or holes to velocities in the range of $v \simeq \mathrm{km/s}$. We note in this context that in normal conductors the velocities are in the range $v \simeq \mathrm{cm/s} - \mathrm{m/s}$. The electrical current depends on the density of the charges, the charge itself and the drift velocities or mobilities:

$$j = nev_d, \qquad v_d = \langle v \rangle = \mu E.$$

In the linear (Ohmic) case, the conductivity is given by $\sigma = ne\mu$. In general mobilities are given in the units $\mathrm{cm}^2/\mathrm{Vs}$. In these units some typical values are:
Amorphous Si: $\mu < 0.5$,
typical organic semiconductors: $\mu < 10$,
silicon at room temperature : $\mu \simeq 1400$,
graphene at low temperature $\mu \simeq 200000$,
special conducting polymers like PDA, PDATS: $\mu \simeq 200000 - 500000$,
two-dimensional degenerated electron gas at low T: $\mu \simeq 3000000$.
In order to get high conductivities we need either high density of the charges (e.g. metals), high velocity of

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** Corresponding author. E-mail: werner_ebeling@web.de
*** e-mail: ChetverikovAP@info.sgu.ru
† e-mail: gerd.roepke@uni-rostock.de
‡ e-mail: mgvelarde@pluri.ucm.es.de

the charges (Tokamaks, new polymer materials), or high charge (dusty plasma). Standard good conductors as metallic Cu, Ag, have high conductivity due to the large density of the degenerate electrons in the conduction band. Standard superconductors have also high electron density but high-temperature superconductivity is not necessarily connected with high densities. High conductivity in materials with low density of itinerant electrons is observed in special conducting polymers as in polyens (polyacetylen, polydiacetylen, etc.). We note that in such crystals drift velocities up to $5\mathrm{km/s}$ were observed experimentally by Donovan and Wilson on samples of PDA- and PDTA-crystals [2–4]. According to several authors the large drift velocities observed may be due to bound states between nonlinear lattice excitations and electrons [3–9].
In previous work we have shown the possibility of enhanced electron transport mediated by supersonic excitations [1]. Here we will consider thermal systems, estimate the density of solectrons by mass-action methods, estimate Wigner momentum distributions analytically and from simulations and calculate transport properties from these non-Maxwellian bimodal distributions.

2 Solitons and solectons in anharmonic chains

For the one-dimensional case analytical results for the problem of supersonic charge transfer in anharmonic chains were obtained first by Davydov and collaborators [6, 9]. Let us assume that we consider a rectilinear axes described by the coordinate z. According to the Davydov theory [6], the probability density of electrons $\rho_e(z,t)$ introduced by doping is closely related to the compression density $\rho(z,t)$ in a nonlinear molecular systems. Let us consider for illustration a chain of Morse molecules with the pair interaction

$$V_M(r) = D\left[\exp(-2b(r-\sigma) - 2\exp(-b(r-\sigma)\right] \simeq -D + (m/2)\omega_M^2(r-\sigma)^2 + (\gamma/3)(r-\sigma)^3 \quad (1)$$

where D, b are the depth and the stiffness, σ the lattice spacing, $\omega_0 = (b/m)\sqrt{2D}$ the oscillation frequency and $\gamma = 3Db^3$ the factor of nonlinearity of the Morse potential. A supersonic soliton creates in a Morse lattice a compression density

$$\rho(z,t) = \rho_0 \mathrm{sech}^2\kappa(\xi - st), \qquad \rho_0 = 3\frac{\omega_M^2(s^2-1)}{2\gamma}. \qquad \kappa = \frac{1}{2}\sqrt{\sigma\rho_0}, \quad (2)$$

Here $\xi = z/\sigma$ is the dimensionless coordinate and $s = v_s/v_0$ the velocity of the soliton v_s related to the sound velocity v_0. Further ρ_0 is the maximum value of the lattice deformation which depends on the soliton velocity v_s and lattice anharmonicity. In thermal systems, solitons will be created depending on temperature with some probability according to the canonical weights. At very low temperatures the density of thermal solitons increases with $AT^{1/3}$ [7, 11, 12]. The coefficient A of the increase was numerically and analytically calculated for Toda systems by several authors (see e.g. [11, 12]) as $A \simeq 0.56/T_0^{1/3}; k_BT_0 = 4a_T/3b_T$. By using the equivalence between Toda and Morse systems $a_T = 2bD/3, b_T = 3b$ we estimated the coefficient in the law $T^{1/3}$ for Morse systems and found $A \simeq 1.06$. At larger temperature the density of thermal solitons increases monotonically but cannot exceed the number of sites in the lattice. Fitting these results to some numerical data [10] we got as an estimate the curve (see Fig. 1)

$$\frac{N_s}{N} \simeq \frac{AT^{1/3} + BT}{1 + AT^{1/3} + BT}, \qquad k_BT/2D \to T. \quad (3)$$

where N is the total number of sites with the fitted constant $B \simeq 20$. Here and in the following T is the dimensionless temperature in units $2D$.

We introduce now an electron into the nonlinear lattice and investigate the bound states electron - soliton. The compression density created by solitons induces a moving potential well which may attract electrons and form rather stable bound states. According to Davydov the potential well may be represented by

$$W(z,t) = -\chi\rho(z,t) = -3\chi\frac{\omega_M^2(s^2-1)}{2\gamma}\mathrm{sech}^2[\kappa(\xi - st)] = 3\chi\frac{\omega_M^2(s^2-1)}{2\gamma}[-1 + \kappa^2(\xi - st)^2 + ...] \quad (4)$$

where χ is the parameter of electron lattice coupling. The wave function may be represented as a phase factor and an envelope function [6, 19]

$$\Psi(z,t) = \exp(i(kz - \omega t)\Psi_0(\xi), \qquad \xi = z - z_0 - v_{se}t; \qquad v_{se} = sv_s \quad (5)$$

where ξ is a running coordinate. In harmonic and adiabatic approximation the envelope of the moving ground state is bell-shaped in coordinate space and is given by

$$\Psi_0(\xi,t) \simeq C_0 \mathrm{sech}(\kappa\xi) \simeq \frac{1}{[2\pi x_0^2]^{1/4}} \exp\left[-\frac{\xi^2}{4\xi_0^2}\right], \qquad \xi_0^2 = \langle\xi_0^2\rangle = \frac{\hbar}{2m\omega_0}. \tag{6}$$

In the supersonic case the energy of our moving ground state is in harmonic approximation [19]

$$E_{se} \simeq 3\chi \frac{\omega_0^2(s^2-1)}{2\gamma}[-1+\hbar^2\kappa^2+..]. \tag{7}$$

This is a ground state for fixed value of the solectron velocity v_{se}. Note that this ground state is degenerated and the energies are the same for right and left running solectrons. The state energy is proportional to the deviation of the square of the solectron velocity from the sound velocity. Let us now estimate the formation of solectrons by mass-action relations. The density of free electrons can be given in several units, the simplest is the so-called relative occupation or doping ν_e which is defined as ratio of the number of sites occupied by an electron to the total number of sites $\nu_e = N_e/N$. Note that within our simple model, the electrons are always associated to one of the sites. In real systems the doping ν_e may vary within certain limits, in general it will not exceed the value 0.3, i.e. not more than 30 percent of sites may be occupied by electrons. Let us denote the number of solectrons by N_{se}. In some approximation we may assume that the number of solectrons and the number of free solitons $N_s - N_{se}$ are related by a mass action factor and get:

$$\frac{N_{se}}{N_s - N_{se}} = \frac{N_e}{N_s} K(T); \qquad K(T) \simeq \left(\frac{T_s}{T}\right)^{1/2} \exp\left[\frac{|E_{se}|}{T}\right]; \qquad \frac{N_{se}}{N_s} = \frac{\nu_e K(T)}{1+\nu_e K(T)} \tag{8}$$

Here $-E_{se}$ is the energy gain in forming a solectron, we may assume that this energy is usually less than 0.1 eV [6]. By using these formulae in combination with eq. (3) we estimated the fraction of solectrons N_{se}/N for two different values of the solectron energy, $|E_{se}| = 0.5D$ and for an in two times smaller value $|E_{se}| = 0.25D$ assuming for the entropic temperature $T_s \simeq 0.2$. The result is shown also in Fig. 1 for a thermal Morse lattice with 30 percent doped sites, i.e. about one third of the sites are occupied with charges. Note also that the temperature is given here in units of $2D/k_B$. We observe that the existence of solectrons on 1d Morse lattices is for realistic values of the binding energy rather concentrated on the region $T \simeq 0.05 - 0.2$. For larger temperatures the potential well of the soliton is not able to bind electrons. We note the existence of two opposite tendencies: The density of thermal solitons increases with T but their ability to bind free electrons decreases with T such, that an optimal temperature range exists.

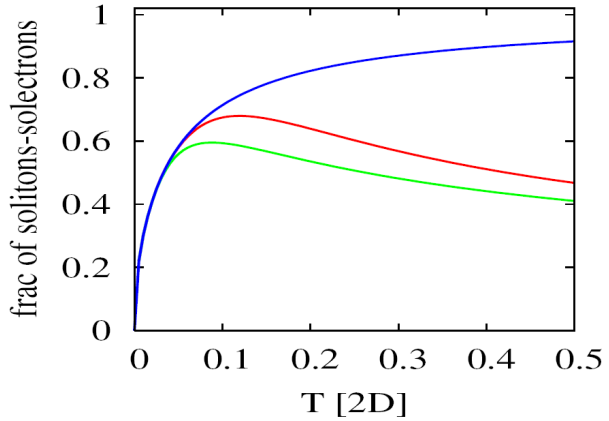

Fig. 1 Estimate of the soliton density in a thermal Morse lattice (eq.(3), upper curve, blue) and the solectron density per site after (eq.(8) (for the assumed binding energies $|E_{se}| \simeq .5D$ - 2nd curve from above, red and $|E_{se}| \simeq .25D$ - 3rd from above, green) for 30 percent doping. The temperature is given in units of $2D$ where $D \simeq 0.1$eV is the depth of the Morse potential.

3 Calculation of solectron momentum distributions

In the ground state the wave function in the momentum space is centered around the solectron momentum $p_{se} = m_{se}v_{se}$. Corresponding to the two possible directions, the ground state is degenerated, i.e. there are two states

with same energy. The wave functions are in first approximation Gaussians

$$\Phi_0^{\pm}(p_z,t) \simeq c_{\pm} \exp\left[-\frac{(p_z \pm p_{se})^2}{2m_{se}\hbar\omega_0}\right] \tag{9}$$

The corresponding density in momentum space is a product of wave functions which in the case that the two states are not overlapping can be approximated by

$$\rho_{se}(p_z,t) \simeq \frac{w_+}{\sqrt{\pi m_{se}\hbar\omega_0}} \exp\left[-\frac{(p_z - p_{se})^2}{m_{se}\hbar\omega_0}\right] + \frac{w_-}{\sqrt{\pi m_{se}\hbar\omega_0}} \exp\left[-\frac{(p_z + p_{se})^2}{m_{se}\hbar\omega_0}\right] \tag{10}$$

For systems in a heat bath at finite temperatures, the effective temperature of the ground state, which is $\hbar\omega_0/2$ has to be generalized and to be replaced by a quantum temperature. For parabolic potentials, the calculations are quite easily performed in the framework of Wigner functions [13–15] and the resulting Wigner momentum distributions for a particle in an oscillator potential at rest is

$$f(p_z) = \frac{1}{\sqrt{2\pi m k_B T_q}} \exp[-\frac{p_z^2}{2mk_BT_q}] \tag{11}$$

with an effective quantum temperature T_q which replaces the classical temperature

$$T_q = \frac{1}{2k_B}\hbar\omega_0 \coth\frac{\hbar\omega_0}{2k_BT} \tag{12}$$

We see easily the limits

$$T_q \to T \qquad \text{if} \qquad T \to \infty, \qquad k_BT_q \to \hbar\omega_0/2 \qquad \text{if} \qquad T \to 0 \tag{13}$$

In other words, this formula contains the classical as well as the quantum-mechanical case. Note that such a simple formula is valid only in the oscillator approximation.
Applying this to solectrons, the momenta have to be shifted. This way we obtain the momentum Wigner function

$$f(p_z) = \frac{w_+}{\sqrt{2\pi m k_B T_q}} \exp\left[-\frac{(p_z - p_{se})^2}{2mk_BT_q}\right] + \frac{w_-}{\sqrt{2\pi m k_B T_q}} \exp\left[-\frac{(p_z + p_{se})^2}{2mk_BT_q}\right]. \tag{14}$$

We see that the momentum Wigner function is bistable and looks very much like the quantum-mechanical density in the ground state. We have to underline however that this expression is an approximation which is valid under the assumption that the overlap of the two Gaussian hills is weak.
In the following we will try to confirm the bimodal distributions which we found by simulations. So far only a few numerical studies of the momentum and distributions for solectrons and for transport enhancement are available. In order to check the theoretical estimates for the momentum distribution given above we compare with simulations for discrete lattices. In earlier work we formulated the Hamiltonian, classical dynamical equations for a nonlinear lattice of Morse atoms as well as Schrödinger equations for the electron [16]. Then we provide numerical evidence that appropriately shaped nonlinear waves on a nonlinear lattice are indeed able to transfer electrons in a controlled way and without dispersion over distances of a few hundred lattice sites. In earlier work we studied moderate temperatures and used kinetic approximations (Pauli equations) for the electron motion [17, 18]. Here we consider the region of rather low to moderate temperatures. We solve directly the Schrödinger equations in the framework of TBA and apply an electronic Hamiltonian with distance-dependent transition probabilities [16]. We study as an example trajectories of solectrons in a 1d lattice obtained from simulations of the tight binding equations

$$\frac{dc_n}{dt} = -i\tau \exp(\alpha b\sigma) \sum_m c_m \exp(-\alpha|z_n - z_m|). \tag{15}$$

Realizations are shown in Fig. 2. Note that $z_n(t)$ is here the time-dependent coordinate of the lattice atom number n in the direction of the 1d-motion, which was calculated by solving classical Langevin eqution for Morse atoms [17, 18]. We consider in the simulation the trajectories of $N = 200$ or $N = 400$ Morse particles which were calculated from solutions of Langevin equations. We note that earlier classical simulations of solectrons described in [10] show also typical Gaussian stochastic trajectories and bimodal distributions.

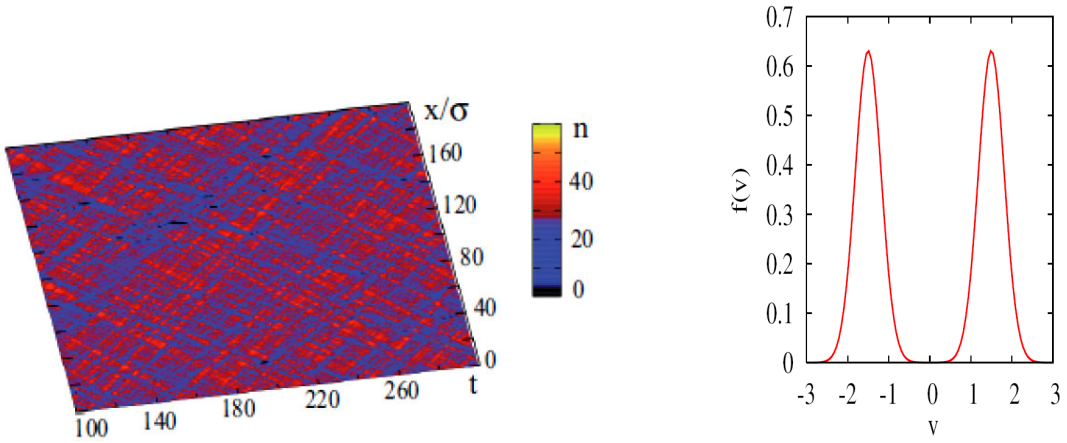

Fig. 2 Typical trajectories in a thermal solectron systems imbedded into a Morse lattice. We show the position (ordinate) over the time (abscissa) and observe left and right running solectrons to be seen as stripes. An estimate of the velocity distribution obtained from the bistable Wigner distribution for $T = 0.1$ is shown on the r.h.s.. The picture of trajectories and the distribution are at least in qualitative agreement. Parameters of simulation: $T = 0.1, b\sigma = 1, \alpha = 1.75, \tau = 10$.

4 Enhancement of transport

On the basis of the Wigner functions in momentum representation several soliton-mediated transport properties may be calculated. The mean one-particle current may be obtained by using the Wigner momentum functions:

$$j_z = \frac{e}{m_{se}} \int_{-\infty}^{+\infty} dp_z p_z f(p_z) \tag{16}$$

Assuming that we generated by appropriate initial and boundary conditions one directed solectron with velocity v_{se} moving in right or left z-direction we get the current

$$j_z^{(0)} = \frac{e}{m_{se}} \int_{-\infty}^{+\infty} dp_z p_z \frac{1}{\sqrt{2\pi m_{se} k_B T_q}} \exp\left[-\frac{(p_z \pm p_{se})^2}{2mk_B T_q}\right] = \pm e v_{se} \tag{17}$$

Here m_{se} is the effective mass of the solectron [6]). The distribution of a directed solectron is in the given approximation Gaussian and the dispersion is given by the quantum temperature. Note that the solectron velocity v_{se} is in general much larger than the Drude velocity of electrons in small and moderate electrical fields E and also larger than the thermal velocity. In thermal equilibrium the solectrons are no more uni-directed but are equally distributed between right and left. Then the fluctuations of solectrons are very large, since the solectrons may have positive and negative sound velocities what leads to current fluctuations of order $e^2 v_{se}^2$. We demonstrate these large fluctuations by simulations in the tight-binding approximation (TBA), (see Fig. 2). The mean squared velocity is in thermal equilibrium

$$\langle v^2 \rangle = \frac{\int_{-\infty}^{+\infty} dp_z (p_z/m_{se})^2 \left[\exp(-\beta_q (p_z - p_{se})^2) + \exp(-\beta_q (p_z + p_{se})^2)\right]}{\int_{-\infty}^{+\infty} dp_z \left[\exp(-\beta_q (p_z - p_{se})^2) + \exp(-\beta_q (p_z + p_{se})^2)\right]} \tag{18}$$

Carrying out the integration gives a generalized Nyquist formula for solectrons.

$$\langle v^2 \rangle = \frac{k_B T_q}{m_{se}} + v_{se}^2; \qquad \beta_q = \frac{1}{2m_{se} k_B T_q} \tag{19}$$

The mean squared velocity is the sum of a thermal part and a solectronic part. These large fluctuations are according to the Taylor-Kubo formulae related to transport. This appears as the physical reason for an enhancement of transport which we want to estimate now. The simplest (classical) estimate due to Drude (1900) and Lorentz (1904) is based on the assumption that the dissipative losses are characterized by an effective collision frequency ν_e for electrons, correspondingly we introduce ν_{se} for solectrons [10]:

$$v_e(t) = v_e(t_0) \exp[-\nu_e (t - t_0)]; \qquad v_{se}(t) = v_{se}(t_0) \exp[-\nu_{se} (t - t_0)] \tag{20}$$

The relaxation time of solectrons is $\tau_{se} = \nu_{se}^{-1}$. The simple Drude model yields for the velocity correlation function

$$A_v(t - t_0) = \langle v(t)v(t_0)\rangle = \exp(-\nu_{se}(t - t_0)]\langle v^2\rangle \tag{21}$$

and for the transport coefficients [10] as the diffusion constant and the conductivities for a single solectron

$$D_{se} = \frac{1}{\nu_{se}}\langle v^2\rangle; \qquad \sigma_{se} = \frac{e^2}{k_B T_q \nu_{se}}\langle v^2\rangle; \qquad \sigma_{se}(\omega) = \frac{e^2\nu_{se}}{k_B T_q(\nu_{se}^2 + \omega^2)}\langle v^2\rangle \tag{22}$$

According to eq. (19), the transport coefficients are enhanced in the presence of solectrons. We denote the coefficient

$$r_1(T, v_{se}) = \frac{D_{se}}{D} = \frac{\sigma_{se}}{\sigma_D} = 1 + \frac{\nu_{se} m_{se} v_{se}^2}{\nu_e k_B T_q} \tag{23}$$

as the transport enhancement factor.
Our elementary approach is consistent with the kinetic theory developed by Gogolin [5] as well as with the fluctuation - dissipation theorem (FDT) for quantum oscillators [14, 15, 20]. According to Balescu the FDT reads in the classical version

$$j_e = \frac{E}{k_B T}\int_0^\infty d\tau\langle j_e j_e(\tau)\rangle \tag{24}$$

For the special case of oscillator states the generalization for quantum oscillators with frequency ω_0 reads [**?**, 20]

$$j_e = \frac{(2/\hbar\omega_0)E}{k_B \coth(\hbar\omega_0 2k_B T)}\int_0^\infty d\tau\langle\hat{j}_e\hat{j}_e(\tau)\rangle. \tag{25}$$

The application to solectrons leads in the (rather crude) relaxation time approximation again to the formula we found in the context of Drude's approach. This way we find the following expression for low-field contribution of one solectron to the current

$$j_{se} = \frac{e^2 E}{k_B T_q \nu_{se}}\langle v^2\rangle \tag{26}$$

This way we are back to the previous formula of the Drude theory. Note that the current may also be calculated for higher fields. As shown already by Gogolin [5], this leads to a saturation with the field which was observed by Wilson [3]. Here we consider only the low field linear approximation.
The enhancement factor $r_1(T, v_{se})$ for a single solectron shows how much transport is enhanced by solectron effects compared to the Drude-Lorentz theory. The physical interpretation of our formulae for the enhancement factor is interesting: The solectronic contribution to the velocity dispersion leads to an additional term proportional to the solectron velocity squared. This shows that the relation between the solectron-driven current and the Drude Lorentz current may be very large and has a maximum for $T \to 0$ as shown in Fig. 3. Assuming as in earlier work [19] the typical set of parameters for a 1d lattice:

$$\omega_0 \simeq 10^{12}\mathrm{s}^{-1}; m_{se} \simeq 5 \cdot 10^{-25} kg: \qquad v_{se} \simeq 10^3 m/s$$

we get for the maximum of the enhancement factor the theoretical estimate (see Fig. 3)

$$r_1(T \to 0) = 1 + \frac{2m_{se}v_{se}^2}{\hbar\omega_0} \simeq 10^2 \tag{27}$$

Note that the maximum is mainly influenced by the sharpness of the minimum of the Morse potential. In a more realistic calculation we have to take into account that the formation of solectrons is bound to the existence of thermal solitons which is temperature-dependent.

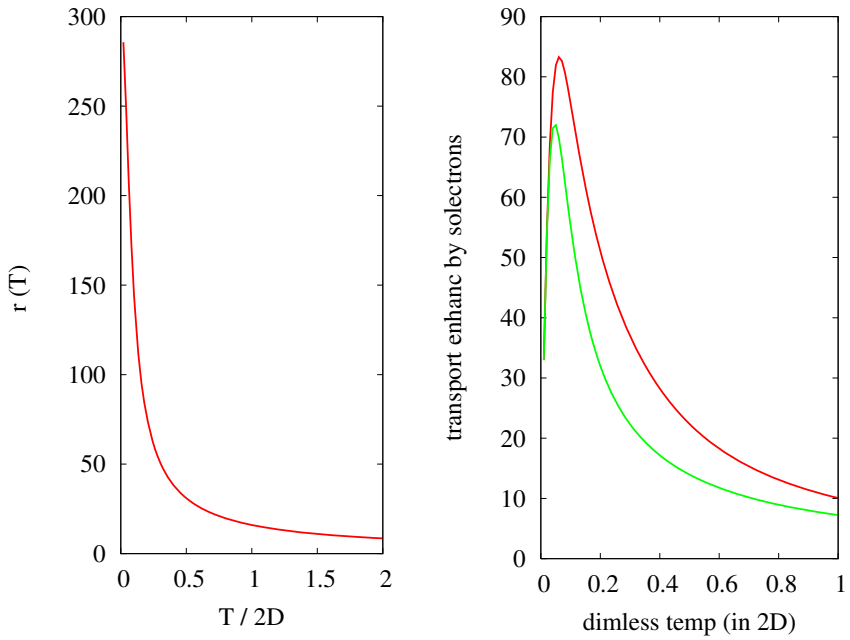

Fig. 3 Solectron-enhancement factor of transport according to the theoretical estimates obtained from Wigner distributions. Left panel: The factor of transport enhancement $r_1(T)$ due to a single solectron compared to electron transport as a function of temperature. Right panel: The enhancement factor multiplied with an estimate of the total fraction of solectrons per site two binding energies, uper curve $|E_{se}| = 0.5D$ (red), lower curve $|E_{se}| = 0.25D$ (green).

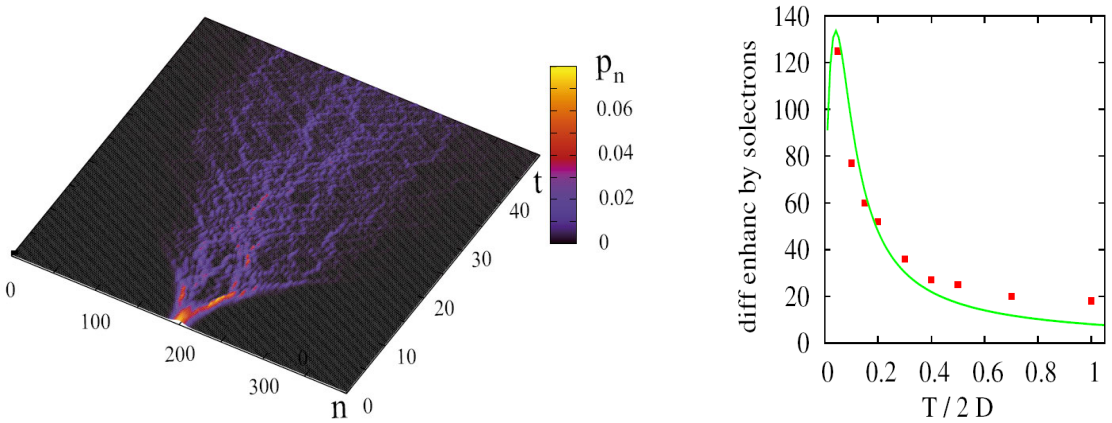

Fig. 4 Solectrons in a Morse lattice. Left panel: Example of the spreading of the electron density for the temperature $T = 0.1$ from simulations with the TBA-Schrödinger equation. The initial density condition is delta-like, concentrated around the center. Parameter values: $N = 400$, $b\sigma = 1$, $\alpha = 1.75$, and $\tau = 10$. Right panel: The points obtained from the TBA-simulations are compared with the theoretical estimate obtained above.

Taking into account the equilibrium between bound solectrons and free electrons, the formula (23) has to be modified taking into account that the enhancement refers only to the solectrons and not to the free electrons.

$$r(T) = 1 + \frac{N_{se}}{N}\frac{\nu_{se} m_{se} v_{se}^2}{\nu_e k_B T_q}; \qquad \frac{N_{se}}{N} \simeq \frac{AT^{1/3} + BT}{1 + BT}\frac{\nu_e K(T)}{1 + \nu_e K(T)}. \tag{28}$$

The factor N_{se}/N provides the relative occupation of sites with solectrons. This way we find the average enhancement per electron which is sometimes much smaller than the enhancement per solectron. We note that so far only estimates for the constants $A, B, |E_{se}|, m_{se}, v_{se}, \nu_{se}$ are known. In order to check transport enhancement

we studied numerically the temperature dependence of the mean square displacement. The problem reduces to solving coupled together both Eqs. (3) and the classical Langevin equations for the lattice for specific conditions: First we heat the system to a given temperature (e.g. $T = 0.1$ in units $2D$ in the example shown in Fig. 4). Then we inject one electron, the electron density concentrated in the center of the sample. Then we switch-off the heat bath and solve the coupled system of lattice and electron equations, in our example for delta-like initial electron densities.

For not too low temperatures the simulations show a stochastic diffusion-like trajectories. With increasing temperature the angle of the opening of the cone is decreasing. The spreading of the electron density is a complex diffusion-like process. and thermal solitons create a diffusive channel which stabilizes the electron dispersion. We compare in Fig. 4 the numerical points for the dispersion with the theoretical estimate obtained above. In the region of mean temperature the agreement is quite good, the large deviations at small temperatures are connected with the fact that at low T the process is not more diffusion- like and the mean-square displacement cannot be obtained with good precision.

5 Discussion and Conclusion

This work is devoted to charge transport, as conductance and diffusion, in thermal systems at moderate to low temperatures say around 10^2 K. We have shown that thermal solitons may be excited which may form with electrons bound states, called solectrons. At moderate temperatures solectrons are rather stable and may provide a considerable enhancement of transport as diffusion and conductance. The enhancement factor depends on the soliton density, the fraction of solectrons and their lifetime. The probability of forming solectrons reaches in the range $T \simeq 0.2 - 0.5D$ (where D is the depth of the Morse well) a maximum and then goes down again, since solectrons are not stable at higher temperatures, We show that at favorable parameter conditions, the enhancement may be considerable and reach values in the range of a factor around 10^2.

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