Towards a Theory of Degenerated Solectrons in Doped Lattices: Problems and Perspectives

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1 Introduction

In the polaron theory developed by Landau, Pekar, Fröhlich, Holstein and others, and successfully used in the study of biomolecules by Davydov, Zolotaryuk and Scott and others [1–7] the self-trapping of the electrons interacting with linear lattice oscillations (phonons) dominates. Davydov exploited the possibility of soliton excitations suitably using the above mentioned nonlinearity. He then identified quasiparticles ("electrosolitons") which move in general with subsonic velocity. Davydov in collaboration with Zolotaryuk also treated the case when the lattice bears a cubic or quartic nonlinearity [3, 5, 7]. This leads to "supersonic electrosolitons", or otherwise "lattice polarons"; excitations growing from the nonlinearity of the lattice itself.

Starting first from semiclassical considerations in several works [8–18] a closely related soliton-mediated form of supersonic charge transfer and electric conduction has been proposed by introducing the concept of "solectron" as a natural extension of both the polaron and the electrosoliton quasiparticles. In the solectron theory the soliton carrier is obtained before an excess electron is added to the system. Classical models and plasma-type Hamiltonians [8–13] and quantum-mechanical models have been studied [14, 18–22]. The quantum theory was developed within the tight-binding approximation (TBA). Besides the general methods which we

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developed in some earlier work [11,14–16,18] the quantum theory has been applied to two different kinds of systems:

(a) Conducting polymers, studies of hopping processes in polymers based on a TBA Hamiltonian [14,18,20–26].
(b) One- and two-dimensional plasmas and solid state plasma layers, studies of the diffusivity and the conductivity by using a plasma Hamiltonian and Pauli-type kinetic equations [12,27].

The first line of research was developed in collaboration with Larissa Brizhik, Leonor Cruzeiro, Dirk Hennig, John Kozak, Oliva Cantu Ros, and Gerd Röpke concentrating on analytical and numerical studies of solectron bound states and recently also on bisolectron bound states [21, 22, 25, 26]. The plasma approach was developed with Gerd Röpke [27, 28]. Here we will study hopping transfer of charges and hopping conductivity in plasma layers. We are using a particular method which has been developed recently in the context of applications to plasmas and charged layers in solids [19,27,29–31]. This approach is based on a generalization of the kinetic equations developed already in 1928 by Pauli [32] and the more recently developed Monte Carlo procedures of doing simulations of many particle systems [33]. As we have shown in [27] by using a particular generalization of the kinetic equations of Pauli-type, the excitations and transport processes based on the coupling of the nonlinear lattice excitations to the hopping transport of the charges may be well described by this method. This procedure is particularly useful for studying the influence of nonlinear excitations of the lattice on electric transfer, conduction and other transport properties.

Let us succinctly summarize the state of art and discuss some open tasks:

The solectron concept offers powerful methods to understand and to control the motion of charges in nonlinear atomic lattices. It is in fact a significant generalization of the polaron concept, extending the latter to nonlinear lattices [47]. This is indeed of some importance, since real atomic interactions are never strictly linear, there are always some nonlinear contributions to the atomic interactions.

In our view, so far the most important results with respect to possible practical applications are:

1. Development of tools to manipulate and control the path of charges, including the so-called vacuum-cleaner effect [20, 23, 31]. This is in fact a new way of controlling charges providing a method to overcome the spreading of probability due Schrödinger evolution and bring electrons in a controlled way from point A to point B in a lattice.
2. Studies of pair formation. It was shown that under appropriate conditions solectron pairs may be formed [21–23,25,26,34].
3. Extension of the one-dimensional solectron concept to two dimensions, i.e. the step from chains to layers [28, 30, 31]. One of the results was the detection of high energetic quasi one-dimensional solectrons running in higher-dimensional systems along the crystallographic axes [31].

Problems not yet treated include:

- Studying the influence of density of doping on physical properties [48],
- The study of nonideality effects in diffusion and conductivity,
- The quantitative treatment of percolation effects,
- The study of the influence of Fermion and Boson effects and the role of the Fermi edge (Fermi net in 2d),
- The investigation of Bose–Einstein condensation in solectron/bisolectron systems and their role in eventual superconducting systems.

As far as we can see, all known systems with high conductance—ranging from usual metals to superconducting materials—operate on the basis of degenerate charges. For this reason we will discuss here the problems which arise in generalizing the existing theory of individual solectrons and bisolectrons to many-body thermal systems.

2 The Temperature-Density Phase Plane and Solectronic Degeneration Effects

Our aim is to extend the existing theory at first in a qualitative way to finite densities and to discuss density—as well as temperature effects. Let us start with some estimates for the relative number of thermal solitons per site N_s/N as a function of temperature. There are several theoretical estimates for Toda lattices [35, 36] as well as estimates from computer simulations for Morse lattices [19]. According to the existing estimates the soliton fraction increases with $T^{1/3}$ and has maximum at certain temperature T_0 which may be in the range of a few hundred Kelvin for biomolecules [19]. For estimates we fitted the existing data with the formula

$$\frac{N_s}{N} \simeq \frac{A\tau^{1/3}}{1 + B\tau^5}, \tag{1}$$

where N is the total number of sites, $\tau = k_B T/2D$ and where $A \simeq 0.5$ and $B \simeq 0.1$ are two fitting constants. For fitting we used the results from simulations showing clearly the existence of optimal temperatures for soliton generation [19, 23]. Let us now study the role of electron density. The electron density can be given in several units, the simplest is the so-called relative occupation or fraction ν_e which is defined as the number of sites occupied by an electron relative to the total number of sites

$$\nu_e = \frac{N_e}{N}.$$

Note that in the simplest model, the electrons are always associated to one of the sites. The relative occupation is denoted as doping.

In real systems the fraction or doping may vary within wide limits, however the fraction/doping will in general not exceed the value 0.2, i.e. not more than 20% of sites are occupied (doping fraction). The number density in charges per unit volume

$$n_e = \frac{N_e}{V},$$

where V is the volume may depend on the dimension and the lattice properties. In 1d the density is given by

$$n_e = \frac{N_e}{aN},$$

where N is again the total number of lattice sites and a is the equilibrium lattice spacing. In a 2d triangular quadratic or triangular lattice the density is given by

$$n_e = \frac{N_e}{Na^2}, \qquad n_e = \frac{N_e}{Na^2(2/\sqrt{3})}.$$

Let us denote the number of solectrons by N_{se}. We assume that the number of solectrons and the number of free solitons $N - N_{se}$ are related by a Boltzmann factor.

$$\frac{N_{se}}{N - N_{se}} = \exp\left[-\frac{\epsilon_{se}}{k_B T}\right]. \tag{2}$$

Here ϵ_{se} is the energy gain in forming a solectron. This energy depends on the specific physical conditions. Following Davydov [3], the ground state energy of a strongly supersonic solectron can be estimated at

$$\epsilon_{se} \simeq \frac{v_{se}}{v_{sound}} \frac{m_e}{m_{se}} [eV], \tag{3}$$

where m_{se} and v_{se} are the mass and velocity of the solectron. For appropriate parameter values, this energy could possibly reach 0.1 eV, which is a very high value. Presumably the above given estimate is an upper bound. In our computer simulations with Morse lattices having a potential well of value D we observe solectrons in a temperature range of 0.1–1 D. Assuming wells of order 0.1–0.5 eV we arrive at temperature intervals of 0.01–0.1 eV. In the following we will assume that the ground state energy is around 0.01 eV. By using this and two smaller values for the binding energy we can estimate the fraction of solectrons as a function of temperature and density. The result is shown graphically in Fig. 1. Not that by using higher values for the binding energy, the densities of solectrons are increasing.

We will now estimate the effects of degeneration assuming that the charges are electrons or holes and are, as well as the corresponding solectrons, Fermions. Systems of Fermions show degeneration effects, if the thermal de Broglie wave length of the charges is about the distance between them. That means the degeneration effects of the charges will begin to play a role at densities satisfying the condition

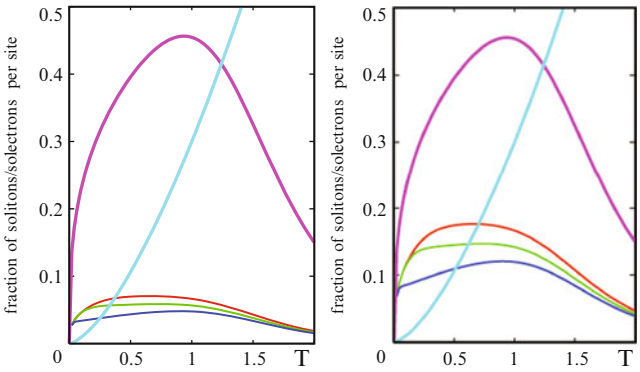

Fig. 1 Estimates of the soliton fraction per site (*upper pink curve* with maximum) and of the solectron fraction for 3 given values of the solectron binding energy (*lower three curves*: $\epsilon_{se} \simeq 0.001, 0.005, 0.01$ eV). *Left panel*: a doping of 20%, *right panel*: a rather high doping of 50%. The magenta lines going up as temperature increases show the border of degeneration effects which are to be expected only above them

$$n_{se}\Lambda_{se}^3 \simeq 1; \qquad \Lambda_{se} = \frac{h}{\sqrt{2\pi m_{se} k_B T}}, \tag{4}$$

where m_{se} is the effective mass of solectron and n_{se} as before is the solectron density. The condition of degeneracy provides us a line in the density-temperature plane

$$n_{se} = const.T^{3/2}, \tag{5}$$

which is displayed in Fig. 1. In the left panel we show the case of a quite an usual doping of 20%, the right panel we have the case of a very high doping of 50%. Only above the magenta lines the effects of degeneration may be expected.

Let us succinctly explain what we mean with a Fermi surface which is in 2d a Fermi net. The Fermi net (Fermi surface in 3d) is defined by the condition that the energy equals the Fermi energy. This corresponds to the transition to degeneration which happens at $n_{se}\Lambda_{se}^3 \simeq 1$.

If the degeneration parameter crosses unity, we expect degeneration effects (Fig. 1). The Fermi net is a set of lines on the plane where, the density corresponds to the degeneration density at the corresponding given temperature. The electron density in the field of atoms is in our case nonuniform and may have a quite complex structure and net structure schematically shown in Fig. 2. As well known from plasma physics and solid state physics most relevant processes, including transitions, diffusion and conductivity occur at the Fermi surface. Therefore it is a primary task, to explore the structure of the Fermi surface. In particular we have to study questions like: Is the Fermi surface connected (percolated) or consisting of non-connected pieces of density regions corresponding to solectrons at the Fermi energy.

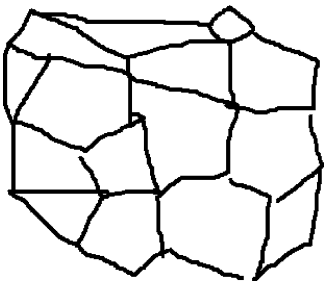

Fig. 2 The Fermi surface (Fermi net in 2d) is defined by the condition that the energy equals the Fermi energy. In other words, the density corresponds to the degeneration density at the given temperature

Our estimates show that it is not easy the cross the border of degeneration. We need strong doping or low temperatures. As far as we can see, it is quite difficult to have conditions for creating degenerate solectrons in real 2d or 3d systems. Probably we need high doping for temperatures beyond 100 K. However one should note that these estimates are conservative, the solectron mass was taken as equal to the electron mass. In reality solectrons are heavier than electrons or holes and tends to behave more classically than electrons. This question was appropriately raised by Alexandrov [37].

3 The Hamiltonian of Our Model and the Equations of Motion

We consider d-dimensional lattices of atoms ($d = 1, 2, 3$) and (added, excess) free electrons which may carry electrical currents. In applications we restrict in most cases to 1d-, or 2d-lattices in order to assess the influence of nonlinear excitations on the electrical properties. The system consists of N classical atoms and one ore several electrons. For the *heavy* atoms we assume that they obey classical Langevin dynamics. We include a phenomenological damping γ_i. In the numerical simulations we consider the lattice units with mass m. The atomic particles are described by coordinates $\mathbf{r}_j(t)$ and velocities $\mathbf{v}_j(t)$, $j = 1, \ldots, N$. We assume periodic boundary conditions. The Hamiltonian consists of three parts, the classical atom/ion Hamilton function H_i, the electron ion interaction function H_{ie} and the rest H_e, accounting for the electrons.

$$H = H_a + H_{ie} + H_e. \tag{6}$$

The atomic part is

$$H_a = \frac{m}{2} \sum_j \mathbf{v}_j^2 + \frac{1}{2} \sum_{ij} V_{ij}(\mathbf{r}_{ij}). \tag{7}$$

The atoms repel each other by strong repulsive forces. The subscript "i" denotes the number of the atom. Let us assume that the characteristic size of the atoms in the

lattice is r_0. In general we will approximate the potential of the forces between two atoms by the Morse-potential

$$V^M(r) = D\left[\exp(2B(r-\sigma)) - 2\exp(-B(r-\sigma))\right]. \tag{8}$$

We note that the characteristic frequency of oscillations around the minima is

$$m\omega_0^2 = V^M(\sigma)''. \tag{9}$$

We introduce now an electron e.g. by doping, and define in TBA the amplitude for being at site j in state n by c_{jn} and the probability to find the electron at the lattice site or atom located at x_j in state n denoted as p_{jn} by

$$p_n = c_n c_n^*. \tag{10}$$

We will show that any displacement of the atoms changes the energetic situation of the electrons, the eigenvalues as well as the transition probabilities. The electron dynamics is influenced by the lattice dynamics and as a result the electron will try to follow up these changes. This is the basic effect leading to the solectron formation. So the essential point is the running local compressions which generate a complex landscape. As shown already by Davydov [3] there exist rather deep potential wells moving (right to left or left to right) along the lattice that strongly influence the local dynamics of the electrons and are able to capture the light electrons. In the TBA the electron Hamiltonian is of hopping type [20–22]

$$H_e = \sum_{jn} E_{jn} c_{jn}^+ c_{jn} + \sum_{jj'n} t_{jj'n} c_{j'n}^+ c_{jn}. \tag{11}$$

Here j denotes the number of the atom and n the quantum numbers of the atomic states. In our adiabatic approach the atomic and the internal positions are assumed to be fixed at R_j. The representation is based on a linear combination of atomic orbitals (LCAO): $|jn>$ which are approximately given by the wave functions of a free atom at position r_j. The matrix elements are related to the operators of kinetic and potential energy. The energy levels E_{jn} fluctuate around the levels of the free atoms. The transition matrix is also a fluctuating quantity depending on the time varying atomic distances $r'_j - r_j$. In a simplified version we neglect the electron–electron interaction. Hence (11) is in fact

$$H_e = \sum_{jn} E_{jn} c_{jn}^+ c_{jn} + \sum_{jj'} t_{jj'n}(R_{j'} - R_j) c_{j'n}^+ c_{jn}, \tag{12}$$

with the matrix elements

$$E_{jn} = < jn|H_0 + V_{ej}|jn >; \qquad t_{jj'n} = < j'n|H_0 + V_{ej}|jn > . \tag{13}$$

We may simplify this expression assuming that the index n uniquely defines the state and set [20–22]

$$H_e = \sum_n E_n c_n^+ c_n + \sum_{nn'} t_{nn'}(r_{n'} - r_n) c_{n'}^+ c_n. \tag{14}$$

In order to estimate the influence of the lattice on the energy levels we consider now the electron–atom interaction.

For 1d-lattices one may consider only nearest neighbor coupling and simplify [20–22]. In the general case the energy landscape shows a complex structure and the dependence of the energy levels on the position has to be taken into account [18, 20]. In the 1d-case the linear Holstein model is

$$E_n \simeq E_n^0 + \chi_0 q_n + \chi_1 \left[q_{n+1} - q_{n-1}\right]. \tag{15}$$

Here, for convenience in notation, q_n denotes a lattice site spatial vibration (relative displacement) coordinate defined by $x_n = n\sigma + q_n/B$. There is the problem that for some values of the deviations (and typical parameter values, $\alpha = 1 - 1.75$) the exponents may take on very large values. The term E_n^0 denotes on-site energy levels of the unperturbed lattice and δE_n is the perturbation due to the lattice vibrations (harmonic as well as anharmonic modes may contribute). In the simplest case the shift is linear in the deformations [38, 39]

$$\delta E_n = \chi(q_n/B), \tag{16}$$

where the "electron-phonon coupling constant", χ, indicates that the on-site energy level E_n, i.e. the local site energy, depends on the displacement of the moving unit; q_n is dimensionless (unit: $1/B$). As shown e.g. in [38, 39], this coupling between lattice deformations and electronic states, leads for large enough values of the parameter χ to the formation of *polarons*. In view of the above given parameter values, the value of the coupling constant is in the range $\chi \simeq 0.1 - 1\,\mathrm{eV/\AA}$. Adapting these assumptions to our model without onsite contributions we have to recall that our model is translationally invariant and we are considering relative lattice displacements.

Recall also that the probability to find the electron at the lattice site or atom located at x_n, i.e. the occupation number p_n is given by (10). The discrete Schrödinger equation for the components of the wave function c_n is then

$$\begin{aligned} i\dot{c}_n \;=\; & [E_n^0 + \chi_1(q_{n+1} - q_{n-1})]c_n \\ & -V_0 \sum_k \{\exp[-\alpha(q_{n+1} - q_n)]c_{n+1} \\ & + \exp[-\alpha(q_n - q_{n-1})]c_{n-1}\}, \end{aligned} \tag{17}$$

where an over-dot denotes time derivative; the energies are dimensionless (unit: 2D).

The corresponding equations for the lattice particles are now

$$\begin{aligned}\ddot{q}_n &= \chi_1[p_{n+1} - p_{n-1}] \\ &+ \{1 - \exp[-(q_{n+1} - q_n)]\} \exp[-(q_{n+1} - q_n)] \\ &- \{1 - \exp[-(q_n - q_{n-1})]\} \exp[-(q_n - q_{n-1})] \\ &- \alpha V_0 \left\{\exp[-\alpha(q_n - q_{n-1})](c_{n+1}^+ c_n + c_{n+1} c_n^+)\right. \\ &\left. + \exp[-\alpha(q_{n+1} - q_n)](c_n^+ c_{n-1} + c_n c_{n-1}^+)\right\}. \end{aligned} \tag{18}$$

The problem reduces, in principle, to solving coupled together both (17) and (18).

Let us study now the two-dimensional case. A standard assumption is, that the interaction is described by a pseudo-potential of polarization type. We assume that the total potential acting on an electron in the field of atoms at positions $r_1, \ldots r_N$ is

$$V_e(\mathbf{r}) = -\sum_j \frac{U_e}{[1 + (\mathbf{r} - \mathbf{r}_j)^2/h^2]^2}. \tag{19}$$

Here h is a characteristic cut-off distance and U_e the maximal polarization energy of the electron. As an estimate we may assume $U_e \simeq 0.1\,\mathrm{eV}$. In earlier work we used also a different pseudopotential approach [27]. In order to be consistent with the pseudopotential formula used above to quadratic terms we can make the choice $h \simeq 0.7\sigma$.

The eigenvalue problem is in general very complicated and practically unsolvable, so we will use the simple assumption that the eigenvalues are shifted like the polarization potential

$$E_n \simeq E_n^0 - \sum_{j=1}^{N} \frac{U_e}{\left[1 + (r_n - r_j)^2/h^2\right]^2}. \tag{20}$$

The discrete Schrödinger equation for the components of the wave function c_n assumes now the form [28, 30]

$$\begin{aligned} i\dot{c}_n &= [E_n^0 - \sum_{j=1}^{N} \frac{U_e}{\left[1 + (R_n - R_j)^2/h^2\right]^2}]c_n \\ &\quad -V_0 \sum_k \{\exp[-\alpha|R_k - R_n|]c_k. \end{aligned} \tag{21}$$

As before the forces between particles are supposed to be of the Morse kind and the friction and random forces accounting for a Langevin model bath in the case of a heated lattice. For convenience in the 2d lattice dynamics we use complex coordinates $Z_n = x_n + iy_n$, where x_n and y_n are Cartesian coordinates of the n-th

particle. Then the Langevin model provides the equations of motion for the lattice units

$$\frac{d^2 Z_n}{dt^2} = \sum_k \left[F^M_{nk}(Z_{nk}) + F^P_{nk}(Z_{nk}) \right] z_{nk} - \alpha V_0 \sum_k \exp\left[-\alpha |Z_{nk}|\right] (c_n^+ c_k + c_k c_n^+) + \left[-\gamma \frac{Z_n}{dt} + \sqrt{2D_v} \left(\xi_{nx} + i\xi_{ny}\right) \right], \tag{22}$$

where index n identifies a particle among all N particles of the atomic ensemble, γ is a friction coefficient, D_v defines the intensity of stochastic forces, $\xi_{nx,y}$ denotes statistically independent generators of the Gaussian noise; $Z_{nk} = Z_n - Z_k$. Further $z_{nk} = (Z_n - Z_k)/|Z_n - Z_k|$ is a unit vector defining the direction of the interaction force F^M_{nk}, corresponding to the Morse potential, and F^P_{nk}, corresponding to the polarization interaction, between the n-th and the k-th particles. The Morse interaction force F_{nk} is here given by

$$F^M_{nk} = 2B[\exp(-2B|Z_{nk}|) - \exp(-B|Z_{nk}|], \tag{23}$$

and the polarization interaction force by

$$F^P_{nk} = 4U_{ek} \frac{p_n |Z_{nk}| - p_k |Z_{kn}|}{[1 + |Z_{nk}|^2/h^2]^3}. \tag{24}$$

Note that to have dimensionless variables we may consider the spatial coordinates normalized to the length σ used in the Morse potential. Time may be normalized to the inverse frequency of linear oscillations near the minimum of the Morse potential well, ω_M^{-1}. The energy is usually scaled with $2D$, where D is the depth of the Morse potential well, a different possibility is to use V_0 as the unit of energy. Further the stiffness parameter B defines the strength of the repulsion between particles. In view of the above only those lattice units with coordinates Z_k, satisfying the condition $|Z_n - Z_k| < 1.5$, are taken into account in the sum in (41). In computer simulations the interaction of particles is considered to take place inside a rectangular cell $L_x \times L_y$ with periodic boundary conditions.

In practice some open problems remain, in particular there is the compatibility between the quantum-mechanical and the classical part of the dynamics. Due to the Langevin sources of noise and friction in the classical part of the dynamics, the dynamics is irreversible. However so far there is no proof that the final distribution corresponds to the correct Gibbs-von Neumann measures. In the following we assume a kinetic description which is irreversible from the very beginning and converges to the correct distributions. The idea we follow is due to Wolfgang Pauli who focused on p_n and not c_n hence disregarding phases. Thus the Pauli averaging excludes a complete description of coherent states hence ruling out a proper treatment of superconducting states.

4 Pauli Kinetics for Nondegenerate Solectrons on Nonlinear Heated Nonlinear Lattices

So far our analysis has been based on the Schrödinger equation for the free electrons in the TBA which is coupled to the Langevin equation for the classical lattice particles. This tacitly assumed the existence of a heat bath in which the lattice particles are embedded. In principle this picture provides a complete description of the coupled lattice–electron dynamics. The irreversibility is guaranteed by the friction-noise terms in the Langevin-equations (23). As earlier shown [14, 18, 20] we may describe this way also irreversible solitonic excitations at finite temperature. However, a serious problem here is the very long relaxation times of the electrons due to the large differences between the time scales of the electrons and the lattice particles. This leads to some difficulties in extensive computer simulations. In the standard theory of electronic transport this problem is solved by Boltzmann-type descriptions or by Fokker–Planck-type equations, which introduce an irreversible behavior [32, 40–43]. The main problem is here to give a correct description of the coupling to the heat bath [41–43]. In the TBA case, the situation is somehow simpler due to the discrete character of the electronic states, which allows a description by discrete Markov chain equations [29, 44]. The Markov approach to electron dynamics goes back to the seminal work of Pauli, Tolman, van Hove and others [32,40–43]. Pauli started from the Schrödinger equation and derived by perturbation theory a Markov chain description and an expression for the transition probabilities. He introduced an irreversible master equation expressing the balance between the transitions in an ensemble. Pauli's equation is valid for a *microcanonical* ensemble and neglects symmetry effects. Further extensions took into account the symmetry of the wave functions and offered a description compatible with the statistics of Bose–Einstein and Fermi–Dirac. Later generalizations are connected with the development of Metropolis algorithms for *canonical* ensembles [33]. Applications to hopping conduction in solids were given since the 1970s of last century by several authors [44]. First applications of the master equation formalism to electron transfer in macromolecules appear in [45]. The system we are studying here is rather difficult and seems to be too complicated to be treated in full detail. We have:

(a) Quantum electrons located in discrete states, which are coupled to a heat bath and to the classical lattice,
(b) Classical lattice particles coupled to the heat bath and to the quantum electrons.
(c) The heat bath with an unspecified nature.

Simplifying this situation we postulate here that the thermal electrons allow a Markov description. Thus we proceed from the *reversible* Schrödinger equation for the tight-binding model to an *irreversible* Pauli master equation description [32, 40–43]. Following Pauli's method [19, 29] we use here a master equation for the occupation probabilities of electrons p_n in a system with the energy levels E_n:

$$\frac{dp_n}{dt} = \sum \left[W_{nn'} p_{n'} - W_{n'n} p_n \right] . \tag{25}$$

The transition probabilities were derived by Pauli using perturbation theory for microcanonical ensembles (transitions in a narrow energy shell). Applications of this formalism to our Schrödinger equation confronts us with the problem of applicability of the perturbation approach to our basic equation. Note that the diagonal part of the interaction operator may not be small in comparison to the nondiagonal elements. We neglect here this problem and assume that we have found already an appropriate unitary transformation which makes the nondiagonal elements sufficiently small to satisfy the conditions of Pauli's perturbation approach. With this assumption the transition probabilities for the 1d-tight-binding model read in a microcanonical ensemble according to Pauli [19, 29, 32] is

$$W_{micro}(n,n') = \frac{V_0}{\hbar}\exp[-2\alpha|q_{n'}-q_n|]2\pi V_0\delta(E_n - E_{n'}), \tag{26}$$

where $n' = n \pm 1$ and $\delta(x)$ is Dirac's delta function. The transitions from state n to a state n' at one of the nearest-neighbor sites should correspond to the same energy level (or to a level within a narrow shell). In the case of a dissipative embedding, the situation is more complicated due the interaction of the electrons with the dissipative heat bath. For a canonical ensemble we assume the transition probabilities

$$W(n,n') = \frac{V_0^2}{\hbar}\exp[-2\alpha|q_n - q_{n'}|]E(n,n',\beta). \tag{27}$$

Instead of a delta-like shell we have now a Lorentz-like profile around it. In the limit of narrow profiles these expressions converge to the Pauli formula with a delta-factor. Temperature effects are to be included. When the electrons are embedded into a heat bath together with the heated lattice particles, the temperature-dependent thermal factors $E(n,n',\beta)$ are not symmetric with respect to the arguments but they are subject to the condition of detailed balance

$$\frac{W(n',n)}{W(n,n')} = \exp[\beta(E_n - E'_n)]. \tag{28}$$

In other words, the relation of the thermal factors should correspond to the relation of Boltzmann factors. The property (28) suggests the symmetry

$$E(n,n') = \exp[-\frac{\beta}{2}(E_n - E'_n)]F(n,n'), \tag{29}$$

$$F(n,n') = F((E_n - E'_n)), \tag{30}$$

where F(n,n') is an even function. There are several variants for this even function $F(x)$ which we will discuss. The simplest is defined by the phenomenological "ansatz" of the Monte-Carlo procedure, where downhill transitions are weighted with $E = 1$ and uphill transitions with a factor less than unity [33]. This corresponds to the F-function.

$$F(E_n - E_{n'}) = \exp[-\frac{\beta}{2}|E_n - E'_n|]. \tag{31}$$

Proper statistical derivations of the thermal factors may be based on certain microscopic models of the heat bath. Assuming that the heat bath is a carrier of phonons which drive transitions by a one-phonon mechanism Böttger and Bryksin [44] studied hopping systems starting from the von Neumann equation for the density matrix. The authors give the following general expression

$$F(E_n - E_{n'}) = \int_{-\infty}^{\infty} \exp[\frac{i}{\hbar}\tau|E_n - E_{n'}|]K(|\tau|)d\tau, \tag{32}$$

where $K(|\tau|)$ is a rapidly decaying memory kernel. The decay of these correlations is connected with the damping of lattice-particle motion. In the simplest case we may assume here an exponential decay with the same damping constant as appears in the above introduced Langevin dynamics. This leads to the Lorentz profile

$$F(E_n - E_{n'}) = \frac{V_0}{\hbar}\frac{\gamma}{\gamma^2 + (|E_n - E_{n'}|)/\hbar)^2}. \tag{33}$$

In the limit of small damping we come back to the delta-function in the Pauli expression for the transition probabilities.

The master equation is a useful tool for computer simulations of electron hopping processes. Since the detailed balance is obeyed, it is guaranteed that in thermal equilibrium the canonical distribution is solution of the master equation. In order to simplify our computer simulations we used so far only the simplest "ansatz", the Monte Carlo procedure. Our basic system of equations contains several approximations, however it provides a rather fast and therefore useful tool for the computer simulations of the electron–lattice dynamics in thermal systems. Figure 3 illustrates results of computer simulations based on this approach. Due to the way we treat electron relaxation effects there are differences between the methodology using the coupled Schrödinger equation and Langevin equation system (23) and that using Pauli's approach albeit they are minor differences at least for small and for intermediate values of adiabaticity $\tau \sim 1$. For large τ, the electron relaxation in the heat bath is very fast and the distribution may be approximated by a local Boltzmann- or Fermi distribution as shown in [23]. For small and intermediate values of the τ-parameter, say for $\tau \simeq 10 - 20$, the approach based on the Pauli equation (25) is most useful, since it provides informations on deviations from the adiabatic approximation. Our approximation based on the Pauli method (25) goes beyond the adiabatic approximation since the lattice dynamics and the electron dynamics are treated independently including their coupling. Recall that in a strict adiabatic approximation one assumes that the electron adapts "instantaneously" to any change in the lattice. In other words one assumes that the electrons follow in a very fast way to the new lattice configuration and may be described at any time by the canonical distribution [46]. In the new approach based on Pauli's method we take into account that the electrons need time to follow the lattice motions what

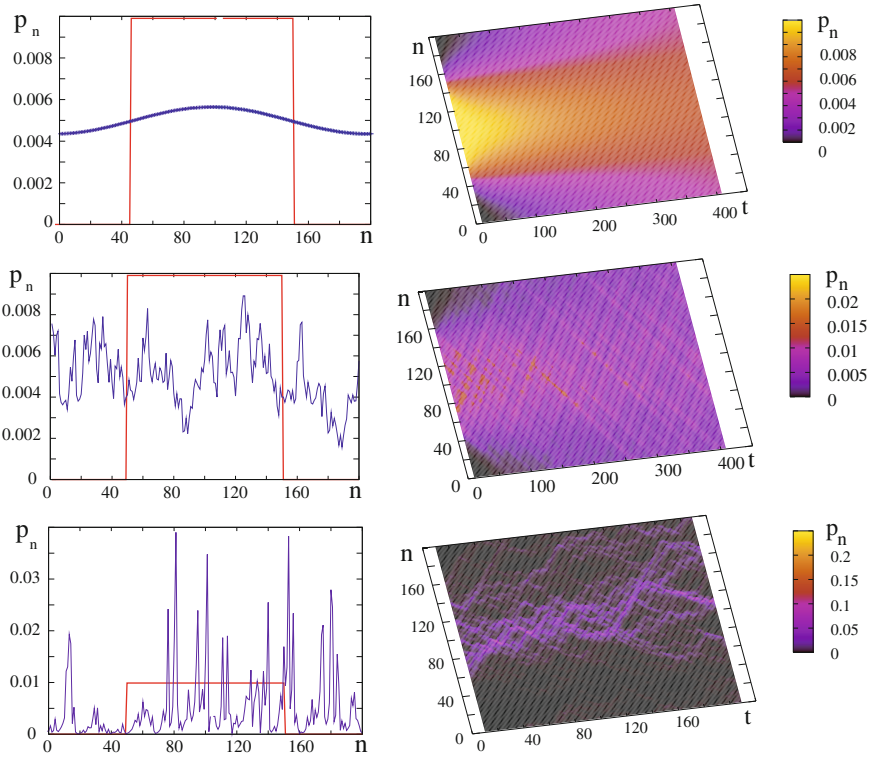

Fig. 3 Time evolution of one-dimensional probability distribution according to Pauli's equation. In the *upper panel* we see the evolution of an initial rectangular distribution, into a uniform distribution without any coupling to the lattice $T = 0$, thus illustrating an H-theorem. In the *center panel* and in the *lower panel* two temperatures different from zero are considered: *upper case*: $T = 0.01$: an initially rectangular distribution tends irreversibly towards homogeneous spreading along the lattice, the wave is weakly structured due to the excitations along the lattice; and *lower case*: $T = 0.5$: the initial rectangular distribution is spreading but at the same time becomes localized around a few peaks thus illustrating the corresponding local formation of solectrons

leads to certain delay in their response and to some deviations from the stationary solution. Qualitatively however the picture remains similar to the results obtained in adiabatic approaches. Figure 3 illustrates how the spreading of the electron density in the 1d case is diffusion-like and strongly influenced by the excitations of solitons in the lattice.

5 Kinetic Equations for Fermi Solectrons with Zero Spin

An advantage of the Pauli approach is, that it can be easily generalized to include the influence of spin and symmetry effects which we have neglected so far, except when using the Hubbard approximation. Following Pauli and Tolman [32, 40] now

we take into account that the electrons are Fermions which are not allowed to occupy a quantum state with more than one particle. In principle there exist the possibility to form bosons by pairing of two electrons but this effect we will considered later on. In a first approach we study electrons without spin, or what is equivalent we consider the case of very low density, where double occupation cannot occur due to the low probability that two electrons meet at the same place. Taking into account symmetry effects for (non-interacting) Fermions without spin the Boltzmann equilibrium distributions are to be replaced by Fermi distributions

$$p_n^0 = \frac{1}{\exp[\beta(E_n - \mu)] + 1}. \tag{34}$$

Here the "plus one" in the denominator expresses the Fermion character. The chemical potential μ marks the border between the occupied and the non-occupied states. Following a procedure described by Tolman and van Hove [40–43] the master equation may be generalized in such a way that Bosonic or Fermionic symmetry effects are included. The idea is to change the transition probabilities in dependence on the occupation of the target state. Let us explain this procedure for Fermions with zero spin. In order to include the Fermi principle we introduce the modified transition probabilities

$$\tilde{W}_{nn'} = (1 - p_n) W_{nn'}. \tag{35}$$

The prefactor reduces the probability of the transition as a function of the occupation of the target state. This way we get a nonlinear master equation

$$\frac{dp_n}{dt} = \sum \left[\tilde{W}_{nn'} p_{n'} - \tilde{W}_{n'n} p_n \right], \tag{36}$$

incorporating the Fermion character. If the spin is different from zero, the prefactor appears only for transitions to states with the same spin direction. The appearance of products like $(1 - p_n) p_{n'}$ leads to the fact that effective hopping is restricted to transitions between states near to the Fermi surface. The meaning is the following: Consider the transitions $n' \to n$. These transitions occur with the weight $p_{n'}$ if and only if the state n is free as expressed by the weight factor $(1 - p_n)$. In Fig. 4 it is demonstrated that according to this weight factor. The states near to the Fermi surface are the major contributors to transport. The new probabilities are still between zero and one i.e. $0 < p_n < 1$ but they are normalized in a different way namely

$$\sum_{n=1}^{N} p_n = N_e \tag{37}$$

where $N_e < N$ is the total number of free electrons in the system. Accordingly, p_n expresses the probability to find one electron in the state $1 \leq n \leq N$. Recall that we assume here one state per atom. This one electronic state per atom may be occupied or not. The prefactors on the r.h.s. of (36) make sure the probabilities p_n cannot grow

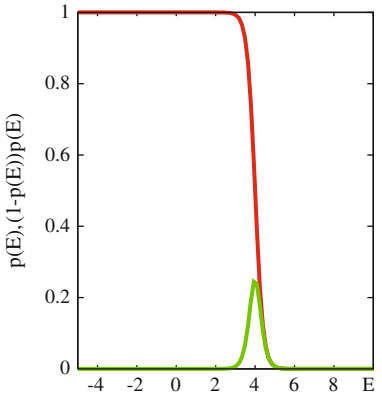

Fig. 4 The Fermi distribution $p(E)$ (upper sharply decreasing *red curve*) and the weight for transitions n' to n (*green curve* with maximum) which is depicted by the function $p(E)(1-p(E)$. The maximum corresponds to the Fermi surface on which transitions have the highest weight

larger than unity. The transition probabilities remain the same as for the Boltzmann case discussed above. The only general condition they have to satisfy is

$$\frac{W(n',n)}{W(n,n')} = \frac{\exp[-\beta E'_n]}{\exp[-\beta E_n]}. \tag{38}$$

In equilibrium the normalization defines the chemical potential by

$$\sum_n \frac{1}{\exp[\beta(E_n-\mu)]+1} = N_e. \tag{39}$$

Clearly the states $E_n = \mu$ play a very special role not only in equilibrium but also for transport.

By taking into account the spin we may easily modify the distribution in such a way that two electrons may occupy the same site. This corresponds to the formation of a (small) bipolaron. However it is not trivial to take the Coulomb repulsion into account, which is significant for the formation of bipolarons.

The master equations are not closed, they still depend on the particle coordinates. The corresponding equations for the lattice particles are in the 1d case given by Chetverikov et al. [29]

$$\begin{aligned}\frac{d^2q_n}{dt^2} &= \chi_1[p_{n+1}-p_{n-1}] + \{1-\exp[-q_{n+1,n}]\}\exp[-q_{n+1,n}] \\ &- \{1-\exp[-q_{n,n-1}]\}\exp[-q_{n,n-1}] - 2\alpha V_0(\exp[-\alpha q_{n,n-1}]\sqrt{p_{n-1}p_n} \\ &+ \exp[-\alpha q_{n+1,n}]\sqrt{p_n p_{n+1}}.\end{aligned} \tag{40}$$

which are phase-averaged modifications of (18).

In the 2d case the equations of motion are more complicated. Assuming the same model about forces and friction as earlier done and using also complex coordinates $Z_n = x_n + iy_n$, where x_n and y_n are Cartesian coordinates of the n-th particle we get the Langevin equations

$$\frac{d^2 Z_n}{dt^2} = \sum_k \left[F_{nk}^M (Z_{nk}) + F_{nk}^P (Z_{nk}) \right] z_{nk} - 2\alpha' \sum_{n'} \exp\left[-\alpha' |R_n - R_{n'}| \right] \sqrt{p_n p_{n'}} + \left[-\gamma \frac{dZ_n}{dt} + \sqrt{2D_v} \left(\xi_{nx} + i\xi_{ny} \right) \right], \tag{41}$$

where as above the index n identifies a particle among all N particles of the atomic ensemble, γ is a friction coefficient, D_v defines the intensity of stochastic forces, $\xi_{nx,y}$ denotes statistically independent generators of the Gaussian noise. Note that the new Langevin equations (41) are different from the previous ones (22), since due to the phase averaging only the variables p_N and not the c_n appear. Further we note that in the classical equations of motion (40) and (41) appear two terms which couple the classical dynamics to the quantum master equations. One is due to the dependence of the energy levels on the coordinates of the atoms and the other on the dependence of the transition probabilities on the atomic distances. Furthermore let us insist on that the description by Pauli TBA equations contains less information than the standard TBA since all phases are lost and only the probabilities p_n appear in the dynamics equations.

6 Spatial Distributions, Energy Spectrum and Energy Distributions

Numerical simulations of our systems of equations (kinetic and dynamic equations) provide snapshots of the spatial distribution of Fermi solectrons on a square of 20×20 triangular lattice at $T = 0.01$. We studied 3 electron numbers $N_e = 16, 200, 300$ on a triangular lattice of 400 sites, whose fractional densities are, respectively, $\nu_e = 0.04, 0.5, 0.75$. Results are shown in Figs. 5 and 6. The corresponding probability and energy distributions are shown in Figs. 7 and 8. Note that the solectrons inside the clusters, stripes or percolated regions are degenerated. Investigating the spatial distributions shown in Figs. 5 and 10, we see interesting structures. We see clustering at the lowest density, striping at the moderate density and a kind of percolation at the highest density. The general trend is that the solectrons tend to cluster rather than remaining isolated. This means that there is a tendency to cluster, hence to pairing in space. This is a point which also needs a further analysis. We have to find the radial distribution function and expect to see a peak at small distances. This would confirm predictions made by Alexandrov [37]. From the informations we have on the energies of the Fermi particles we calculated the distributions by averaging.

Investigating the energy distributions shown in Figs. 7–10, we see also interesting structures. The general trend is that the probabilities decrease with energies. The energies are given here relative to the minimal energy and are ordered

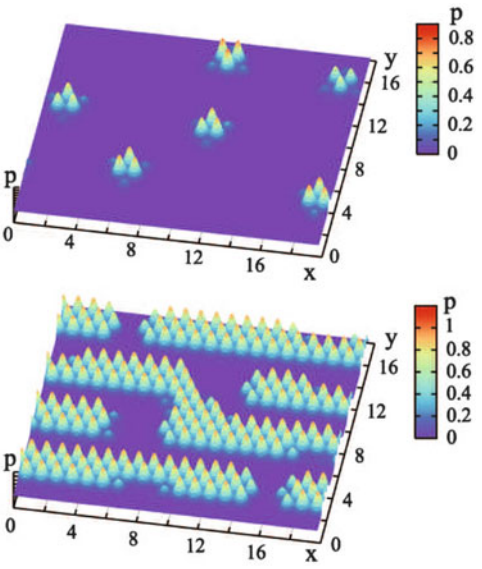

Fig. 5 Snapshot of the spatial distribution of Fermi solectrons on a versus sites 20×20 triangular lattice at a low temperature $T = 0.01$. We study 2 electron numbers $N_e = 16, 200$ on a triangular lattice of 400 sites. This corresponds to the (fractional) doping densities $\nu_e = 0.04, 0.5$. We see clustering at the lowest density and striping on the moderate density

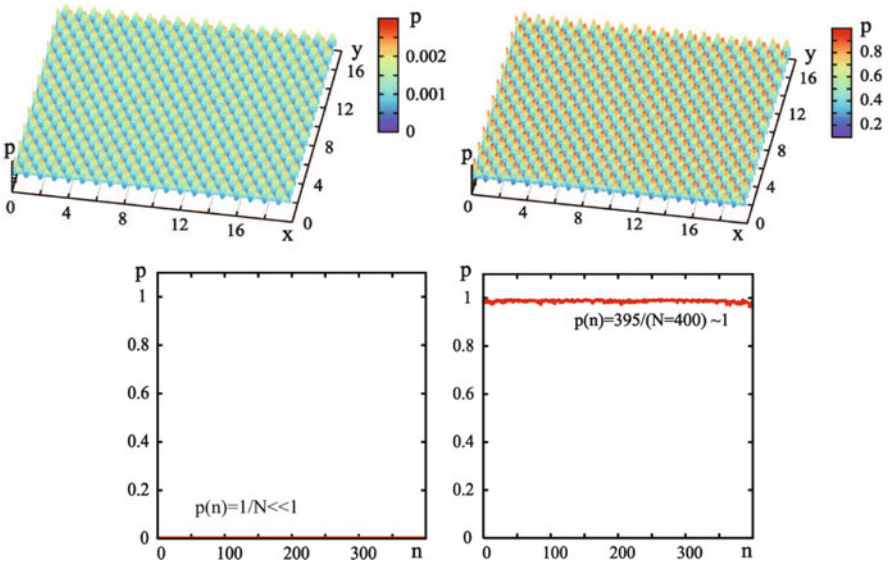

Fig. 6 Probability distribution of Fermi solectrons on a versus sites 20×20 triangular lattice at a very low temperature $T = 0.001$ for two extreme cases. *Left panel* for $N = 1$ shows the expected equal distribution of quantum probability. In the *right panel* for $N = 395$ we see a nearly equal distribution for the case of a near to full occupation

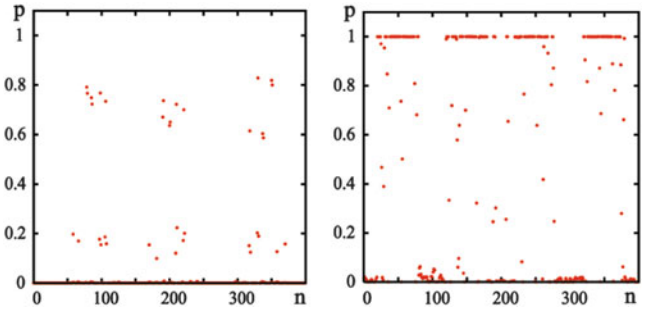

Fig. 7 Snapshot of the probability distribution of Fermi solectrons on a versus sites 20×20 triangular lattice at a very low temperature $T = 0.001$ for two intermediate densities. *Left panel* $N = 16$ and *right panel* $N = 200$

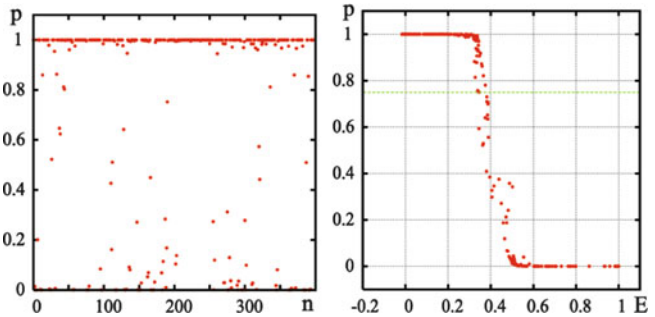

Fig. 8 Probability distribution for $\nu_e = 300/400 = 0.75$ at a low temperature $T = 0.001$. First we see versus sites and then the distribution versus energies (energy distribution). In the latter we observe (the lowest energies are left) the formation of a Fermi edge and may identify the Fermi energy

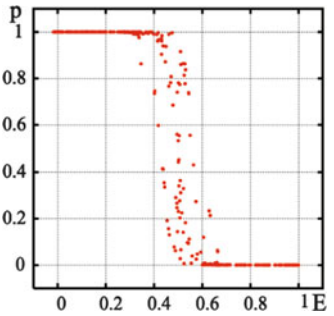

Fig. 9 Typical probability distribution versus energies (energy distribution) of Fermi solectrons at a low temperature $T = 0.001$ for the moderate doping density $\nu_e = 200/400 = 0.5$. We observe again the formation of a Fermi edge and may identify the Fermi energy

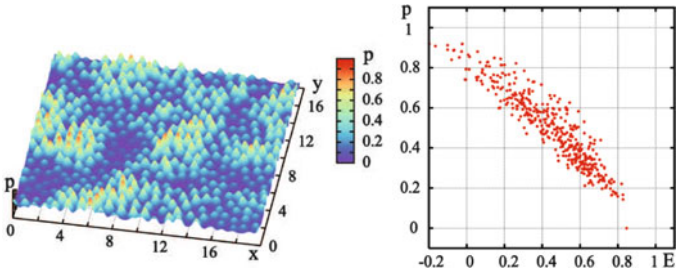

Fig. 10 Another example for the probability distribution versus energies (energy distribution) of Fermi solectrons at an intermediate temperature $T = 0.5$ for the moderate doping density $\nu_e = 200/400 = 0.5$. We observe that the Fermi distribution tends to a Boltzmann distribution. In the *left panel* we see a snapshot of the corresponding spatial electron distribution

in a way that on the left are the lowest energies for a given snapshot. At low temperatures and higher densities (region of degeneracy) a typical Fermi distribution appears which transforms at higher temperatures into a Boltzmann distribution. This transition from degeneration to Boltzmann behavior occurs at

$$n_e \Lambda_e^3 \simeq 1, \qquad \Lambda_e = \frac{h}{\sqrt{2\pi m_e k_B T}}, \qquad n_e = \frac{N_e}{Na^2/2}.$$

Besides this general trend we see an interesting fine structure including steps and gaps. This is a point which needs a further analysis. We cannot exclude the possibility that the gap-like phenomena are connected with the existence of pseudo gaps, but this needs more accurate computer simulations.

Our approximations provide a rather fast and therefore useful tool for the computer simulations of the electron–lattice dynamics in heated systems. Figures 3 and 5 illustrate results based on this approach. Due to the way we treat the electron dynamics, there are differences between the methodology using the coupled Schrödinger equation and Langevin equation system and that using Pauli's approach albeit they are minor differences. An advantage of the Pauli approach is, that it can be generalized to include the influence of spin, and Bose effects which we have neglected so far.

The qualitative difference between the Boltzmann distributions and the Fermi distributions is that Fermi distributions distinguish sharply between electrons below and above the Fermi level μ. The chemical potential (Fermi level) may be estimated from our energy distributions.

The states below the Fermi level are occupied and the states above are empty or weakly occupied. This way the Fermi level acts as the sea level in a country with many mountains. Lowering the sea level decreases the area occupied by the sea and increasing the sea level increases the area of the sea and reduces the part of the mountains. Note that transfer and transport happens only at the Fermi level (Fig. 2). Finally the "land" consists of separated islands. When this happens we have a percolation transition as seen in Fig. 11. The possible Fermi levels are

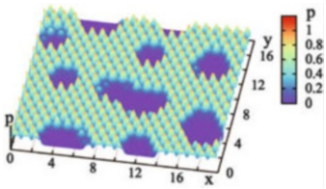

Fig. 11 Percolation is illustrated by a snapshot for a rather high level of doping density of 75% and a rather low temperature $T = 0.01$

given here by the colors. Clearly, for the given potential landscape the Fermi level $\mu \simeq -1$ hints at percolation. We see that the regions $E < \mu \simeq -1$ are connected, this is what we mean by percolation. With increasing density the Fermi level raises, and increasing Fermi levels may lead to percolation of the electronic density corresponding to a sudden increase of diffusion, conductivity and other macroscopic transport properties, from side to side of the system like, indeed, in the Italian coffee percolator when making expresso (Fig. 11). In this respect the 2d- as well as the 3d-systems are fundamentally different from the 1d-systems.

By analyzing the Pauli equation we see that due to the existence of a factor $(1-p_n)\,p_{n'}$ only the states near to the Fermi level the regions $E_n \simeq \mu$ may contribute to transport.

7 Discussion and Outlook

We have investigated the role of Fermi degeneration for a system with nonlinear anharmonic excitations. This may be significant for a theory of conducting lattices. Solitons are hard excitations of the lattice which have a long lasting time and influence the local density and this way the Fermi level. Solitons are local deformations—peaks of the density—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 [31] (Fig. 12).

An evaluation of the influence of solitons predicts for 1d-lattices a conductivity increase in the temperature region where most thermal solitons are excited. For 2d-lattices we find an eventual percolation transition to connected conducting regions. We have shown that the Fermi level of the electrons determines the percolation effects.

A few remarks are worth recalling:

(a) As our simulations show, there is a general tendency for formation of pairs. In recent work [25, 26, 34] we have shown that the soliton mediated pair

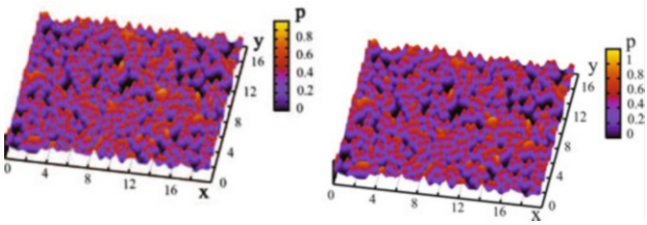

Fig. 12 The case of high temperatures: Snapshots of the electron density in a 2d Fermi system with zero spin and $N = 400$ sites at the temperature $T = 2.5$ for two different doping situations $N_e = 250$; $\nu_e = 0.625$ and $N_e = 300$; $\nu_e = 0.75$

formation is energetically favorable. However as well known this proves only, that pairs will form at $T = 0$; at higher T one has to estimate the thermodynamic probability. This is done for example by our simulations which clearly show that at moderate T, pairs can be formed. According to Alexandrov [37] the existence of local pairs is relevant for high T_c superconductors. Therefore the present study may be useful to start solving this question. However the proper treatment of pairs at finite temperatures requires first an extension of the theory to Bose systems [49].

(b) If solectrons (polarons) are dominant, the Fermi surface of the solectrons determines the electrical conductivity. That means that in order to get high conductivities, we need high enough densities of solectrons near to the Fermi surface.

(c) In certain regions (Fig. 3) bi-solectrons may be more frequent than solectrons. Note that what matters for Bose–Einstein condensation is not the Fermi levels but the lowest energy levels. Since bisolectrons are bosons, Bose condensation is then at least in principle possible. However a problem in this respect is the relatively large mass of solectrons and bisolectrons, which make it difficult to reach the conditions for Bose–Einstein condensation.

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