

# Hopping Transport and Stochastic Dynamics of Electrons in Plasma Layers

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We investigate the stochastic dynamics and the hopping transfer of electrons embedded into two-dimensional atomic layers. First we formulate the quantum statistics of general atom - electron systems based on the tight-binding approximation and express - following linear response transport theory - the quantum-mechanical time correlation functions and the conductivity by means of equilibrium time correlation functions. Within the relaxation time approach an expression for the effective collision frequency is derived in Born approximation, which takes into account quantum effects and dynamic effects of the atom motion through the dynamic structure factor of the lattice and the quantum dynamics of the electrons. In the last part we derive Pauli equations for the stochastic electron dynamics including nonlinear excitations of the atomic subsystem. We carry out Monte Carlo simulations and show that mean square displacements of electrons and transport properties are in a moderate to high temperature regime strongly influenced by soliton-type excitations and demonstrate the existence of percolation effects.

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## 1 Introduction

In preceding works [1–8] a soliton-mediated new form of non-Ohmic fast electric conduction has been proposed and studied in detail albeit mostly for one-dimensional (1d-) systems. In recent work we extended these studies to two-dimensional systems of electrons and atoms using adiabatic semi-classical approximations [4, 5, 7–11]. Here we formulate the quantum statistics based on the tight-binding approximation (TBA) and derive Pauli-type kinetic equations. We consider a highly disordered atomic system, e.g. an atomic monolayer on a surface or a layer imbedded into a 3d-system in which an electronic plasma system is embedded. The electron concentration is in our model rather low and assumed to be generated by doping, the dynamics is mainly determined by the electron-atom and by the atom-atom interactions.

Here we do not have in mind any kind of concrete system but we may think about the electron plasma in the Cu O<sub>2</sub> layers of Cuprates which are coupled to nonlinear oscillations of the oxygen atoms [12]. One may hope that a better understanding of the nonlinear excitations of such two-dimensional plasmas may contribute to the better understanding of the electronic properties of such systems [13]. Indeed there is some experimental evidence suggesting that in this type of conducting systems, anharmonic effects may play a key role [12–17].

As we have shown in [6] by using a generalization of the Kubo-Zubarev method [18–23], the complete information on the lattice excitations may be taken into account by the dynamic structure factor. This procedure is particularly useful for studying the influence of nonlinear excitations of the atomic lattice on conductive properties.

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In difference to earlier work [2, 6] we use here the tight-binding approximation [24–26] as more appropriate to the kind of problems treated here [26].

The central physical problem we study is the coupling of the nonlinear atomic lattice excitations to the dynamics of the electrons. The physical basis for such a coupling is the polarization interaction between electrons and atoms. As in our earlier works [6, 8, 11] we assume the Buckingham model potential for the polarization interaction between the atoms and the electrons,

$$V_{ea}^{\text{pol}}(r) = -\frac{U_e h^4}{(r^2 + h^2)^2}. \quad (1)$$

The long-range behavior is given by the polarizability of the atom,  $V(r) \propto r^{-4}$ , whereas a cut-off parameter  $h$  is introduced to obtain a finite potential energy  $U_e$  at zero distance. Considering an atomic configuration  $\{\mathbf{R}_n\}$ ,  $n = 1 \dots N$ , where the position  $\mathbf{R}_n$  of the  $n$ th atom may change with time, the total electron potential due to the atoms is  $V_{ea}(\mathbf{r}) = \sum_n V_{ea}^{\text{pol}}(\mathbf{r} - \mathbf{R}_n)$ . We assume that the density of the electrons is low so that their interaction and quantum degeneracy can be neglected. Since the polarization potential is attractive, in equilibrium the electrons will be concentrated around regions of highest atomic density.

The atoms interact with an anharmonic potential. We use here the Toda-Morse like exponential interaction [4]. Our aim is to show that the electron carriers form a *supersonic* solitary wave that builds upon the anharmonicity of (positive) ion interactions. The supersonic soliton carrier proposed in Refs. [3–10] 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 e.g. the Toda-Morse exponential interaction [4].

In view of the above in the present work we look at the problem from the general approach provided by the linear response transport theory [18, 19], 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 two-dimensional materials in a heat bath without assuming external driving of the excitations. Before embarking in such an approach it is worth recalling a few features about electric transport in electron-atom systems.

Present-day theories of thermal and electric transport processes in electron-atom systems like solids or plasmas do take into account different elementary excitations like phonons, polarons, plasmons, and excitons [33, 34, 37, 38]. For a survey of transport theory of dense Coulombic systems including solids and dense plasmas we refer to [20–23, 39]. As the coupling of electron modes with phonon modes is well understood it is thus clear why we here explore the possibility of interaction of electrons with soliton modes.

## 2 Hopping dynamics of the electron - atom system

### 2.1 Hamiltonian in tight-binding approximation

We study a  $d$ -dimensional system of atoms ( $d = 1, 2, 3$ ) and embedded electrons which may carry electric current. For illustration we restrict to 1d-, or 2d- lattices in order to assess the influence of nonlinear excitations on the conductivity. The system consists of  $N$  atoms forming a disordered lattice with rest positions  $\mathbf{R}_n^{(0)}$ ,  $n = 1 \dots N$ , and one or several electrons with periodic boundary condition. Electroneutrality is given by a compensating homogeneous background charge density. The dynamics of the system is given by the Hamiltonian

$$H = H_{\text{lattice}} + H_{\text{el}} + H_{\text{lattice-el}}. \quad (2)$$

The lattice part of the Hamiltonian,  $H_{\text{lattice}}$ , models dynamical changes of the equilibrium positions of the atoms,

$$H_{\text{lattice}} = \sum_n^N \frac{p_n^2}{2M} + \frac{1}{2} \sum_{m,n} V_{aa}(\mathbf{R}_n - \mathbf{R}_m). \quad (3)$$

We approximate the potential of the forces between two atoms by the Morse-potential

$$V_{aa}^{\text{Morse}}(r) = D [\exp(-2B(r - r_0)) - 2 \exp(-B(r - r_0))]; \quad (4)$$

$D$  is the breakup energy of a bond,  $B$  is the range parameter of the Morse potential (otherwise called the lattice stiffness), and  $M$  denotes the mass of an atomic unit. Instead of the stiffness  $B$  we will use later the dimensionless stiffness  $b = B\sigma$ , which usually has values in the range  $b = 1 - 10$ . Alternatively, we can also introduce  $\mathbf{R}_n - \mathbf{R}_n^{(0)}$  that quantify the relative displacements of the atoms from their equilibrium positions. The atoms are composed of the ion cores with strongly bound electrons that are not excited to higher states. In general, they have a spin as additional degree of freedom, for instance in the case of hydrogen. We will not consider spin states in the present calculation. The electron part of the Hamiltonian,  $H_{\text{el}}$ , describes the electrons that are added to the atomic system. Instead of free electron states interacting via the Coulomb potential, we start from the tight binding approximation where the additional electrons are localized at atom sites so that they are coupled to the lattice degrees of freedom.

The interaction of the additional electrons with the neutral atoms is given by the polarization potential, that has for large distances the asymptotic form  $V^{\text{pol}}(r) \sim \alpha e^2 / (2\epsilon_0 r^4)$  with the atomic polarizability  $\alpha$ . For example, in the case of hydrogen we have  $\alpha = 4.5a_B^3$ . Here a bound state is found in the singlet channel of the bound and attached electron, with binding energy 0.754 eV. Because of the Pauli principle, no bound state is observed in the spin triplet state. As a specification of the polarization potential discussed in the Introduction, we will adapt the screened Buckingham potential for the electron-atom interaction [22],

$$V_{ea}(r) = -\frac{\alpha e^2}{2\epsilon_0(r^2 + h^2)^2}(1 + \kappa r)e^{-2\kappa r}. \quad (5)$$

For hydrogen, different values of the cut-off parameter  $h$  can be found. To reproduce the exact value of the interaction potential at  $r = 0$ , Buckingham found  $h = 1.4565a_B$  [22]. To reproduce the correct binding energy of  $\text{H}^-$ , the value  $h = 1.033a_B$  has been obtained [28]. The factors containing the screening parameter  $\kappa$  reduce the polarization potential, as given by the Debye screening. Note that we neglect here screening effects ( $\kappa = 0$ ) assuming a low enough density of electrons. Note further that different mechanisms are possible if the neutral system interacts with a charged particle. The polarization of neighboring atoms is related to the polarization of the lattice leading to the polaron. In the case of ideal plasmas, Debye screening accounts for the polarization of the surroundings.

To study the evolution of the additional electrons interacting with the atoms, we assume a tight-binding model Hamiltonian of hopping type [21, 24–26]

$$H_{\text{el}} = \sum_{n,m} E_{n,m} c_{n,m}^+ c_{n,m} + \sum_{n,n',m} t_{n,n',m} (\mathbf{R}_{n'} - \mathbf{R}_n) c_{n',m}^+ c_{n,m} \quad (6)$$

with the matrix elements

$$E_{n,m} = \langle n, m | H_0 + V_{ea} | n, m \rangle; \quad t_{n,n',m} = \langle n', m | H_0 + V_{ea} | n, m \rangle, \quad (7)$$

$m$  denotes the internal quantum number of the electron state that is bound to the atom at site  $\mathbf{R}_n$ . In the following we will assume for simplicity, that there is only one internal quantum state per atom. In particular, the additional electrons can be in a localized, bound state, but they can also form extended states when they are excited above the edge of continuum. We will drop the internal quantum number  $m$  in the following. If necessary, the internal state that characterizes the orbit as well as spin, can be included in the quantum number  $n$ . Now, we get [29]

$$H_{\text{el}} = \sum_n E_n c_n^+ c_n + \sum_{n,n'} t_{n,n'} c_{n'}^+ c_n, \quad (8)$$

The matrix elements  $E_n, t_{n',n}$  are functions of the atomic configuration  $\{\mathbf{R}_1, \dots, \mathbf{R}_N\}$  that describe the coupling to the lattice. The diagonal terms contain in addition to the atomic binding energy  $E_0$  also the polarization interaction with the other atoms. We will use the simple assumption that the eigenvalues are shifted like the polarization potential

$$E_n \simeq E_0 - \sum_{n'=1}^N \frac{U_e h^4}{[(\mathbf{R}_n - \mathbf{R}_{n'})^2 + h^2]^2}. \quad (9)$$

As a consequence, the energies  $E_n$  form a rather complex landscape that is determined by the atomic positions  $\{\mathbf{R}_1, \dots, \mathbf{R}_N\}$  and leads to a distribution of the energy levels with density of states  $D(E)$ . In the 1d-case in a first order approximation a linear Holstein model may be used [4, 5]. Note that this coupling to the lattice is closely related to the contribution to the electron-lattice interaction introduced by Davydov [4, 5]. The transition matrix  $t_{n,n'}$  is a fluctuating quantity depending on the atomic distances,  $t_{n,n'} = t(\mathbf{R}_{n'} - \mathbf{R}_n)$ . In the following we will assume an exponential decrease, as earlier suggested by Slater [30]

$$t_{n,n'} = t_0 \exp[-\alpha_{\text{hop}}|\mathbf{R}_n - \mathbf{R}_{n'}|]. \quad (10)$$

The range parameter  $\alpha_{\text{hop}}$  can be related to the tunneling probability that decreases exponentially with distance.

## 2.2 Dynamics of the atom subsystem

For the *heavy* atoms, mass  $m$ , we assume that they obey classical Langevin dynamics. We include a phenomenological damping  $\gamma_n$ . In the presence of random forces  $\xi_n(t)$  (hence non zero temperature that determines the strength  $2D_v$ ) and also external forces, the evolution of the  $n$ th atom is described by the Langevin equations ( $n = 1, 2, \dots, N$ )

$$\frac{d\mathbf{v}_n}{dt} + \frac{1}{m} \frac{dH}{d\mathbf{R}_n} = -\gamma_n \mathbf{v}_n + \sqrt{2D_v} \xi_n. \quad (11)$$

The stochastic forces (with diffusion coefficient  $D_v$ ) model a surrounding heat bath (Gaussian white noise). The factor  $\gamma$  describes the standard friction frequency acting on the atoms from the side of the surrounding heat bath. The validity of an Einstein relation  $D_v = k_B T \gamma / m$  is assumed, where  $T$  is the temperature of the heat bath and  $k_B$  is the Boltzmann constant.

Let us assume that the atoms are randomly distributed according to the canonical ensemble. The atomic dynamics in nonlinear lattices is described by the *dynamic structure factor*, which is defined as

$$S(\mathbf{q}, t) = \sum_{n,n'} \exp\{i\mathbf{q} \cdot [\mathbf{R}_n(t) - \mathbf{R}_{n'}(0)]\}. \quad (12)$$

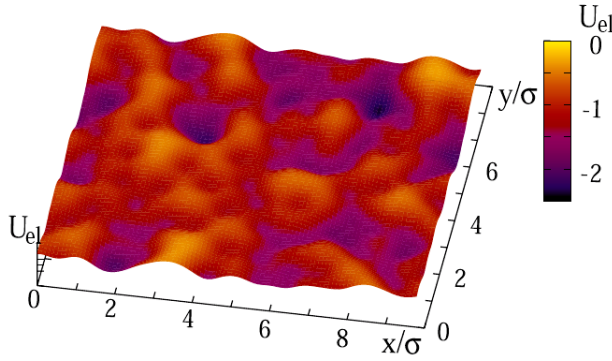
The Fourier transform with respect to time is given by

$$S(\mathbf{q}, \omega) = \int dt \exp(i\omega t) S(\mathbf{q}, t). \quad (13)$$

More information on this function is given elsewhere (see Refs. [3, 6, 40]). The function  $S(q, \omega)$  for classical systems of particles is known from theoretical estimates and from experimental studies based on investigations of inelastic neutron scattering. It contains the harmonic excitations (phonons) as well as non-linear excitations (solitons). Note, however, that the knowledge about dynamic structure factors for two- and three-dimensional conductors is quite limited [23, 41, 42]. The Hamiltonian describes the influence of the atomic motion to the electron dynamics, the feedback of the electron dynamics on the atomic motion is neglected. Any cluster of moving atoms generates a potential hole in which electron density might be concentrated and any displacement of the atoms changes the polarization energy. The electron will follow these changes. This means that the running local compressions generate a complex landscape with rather deep moving potential wells, which strongly influence the local dynamics of the electrons and possibly even capture the light electrons. In order to illustrate these structures we may use the simplest classical approximation and assume that the electron density follows the Boltzmann distribution (normalized to 1)

$$n(\mathbf{r}) = \frac{\exp(-\beta V_{ea}(\mathbf{r}))}{\int d\mathbf{r}' \exp(-\beta V_{ea}(\mathbf{r}'))}. \quad (14)$$

where  $V_{ea}(\mathbf{r})$  is the total local potential at the position  $\mathbf{r}$  of an electron. An example of the distribution of the polarization potential is shown in Fig. 1.



**Fig. 1** Snapshot of typical landscape of the polarization potential on a thermal lattice, created by the solitonic excitation in a 2d-lattice with  $10 \times 10$  particles (parameter values  $b = B, \sigma = 3, T = 2$ ). The colors represent the levels of potential, only the highest peaks are displayed. (Online color: [www.cpp-journal.org](http://www.cpp-journal.org)).

### 3 Transport theory of electron hopping in nonlinear lattices

#### 3.1 Linear response theory

In our previous work we studied already the influence of solitonic excitations on the conductivity of electron plasmas in the framework of classical and semiclassical descriptions [6]. As the most important result we may consider that the solitonic excitations may lead to an increase of the conductivity. This is due to an increase of the long correlations in the dynamics of the electrons and a corresponding decrease of the collision frequency in the plasma. Note that the mechanism of hopping conductivity is somewhat opposite to the mechanism of plasma conductivity. In plasma conductivity the unperturbed state is the free motion of the electrons, the perturbations are the acts of scattering. In the case of hopping, the unperturbed state is the rest of the electron in one of the bound states, the perturbation is the transition, the hopping to a different state.

In linear response theory, transport coefficients are obtained from equilibrium time correlation functions. In the framework of quantum statistics an average is defined as [6]

$$\langle A; B \rangle_{\omega - i\eta} = \int_0^{\infty} d\tau \exp[-(\eta + i\omega)\tau] \frac{1}{\beta} \int_0^{\beta} d\lambda \text{Tr} [\rho_0 B(\tau - i\hbar\lambda) A]. \quad (15)$$

where  $\omega$  denotes the frequency of the external perturbation, and  $\eta \rightarrow +0$  after the thermodynamic limit is taken. The time dependence is according to the Heisenberg picture with respect to the system Hamilton  $H_s$ ,  $B(t) = \exp(iH_s t/\hbar) B \exp(-iH_s t/\hbar)$ , and  $\rho_0 = Z^{-1} \exp(-\beta H_s + \beta\mu)$  is the grand canonical distribution. In the classical, nondegenerate limit, the operators are commuting variables so that the  $\lambda$ -integral can be dropped.

The time correlation function of the electron is the essential quantity which determines transport properties as e.g.:

- (i) conductivity,
- (ii) diffusion and mean square displacement,
- (iii) reaction rates.

Most transport properties are determined by the correlation time or more general by the integral over the velocity correlation function, as e.g. the diffusion coefficient, the static conductivity and the mean square displacement:

$$D \simeq \langle v; v \rangle_0, \quad \sigma = \frac{e^2}{k_B T} \langle v; v \rangle_0, \quad \langle \delta x(t)^2 \rangle \simeq \langle v; v \rangle_0 t. \quad (16)$$

#### 3.2 Hopping conductivity

Let us study now the velocity-velocity correlation function. The position operator of the  $N_e$  electrons embedded into the atomic subsystem is denoted by  $\mathbf{R} = \sum_j^{N_e} \mathbf{r}_j$ . Following [21] we proceed as follows. We start from the average velocity

$$\langle \dot{\mathbf{R}} \rangle^t = \text{Tr}(\rho(t) \dot{\mathbf{R}}) \quad (17)$$

and represent the position operator in the hopping form

$$\mathbf{R} = \sum_n \mathbf{R}_n c_n^\dagger c_n. \quad (18)$$

This way we find for the derivative

$$\dot{\mathbf{R}} = \frac{i}{\hbar} [H_{\text{lattice-el}}, \mathbf{R}] = \frac{i}{\hbar} \sum_{nn'} t_{n,n'} (\mathbf{R}_n - \mathbf{R}_{n'}) c_{n'}^\dagger c_n. \quad (19)$$

In the framework of an adiabatic approximation we assume now that the positions of the lattice particles are fixed for a moment, so that we have to follow only the fast electron dynamics. The coupling of the electrons to the external field  $\mathbf{E}$  is described by

$$H_E = -e\mathbf{E} \cdot \mathbf{R}. \quad (20)$$

Following [24–27, 29] we have

$$\langle \mathbf{j} \rangle = \text{Tr}(\rho \mathbf{j}) = \frac{e}{V} \text{Tr}(\rho \dot{\mathbf{R}}) = \sigma \mathbf{E} \quad (21)$$

and represent this in the hopping form. In a first approximation we neglect dynamical disorder, in particular solitonic excitations, and consider the atoms on a lattice. Then by introducing the derivative into eq.(21) we find [29] the first contribution to the current

$$\mathbf{j}_1 = \frac{\beta e^2}{2\epsilon_0 \hbar V} \sum_{n,n'} |t_{n,n'}|^2 (\mathbf{R}_n - \mathbf{R}_{n'}) \mathbf{E} (\mathbf{R}_n - \mathbf{R}_{n'}) f_{n'} (1 - f_n) E(n, n'). \quad (22)$$

Two comments are needed:

1) In our expression for the current appears a term  $f_{n'}(1 - f_n)$ . This is a weight factor for the transitions  $n' \rightarrow n$ . These transitions occur with the weight  $f_{n'}$  if and only if the state  $n$  is free as expressed by the weight factor  $(1 - f_n)$ . The factor  $f_{n'}(1 - f_n)$  is responsible for the fact that the biggest contribution to the integrals comes from the region around the Fermi level. Effects connected with degeneration will be discussed in a subsequent work.

2) We separated a term  $E(n, n')$  which denotes the energy conservation and is defined by

$$E(n, n') = 2\pi \delta(E_n - E_{n'}) \quad (23)$$

Corresponding to eq. (22) we get a contribution to the conductivity

$$\sigma_1 = \frac{\beta e^2}{2\epsilon_0 \hbar V} \sum_{n,n'} |t_{n,n'}|^2 (\mathbf{R}_n - \mathbf{R}_{n'})^2 f_{n'} (1 - f_n) E(n, n') \quad (24)$$

We will call this the direct conductivity induced by the external field. The problem is that the expression (24) gives the correct conductivity only for "regular" lattices. Our atom distributions, however, are very nonuniform, and we may have therefore a second contribution to the conductivity which stands for the nonuniformity [24–27]

$$\mathbf{j}_2 = \frac{\beta e^2}{2\epsilon_0 \hbar V} \sum_{n,n'} (\mathbf{R}_n - \mathbf{R}_{n'}) [\delta\mu_{n'} - \delta\mu_n] t_{n,n'} f_{n'} (1 - f_n) E(n, n') \quad (25)$$

Here the quantity  $\delta\mu_n$  describes a kind of chemical potential change due to the redistribution of the particles at the  $n$ th site. In a system with regular lattice, i.e. in the presence of translational symmetry, such a redistribution does not occur, i.e. we have  $\delta\mu_n = 0$  for all sites. However in the nonuniform case, applying a field the charges are redistributed as a reaction of the external field. According to the principle of minimum entropy production of Prigogine, this reaction of the system will enhance the conductivity obtained from eq.(24). Because the estimation of the additional, diffusive current is a nontrivial task that needs the self-consistent determination of  $\delta\mu_n$ , see [21], we will restrict our study to the direct current, thus limiting the validity of our results to the region of not too strong deformations of the lattice.

### 3.3 Open systems

The formulae derived so far, correspond to a closed system which conserves energy in each microscopic act which is expressed by the delta function  $E(n, n')$ . Our system is open since the lattice is embedded in a heat bath modeled by the damping and the noise in the Langevin equation. In order to realize the transition to open systems we replace the delta-function  $E(n, n')$  by some temperature function which should model the influence of the heat bath similar to that proposed in [8] and following the lines developed in [24, 26]. We use the following "ansatz"

$$E(n, n') = \exp\left[-\frac{\beta}{2}(E_n - E_{n'})\right]F(n, n'), \quad (26)$$

$$F(n, n') = F(E_n - E_{n'}) \quad (27)$$

where  $F(E_n - E_{n'})$  is an even function of the difference of the energy levels. There are several variants for this even function  $F(x)$  given in the literature [26]. 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 [32]. This corresponds to the  $F$ -function.

$$F(E_n - E_{n'}) = \exp\left[-\frac{\beta}{2}|E_n - E_{n'}|\right] \quad (28)$$

Proper statistical derivations of the thermal factors may be based on specific microscopic models of the heat bath. Böttger and Bryksin [24, 26] derived the following general expression

$$F(E_n - E_{n'}) = \int_{-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\tau|E_n - E_{n'}|\right]K(|\tau|)d\tau, \quad (29)$$

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 obtained also in other work [43]

$$F(E_n - E_{n'}) = \frac{V_0}{\hbar} \frac{\gamma}{\gamma^2 + (|E_n - E_{n'}|/\hbar)^2} \quad (30)$$

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

The same argument can also be given in the quantum statistical approach where correlation functions  $\langle A; B \rangle_{\omega - i\eta}$  have to be evaluated, see [44]. The parameter  $\eta$  can be interpreted as inverse relaxation time to bring the statistical operator to the relevant distribution. Such relaxation processes are due to all interactions that are not explicitly treated in the Hamiltonian  $H_s$ . In particular, the excitation of phonons or the Langevin dynamics of the atoms are such processes. As long as they are not explicitly included in  $H_s$ , they can be accounted for by an effective relaxation time, i.e. a finite value of  $\eta$ . A finite value of  $\eta$  gives immediately the Lorentz profile (30) calculating  $\int_0^{\infty} d\tau \exp[-(\eta + i\omega - (i/\hbar)(E_n - E_{n'}))\tau]$ . Another simple approximation for the thermal factor is the Monte Carlo procedure, which we will use in the next section.

So far we formulated all equations in the framework of an adiabatic approximation with respect to the lattice dynamics. All quantities appear as slow functions of the atomic positions in the lattice. That means all quantities have still to be averaged over lattice positions following the dynamics over certain time interval. In particular, the configurational average gives the probability  $D(E)$  of the energy levels (diagonal disorder) that has to be considered for the energy conservation discussed above.

In principle this averaging may be avoided, if the structure factors of the lattice are known. In order to introduce the structure factors into the transport theory we may proceed as shown in our previous work [6] replacing the plasma Hamiltonian by the hopping-type Hamiltonian (8).

We consider the transition matrix

$$t_{n,n'} = t(\mathbf{R}_{n'}, \mathbf{R}_n) = t(\mathbf{r}_{n,n'}); \quad \mathbf{r}_{n,n'} = \mathbf{R}_{n'} - \mathbf{R}_n \quad (31)$$

and introduce the Fourier transform of the transition matrix  $t(\mathbf{q}) = \int d^3r \exp(i\mathbf{q} \cdot \mathbf{r})t(\mathbf{r})$ . We proceed as above by perturbation theory and introduce the *dynamic* structure factor as defined above and the corresponding Fourier transform  $S(\mathbf{q}, \omega)$ . This way we find within perturbation theory the generalization of Eq. (24)

$$\sigma = \frac{\pi\beta e^2}{\epsilon_0 \hbar V} \sum_{nn'} \int d\mathbf{q} |t(\mathbf{q})|^2 f_{n'}(1 - f_n) \frac{d^2}{dq^2} S \left[ \mathbf{q}, \frac{1}{\hbar}(E_{n'} - E_n) \right] \frac{\exp(\beta(E'_n - E_n)) - 1}{\beta(E'_n - E_n)}. \quad (32)$$

#### 4 Stochastic electron dynamics on thermal lattices

So far our analysis has been based on the Schrödinger equation for the electrons in the tight binding approximation which is coupled to the Langevin equation for the classical lattice particles. This tacitly assumes 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 (3). As shown in [4, 5] we may describe this way also irreversible solitonic excitations at finite temperature. However, a serious problem connected with this approach are 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 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 [18, 19]. The main problem is here to give a correct description of the coupling to the heat bath. In our case of the tight binding systems, the situation is somehow simpler due to the discrete character of the electronic states, which allows a description by discrete Markov chain equations [8, 24, 26, 43]. The Markov approach to electron dynamics goes back to Pauli's (1928) seminal work [31]. 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 or Fermi-Dirac. Later generalizations are connected with the development of Metropolis algorithms for *canonical* ensembles [32]. Applications to hopping conduction in solids were given since the seventies by several authors [24, 26]. First applications of the master equation formalism to electron transfer in macromolecules are due to [43]. The system we are studying here is rather difficult and seems to be too complicated to be treated in full detail. We have:

- (i) quantum electrons located in discrete states, which are coupled to a heat bath and to the classical lattice,
- (ii) classical lattice particles coupled to the heat bath and to the quantum electrons.
- (iii) the heat bath with an unspecified internal dynamics.

An additional difficulty is connected with the very large difference between the electronic and the lattice time scales which was mentioned above.

To simplify this situation we postulate here that the thermal electrons allow a Markov description. Thus we move from the *reversible* Schrödinger equation for the occupation numbers in the tight-binding model to an *irreversible* Pauli master equation description [19, 31]. Following Pauli's method we postulate a master equation for the occupation probabilities of electrons  $p_n$  of the state  $n$ , given here by the position  $\mathbf{R}_n$  with the energy  $E_n$ :

$$\frac{dp_n}{dt} = \sum_{n'} [W_{nn'} p_{n'} - W_{n'n} p_n]. \quad (33)$$

The transition probabilities were derived by Pauli using perturbation theory for microcanonical ensembles (transitions in a narrow energy shell). For comparison, in the Schrödinger equation approach also nondiagonal elements of the density matrix occur that are in general not small. 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 the perturbation approach. With this assumption the transition probabilities for the tight-binding model read [8, 31, 43]

$$W_0(n, n') = \frac{t_0^2}{\hbar} \exp[-2\alpha_{\text{hop}}|\mathbf{R}_{n'} - \mathbf{R}_n|] 2\pi\delta(E_n - E_{n'}), \quad (34)$$



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. Taking into account the heat bath we assume the structure

$$W(n, n') = \frac{t_0^2}{\hbar} \exp[-2\alpha_{\text{hop}}|\mathbf{R}_n - \mathbf{R}_{n'}|] E(n, n', \beta). \quad (35)$$

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-like factor. Temperature effects are to be included. When the electrons are embedded into a heat bath together with the thermal lattice particles [24, 26], 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

$$\frac{W(n', n)}{W(n, n')} = \exp[\beta(E_n - E_{n'})]. \quad (36)$$

corresponding to the relation of Boltzmann factors.

The simplest way to satisfy the condition of detailed balance is the Monte Carlo algorithm which we will use here. For the transition rates (35) we take, see Eq. (28),

$$E(n, n') = 1 \quad \text{if} \quad E_n < E_{n'}, \quad (37)$$

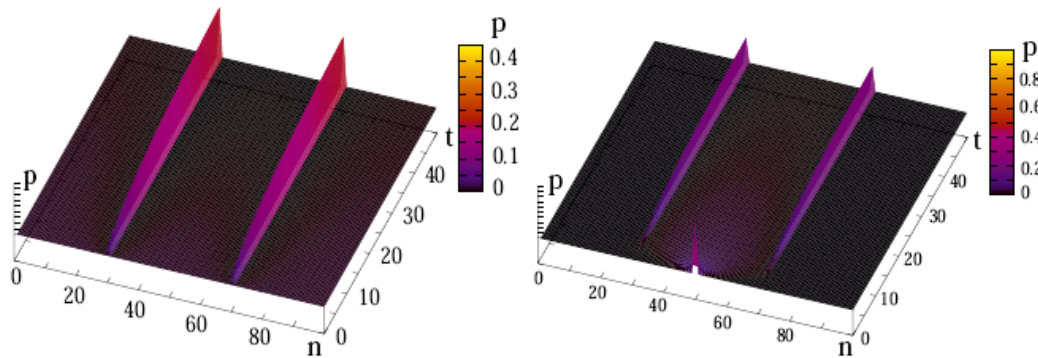
$$E(n, n') = \exp[-\beta(E_n - E_{n'})] \quad \text{if} \quad E_n > E_{n'}. \quad (38)$$

A simplified form for the 1d-case was used in ref. [8]. The master equation in the given form is a useful tool for computer simulations of irreversible (non-coherent) electron hopping processes. Since the detailed balance is obeyed, it is guaranteed that in thermal equilibrium an H-theorem is valid and any initial distribution converges to the canonical distribution, which is the target distribution of the master equation.

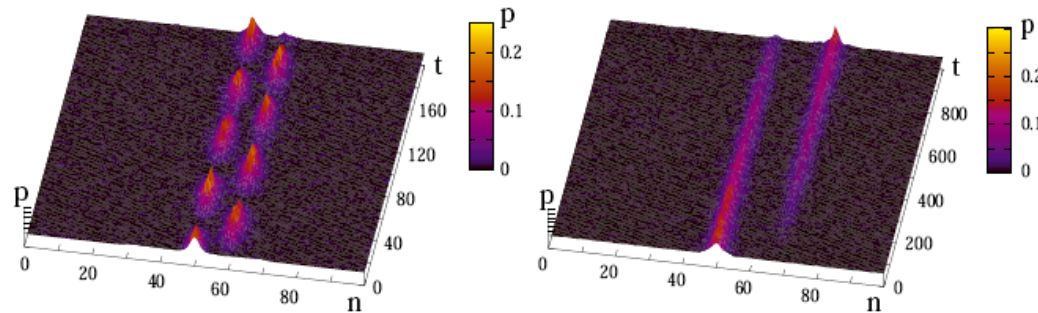
In order to simplify our computer simulations we used so far only the simplest "ansatz", the Monte Carlo procedure described above. The Pauli system of equations contains several approximations, however it provides a rather fast and therefore useful tool for the simulations of the electron-lattice dynamics in thermal systems. Fig. 2 illustrates results of computer simulations for the case that two fixed wells, depth 2 (in our units 2D), at the atoms with positions  $n = 30$  and  $n = 70$  are present. We studied two different initial conditions. In the first case the initial electron density is uniformly distributed. In the second case we initially have a delta-like distribution in between both wells at position  $n = 50$ . We see that the relaxation to a canonical distribution with two peaks around the positions of energy wells is rather fast, in a few time units the final distribution is reached. In this respect the Pauli equation describes a basically different behavior as the Schrödinger equation, see Fig. 3. In the latter we have a reversible description and see a periodic return to the initial state. In the Pauli description the behavior is irreversible which is due to the neglect of non-diagonal terms of the density matrix. As reason for the decay of non-diagonal elements the coupling to a surrounding heat bath may be considered.

We show the difference between a Pauli dynamics and a Schrödinger dynamics in Figs. 2 and 3. The evolution of densities in time is irreversible in the Pauli description and is quasiperiodic in the Schrödinger picture. The quasiperiodicity is due to the reversibility of the Schrödinger equation which is in our example only weakly disturbed by the coupling to the irreversible low-temperature Langevin dynamics. We observe coherent motions of the electron density between the two wells which is tunneling-like. In the Pauli dynamics the coherence between the phases is destroyed and we see an irreversible approach to canonical distributions. This is a major difference and the choice of the description might depend on the question we ask. Here we concentrate on transport processes based on irreversible phenomena.

We mention also that due to the way we treat electron relaxation effects there are also differences between the methodology using the coupled Pauli and Langevin equation system and that using adiabatic approximations at least for small and for moderate values of adiabaticity  $\tau \sim 1$ . Here the parameter of adiabaticity  $\tau = V_0/\hbar\omega_0$  denotes the relation between the characteristic time of lattice oscillations  $1/\omega_0$  and the electron hopping time  $\hbar/V_0$ . For large  $\tau$ , the electron relaxation in the heat bath may be considered as very fast and the distribution



**Fig. 2** Morse lattice. The Pauli equation evolution of the electron density for a one-dimensional lattice with 2 energy wells and the temperature  $T = 0.01$  for two initial electron distributions. The irreversible dynamics is illustrating the H-theorem. We study the dynamics of the electron density for the case that the fixed wells are located at  $n = 30$  and  $n = 70$  and have the depth  $E_n = -2$ . Left panel: The initial electron density is uniform.: Right panel: A “localized” (delta-like) initial condition, as time proceeds, splits into two peaks around the wells. Parameter values  $T = 0.01$ ,  $N = 100$ ,  $\alpha = 0$ . The parameter of adiabaticity has the value  $\tau = V_0/\hbar\omega_0 = 10$ . (Online color: www.cpp-journal.org).



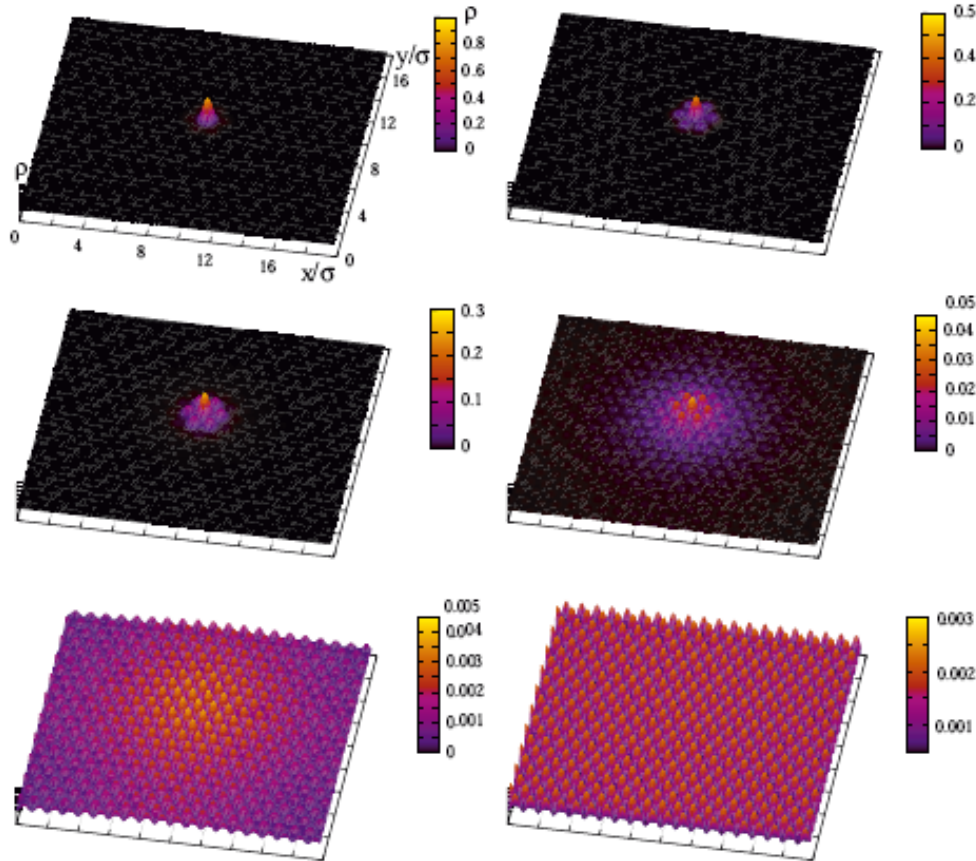
**Fig. 3** Morse lattice. The tight-binding Schrödinger evolution of the electron density on a one-dimensional Morse lattice at the temperature  $T = 0.01$  with two energy wells and delta-like initial electron distributions. The plots illustrate the quasi-reversible dynamics including coherent motions. The electron density corresponds to two fixed wells with depth  $\epsilon_0 = -5$  and a distance 10 (left panel) and a distance 18 (right panel). Parameter values  $T = 0.01$ ,  $N = 100$ ,  $\alpha = 0.1$ ,  $V_0 = 0.1$  and  $\tau = 10$ . (Online color: www.cpp-journal.org).

may be approximated by a local Boltzmann- or Fermi distribution as shown in ref. [8]. For small and moderate values of the  $\tau$ -parameter, say for  $\tau \simeq 10 - 20$ , the approach based on the Pauli equation is most useful, since it provides information on deviations from the adiabatic approximation. Our approximation based on the Pauli method 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 electrons adapt “instantaneously” to any change in the lattice. In other words one assumes that the electrons follow in a very fast way to the new atomic configuration and may be described at any time by the canonical distribution [9]. In the present approach based on Pauli’s method we take into account that the electrons need time to follow the lattice motions what leads to certain delay in their response and to some deviations from the stationary solution.

## 5 Mean square displacement and transport coefficients

The simplest transport property is diffusion. Many other properties are simply related to this as explained above. Our access to diffusion is through the Einstein relations for the mean square displacement. Let us first discuss some basic aspects. As well known, the spreading of the wave packets according to the Schrödinger equation is not a diffusion process. In the Pauli-type description the irreversible aspect of the diffusion process of the electron

density is correctly described as discussed above. Therefore we will concentrate here on the Pauli description. Figs. 4 and 5 obtained from Pauli dynamics simulations illustrate how the spreading of the electron density, which is diffusion-like, is strongly influenced by the excitations of solitons in the lattice. We observe that the thermal solitons create a kind of diffusive channel which stabilize the diffusive character of the spreading as earlier noted for the 1d-case. In order to investigate the diffusive transport we made several simulations with a delta-like initial distribution of the electrons for different times and calculated by averaging the "effective" diffusion coefficient. An example for the spreading of the wave function in the 2d case is shown in Figs. 4 and 5.



**Fig. 4** Morse lattice. The spreading of the electron density in a two-dimensional cold lattice ( $T = 0.001$ ) for a "localized" (delta-like) initial distributions at 6 subsequent time instants:  $t = 0.001, 0.01, 0.1, 1.0, 2.0, 4.0$ . Parameter values  $N = 400$ ,  $b = B\sigma = 4$ ,  $\alpha = 0.1$ , and  $\tau = 20$ . (Online color: [www.cpp-journal.org](http://www.cpp-journal.org)).

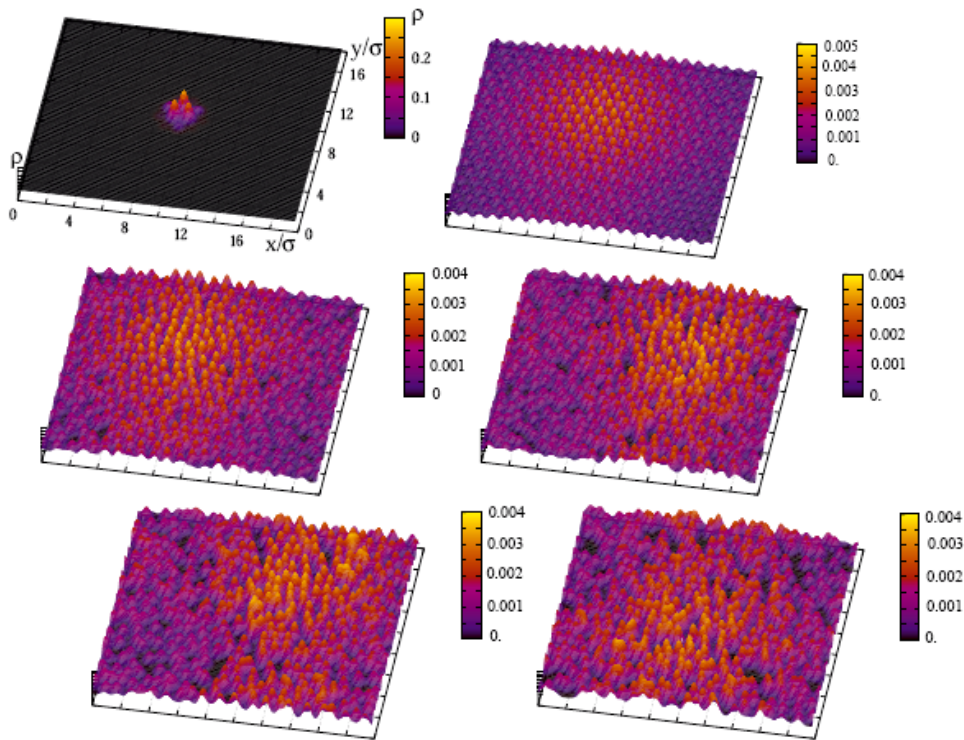
This "effective" diffusion coefficient may be estimated on the basis of the Einstein relation for the mean square displacement. For the one-dimensional case the mean square displacement is connected with time and effective diffusion constant by the relation

$$\langle(\delta n)^2\rangle_t = 2D_{\text{eff}}t. \quad (39)$$

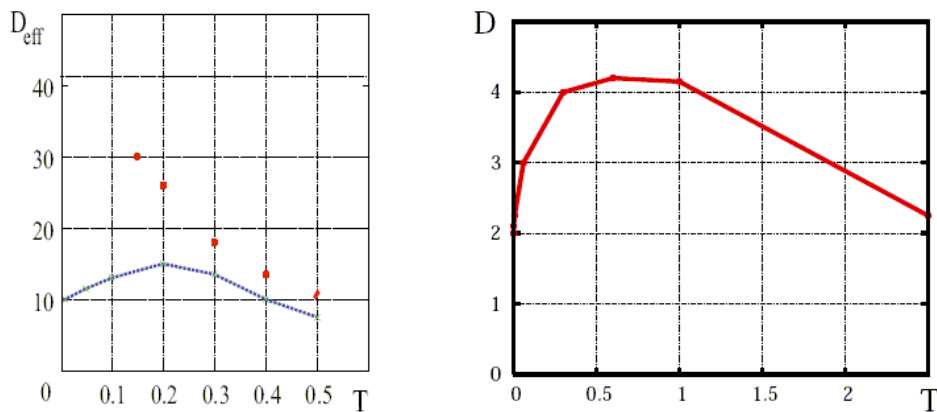
Here  $n(t)$  is the position (the site) for an electron which starts at  $n_0$  at  $t = 0$ . The average is to be done as follows. First, the average with respect to the distribution is to be taken

$$\langle(\delta n)^2\rangle_t = \sum_n (n - n_0)^2 p_n(t). \quad (40)$$

Further we have to average over many realizations of the lattice dynamics. Some results for the 1d-case are given in Fig. 6.



**Fig. 5** Morse lattice. The spreading of the electron density for “localized” (delta-like) initial electron distributions on a 2d-lattice for a fixed time instant  $t = 1$  after the start for 6 increasing temperatures  $T = 0.0006, 0.006, 0.3, 0.6, 1.0, 1.54$ . Parameter values:  $N = 400$ ,  $\alpha' = 0.5$  and  $\tau' = 10$ . (Online color: www.cpp-journal.org).



**Fig. 6** Estimate of the diffusion constant as a function of temperature for Morse lattices. Left panel: Data obtained in ref. [8] for 1d-Morse lattices by simulations with the Master equation in combination with the Langevin equation. Particle number  $N = 200$ , stiffness of the Morse atoms  $b = B\sigma = 1$ , parameters of the electron-lattice interactions  $\alpha = 1, \chi_1 = 0.1$ . The few points outside the main curve were obtained within the Langevin -Schrödinger-TBA-model for the electron-lattice parameters  $\alpha = 1.75, \chi_1 = 0$ , the increase of the values in comparison to the curve are due to contributions of coherent transport. Right panel: Estimate of the diffusion constant as a function of temperature for two-dimensional lattices obtained by simulations with the master equation in combination with the Langevin equation. Parameter values:  $\alpha = 0.5, \tau = 10, N = 400, b = B\sigma = 4$ . (Online color: www.cpp-journal.org).

In the 2d-case the mean square displacement is defined as

$$\langle (\mathbf{R}(t) - \mathbf{R}(0))^2 \rangle = \sum_n (\mathbf{R}_n - \mathbf{R}_0)^2 p_n(t). \quad (41)$$

Finding this expression as a function of time we may estimate the effective diffusion coefficient from

$$\langle (\mathbf{R}(t) - \mathbf{R}(0))^2 \rangle = 4D_{\text{eff}}t. \quad (42)$$

We note that the master equations are not closed, they still depend on the particle coordinates. The corresponding equations for the lattice particles was investigated for the 1d case in Ref. [8]. We calculated the mean square displacement for several temperatures and represented the mean square function  $d(t)$  from simulations by a linear fit. For  $T < 0.1$  no good approximation by a straight line could be achieved since the shape of the curves  $d(t)$  is not a linear function of time. For  $0.1 < T < 0.5$  we found a nice quasi-linear shape for all  $t$ . On the basis of several sets of computer simulations with the master equation we obtained the curve shown in Fig. 6 (left panel). The values of  $D_{\text{eff}}$  below  $T \simeq 0.1$  have to be considered as extrapolations. The effective diffusion shows a maximum around  $T \simeq 0.4$ . This observed maximum is compatible with some predictions given in earlier work based on a different semiclassical model [6]. The prediction based on the semiclassical model was that solitonic excitations are expected to significantly enhance diffusivity first, then reaching a maximum and then going to a decrease [6, 8]. The maximum was expected at temperatures where the specific heat has a turning point that is around  $T \simeq 0.1 - 0.5$ .

For comparison we did also some simulations on the basis of the Langevin-equation coupled to the TBA-Schrödinger equation. The results for several temperatures are depicted in Fig. 6 by dots. Here we observe a continuous decrease of  $D_{\text{eff}}(T)$  with  $T$  which looks as a hyperbola. The diffusion coefficient as a function of temperature was estimated for the Schrödinger-TBA-model with the parameter values  $\alpha = 1.75$ ,  $\chi_1 = 0$ ,  $N = 200$ ,  $B\sigma = 1$ . The increase of the values for the diffusion constant might be interpreted by contributions by coherent transport which is not taken into account in the Pauli equation.

From the physical point of view the most interesting result is the decrease of the effective diffusivity with the increase of temperature. We believe that the pole near  $T = 0$  may be an artefact due to the problems of consistency between the TBA-Schrödinger equation and the classical Langevin equation. Beyond the maximum the two descriptions are more or less compatible, taking into account the different value of the  $\alpha_{\text{hop}}$ -parameter.

In the two-dimensional case the equations of motion are more complicated [11]. Again we assume that the forces between particles which 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 coupled to the stochastic dynamics provides the equations of motion for the lattice units

$$\begin{aligned} \frac{d^2 Z_n}{dt^2} = \sum_k [F_{nk}^M(Z_{nk}) + p_k F_{nk}^P(Z_{nk})] z_{nk} - 2\alpha_{\text{hop}} \frac{t_0}{\hbar} \sum_k \exp[-\alpha_{\text{hop}}|Z_{nk}|] \sqrt{p_n p_k} \\ + \left[ -\gamma \frac{Z_n}{dt} + \sqrt{2D_v} (\xi_{nx} + i\xi_{ny}) \right], \end{aligned} \quad (43)$$

where an index  $n$  identifies a particle among all  $N$  particles of the atomic ensemble,  $\gamma$  is a friction coefficient,  $D_v$  defines the intensity of stochastic forces,  $\xi_{n,x,y}$  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  $F_{nk}^M$ , corresponding to the Morse potential, and  $F_{nk}^P$ , corresponding to the polarization interaction, between the  $n$ -th and the  $k$ -th particles. To have dimensionless variables we consider the spatial coordinates normalized to the length  $r_0$  used in the Morse potential. Time is normalized to the inverse frequency of linear oscillations near the minimum of the Morse potential well,  $\omega_M^{-1}$ . The energy is scaled with  $2D$ , where  $D$  is the depth of the Morse potential well. Further the parameter  $b$  defines the strength of the repulsion between particles. The Morse interaction force  $F_{nk}$  is given by

$$F_{nk}^M = F_{nk}^M(|Z_{nk}|) = -\frac{dV^M(r)}{dr} \Big|_{r=|Z_{nk}|}, \quad (44)$$

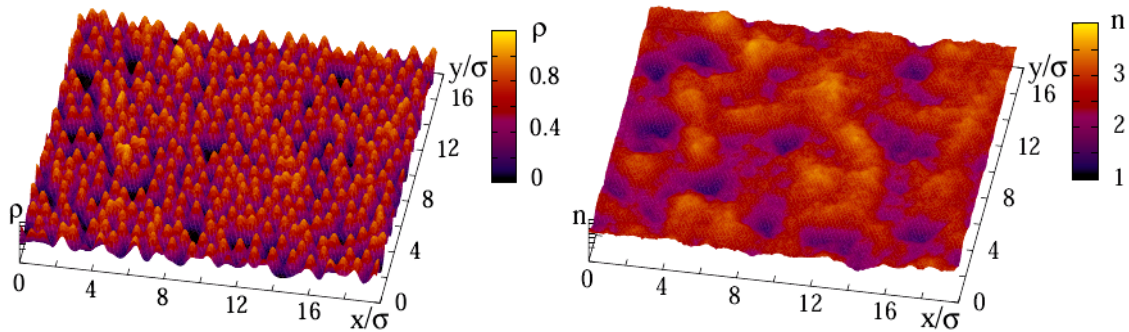


and the polarization interaction force by

$$F_{nk}^P = F_{nk}^P(|Z_{nk}|) = -\frac{dV_{ea}(r)}{dr}\Big|_{r=|Z_{nk}|}. \quad (45)$$

Here,  $V_e$  is the polarization potential defined by Eq. (5) which depends on the characteristic distance  $h$  and the maximal polarization energy  $U_e$ . 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 Eq. (43). 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. We note that in the essentially classical eqs. of motion (43) there appear 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  $R_n$ .

In the two-dimensional case the calculation of the MSD is a very hard task which requires many simulations to find valid averages. A first estimate is given in Fig. 6 (right panel). Typical is again a maximum at some intermediate temperatures. At moderate and at higher temperatures the electronic density fluctuates all the time. A snapshot of a typical landscape of the quasi-stationary electron density in a thermal lattice, created by the solitonic excitation in a 2d- lattice with  $10 \times 10$  particles. Results of simulations for the stiffness parameter  $b = B\sigma = 3$  and the temperature  $T = 0.1$  are shown in Fig. 7.



**Fig. 7** Morse lattice. Typical snapshots of electron densities in a 2d-system of  $20 \times 20$  Morse atoms with stiffness  $b = B\sigma = 3$  and temperature  $T = 0.1$  Left panel: Distribution of atomic core densities. Right panel: The Boltzmann distribution of free (external) electrons in the field of polarized nonuniformly distributed atoms. (Online color: www.cpp-journal.org).

## 6 Discussion

The system of Pauli equations for the electron dynamics coupled to a classical nonlinear lattice is a very useful tool to study short time electronic processes in monatomic layers and to estimate transport properties through the mean square displacement. The Pauli hopping dynamics which we used in this work contains several approximations. In particular we have in mind the perturbation approximation which restricts our study to not too strong electron-lattice couplings. Further we neglected screening and Fermi effects, restricting this way our study to low enough electron concentrations (low doping), such that in particular the difference between the Fermi- and the Boltzmann distribution can be neglected. In its range of validity, the present method provides a rather fast and therefore useful tool for the computer simulations of the electron-lattice dynamics in thermal systems. Figs. 1 and 7 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. An advantage of the Pauli approach is, that it takes into account the coupling to the surrounding modeled as a heat bath. This coupling might be quite essential in the temperature range we are interested here which is  $T > 10^2 K$ . Another advantage of the Pauli method is that it can be easily generalized to include the influence of spin and symmetry effects. This will be done in a subsequent work. In comparison to the adiabatic approach used in some previous works [9–11] for one and for two-dimensional systems, the great advantage is here that we describe directly fast kinetic processes in the layer and can estimate transport processes as demonstrated for the case of diffusion here. We assumed so far that the electron concentration is generated by

doping and is rather low, the dynamics is mainly determined by the electron-atom and by the atom-interactions. Effects of strong Coulomb coupling are not taken into account. A different effect, which is still to be explored are transition probabilities, which are more interesting than the Monte Carlo algorithm. An open problem is, that then all results are becoming very sensitive to details of the physical model for the electron coupling to the heat bath.

The model which we developed here, is rather general and in this sense more or less universal. We do not have in mind any kind of concrete system. However, as far as we see, the plasma physics of realistic two-dimensional systems is still underdeveloped, having in mind many important applications. Several known models of 2d-plasmas are rather abstract, dealing mostly with the 2d- electron gas. Further there exist a lot of work about quantum Monte Carlo simulations for parabolic confinement. Here we try to simulate a time-dependent nonuniform confinement. Further our aim is here to treat plasmas which are embedded into a heat bath located above or below, or at both sides. This is, as we believe much more interesting as the treatment of mathematical two-dimensional plasmas. The price to pay is however, the extreme complexity of the embedding, i.e. the coupling to an external heat bath. As possible future applications we may think about the electron plasma in the  $CuO_2$  layers of Cuprates which are coupled to nonlinear oscillations of the oxygen atoms (as confirmed experimentally). One may hope that a better understanding of the nonlinear excitations of such two-dimensional plasmas may contribute to the better understanding of the electronic properties of such systems, which are in part rather unusual, including in particular the possibility of high-temperature superconductivity, but this is not our target here. Our aim is a better understanding of the influence of nonlinear oscillations and waves on the transport properties of such dimensional plasmas. Beside details of the mechanism, there is indeed some experimental evidence suggesting that in this type of conducting systems, anharmonic effects may play a key role [12–17].

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