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Contributions to Plasma Physics

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WILEY-VCH

REPRINT

Contrib. Plasma Phys., No. 4-5, 355 – 359 (2013) / **DOI** 10.1002/ctpp.201200124

Electron Transport Mediated by Nonlinear Excitations in Atomic Layers*

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Received 10 December 2012, revised 11 January 2013, accepted 11 January 2013
Published online 13 May 2012

Key words Plasma layers, controlling electrons, solitonic excitations.

We study the quantum dynamics in tight-binding approximation (TBA) of an electron interacting with a classical nonlinear lattice of atoms. By computer simulations we show the existence of fast and nearly loss-free motions of electrons along crystallographic axes of a two-dimensional dynamic triangular lattice. Moving bound states between electrons and lattice solitons are formed. These so-called solectrons allow to transfer charge which initially is localized at certain site to a different place along the same crystallographic axis, with negligible spreading of probability density. The relation to experimental findings about controlling electrons by surface acoustic waves (SAW) in piezoelectric materials is pointed out.

1 Introduction

The electron circuits of the future may consist of networks of quantum dots. This structure will require a mechanism to transport electrons from one node to another distant node. In practice this is done at present by imprinting certain wafer masks prescribing the way along which the electrons can go. Several teams of researchers have succeeded in transporting a single electron from one quantum dot at solid interfaces like GaAs-layers to another dot using a surface acoustic wave [1, 2, 3].
For the one-dimensional case analytical results for the problem of supersonic charge transfer in anharmonic chains were obtained first by Davydov [4, 5]. Since for the two-dimensional case no analytical solutions for this problem are available, we decide to carry out computer simulations. Here we formulate the Hamiltonian, classical dynamical equations for a nonlinear lattice of Morse atoms as well as Schrödinger equations for the electron in tight-binding approximation (TBA) [6]. Then we provide numerical evidence that appropriately shaped nonlinear waves on a twodimensional lattice are indeed able to transfer electrons in a controlled way and without dispersion over distances of a few hundred lattice sites.
In earlier work we studied finite temperatures and used kinetic approximations (Pauli equations) for the electron motion [7, 8, 9]. Here we consider similar as in the mentioned experiments the region of very low temperatures. We solve directly the Schrödinger equations in the framework of TBA and apply an electronic Hamiltonian with distance-dependent transition probabilities [6] .

2 Hamiltonian and dynamic equations

We consider a system consisting of atoms arranged initially on a triangular lattice and additional excess electrons moving from site to site and interacting with the atoms. In order to study the evolution of the quantum states of

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the additional electrons, we assume a standard TBA [4, 6, 7, 8, 9]. Let n, m denote the internal quantum numbers of the states of electrons bound to the corresponding atoms at sites r_n and r_m, respectively. We will assume, for simplicity, that there is only one quantum state per atom with Gaussian shape, which can be occupied by the added electron. The internal state that characterizes the orbit as well as spin, can be included in the quantum number n. We set the electron wave function and Hamiltonian as follows

$$\psi(\mathrm{r}) = \sum_n c_n \psi_n(\mathrm{r}); \qquad H_e = \sum_e E_n c_n^+ c_n + \sum_{n,m} t_{n,m} c_m^+ c_n \tag{1}$$

The energy levels E_n will be approximated by constant values $E_n = E_0$. The coupling to the lattice is given by the transition matrix elements $t_{n,m}$, which depend on the atomic distances, $t_{n,m} = t(\mathrm{r}_m - \mathrm{r}_n)$. Following Slater we take an exponential dependence

$$t_{n,m} = V_0 \exp[-\alpha|\mathrm{r}_n - \mathrm{r}_m|]\,. \tag{2}$$

The range parameter α can be related to the tunneling probability. For the atomic lattice part, the Hamiltonian with Morse interactions reads

$$H_a = \frac{M}{2}\sum_k v_k^2 + \frac{D}{2}\sum_{k,l}\{\exp[-2b(r_{kl}-\sigma)] - 2\exp[-b(r_{kl}-\sigma)]\}\,. \tag{3}$$

The subscripts locate the atoms all with equal mass, M, at lattice sites and the summations run from 1 to N. We shall assume that the lattice units repel each other with exponentially repulsive forces of range $1/b$ (b-stiffness) and binding energy strength D and attract each other with weak dispersion forces. The characteristic distance of our initially equilateral triangular lattice σ is used as length unit. Time is measured in units of the reciprocal frequency of oscillations around the minimum of the Morse potential $1/\omega_0 = \sqrt{M/2Db^2}$. Note that the 1dsound velocity is $v_s = \sigma\omega_0$. We limit the interaction to nearest-neighbors only using the relative distance with $r_{kl} = |\mathrm{r}_k \mathrm{r}_l|$. By imposing the cut-off of the forces at 1.5σ, we exclude unphysical cumulative interaction effects arising from the influence of lattice units outside the first neighborhood of each atom [9]. Introducing complex coordinates $Z_n = x_n + iy_n$ we write the Newton equations for the atoms and the Schrödinger equation in TBA for the electrons on the lattice in the form:

$$\begin{aligned}\frac{d^2 Z_n}{dt^2} = \sum_m [&\exp(b\sigma - |Z_n - Z_m|)(1 - \exp(b\sigma - |Z_n - Z_m|)) \\ &+2\alpha V_0 \exp(b\sigma - |Z_n - Z_m|)\mathrm{Re}(c_n^* c_m)]\frac{Z_n - Z_m}{|Z_n - Z_m|}\end{aligned} \tag{4}$$

$$\frac{dc_n}{dt} = E_0 c_n - i\frac{V_0}{\hbar}\tau\exp(\alpha b\sigma)\sum_m c_m \exp(-\alpha|Z_n - Z_m|), \qquad \tau = V_0/\hbar\omega_0\,. \tag{5}$$

Strictly speaking our numerical algorithm for the motions of the atoms models a Langevin equation including also a weak white noise source corresponding to a weak heat bath which can be switched on or off [9]. Here we study very low temperatures so that these terms do not play an essential role except in creating the initial velocities.

3 Simulations

In the initial state the atoms are positioned at the nodes of an equilateral triangular lattice. Note that we use in the figures the characteristic distance of the lattice σ as the length unit, and the reciprocal frequency $1/\omega_0$ of the oscillations around the potential minimum of atom-atom interactions as the time unit. The initial velocities are generated by a short but strong contact to a heat bath at very low temperature $T \simeq 1\ K$. Then the heat bath is switched off, so that the atoms start with a thermal distribution of the velocities. In order to generate a soliton, one of the lattice units gets a kick along the x-axis which is a crystallographic axis which generates an initial velocity of about two times the sound velocity. Then the atoms are left free and move according to the dynamical equations (4). The excited atoms kicks the next neighbor along the axes and generates a solitonic excitation as

seen in Fig. 1. For purpose of a better visualization we replace all points resulting from the simulations by small Gaussian distributions.

The simulations are carried out by solving numerically the set of equations given above for 400 atoms and 1 electron starting at the center. We use for the dimensionless parameters the values $b\sigma = 4$, $(V_0/\hbar) = 20\ D$. The noise strength in the Langevin equation corresponds to a a rather small temperature $T \simeq 0.002\ D$ (where D is the depth of the Morse well). The initial electron density is set as a narrow Gaussian distribution around the center of the lattice. In the first time period up to $t \simeq 0.5$ we see the typical spreading of free wave functions (see Figs. 2 and Fig. 3). In Fig. 2 the interaction with the atoms is switched off and we see a continuation of free spreading including some structures reflecting the triangular lattice symmetry and the periodic boundary conditions.

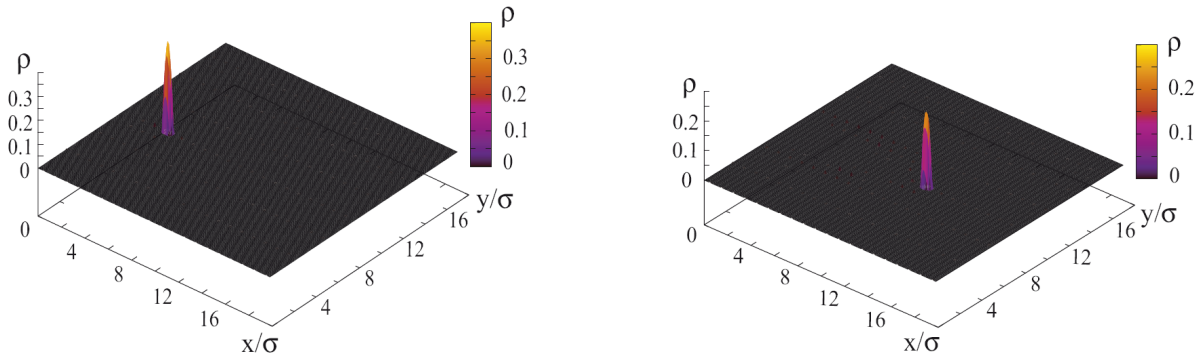

Fig. 1 Triangular Morse lattice without electrons: A supersonic soliton is created moving along the x-axis which is a crystallographic axis. The moving compression density is shown at time $t = 0$ and at time $t = 1$ ($N = 400$, $b\sigma = 4$).

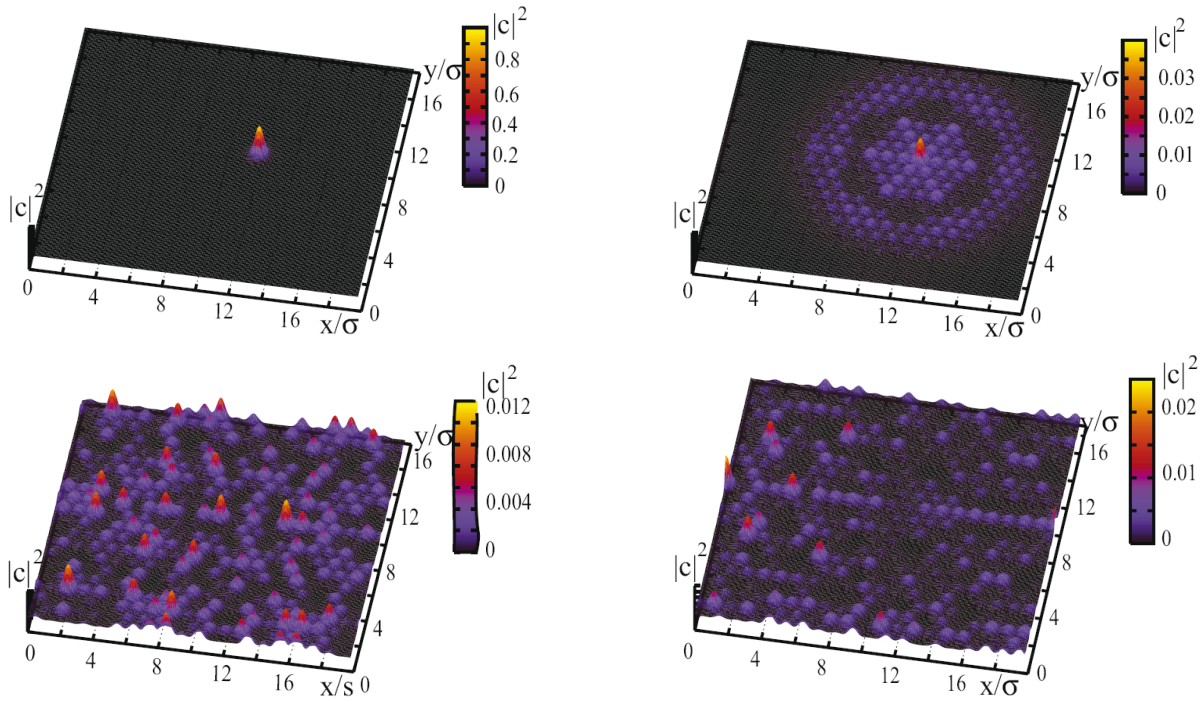

Fig. 2 Density distribution of a free excess electron starting at $t = 0$ near the center of the triangular lattice evolving according to the Schrödinger equation in tight-binding approximation. The interaction with the atoms is switched off. We show the fast spreading of the density at the times $t = 0$; 0:2; 0:8; 1:0. Beside the typical spreading of the wave function, we see some structure due to the symmetry of the triangular lattice with 3 crystallographic axes and in part also due to the periodic b.c. ($N = 400$).

In Fig. 3 we demonstrate the effect of the electron - lattice interaction. At the times $t > 0.5$ when the soliton crosses the center of the lattice, we observe some effects of structuring of the electron density. Finally we see for larger times $t > 0.8$ that the electron density is catched by the soliton forming a moving quantum bound state (the solectron). The supersonic velocity is in physical units around $\mathring{A} = ps$ which corresponds to km/s. This is a rather fast electron motion in comparison to the standard velocity of conducting electrons which is usually in the range of cm/s or m/s. We are well aware that simulations for a matrix of 400 lattice sites still needs a careful check to rule out size effects. Preliminary tests have shown that the basic effect demonstrated here, the formation of moving bound states between lattice excitations and electrons is only weakly size-dependend. We note that on real time and length scales we work in the region of ps and nm, in the SAW experiments the scales are about thousand times larger, i.e. on scales of ns and μm [1, 2, 3]. Thus a direct comparison of our simulations for small lattices on the nanometer and picosecond scale with the experiments performed on larger scales is not possible. However one may assume that the basic effects are scale-independent and remain the same. Indeed in both cases is the electrical polarization field associated to the mechanical wave (soliton or SAW) the responsable carrier of the electron.

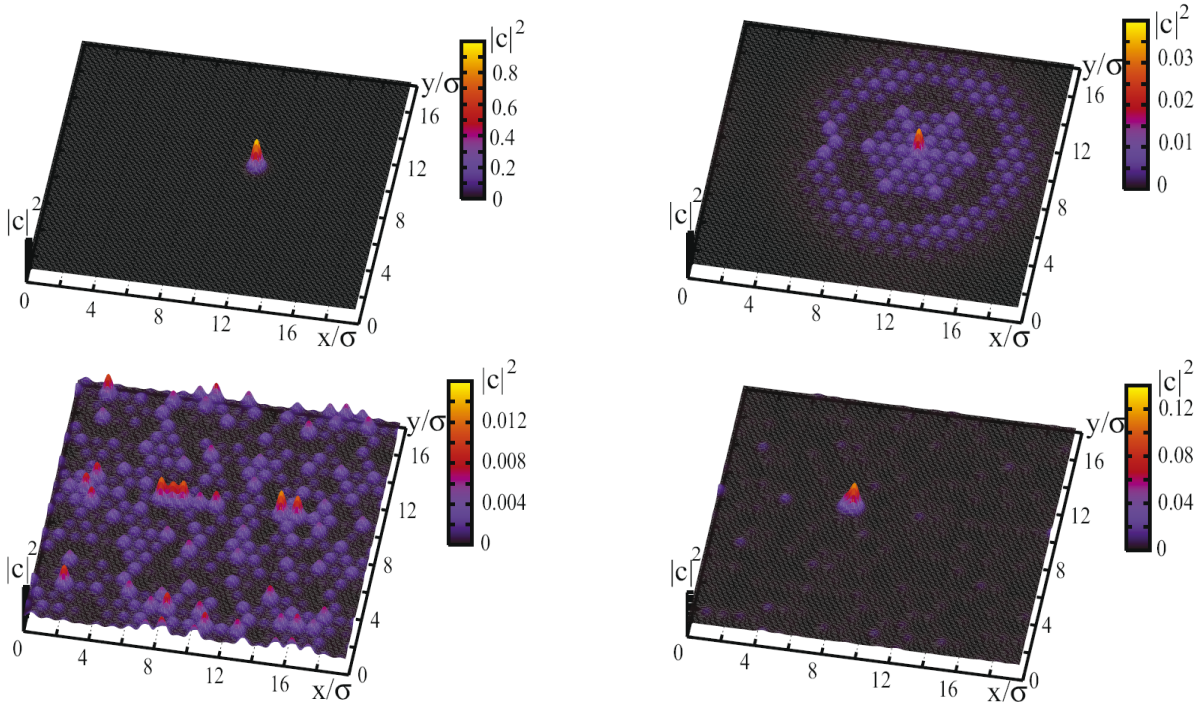

Fig. 3 Electron density on a Morse triangular lattice: We show the evolution of the density of an electron interacting with a soliton moving as in Fig. 1. After switching on in eqs. (4 - 5) the interaction terms electron - lattice we show the mean electron density at the times (τ = 0, 0.2, 0.8, 1.0). The electron density remains nearly unchanged for small times (in comparison to Fig. 2, but then the electron feels the compressions created by the soliton and starts to concentrate around the peaks of the compression density of the soliton. With increasing time (in particular from t = 0:8 on) the electron density is more and more concentrated around the compression density leading to the formation of a moving solectron.

4 Discussion and Conclusion

We study the electron transfer mediated by solitons at low, near to zero, temperatures. In difference to previous work carried out for finite temperatures [8, 9] the main factor influencing the transfer is at low temperatures the distance-dependence of hopping modelled by the Slater factor. In the computer simulations we launched an electron at rest at the center of the sample and started on the same axis by a kick a soliton which passes the electron position. Electrons are guided by the moving amplitude of the soliton-like acoustic excitations and follow their path. This way electrons introduced into a triangular lattice can be transported at least a few hundred lattice sites

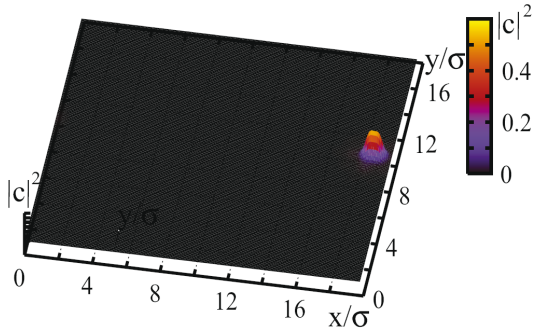

Fig. 4 Electron density on a Triangular Morse lattice: At long times t = 6.0, still more electron density is collected around the peak and the electron - soliton bound state is quite clearly seen. The quasiparticle called solectron is rather stable and moves with supersonic velocity along the selected crystallographic axes.

along crystallographic axes. This is qualitatively the same picture observed on a larger spatial scale in the experiments with surface acoustic waves. We expect that corresponding computer simulations for pairs of electrons [10] will be ready soon.

This research was supported by the Spanish *Ministerio de Ciencia e Innovacion*, under Grant MAT2011-26221 and by the Ministry of Education and Science of the Russian Federation within FTP "Scientific and scientificpedagogical personnel of the innovative Russia", 2009-2013, grant 14.B37.21.0751.

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