ANHARMONICITY AND SOLITON-MEDIATED ELECTRIC TRANSPORT. IS A KIND OF SUPERCONDUCTION POSSIBLE AT ROOM TEMPERATURE?

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We discuss here models for soliton-mediated electron transport that may underlie the possibility of superconductivity.

Keywords: Morse interaction, anharmonicity, lattice solitons, solectrons, electron transfer, high T superconductivity.

1. Introduction

It is customary to denote by *solitary* waves certain localized (single-event) nonlinear waves of translation, i.e., waves that cause a net displacement of e.g. the liquid in the direction of the wave motion like tsunami in the ocean or bores in rivers. This denomination may also apply to nonlinear periodic waves or wave trains. Surfing on a river bore or on a huge wave approaching the sea-shore is a form of wave-mediated transport. Some of those single waves or wave peaks may exhibit particle-like behavior upon collision among themselves or reflection at walls as already noted long ago by the pioneer Russell. Their particle-like behavior led Zabusky and Kruskal to introduce the concept of soliton (bores or hydraulic jumps or even kinks are also called "topological" solitons, whereas waves of "elevation" or "depression" are denoted as non-topological solitons -aka "bright" and "dark" solitons, respectively- in condensed matter physics). We also wish to highlight the work done by Toda on a lattice (he invented) with an exponential interaction (with repulsion akin to Morse and Lennard-Jones potentials) that due to its integrability permitted obtaining exact explicit analytical solutions. The Toda interaction yields the hard rod impulsive force in one limit (the fluid-like or "molten" phase) while in another limit it becomes a harmonic oscillator (the lattice crystal-like solid phase). Worth also mentioning is that Schrieffer, Heeger, and collaborators have used (topological) solitons to explain the electric conductivity of polymers though in this case solitons come from the degeneracy of the ground state and not from an originally underlying lattice anharmonicity. The present authors have shown that lattice solitons like in a Toda lattice can trap electrons thus forming dynamic bound states called solectrons. The latter may act as electric carriers thus generalizing the polaron concept and quasiparticle introduced by Landau and Pekar.

2. One-dimensional (1D) models

We consider a 1D nonlinear lattice which is treated classically, augmented with an added excess electron that will be considered within the quantum tight binding approximation (TBA). The lattice interactions are assumed to be of Morse type, hence allowing for phonon -and soliton- longitudinal vibrations with compressions governed by the repulsive part of the potential. Thus we consider the Hamiltonian $H = H_{lattice} + H_{electron}$, with

$$H_{lattice} = \sum_n \left\{ \frac{p_n^2}{2M} + D\left(1 - exp\left[-B\left(q_n - q_{n-1}\right)\right]\right)^2 \right\}, \tag{1}$$

and

$$H_{electron} = E_n\left(q_k\right) c_n^* c_n - \sum_n V_{nn-1}\left(q_k\right)\left(c_n^* c_{n-1} + c_n c_{n-1}^*\right), \tag{2}$$

with n denoting the lattice site where the electron is (in probability density) "placed"; the complex quantities c_n give the n-th component of the electron wave function, and $p_n = |c_n|^2$ gives the probability of finding the electron at site n. The state energy at site n may depend on the particle displacements of the neighbors. We can use the linear ansatz

$$E_n = E_n^0 + \chi_0 q_n + \chi_1\left(q_{n+1} - q_{n-1}\right), \tag{3}$$

for rather low values of χ_0 and χ_1 as we want to neglect effects owing to energy shifts relative to hopping effects controlled by V_{nn-1}, the transfer matrix elements along the chain (considering only nearest neighbors). A reasonable choice for V_{nn-1} is

$$V_{nn-1} = V_0 exp\left[-\alpha\left(q_n - q_{n-1}\right)\right], \tag{4}$$

where α accounts for the strength of the electron-lattice coupling. We shall measure all energies in units 2D except the energy levels which are scaled with $\hbar\omega_0$ (quantum of the oscillations around the minimum of the Morse potential). Further we consider the system in a "thermal bath" characterized by a Gaussian white noise, ξ_j, of zero mean and time delta correlated.

We take ω_0^{-1} and B^{-1} as unit of time and displacements, respectively. Then $\tau = V_0/\hbar\omega_0$ gives the ratio of the two time scales involved in the dynamics. The system (1)-(2) permits both phonon and soliton (solectron) assisted hopping. An important role plays the temperature T. Indeed, for solitons to be sustained moving unaltered along the lattice the temperature must be high enough. According to the specific heat characteristics of the lattice the solitons are expected beyond the Dulong-Petit plateau (for biomolecules this corresponds to room temperature). When the lattice is heated both phonons (infinitessimal, linear disturbances) and solitons (finite amplitude, nonlinear disturbances) may be excited. However, we do not have just one or two solitons, but many of them with a finite life-time up to a few picoseconds. The solectron picture is now that the electron probability density is concentrated in local "hot spots" created by the local soliton thermal excitations.

Using the corresponding classical and quantum evolution equations obtained from (1) and (2), respectively, in a series of computer experiments we released an electron into a lattice already appropriately heated by means of the friction and noise sources. These sources were switched-off at $t = 0$. Then the electron was "placed" at a lattice site. The result is shown in Fig. 1 in which we represent the evolution of the electron probability density in a lattice heated to $T = 0.2$ (in our dimensionless units). The electron probability density evolves in time confined in a kind of cone. Clearly the electron probability density splits into many small spots bound at the thermally excited solitons. These "hot spots" may comprise up to 10 lattice sites. The overall process is time-dependent as the "hot spots" are erratically created and annihilated in the thermal process. Recall that the spots denote only probability density. We have done computer simulations also at low and at high temperatures. It occurs that at $T = 0.2$ there is some kind of optimum for the creation of solectron spots. We understand that such process is not fully diffusion-controlled. There are other tunneling contributions. "Surfing" of the electrons on thermal solitons provides not a fast transport mechanism, due to the quick and erratic changes of thermal soliton directions. However this ride is for free since thermal solitons are always present in real systems. Another important finding is that solectrons may form bosons with the peculiarity that electron pairing occurs both in momentum space and in real space due to the above mentioned solectron bound states.

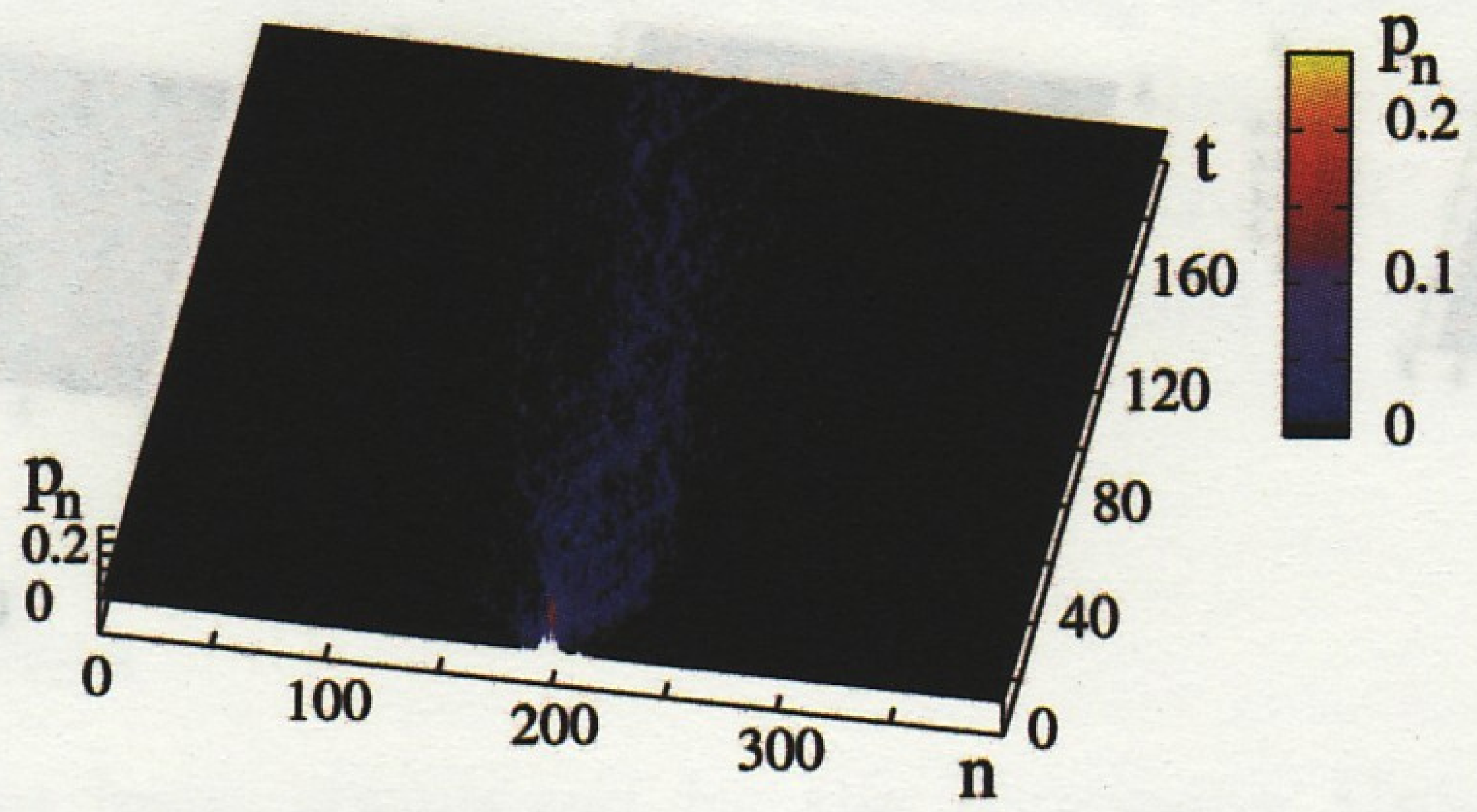

Fig. 1. Heated Morse lattice. An electron is placed (in probability density) at site 200 of a heated lattice ($T = 0.2$, $\tau = 10$, $\alpha = 1.5$, $V = 0.4$). The probability density tends to be concentrated at places of local soliton excitations (embracing up to 10 lattice sites) and survives there for a finite time (a few picoseconds). Subsequently, it moves to another "hot spot" and so on.

3. Two-dimensional (2D) models

Due to the difficulty of defining (stable) solitons and their evolution in 2D lattices and the fact that specifying lattice symmetry may jeopardize the "universality"of our predictions we prefer now to explore an alternative path. Using again the Morse interaction but not in the frame of a "lattice-kind" model but in the frame on an "ensemble-kind" of 2D system by considering the evolution of the n-th particle with coordinates $(x_n,\, y_n)$ on the complex plane $Z = x + iy$, as a result of interaction with the other $(N-1)$ particles of the ensemble we can write

$$\ddot{Z}_n = \sum_k F_{nk}\left(|Z_{nk}|\right) z_{nk} + \left[-\gamma \dot{Z}_n + \sqrt{2D_v}\left(\xi_{nx} + i\xi_{ny}\right)\right], \qquad (5)$$

with $Z_{nk} = Z_n - Z_k$, $z_{nk} = \frac{Z_n - Z_k}{|Z_n - Z_k|}$ and $F_{nk}\left(|Z_{nk}|\right) = -\frac{dU^M(r)}{dr}|r = |Z_{nk}|$.

Based on trajectories of particles $Z_n(t)$ derived as a result of computer simulations of (5) we restrict the interaction of atoms with electrons within a "polarization" radius r_0

$$U(Z) = \sum_n U_{el}\left(|Z - Z_n|\right), \qquad (6)$$

where $U_{el}(r) = -U_e\left[r_0^2/\left(r^2 + r_0^2\right)\right]^2$. Further we use the Boltzmann approximation for the lattice particles distribution

$$\rho_{el}(Z) = exp\left[-U(Z)/k_B T\right]. \qquad (7)$$

In Fig. 2 we show a typical illustration of the evolution of the lattice particles density in the 2D system.

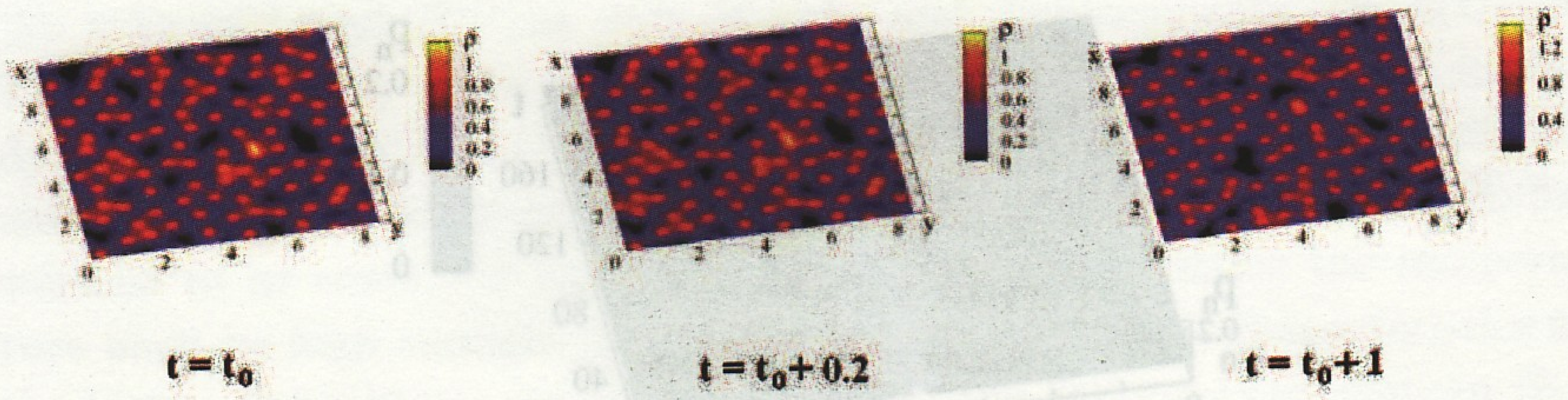

Fig. 2. Time evolution of density landscape of Morse lattice particles for a 2D system illustrating solectron islands that may lead to percolation and hence to a form of second-order phase transition and thus a solectron (soliton-mediated) kind of superconduction (at least supersonic).

4. Possibility of superconducting (SC) states. What is to be done

As it is known and earlier noted, handling solitons and their evolution in 2D systems is a hard task. The exploration sketched in the previous Section points as way out to the problem using a phenomenological approach to the dynamics (and thermodynamics). Following Landau one assumes that the Gibbs free energy of the system is a function $G(T,p,\psi)$ [where ψ is the order parameter]:

$$G(T,p,\psi) = G_0(T,P) + A(p)(T-T_c)\psi^2 + C\psi^4 + \ldots \quad (8)$$

Then following Ginzburg and Landau (GL) ψ is considered as a kind of macroscopic wave function. Then the free energy density is

$$g(T,p,\psi(r)) = g_0(T,P,r) + A(T)|\psi(r)|^2 + \frac{1}{2}|\psi(r)|^4 + \frac{\hbar^2}{2m^*}|\nabla\psi|^2 + \ldots \quad (9)$$

By minimization one can obtain from (9) a *nonlinear* Schroedinger equation for the wave function ψ which describes the SC phase. Could such an approach work with our solectrons?: (i) solectrons are the new charge carriers (quasiparticles) stable up to high temperatures (room temperatures for biomolecules). They permit forming bosons with appropriate electron pairing occurring both in momentum space and in real space! (ii) in 1D the solectrons form charged islands and there is no chance to unify them to a highly conducting path. However, in 2D we may obtain connected conducting regions leading to percolation and hence a new conducting phase, which could be taken as a candidate for SC phase; (iii) the solectron equations may be derived from a variational principle for two fields, the soliton density $\Phi(r)\psi$ and the charge density $\rho(r)$, thus offering the possibility of a *nonlinear* Schroedinger equation permitting a kind of soliton-bearing equation for the two fields $\Phi(r)$ and $\rho\,(r)$. Thus the phenomenological GL approach offers a sound path to understand solectron SC.

Details about some of the results so far obtained can be found in Refs. [1–13].

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