

From macrosurf (hydrodynamics) to nanosurf (electron transfer in crystals): a common line of nonlinear thinking with useful consequences

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Soliton-assisted transport (with commercial purposes) was invented in modern times by the ship-building architect engineer J. S. Russell who in mid-XIXth Century made the discovery of the solitary wave at Union Canal near Edinburgh. Indeed, solitary waves, e.g., at the sea shore, and bores in rivers, permit matter transport and surfing (upstream!). Bores had been observed and used by peasants in China several centuries ago. They used them to transport goods surfing upstream, with small boats, and getting back to origin with the downstream river flow. In the later quarter of the XIXth century, such waves received a good theoretical explanation by Boussinesq and Lord Rayleigh (who acknowledged Boussinesq's earlier achievements). Later on came Korteweg and de Vries who rediscovered the solitary wave evolution equation (fifteen years after Boussinesq). Their achievement was to also provide besides the solitary wave, another solution in the form of periodic cnoidal wave-train (their stability analysis was not correct). It was not until mid-XXth Century that the curiosity of the solitary wave attracted the interest of Zabusky and Kruskal who numerically explored the solutions of the BKdV equation, and their (overtaking) collisions, and coined the soliton word and concept. Their research was motivated by earlier work of Fermi, Pasta and Ulam (FPU) on heat transfer and equipartition in (anharmonic) lattices. One of the lattice cases treated by FPU, i.e., with cubic potential interactions, was shown to have as continuum equivalent the BKdV equation. Eventually, subsequent mathematical work about BKdV and other soliton-bearing equations led to a new area

in Applied Mathematics and General Physics (of conservative and, mostly, Hamiltonian integrable systems). The soliton concept has been a powerful paradigm to provide a unifying understanding of a disparate collection of phenomena found in several branches of Science and not just Physics (Fluid Physics, Nonlinear Optics and Lasers, Optical Fiber transmission, Acoustics, Plasmas, Neuro-dynamics, etc).

The BKdV equation is peculiar in the sense that it possesses a (local) balance between nonlinearity (velocity depends on amplitude) and dispersion (velocity depends on wavelength/color) that permits maintaining alive the solitary wave (or the cnoidal wave-train) as time proceeds. Dissipation or damping alone generally tends to destroy solitons, mostly through a leaking (linear) radiation, a capillary-gravity wave-tail/head where viscosity eventually kills all wave motion. In the 20s of past century, Taylor and Burgers argued that waves could survive damping if an appropriate nonlinear-dissipation balance existed (another possibility is an input-output dynamic energy balance, much later studied). The TB equation has heteroclinic solutions in the form of (supersonic) shocks in compressible gases (with local Mach number above unity) and bores (with corresponding Froude number above unity) in hydraulics. This (1D)-compressible gases-(2D)-hydraulics similarity had been known and exploited by Mach in the late XIXth century. Shocks, bores (mascarets, in French), hydraulic jumps, kinks, are also called topological solitons (to discriminate from e.g. Sech2-like solitons of the BKdV equation).

In the second half of the XXth century, room temperature soliton-assisted electron transport (ET and positive hole) was experimentally observed and theoretical described in polymers like trans-polyacetylene (tPA). Their discovery led to the Nobel Prize for Chemistry awarded to A. J. Heeger, A. G. MacDiarmid and H. Shirakawa, in 2000. The supporting theory is based on a harmonic backbone Hamiltonian (as relative displacements are of the order of 0.04 Angstroms while the equilibrium inter-atomic lattice distance is about 1.22 Angstroms). As the ground state of tPA is degenerate, in the theory this is accounted by means of an additional double-well quadratic potential. This together with the nonlinear electron-lattice interaction brings the possibility of solitons in the form of kinks. Most important feature of tPA and relatives is that they are easily doped thus offering very attractive features for electronic devices.

At about the same time, Davydov introduced the concept of electro-soliton to describe ET along bio-(macro)-molecules. He also used a harmonic backbone Hamiltonian (though he studied, albeit fragmentarily, anharmonic cases). His clever use of the nonlinearity of the electron-phonon interaction together with suitable way of transition to the continuum description, permitted him to building a soliton-bearing system. Many other scientists followed Davydovs ideas but, apparently, his predictions were shown not to survive above 10K and have not yet found support by experiment.

I shall present another possibility for soliton-assisted ET arising from starting with a soliton-bearing anharmonic lattice (using e.g. Morse interactions) and, as in the above mentioned theories, treating the electron in the standard quantum mechanical tight-binding approximation. The interaction between the electron and the lattice vibrations

provides the dependence of the hopping electron transfer-matrix elements on the relative, time-dependent distance between neighboring lattice units (of particular interest are strong enough compressions, say, about half the equilibrium inter-atomic distance). It appears that when adding an excess electron there is electron trapping by the, generally supersonic moving, lattice soliton. This has been called a solelectron which, depending on parameter values, provides (sub- and supersonic) electron surfing at the nano-level. The solelectron appears as a natural extension to anharmonic lattices of both the Landau-Pekar polaron (for harmonic lattices) and the Davydovs electro-soliton. It has also been shown that such lattice solitons (in the absence of added electron and solelectrons) survive up to ambient temperatures (ca. 300K) for parameter values typical of bio-(macro)-molecules. I shall discuss the role of an external electric field thus showing features of a novel form of ET that appears valid to support thirty-year old outstanding experimental results obtained by K. Donovan and E. G Wilson on highly crystalline polymers like poly-diacetylene (PDA) crystals which behave quite differently from tPA (no doping allowed).

I shall also present work on controlling ET from say a source to a drain, like in a transistor, along natural channels (crystallographic axes) in e.g. triangular lattices. This ET bears similarity to electron surfing on surface acoustic waves in piezoelectric materials, like GaAs layers and other systems and I shall also comment on this item.

Finally, I shall comment on the relationship between lattice solitons and DB/ILM (kind of unification with differences).

Keywords: lattice solitons, electron transport, solelectrons.