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SOLITON-MEDIATED ELECTRON PAIRING

MANUEL G. VELARDE* and CHRISTIAN NEIßNER†
Instituto Pluridisciplinar,
Universidad Complutense de Madrid,
Paseo Juan XXIII, 1, 28040 Madrid, Spain
**mvelarde@pluri.ucm.es*
†*neissner@pluri.ucm.es*

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We study electron-electron pairing in an one-dimensional model lattice system embedded into a three-dimensional environment. The electron pair potential is lowered by a single, localized lattice deformation. Such a deformation is related to solitons moving along the lattice. Yet the exact form and the time evolution of the lattice excitation are of secondary relevance as the electron pair is stable for sufficiently wide deformations which propagate on molecular time scales, e.g. velocity of sound $\ll$ electron velocity. The spatial structure of the pair potential and the electron-electron wave function bring a mechanism of pairing different from the exchange of phonons between the electrons and the lattice which leads to Cooper pairs, and different also from the formation of bipolarons.

Keywords: Solitons; electron pairing; electron-soliton interaction.

Recently, it has been shown that an one-dimensional (1D) electrically conducting *anharmonic* lattice allows both ohmic and a faster, eventually supersonic, non-ohmic form of conduction [Velarde *et al.*, 2005; Velarde *et al.*, 2006; Chetverikov *et al.*, 2006a; Hennig *et al.*, 2006; Makarov *et al.*, 2006; Chetverikov *et al.*, 2006b]. The latter is a soliton-mediated transport exhibiting striking features like current-field characteristics where the current becomes field-independent as we suitably lower the field strength. Hence the field's role is that of symmetry breaking to merely orient conduction. Consequently, at vanishing field strength the lattice differential conductivity passes from zero to very high. This finding appears as a consequence of electron-soliton binding irrespective of the classical or quantum nature of the electron-lattice dynamics interaction and hence shows a kind of universality. In [Velarde *et al.*, 2005; Chetverikov *et al.*, 2006a; Makarov *et al.*, 2006; Chetverikov *et al.*, 2006b] the coupling is classical while in [Velarde *et al.*, 2006; Hennig *et al.*, 2006] quantum tight-binding is used. On the other hand, when temperature is added to the dynamics the electric current exhibits a significant increase when the lattice solitons appear in the system [Velarde *et al.*, 2005; Chetverikov *et al.*, 2006a, 2006b]. The above features have been shown to survive up to room temperature, e.g. 300 K [Velarde *et al.*, 2006; Hennig *et al.*, 2006]. The onset of the soliton carriers in the lattice due to strong anharmonic compressions appears as a necessary albeit not sufficient condition for the findings described above. In view of this, in the present communication we take up the same problem from a different perspective. We here address the question of electron-soliton trapping and soliton-mediated electron pairing from the quantum dynamics viewpoint. Such an approach, on the one hand, brings us to current views on electric superconduction and, on the other hand, to revisiting an old idea suggested by Fröhlich about the possible role played by the lattice dynamics in electron pairing and superconduction

[Fröhlich, 1950, 1952, 1954]. Fröhlich theory invoked phonon excitations only. Note that although anharmonicity in lattice interactions had been invoked for some time to understand thermal expansion and heat transfer in solids the soliton concept was introduced in 1965 [Zabusky & Kruskal, 1965; Payton *et al.*, 1967; Christov & Velarde, 1995]. Here we invoke solitons and hence we also generalize the polaron concept to account for strongly localized excitations in the form of solitons.

Since electron pairing was shown to be the fundamental ingredient of superconductivity, it is worth to investigate different possible mechanisms of pairing. In general the electron-electron interaction is modified by the interaction of the electrons with lattice excitations. Under certain circumstances the electron-electron interaction shows attractive parts under the influence of lattice excitations [Bardeen & Pines, 1955]. There are several accepted mechanisms of electron pairing. The best known mechanism is based on the Cooper instability [Cooper, 1956] leading to the Bardeen–Cooper–Schrieffer (BCS) theory [Bardeen *et al.*, 1957]. For polarons [Firsov, 1975], compounds of electrons and lattice deformations, the pairing occurs due to the correlation of two localized electrons to form bipolarons. The condensation of bipolarons has been shown in [Alexandrov, 2000].

Here we address the question of electron-electron correlations. We take an electroneutral system of N electrons and N ions. But not all degrees of freedom are crucial to account for soliton-mediated electron-electron pairing. First, we assume that ions or ion cores are compound to atoms or molecules that interact via an appropriate model potential V_{ii}, such as the Morse potential [Morse, 1929] or another strongly repulsive potential. Then, if the interaction is nonlinear, its repulsive part may allow the existence and propagation of solitons. For a Toda interaction [Toda, 1989] we know the exact form of the solitons or nonlinear periodic waves running along a lattice (tanh-like or topological soliton for displacements and sech^2-like or periodic conoidal waves for displacement gradients or force). The Toda's repulsive part is akin to the Morse interaction and to the repulsive part of the Lennard–Jones interaction. The attractive component of the Toda potential is unphysical but we are interested only in strong repulsion and strong lattice compressions. If the electrons interact with the ionic core of the molecules via a Coulomb-like pseudopotential V_{ei} we may classically have electron trapping by the solitons [Velarde *et al.*, 2005; Chetverikov *et al.*, 2006a, 2006b].

In an unperturbed lattice the separation between the units is given by the equilibrium distance σ (taken as $\sigma = 5a_B$ for the model, with a_B being the Bohr radius). The resulting periodic structure of the potential V_{ei} leads to extended single-electron excitations represented by Bloch states [Ashcroft & Mermin, 1976]. A soliton-like deformation of the lattice leads to a localization of the single-electron wave function [Velarde *et al.*, 2006; Hennig *et al.*, 2006]. Let us see how this localized compound influences the electron-electron interaction. For two electrons at x_1 and x_2 we can write down the interaction

$$\begin{aligned} V_{ee}(x_1, x_2, t) = V_{ee}^{(0)}(x_1 - x_2) + \sum_n \{ & V_{ei}(x_1 - Q_n^{(0)} \\ & - \Delta_n(t)) - V_{ei}(x_1 - Q_n^{(0)}) \\ & + V_{ei}(x_2 - Q_n^{(0)} - \Delta_n(t)) \\ & - V_{ei}(x_2 - Q_n^{(0)}) \}. \end{aligned} \tag{1}$$

Here the first term describes the direct electron-electron interaction and the second one the influence of the lattice deformation. The equilibrium position of the nth ion core is given by $Q_n^{(0)} = n\sigma$ and its time-dependent deviation by $\Delta_n(t)$. The latter variable is given by the displacement function of the soliton. The displacement function is characterized by its width w_{sol}, its maximum amplitude $A_{\max}$, and the position of its maximum x_{sol}. For illustration we use a Gaussian displacement with $w_{\mathrm{sol}} = 1.5\sigma$ and $A_{\max} = 0.1\sigma$.

Since the soliton may bind hence localize a single electron, the screening of the electron-ion potential V_{ei} near the soliton will be enhanced. Therefore, when calculating (1) one has to use the locally corrected screening parameter $\kappa(x) = \kappa_0(1 + \Delta n(x)/n_0)^{1/2}$, with the screening κ_0 of the system without the soliton. For the calculations we have used $\kappa_0 = 0.3\sigma^{-1}$. The quantity $\Delta n(x) = |u_0(x)|^2$ is the density deviation given by the ground state wave function $u_0(x)$ of the localized electron and n_0 is the particle density in dimension one (1D), the only case here considered. The local screening correction is lowered with the increase of the density. Further the shape of wave function $u_0(x)$ can be taken as Gaussian with the same width w_{sol} as the displacement function of the soliton. A snapshot of the effective electron-electron potential is given in Fig. 1. The potential (1) expresses

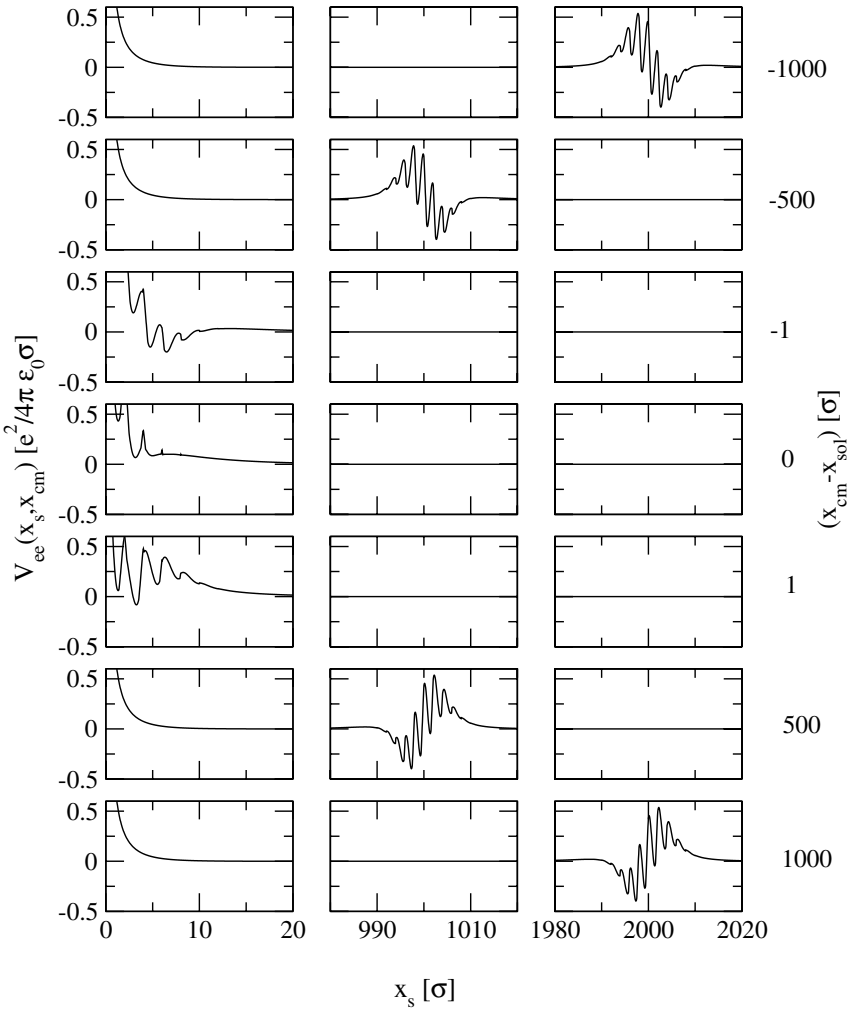

Fig. 1. Electron-electron potential under the influence of a localized, single lattice deformation. The parameters of the displacement function of the lattice units are: $x_{\mathrm{sol}} = 0$, $w_{\mathrm{sol}} = 1.5\sigma$ and $A_{\max} = 0.1\sigma$.

sequences of potential wells and walls along the lines $(X - x_{\mathrm{sol}})^2 - x^2/4 = 0$, with the center-of-mass position $X = (x_1 + x_2)/2$ and the separation $x = x_1 - x_2$, if a soliton is excited in the lattice. We found that the sequences are suppressed for absolute values of the pair separations below 20σ. On the other hand, they are stable for arbitrary large separations. This leads to some conclusions for the electron pairing. Namely (i) the pairing is suppressed near the soliton position, (ii) the localized electron at the soliton position is always involved into the pairing, (iii) the pair wave function is extended to arbitrary large separations. The latter point implies the existence of long-range correlation. Although we are aware of the fact that those correlations may decay because of many-particle effects in the quantum mechanical description the long-range correlations exist and may survive at least for small densities. Then one can make an ansatz for the ground state wave function depending on the separation x and the center-of-mass position X:

$$\psi_0(x, X) \sim \Theta(X - x_{\mathrm{sol}} - B)\,\{\phi_0(x) \pm \phi_0(-x)\} + \Theta(x_{\mathrm{sol}} - X - B)\,\{\varphi_0(x) \pm \varphi_0(-x)\}. \tag{2}$$

Here Θ is the Heaviside step function and B defines the radius of pair suppression around the soliton position. The wave functions ϕ and φ are not identical because the lattice symmetry is broken by the soliton. Because ϕ and φ depend only on the electron-pair separation, they are solutions of the eigenvalue equations

$$\left\{-\frac{\hbar^2}{2\mu}\,\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_{ee}(x, X)\right\}\phi_k(x) = E_k\,\phi_k(x) \quad \text{with } X - x_{\mathrm{sol}} > B \tag{3}$$

and

$$\left\{-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V_{ee}(x,X)\right\}\varphi_k(x)=E_k\,\varphi_k(x)$$
$$\text{with } x_{\mathrm{sol}}-X>B, \qquad (4)$$

where X appears as a parameter. Further, $\mu = m_e/2$ represents the reduced mass of the electron-electron pair. Figure 2 shows a numerical result of the pair wave function. An interesting detail is the independence of the ground state on the spin. Because of the quite large separation ($>20\sigma$) of the pair the eigenvalue is the same for the symmetric and antisymmetric spatial wave functions. Therefore the pair could also have a magnetic moment.

The dependence of the wavefunction on the center-of-mass position and the separation has an interesting effect if one thinks about a many-pair problem. If we assume many pairs formed in the system they would be highly correlated because all electrons sufficiently far away from the soliton position form a pair with one and the same electron trapped by the soliton. Therefore an ansatz for a N-electron ground state wave function of paired electrons reads like

$$\begin{aligned}\Psi_0(x_1,s_1;\ldots;x_N,s_N)&\\ =\mathcal{A}\{&\psi_0(x_1,s_1;x_2,s_2)\psi_0(x_1,s_1;x_3,s_3)\cdots\\ &\psi_0(x_1,s_1;x_N,s_N)\},\end{aligned} \qquad (5)$$

with the electron positions x_i and the spin variables s_i. The operator $\mathcal{A}$ represents the antisymmetrization procedure which has to act on the product. Although one pair can be treated as a boson the internal degrees of freedom are of fermionic nature. The exchange of two of these internal variables results in a change of the sign in the expression for the wave function.

The considerations above rest on an adiabatic approximation. The electron does not influence the lattice dynamics. Although we believe that due to the large ratio between the electron and ion masses the dynamics decouple, there is an additional problem due to the discreteness of the lattice. During the soliton propagation (i) the maximum of the displacement function coincides with the equilibrium position of the nth lattice ion core: $x_{\mathrm{sol}} = Q_n^{(0)}$, (ii) the maximum lies between two neighboring equilibrium positions: $Q_n^{(0)} < x_{\mathrm{sol}} < Q_{n+1}^{(0)}$, and (iii) the maximum of the displacement function coincides with the equilibrium position of the $(n+1)$th ion core: $x_{\mathrm{sol}} = Q_{n+1}^{(0)}$. This configuration is equivalent to (i).

All possible configurations are related to different eigenvalues of the electron-electron bound state. When propagating along the lattice this eigenvalue would change. Unfortunately, this would also change the shape of the wave function. However, for a large enough width w_{sol} of the displacement function of the soliton the eigenvalues of all possible configurations are equal. The effect of discreteness vanishes for wide solitons. The consequence is that the motion of a wide enough soliton does not influence the electron-electron wave function anymore, its shape or its eigenvalue.

Finally, let us discuss the effects of temperature on the stability of the quantum mechanical two-electron bound state. Once the eigenvalue of the ground state is given one could ask at what temperature thermal "ionization" may occur. This question leads to the inequality $T > |E_0|/k_B$. In the example given above we have obtained an eigenvalue E_0 of approximately $-0.04Ry$ which

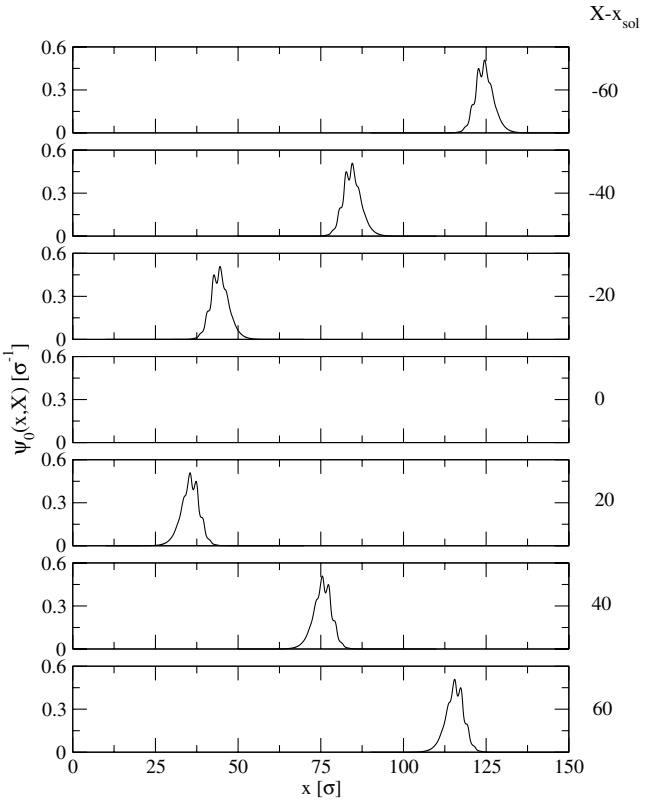

Fig. 2. Wave function (2) of a electron-electron pair that is created due to a localized lattice deformation. The wave function vanishes for small absolute values of the separation. For large separations the wave function shows a constant form. As the spatial wave function is symmetric or antisymmetric under the exchange of the particles only the solution for positive x is shown.

corresponds to a temperature of about 5200 K. Because of this very high temperature the thermal "ionization" cannot be responsible for the destabilization of the ground state with increasing temperature. On the other hand, the thermal motion of the ion cores will also affect the two-electron bound state. We can assume the probability of finding the nth ion core at position Q as

$$P_n(Q) = \frac{\exp\left\{-\dfrac{(Q - Q_n^{(0)})^2}{2\Delta Q^2}\right\}}{(2\pi\,\Delta Q^2)^{1/2}}, \tag{6}$$

with $\Delta Q = (k_B\,T/(M\Omega^2))^{1/2}$. Here ΔQ gives the thermal deviation of the ion core position depending on the temperature T, the molecular mass M and the frequency Ω of low-amplitude oscillations of an ion pair around its equilibrium separation σ. The frequency is determined from the harmonic approximation to the interaction potential V_{ii}. Let us refer to the soliton induced potential at $T = 0\,\mathrm{K}$ as the coherent part because it is stable under the soliton propagation. For higher temperatures this coherent part is disturbed by incoherent thermal fluctuations. In our case the thermal fluctuations dominate already at a little more than $T = 30\,\mathrm{K}$. Although those fluctuations can create new and even deeper minima in the effective electron-electron potential those additional structures are not coherent. Therefore, they have a destabilizing effect on the electron-electron ground state. Of course, this depends strongly on the system under investigation.

Let us estimate the relation between "critical temperature" and amplitude of lattice displacement in a more analytical form. We recall that $A_{\max}$ is the maximum deviation of the ion position induced by the soliton. One could ask at what temperature the thermal deviation of the ion positions reaches 10 per cent of $A_{\max}$. The inequality reads

$$\frac{A_{\max}^2}{T} > \frac{100 k_B}{M\Omega^2}. \tag{7}$$

Hence the ratio of deformation to the "critical temperature" is given only by material constants. In our case we obtain a "critical temperature" $T_c = 35\,\mathrm{K}$, which is in agreement with the numerical result. On the other hand, if we would like to extend the range of validity to room temperature ($T = 300\,\mathrm{K}$), we have to realize larger lattice deformations ($A_{\max} = 0.3\sigma$ instead of $A_{\max} = 0.1\sigma$ used for the model system).

A new quantum mechanical mechanism of electron pairing has been described. This pairing originates in a localized deformation of the lattice in the form of solitons. Although, the electron pair is a quantum mechanical compound where many-particle effects are not considered and its solution is valid only at zero temperature, we can estimate a thermal criterion of finding the electron pair. It makes sense to consider the thermal motion of the classical ions. Since the electron pairing is bound to the existence of the soliton and the thermal ion motion tends to disturb the soliton, the electron pairing is also destabilized by the increase of temperature. We wish to emphasize once more the spatial structure of the electron pair. A dynamic bound state of a soliton and an electron (called, for simplicity, solectron) propagates along the lattice. Meanwhile, the localized electron can form pairs with electrons at arbitrary large absolute values of the separation. This point is crucial to distinguish the mechanism from those leading to the formations of bipolarons.

For decades the formation of bipolarons has been assumed to be a mechanism that may lead to superconductivity [Schafroth, 1955] even for high-temperature superconductors [Bednorz & Mueller, 1986]. The polaron formation is based on the short-range electron-lattice interaction [Holstein, 1959] or the long-range electron-lattice interaction [Fröhlich, 1954]. Both methods are successful in describing single polarons. The first model tends also to form strongly localized ("small") bipolarons [Emin, 1987]. Since the localization reduces the mobility of the pair small polarons are not expected to contribute to superconductivity. On the other hand, only long-range electron-lattice interactions do not tend to generally form bipolarons [Emin & Hillery, 1989]. However, the existence of "large" bipolarons (induced by long-range electron-lattice interactions) has been shown at least for large coupling strengths between the electron and the lattice [Verbist *et al.*, 1991]. But large coupling strengths are known to suppress the polaron motion [Hennig *et al.*, 2006]. Nevertheless, the possibility of bipolaron-induced superconductivity has been shown in [Alexandrov & Ranninger, 1981]. There the fermionic electron-phonon system has been reduced to a bosonic bipolaron system.

Here we have described the coherent motion of an electron on top of a solitonic lattice excitation (in fluid flows this is similar to the surfing on the bore of certain rivers). While the electron is trapped, the

strength of the deformation and the energy of the soliton do not allow the electron to influence the propagation of the soliton significantly. When there is a mechanism of pairing as we have shown here the motion of the pair is also coherent with the motion of the soliton.

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