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Zero-sound solitons in an interacting electron gas in one dimension

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It is shown that the semiclassical approximation may apply to the interacting electron gas in one dimension, in which case the zero-sound oscillations may give rise to classical solitons. They appear as kink solutions of the backward-scattering and the umklapp-scattering sine-Gordon equation.

The momentum distribution of the interacting electrons in one dimension is continuous at the Fermi wave vector k_F.[1-3] One can easily check that the Fermi distribution in one dimension is a slowly decreasing function at the chemical potential for any finite temperature in the high-density limit. This implies a great uncertainty in the electron momentum near $\hbar k_F$ and an appreciable tendency toward localization for the electrons in one dimension. The density-response function exhibits a singularity near $2k_F$ in one dimension,[4] indicating the instability of the system (overscreening). This is a consequence of the extent to which the system distributes the energy among the one-electron states near the Fermi wave vector $d\varepsilon/dn = \pi\hbar^2 k_F/2m$ (reciprocal of the Fermi density of states), which increases indefinitely in the high-density limit, in contrast, for example, to the three-dimensional case, where it vanishes ($d\varepsilon/dn = \pi^2\hbar^2/mk_F$). All this may constitute evidence that the Fermi-liquid theory breaks down in one dimension. In fact, the boson representation of the fermion fields in one dimension[5,6] shows that the one-dimensional electron gas possesses a Bose-type spectrum. It is shown in this paper that the semiclassical approach applies to the interacting electrons in one dimension, leading to classical (kink) solitons associated with the zero-sound disturbances of the backward-scattering and the umklapp-scattering interactions.

The electrons with mass m and spin $\sigma = \pm$ are divided, as is usual in one dimension, into right-moving ($j=1$) and left-moving ($j=2$) electrons, with the density $n_{j\sigma} = n/4 = k_F/2\pi$ and energy $E_{j\sigma} = \hbar^2 k_F^3/12\pi m$. Suppose that the electrons are subjected to a displacement field $u_{j\sigma}(x,t)$, slowly varying in space ($|\partial_x u_{j\sigma}| \ll 1$) and much larger than the average interelectron distance $a \sim 1/k_F$, $|u_{j\sigma}| \gg a$ (collective motion). This displacement field yields a density variation $\delta n_{j\sigma} = -(n/4)\partial_x u_{j\sigma}$ (much lower than the average density $n/4$), whose time variation is related to the velocity $\dot{u}_{j\sigma}$ of the displacement field by the continuity equation $\partial_t \delta n_{j\sigma} + (n/4)\partial_x \dot{u}_{j\sigma} = 0$. The kinetic energy of the displacement field $(nm/8)(\partial_t u_{j\sigma})^2$ and the variation of the Fermi energy $\delta E_{j\sigma} = (nm/8)v_F^2[(\partial_x u_{j\sigma})^2 - \partial_x u_{j\sigma}]$ provide the noninteracting Hamiltonian

$$H_0 = \sum_{j\sigma} \int dx\,(nm/8)\{(\partial_t u_{j\sigma})^2 + v_F^2[(\partial_x u_{j\sigma})^2 - \partial_x u_{j\sigma}]\}\,, \tag{1}$$

which describes the zero-sound oscillations $\delta k_F = -(\pi n/2)\partial_x u_{j\sigma}$ propagating with the Fermi velocity v_F.

The wave vectors of the electron states affected by the displacement field are, therefore, $k_{Fj\sigma} = (-1)^{j+1}k_F - (\pi n/2)\partial_x u_{j\sigma}$. In the semiclassical approximation these electrons are described by wave functions built up with the mechanical action

$$\hbar \int_0^x dx'\,k_{Fj\sigma}(x',t) = (-1)^{j+1}k_F x - (\pi n/2)u_{j\sigma}(x,t)\,, \tag{2}$$

where $u_{j\sigma}(0,t)$ is set equal to zero. One gets

$$\psi_{1\sigma} = (n/4e)^{1/2}\exp[ik_F x - (i\pi n/2)u_{1\sigma}]\,,$$
$$\psi_{2\sigma} = (ne/4)^{1/2}\exp[-ik_F x - (i\pi n/2)u_{2\sigma}]\,, \tag{3}$$

where we have chosen to compute the electron density by

$$\psi_{j\sigma}^*(x+ia/2)\psi_{j\sigma}(x-ia/2) = (n/4)\exp(-\partial_x u_{j\sigma}) = n/4 + \delta n_{j\sigma}\,. \tag{4}$$

(Recall that $ak_F = 1$ and $|\partial_x u_{j\sigma}| \ll 1$.) This is nothing but the classical counterpart of the boson representation of the fermion fields in one dimension.[7] It holds as long as the relative variation of the wave vector is small, i.e., $|\partial_{xx} u_{j\sigma}| \ll k_F$ (geometrical-optics condition).

The local two-body interaction reads

$$H_{\rm int} = (U/2)\sum_\sigma \int dx\,\psi_\sigma^*(x)\psi_\sigma(x)\psi_{-\sigma}^*(x)\psi_{-\sigma}(x)\,, \tag{5}$$

where the electron amplitude of probability $\psi_\sigma = \psi_{1\sigma} + \psi_{2\sigma}$ and the parallel-spin contribution disappears by the Pauli exclusion principle. According to (4) the density of the electrons with spin σ acquires the usual charge-density-wave (CDW) form

$$\psi_\sigma^*(x)\psi_\sigma(x) = n/2 - (n/4)\partial_x(u_{1\sigma}+u_{2\sigma}) + (n/2)\cos[2k_F x - (\pi n/2)(u_{1\sigma}-u_{2\sigma})] , \tag{6}$$

which contains, beside the slowly varying components $\partial_x(u_{1\sigma}+u_{2\sigma})$, the rapidly varying contribution with wave vectors near $\pm 2k_F$, due to the interference of the $\pm k_F$ states. These states may interfere constructively in the interaction processes, bringing nontrivial contributions to the Hamiltonian. Passing to the normal-mode coordinates

$$\begin{aligned} u_{++} &= (\tfrac{1}{2})(u_{1+}+u_{2+}+u_{1-}+u_{2-}) , \\ u_{+-} &= (\tfrac{1}{2})(u_{1+}+u_{2+}-u_{1-}-u_{2-}) , \\ u_{-+} &= (\tfrac{1}{2})(u_{1+}-u_{2+}+u_{1-}-u_{2-}) , \\ u_{--} &= (\tfrac{1}{2})(u_{1+}-u_{2+}-u_{1-}+u_{2-}) , \end{aligned} \tag{7}$$

the Hamiltonian given by (1) and (5) reads

$$H = (nm/8)\int dx [(\partial_t u_{++})^2 + v_+^2(\partial_x u_{++})^2 - 2(v_F^2 + Un/m)(\partial_x u_{++}) + (\partial_t u_{+-})^2 + v_-^2(\partial_x u_{+-})^2 + (\partial_t u_{-+})^2 + v_F^2(\partial_x u_{-+})^2 + (\partial_t u_{--})^2 + v_F^2(\partial_x u_{--})^2 + (Un/m)\cos(\pi n u_{--}) + 2Un/m] , \tag{8}$$

where $v_{+,-} = v_F(1 \pm U/\pi\hbar v_F)^{1/2}$. This is the classical counterpart of the quantum phase Hamiltonian,[8] which, apart from the zero-sound oscillations propagating with the velocities $v_{+,-}$ and v_F, contains classical sine-Gordon solitons of the u_{--} coordinate corresponding to the backward-scattering interaction [$\psi_{1\sigma}^*\psi_{2\sigma}\psi_{2-\sigma}^*\psi_{1-\sigma}$ in (5)].

With the notation $\phi = \pi n u_{--}$ the backward-scattering part of (8) becomes

$$H_b = (\hbar/16\pi v_F)\int dx[(\partial_t\phi)^2 + v_F^2(\partial_x\phi)^2 + (2\pi/\hbar)Uv_F n^2\cos\phi] , \tag{9}$$

which describes the well-known kinks propagating with the velocity u. The phase ϕ is given by $\phi = 2\theta + \pi$ for $|u| < v_F$ where

$$\theta = 2\tan^{-1}\exp[(s-s_0)/l] , \tag{10}$$

$s = x - ut$, the characteristic length $l = (\pi g\gamma n)^{-1}$, $\gamma = (1-u^2/v_F^2)^{-1/2}$, $g = (U/\pi\hbar v_F)^{1/2}$ being the interaction parameter (the interaction is assumed repulsive, $U > 0$). The kinks extend over $\Delta s \sim \pi l$ around s_0 and involve a phase slip $\Delta\phi = 2\pi$ (solutions with l changed formally into $-l$ have a phase slip $\Delta\phi = -2\pi$ and are described as antikinks). A kink soliton of the backward scattering implies an imbalance of the spin density of one-half. Indeed, according to (7),

$$\frac{1}{2}\int dx(\delta n_{1+} - \delta n_{2+} - \delta n_{1-} + \delta n_{2-}) = -(n/4)\Delta u_{--} = (1/4\pi)\Delta\phi = -\tfrac{1}{2} . \tag{11}$$

The soliton energy is readily obtained from (9) and (10) as

$$\varepsilon = \hbar v_F/\pi l = \Delta\gamma , \tag{12}$$

where $\Delta = \hbar v_F g n$ is the soliton energy gap. For $|u| \ll v_F$, the soliton energy (12) is $\varepsilon \simeq \Delta(1 + u^2/2v_F^2)$ and the soliton mass may be defined as $\mu = \Delta/v_F^2 = (2g/\pi)m$.

The condition for slowly varying density disturbance $|\partial_x u_{j\sigma}| \ll 1$ implies $|\partial_x\phi| \ll 2\pi n$, while the condition for the validity of the semiclassical approximation $|\partial_{xx}u_{j\sigma}| \ll k_F$ reads $|\partial_{xx}\phi| \ll \pi^2 n^2$. Both are ensured by $\pi l n \gg 1$, i.e., $\gamma g \ll 1$. First, one notices that backward-scattering kinks propagating with velocity near the Fermi velocity v_F do not exist in the interacting electron gas in one dimension. Indeed, in this case both the semiclassical approach and the collective-mode conditions break down, the classical soliton crumbling away into quantum solitons.[9] This corresponds to the Landau damping of the collective modes by the one-particle excitations. The standard quantization scheme[10,11] may be applied in this $u \sim v_F$ region. In this connection we remark that other nonlinear solutions of the sine-Gordon equation (like breathers or kinks propagating with velocity greater than v_F) are disregarded as being unstable in real quasi-one-dimensional materials. Second, one can see from $g\gamma \ll 1$ that $g < 1$ is a necessary condition for the existence of the zero-sound solitons. For the quasi-one-dimensional materials the electronic bandwidth $E_b \sim \pi\hbar v_F n/4$, and nU may be taken as the Hubbard repulsion U_H plus the intersite Coulomb repulsion V. The interaction parameter g may therefore be expressed as $g^2 \sim (U_H + V)/4E_b$. For organic materials, like the charge-transfer salts of the tetrathiofulvalene-tetracyanoquinodimethane (TTF-TCNQ), $U_H \sim V/2 \sim 2E_b \sim 1$ eV,[12] so that $g^2 \sim \frac{3}{2}$. Backward-scattering solitons hardly may exist in these compounds. In addition, one notices that the zero-sound oscillations of the u_{+-} coordinate are unstable for $g > 1$ ($v_-^2 < 0$), which implies that inhomogeneities of the spin density may be built up in the highly interacting electron gas in one dimension. A similar situation seems to occur in the blue bronzes. A possible exception could be the inorganic one-dimensional conductors, where the screening effects may reduce considerably the Coulomb interaction. In the highly interacting case $g \sim 1$ one may say that the backward-scattering solitons are very energetic ($\Delta \sim E_b$), narrow ($l \sim a$), and heavy ($\mu \sim m$). They contribute an extremely low exponentially activated specific heat in the limit of low temperatures, and require an extremely high magnetic field to be seen in the magnetic susceptibility.

The situation may be different in the case of the umklapp-scattering solitons. For electrons moving on a latticial, rigid background the semiclassical wave functions (3) must be multiplied by the Bloch functions $w(x)$ corresponding to $\pm k_F$ (and normalized to unity). In this case the interaction (5) may contain an additional contribution of the sine-Gordon type, coming from the G component of $w^4(x)$, providing the reciprocal vector $G=4k_F$ (half-filling case). This is the umklapp-scattering Hamiltonian [corresponding to $\psi_{1\sigma}^*\psi_{2\sigma}\psi_{1-\sigma}^*\psi_{2-\sigma}$ in (5)], which can be obtained formally from (9) by replacing ϕ by $\psi=\pi n u_{-+}$ and U by $W=U(w^4)_G$. For weak electron-lattice interaction $w(x)\sim 1+2w_G\cos Gx$, where $w_G \ll 1$ (it is of the order of the ratio of the electron-lattice interaction to the Fermi energy), so that $W\sim 4Uw_G \ll U$. The interaction parameter g may be much lesser than unity in this case, which means that the umklapp-scattering solitons may well exist. They are much lower in energy, more shallow, and lighter than the backward-scattering solitons. The umklapp-scattering solitons correspond to an electric charge imbalance equal to an electron charge (CDW commensurability index $M=G/2k_F=2$). According to the classical dynamics[13] they may contribute an appreciable conductivity $\sigma\sim W^{-1/2}$ to the current-voltage characteristic. On the other hand, their characteristic length $l\sim W^{-1/2}$ being large, they are more difficult to be seen in the nearly commensurate case where the soliton lattice with the spacing $2\pi/|G-4k_F|$ establishes.

For a nonlocal interaction extended over the interelectron distance a the interacting Hamiltonian (5) contains an additional spin-independent coupling constant V (which may simulate the intersite Coulomb repulsion). In this case the coupling constant U in the backward-scattering and the umklapp-scattering Hamiltonians is replaced by $U+V$, the zero-sound velocity v_+ becomes $v_+=v_F[1+(U+2V)/\pi\hbar v_F]^{1/2}$, while v_- remains unchanged. The phase Hamiltonian (8) corresponds in this case to the g-ology model[14] with the identifications $g_{4\parallel}=g_{2\parallel}-g_{1\parallel}=V$, $g_{4\perp}=g_{2\perp}=-g_{1\perp}=V+U$, and $2g_3=W$.[15]

Finally, it is worth noting that the semiclassical approach can be used to describe the coupling of the classical electronic solitons derived in this paper to the phasons and the amplitudons of the Peierls-Fröhlich lattice distortion. A classical dynamics is thereby obtained for the electron-lattice coupling in one dimension, in agreement with the adiabatic hypothesis.[8] Similarly, the interaction of the classical electronic solitons with impurities, either randomly or regularly distributed, can be treated along the same lines, with nontrivial consequences regarding the electronic transport and localization in one dimension.[16] The semiclassical representation of the wave functions in terms of the classical-mechanical action, though not restricted, in principle, to one dimension, comes upon certain difficulties in higher dimensions. All these issues will be discussed elsewhere.

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