Wigner Crystal in One Dimension

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A one-dimensional gas of electrons interacting with long-range Coulomb forces [$V(r) \approx 1/r$] is investigated. The excitation spectrum consists of separate collective charge and spin modes. For arbitrarily weak Coulomb repulsion density correlations at wave vector $4k_F$ decay extremely slowly and are best described as those of a one-dimensional Wigner crystal. Pinning of the Wigner crystal then leads to the nonlinear transport properties characteristic of charge density waves. The results allow a consistent interpretation of the plasmon and spin excitations observed in one-dimensional semiconductor structures, and suggest an interpretation of some of the observed features in terms of "spinons."

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The properties of models of one-dimensional interacting electrons have been studied in great detail. Examples are the so-called "g-ology" model of fermions moving in a continuum [1,2], or the one-dimensional Hubbard model [1,3,4]. In these models, one usually assumes short-ranged (effective) electron-electron interactions. The so-called "Luttinger liquid" [5] behavior in this type of model is characterized by separation between spin and charge degrees of freedom and by power-law correlation functions, with interaction-dependent exponents. Short-range interactions are a reasonable assumption for applications, e.g., to quasi-one-dimensional conductors, where screeening between adjacent chains leads to effectively short-range interactions within one chain [6]. However, the situation can be quite different if an isolated system of electrons moving in one dimension is considered. There then is no interchain screening, and the true long-range character of the Coulomb forces [$V(r) = e^2/r$] needs to be taken into account. This appears to be the case, e.g., in certain one-dimensional semiconductor structures, where the effects of one-dimensional Coulomb forces have indeed been observed [7].

The purpose of the present paper is to investigate the effects of the long-range Coulomb interaction in a one-dimensional model, using the bosonization method [1,2]. This allows in particular a rather straightforward and asymptotically (for low energies and wave numbers) exact description of excitation spectra and correlation functions. The main conclusion is that the long-range force, even if it is very weak, leads to a state characterized by quasi-long-range order much closer to a one-dimensional Wigner crystal [8] than to an electron liquid. The calculations presented here provide a rather simple microscopic description of the Wigner crystal, a problem that in higher dimensions has been difficult to treat by many-body techniques.

I will start by considering the particular case of one-dimensional electrons with a linear energy-momentum relation interacting with long-range Coulomb forces, described by the Hamiltonian

$$H = \sum_{k,s} v_F[(k-k_F)a^\dagger_{k,s}a_{k,s} + (-k-k_F)b^\dagger_{k,s}b_{k,s}] + \frac{1}{2L}\sum_q V(q)\rho_q\rho_{-q} + H_{\rm bs} \ . \quad (1)$$

Here $a^\dagger_{k,s}$ ($b^\dagger_{k,s}$) creates a right- (left-) moving electron with momentum k and spin projection s and v_F is the Fermi velocity. In the interaction term $\rho_q = \rho_{a,q} + \rho_{b,q}$ is the Fourier component of the total particle density, and $V(q)$ is the Fourier transform of the interaction potential. In strictly one dimension, a $1/r$ Coulomb interaction does not have a Fourier transform because of the divergence for $r \to 0$, however, in a system of finite transverse dimension d, the singularity is cut off at $r \approx d$ [9]. Using the approximate form $V(r) = e^2/\sqrt{r^2+d^2}$, one has $V(q) = 2e^2K_0(qd)$. Finally, the backward scattering term $H_{\rm bs}$ describes processes where particles go from the right- to the left-moving branch and vice versa. This involves a nonsingular interaction matrix element at $q \approx 2k_F$, called g_1.

The linear energy-momentum relation makes the model (1) exactly solvable using standard bosonization methods. Moreover, at least for weak Coulomb interactions, when states near the Fermi energy play the major role, linearizing the spectrum is not expected to change the physics drastically, and one therefore expects that the model (1) correctly represents the low-energy physics even for more realistic band structures. The model can be easily solved introducing the phase fields

$$\phi_\nu(x) = -\frac{i\pi}{L}\sum_{p\neq 0}\frac{1}{p}e^{-ipx}[\nu_+(p) + \nu_-(p)] \ , \quad (2)$$

where $\nu = \rho, \sigma$, and $\rho_r(p)$ [$\sigma_r(p)$] are the usual charge [spin] density operators for right- ($r = +$) and left- ($r = -$) going fermions. The Hamiltonian then decomposes into commuting parts for the charge and spin degrees of freedom. The charge part takes the simple quadratic form

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$$H_\rho = \frac{v_F}{2\pi}\int dx\,[\pi^2(1+\tilde{g}_1)\Pi_\rho^2 + (1-\tilde{g}_1)(\partial_x\phi_\rho)^2] + \frac{1}{\pi^2}\int dx\,dx' V(x-x')\partial_x\phi_\rho\,\partial_{x'}\phi_\rho. \quad (3)$$

Here Π_ρ is the momentum density conjugate to ϕ_ρ, and $\tilde{g}_1 = g_1/2\pi v_F$. The Hamiltonian (3) is quadratic in the bosonic fields and therefore can be diagonalized straightforwardly. The elementary excitations are then found to be charge oscillations (plasmons), with energy-momentum relation

$$\omega_\rho(q) = v_F|q|\{(1+\tilde{g}_1)[1-\tilde{g}_1+2\tilde{V}(q)]\}^{1/2}, \quad (4)$$

where $\tilde{V}(q) = V(q)/\pi v_F$. The long-wavelength form, $\omega_\rho(q) \approx |q^2 \ln q|^{1/2}$, agrees with RPA calculations [9,10]; however, the effect of g_1, which is a short-range exchange contribution, is usually neglected in those calculations.

The spin part of the Hamiltonian does not involve the long-range part of the interaction and only depends on the backward scattering amplitude g_1. For repulsive interaction, the long-wavelength spin excitations are then described by a Hamiltonian similar to the first term in (3), giving rise to collective spin oscillations with $\omega_\sigma(q) = u_\sigma|q|$, and spin wave velocity $u_\sigma = v_F\sqrt{1-\tilde{g}_1^2}$. Together with the charge oscillations (4), these excitations are the complete spectrum of the model.

The bosonization method makes the calculation of correlation functions rather straightforward. Here, the charge-charge correlations are of particular interest. Using the expression

$$\rho(x) = -(\sqrt{2}/\pi)\partial_x\phi_\rho(x) + \frac{1}{2\pi\alpha}e^{2ik_Fx}e^{-i\sqrt{2}\phi_\rho(x)}\cos[\sqrt{2}\phi_\sigma(x)] + \text{const}\,e^{4ik_Fx}e^{-i\sqrt{8}\phi_\rho(x)} + \text{H.c.}\,, \quad (5)$$

the evaluation of the charge correlation function reduces to the calculation of averages of the type

$$\langle[\phi_\rho(x)-\phi_\rho(0)]^2\rangle = \int_0^\infty \frac{dq}{q}\left[\frac{1+\tilde{g}_1}{1-\tilde{g}_1+2\tilde{V}(q)}\right]^{1/2}(1-\cos qx) \approx c_2\sqrt{\ln x}\,, \quad (6)$$

with $c_2 = \sqrt{(1+\tilde{g}_1)\pi v_F/e^2}$. One thus obtains

$$\langle\rho(x)\rho(0)\rangle = A_1\cos(2k_Fx)\exp(-c_2\sqrt{\ln x})/x + A_2\cos(4k_Fx)\exp(-4c_2\sqrt{\ln x}) + \cdots, \quad (7)$$

where $A_{1,2}$ are interaction-dependent constants, and only the most slowly decaying Fourier components are exhibited. The most interesting point here is the extremely slow decay (much slower than any power law) of the $4k_F$ component, showing an incipient charge density wave at wave vector $4k_F$ (instead of the usual $2k_F$ of the Peierls instability). This slow decay should be compared with the case of short-range interactions, where the $2k_F$ and $4k_F$ components decay as with the power laws x^{-1-K_ρ} and x^{-4K_ρ}, respectively, with an interaction-dependent constant K_ρ [1,2,4]. The $4k_F$ oscillation period is exactly the average interparticle spacing; i.e., the structure is that expected for a one-dimensional *Wigner crystal*. Of course, because of the one-dimensional nature of the model, there is no true long-range order; however, the extremely slow decay of the $4k_F$ oscillation would produce strong quasi-Bragg peaks in a scattering experiment. It is worthwhile to point out that this $4k_F$ contribution arises even if the Coulomb interaction is extremely weak and depends only on the long-range character of the interaction. On the other hand, any $2k_F$ scattering is considerably weaker, due to the $1/x$ prefactor in (7) which has its origin in the contribution of spin fluctuations.

Other correlation functions are easily obtained. For example, the spin-spin correlations are

$$\langle\mathbf{S}(x)\cdot\mathbf{S}(0)\rangle \approx B_1\cos(2k_Fx)\exp(-c_2\sqrt{\ln x})/x + \cdots, \quad (8)$$

where there is no $4k_F$ component. On the other hand, correlation functions that involve operators changing the total number of particles (e.g., the single particle Green's function) decay like $\exp[-\text{const}(\ln x)^{-3/2}]$, i.e., *faster* than any power law. This in particular means that the momentum distribution function n_k and all its derivatives are continuous at k_F, and there is only an essential singularity at k_F. The calculations are also straightforwardly generalized to finite frequency and temperature [1,2], however, the rather complicated formulas are not of immediate interest here.

The presence of metallic screening changes the above behavior: a finite screening length ξ_s would lead to a saturation of $V(q)$ for $q \to 0$ at $2e^2\ln(\xi_s/d)$. One then would have, for $x > \xi_s$, power law decay of the type discussed above for short-range interactions, with $K_\rho \approx 1/\sqrt{\ln\xi_s}$. On the other hand, if the interaction potential decays more slowly than $1/r$ (a rather hypothetical case), the integral (6) remains finite for $x \to \infty$, and therefore there then is real long-range order of the Wigner crystal type.

It is instructive to compare the above result (7), obtained in the limit of weak Coulomb interactions, with the case of strong repulsion (or, equivalently, heavy particles). The configuration of minimum potential energy is one of a chain of equidistant particles with lattice constant a, and quantum effects are expected to lead only to small oscillations in the distances between particles. The

Hamiltonian then is

$$H = \sum_l \frac{p_l^2}{2m} + \frac{1}{4}\sum_{l\neq m} V''(ma)(u_l - u_{l+m})^2 \ , \qquad (9)$$

where u_l is the deviation of particle l from its equilibrium position. In the long-wavelength limit, the oscillation of this lattice have energy $\omega(q) = \sqrt{2/(ma)}eq|\ln(qa)|^{1/2}$. The most slowly decaying part of the density-density correlation function is then

$$\langle\rho(x)\rho(0)\rangle \approx \cos(2\pi x/a)\exp\left[-\frac{4\pi}{(2me^2a)^{1/2}}\sqrt{\ln x}\right] \ . \qquad (10)$$

Noticing that $k_F = \pi/2a$, one observes that the results (7) and (10) are (for $g_1 = 0$) identical as far as the long-distance asymptotics are concerned, *including the constants in the exponentials.* Equation (7) was obtained in the weak interaction limit, whereas (10) applies for strong Coulomb forces. Similarly, the small-q limit of the charge excitation energies is identical. We are thus led to the rather remarkable conclusion that the long-distance behavior of correlation functions is independent of the strength of the Coulomb repulsion, provided the interaction is truly long ranged.

In recent experiments, one-dimensional structures with two partially filled subbands have been investigated [7]. If only the long-range part of the Coulomb interaction is considered, the appropriate generalization of the model (3) to that case is described by the Hamiltonian

$$H_\rho = \sum_{i=0,1}\frac{v_i}{2\pi}\int dx\,[\pi^2\Pi_{\rho,i}^2 + (\partial_x\phi_{\rho,i})^2] + \frac{1}{\pi^2}\int dx\,dx' V(x-x')\partial_x(\phi_{\rho,0}+\phi_{\rho,1})\partial_{x'}(\phi_{\rho,0}+\phi_{\rho,1}) \ ,$$

where v_i is the Fermi velocity of band i, and $\phi_{\rho,i}, \Pi_{\rho,i}$ are the charge fields of band i. In the long-wavelength limit the charge oscillation eigenmodes have energies

$$\omega_+(q) = |q|\sqrt{2(v_0+v_1)V(q)/\pi}, \quad \omega_-(q) = \sqrt{v_0v_1}|q| \ .$$

The ω_+ mode represents in-phase oscillations of the two bands and has the typical $|q^2\ln q|^{1/2}$ behavior of one-dimensional plasmons, whereas the ω_- mode is an out-of-phase oscillation. In addition there are two spin modes, at energies $v_{0,1}|q|$. If the various possible interaction processes involving momentum transfer of order $2k_{F,i}$ are included, the velocities of these modes are renormalized, similar to the effect of g_1 in the one-band model above.

For the density correlations of the two-band model I find

$$\langle\rho(x)\rho(0)\rangle = C_2\cos[4(k_{F,0}+k_{F,1})x]\exp(-4c_2\sqrt{\ln x}) + x^{-K}\sum_{i=0,1} C_i\cos(4k_{F,i}x)\exp(-c_i\sqrt{\ln x}) \ ,$$

where now $c_2 = \sqrt{\pi(v_0+v_1)/e^2}$, $c_i = 4v_i^2c_2/(v_0+v_1)^2$, $K = 4\sqrt{v_0v_1}/(v_0+v_1)$, and again only the most slowly decaying Fourier components are exhibited. The most slowly decaying part of (10) [$q = 4(k_{F,0}+k_{F,1})$] is again the one that corresponds to Wigner-crystal-type ordering; e.g., the electrons order approximately equidistantly. In fact, this type of ordering is determined only by the ω_+ mode, whereas all other Fourier componets contain contributions from the ω_- mode, which lead to power law decay.

To compare the present results with experiment [7] one can first notice that, provided that $2k_Fd < 1$ and including the background dielectric screening, one has $\tilde{g}_1 < 0.2$, and consequently to within a few percent $u_\sigma = v_F$; i.e., the triplet spin mode [spin density excitiation, (SDE)] is expected at v_Fq, as experimentally observed. Further, in the experimentally accessible range $q < 0.2k_F$ the plasmon energies found here are indistinguishable from RPA results, and thus the present results provide a good fit to the experimental plasmon dispersion.

More difficult to explain is the extra feature which has been interpreted as an electron-hole continuum [single particle excitation, (SPE)] [7]: in fact in the present model with its linear electron dispersion relation, there is no such continuum (and it would not exist in an RPA calculation either). However, the model offers an alternate possibility: together with the triplet spin mode, there is also a *singlet* mode [11]. The existence of the singlet mode is a consequence of spin-charge separation in one-dimensional fermion systems, and in particular it is degenerate with the triplet mode. This mode can be found, e.g., in energy density correlation functions (as opposed to the spin mode, which appears as a pole of the spin density correlation function), and therefore is also expected to be seen in the polarized Raman spectra. This interpretation requires the SDE and SPE features to appear at the same energy, which seems to be consistent with the results published in Ref. [7]. It is noteworthy that, if correct, this interpretation would mean that these results constitute the first direct spectroscopic evidence for the existence of individual spin-1/2 objects ("spinons"): the simplest explanation for the observation of degenerate triplet and singlet modes is that they both correspond to an excitation of a pair of spin-1/2 objects, with the degeneracy due to the absence of interaction between them.

One might argue that the existence of the particle-hole continuum is due to effects of band curvature, which is neglected in the present model. RPA calculations including band curvature certainly predict both a plasmon and a particle-hole continuum [9,10]. However, within RPA the total spectral weight for the continuum is about 2 orders of magnitude smaller than that of the plasmon, whereas in Ref. [7] plasmon and SPE have compara-

ble weight. Moreover, in exactly solved one-dimensional models like the Hubbard model [3], one finds both a plasmonlike collective mode and the singlet mode discussed above, but no separate particle-hole continuum [12]. There thus seems to be little theoretical evidence in favor of an interpretation of the SPE feature in terms of a particle-hole continuum.

The nearly long-range Wigner-crystal-type order should have important consequences for transport properties: in fact, in the presence of disorder, a classical charge density wave (which has real long-range order at $T = 0$) becomes disordered [13], with a "pinning length" describing the decay of spatial correlations given by

$$\xi_{\text{pin}} \approx [(V/v_F)^2 n]^{-1/3} , \tag{11}$$

where n is the density of impurities, and V the Fourier component of the impurity potential at the wave vector of the charge density wave (CDW) ($4k_F$ in our case). Inclusion of quantum effects in systems with short-range interaction only leads to corrections to the exponent 1/3 in (11) [14]. Following the same arguments, I expect (11) to be valid for the Coulomb system too (up to logarithmic corrections); i.e., as far as low-frequency phenomena are concerned, the system of electrons interacting with Coulomb forces *behaves like a classical charge density wave*. In particular, all the unusual dynamical properties associated with nonlinear transport in CDW systems should also occur in the one-dimensional electron system.

At finite temperature, thermal agitation can become sufficiently strong to depin a CDW. In the present case, this is expected to happen when the thermal correlation length, ξ_T, in the absence of impurities, given by $\omega_\rho(1/\xi_T) \approx T$, becomes shorter than ξ_{pin}.

Nonlinear current-voltage relations characteristic of CDW transport have been observed in one-dimensional semiconductor structures [15]. In these experiments, strong variations of the *linear* conductance with carrier density have been interpreted in terms of the Coulomb blockade [16], implying the existence of a pair of strong impurity potentials. It seems certainly conceivable that the *nonlinear* behavior should be due to collective motion of a pinned CDW, possibly in parts of the sample where there is only a weak random potential. The fact that the order of magnitude of the nonlinear conductance is independent of the value of the linear conductance suggests that different mechanisms are involved in the two phenomena. The present calculation then demonstrates that Coulomb interactions do not have to be particularly strong to create nearly classical CDW type behavior. It would clearly be interesting to investigate the possible interplay between Coulomb blockade and CDW-like behavior.

In conclusion, using the bosonization technique a consistent microscopic picture of the excitation spectrum and the correlation functions of a one-dimensional electron gas interacting with long-range Coulomb forces has been obtained. The density correlations are those of a nearly perfect one-dimensional Wigner crystal. The results are in agreement with excitation spectra observed in one-dimensional semiconductor structures and provide a possible explanation for nonlinear transport properties.

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