Transition from a One-Dimensional to a Quasi-One-Dimensional State in Interacting Quantum Wires

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Upon increasing the electron density in a quantum wire, the one-dimensional electron system undergoes a transition to a *quasi*-one-dimensional state. In the absence of interactions between electrons, this corresponds to filling up the second subband of transverse quantization, and there are two gapless excitation modes above the transition. On the other hand, strongly interacting one-dimensional electrons form a Wigner crystal, and the transition corresponds to it splitting into two chains (zigzag crystal). We show that the soft mode driving the transition to the zigzag state is gapped, and only one gapless mode exists above the transition. Furthermore, we establish that in the vicinity of the transition already arbitrarily weak interactions open a gap in the second mode. We then argue that only one gapless mode exists near the transition at any interaction strength.

Transport properties of quantum wires have attracted much attention over recent years [1–7]. Because of their quasi-one-dimensional structure, conductance is expected to be quantized in units of the conductance quantum $G_0 = 2e^2/h$, where e is the elementary charge and the factor of 2 accounts for spin degeneracy. This property of noninteracting electrons is insensitive to the inclusion of interactions within the Luttinger-liquid description. However, a number of experiments show deviations from perfect conductance quantization, such as the so-called 0.7-structure observed below the first plateau [3–7]. These experiments have stimulated much theoretical interest in the physics of one-dimensional conductors not captured by the Luttinger-liquid theory, such as that of the spin-incoherent regime characterized by very weak coupling of the electron spins [8–10]. Here we consider another important problem in this category: the transition of the one-dimensional electron system in a quantum wire into a quasi-one-dimensional state.

Whether or not an electron system can be viewed as one-dimensional crucially depends on the strength of interaction [11]. In the absence of interactions, electrons occupy subbands of transverse quantization, and the system is one-dimensional until the chemical potential reaches the bottom of the second subband. On the other hand, at strong interactions, the electrons form a Wigner crystal, and the subband picture is no longer applicable. The system remains one-dimensional until the interaction energy overcomes the confining potential, and the crystal splits into two chains, forming a zigzag structure [12].

There is an important difference in the behavior of the system in the vicinity of the transition between the limits of noninteracting and strongly interacting electrons. In the noninteracting case the two subbands are independent and therefore represent two gapless modes. By contrast, at strong interactions one expects that the two chains of the

classical Wigner crystal are locked, and only one gapless mode (the plasmon) remains. In this Letter we address the fate of the second low-energy mode in the vicinity of the transition as the interaction strength varies. First we establish that the second excitation mode of the zigzag crystal remains gapped in the presence of quantum fluctuations. Then we show that in the vicinity of the transition already arbitrarily weak interactions open a gap in the second mode. We subsequently argue that a gap exists at any interaction strength.

For simplicity we consider spinless electrons and assume that they interact via long-range Coulomb repulsion,

$$V_{\text{int}} = \frac{e^2}{2\epsilon} \sum_{k \neq l} \frac{1}{|\mathbf{r}_k - \mathbf{r}_l|}. \qquad (1)$$

Here $\mathbf{r}_k$ are the two-dimensional position vectors of the electrons, and ϵ is the dielectric constant of the material. If the electrons in the wire are confined to one dimension by a strong external potential $V_{\text{conf}}(y_k)$, their physics is controlled by the one-dimensional electron density n_e. Since at $n_e \rightarrow 0$ the kinetic energy of an electron $\sim(\hbar^2/m)n_e^2$ scales to zero faster than the interaction energy $\sim(e^2/\epsilon)n_e$, at low densities the Coulomb repulsion dominates. In this limit electrons behave classically. In order to minimize their mutual interaction, they form a periodic one-dimensional structure—the so-called Wigner crystal. At small but finite density, quantum fluctuations smear the long-range order [13], but the short-range order remains as long as the distance between electrons n_e^{-1} is greater than the Bohr radius $a_B = \epsilon\hbar^2/me^2$.

The above picture is valid if the width w of the wire is small, $w \ll a_B$. In wider wires, or, equivalently, at stronger interactions, the opposite regime $w \gg a_B$ can be achieved. In this case the electrons may form a two-dimensional structure while remaining essentially classical. The struc-

ture of the classical Wigner crystal can be studied in detail
(cf. Ref. [12]), if the confining potential is quadratic,

$$V_{\text{conf}} = \frac{1}{2} m\Omega^2 \sum_k y_k^2. \tag{2}$$

Here the frequency Ω determines the width of the wire,
$w \sim \sqrt{\hbar/m\Omega}$. The positions of all electrons are found by
minimizing the energy $V_{\text{int}} + V_{\text{conf}}$ over $\mathbf{r}_k$ keeping the
one-dimensional electron density n_e fixed. The geometry
of the classical crystal is controlled by the dimensionless
electron density $\nu = n_e r_0$, where $r_0 = (2e^2/\epsilon m\Omega^2)^{1/3}$ is
the sole length scale of the problem [12]. At ν below the
critical value $\nu_c = \sqrt[3]{4/7\zeta(3)} \approx 0.780$ the energy is mini-
mized when electrons form a one-dimensional crystal, in
which $x_k = k/n_e$ and $y_k = 0$. At $\nu > \nu_c$ the crystal splits
into two rows. The distance between rows vanishes at the
transition; just above the critical value, when $\delta\nu = \nu - \nu_c \ll 1$, it grows as $c = [\sqrt{24/93\zeta(5)}/\nu_c^2]\sqrt{\delta\nu}$ (in units
of r_0).

Let us consider the low-energy phonons in the zigzag
Wigner crystal. Regardless of the density, the crystal has
the usual plasmon excitation mode with acoustic spectrum.
In the limit of zero wave vector, this excitation corresponds
to translation of the crystal along the wire, $\delta x_k = \eta$, $\delta y_k = 0$ for any k. In addition, at the zigzag transition point a
transverse soft mode appears, for which $\delta x_k = 0$ and
$\delta y_k = (-1)^k \varphi$. One can easily show that near the zigzag
transition, when $\delta\nu \ll 1$, the coupling of the two low-
energy excitation modes is weak, and they can be treated
separately. The action describing the soft transverse mode
takes the form

$$S = A\hbar \sqrt{\frac{r_0}{a_B}} \int d\tau dx [(\partial_\tau \varphi)^2 + (\partial_x \varphi)^2 - \delta\nu \varphi^2 + \varphi^4]. \tag{3}$$

Here x, τ, and the field φ have been rescaled so as to yield
the simplest form of the action possible; $A = [7\zeta(3)]^{3/2} \times \sqrt{\ln 2}/31\zeta(5)$. The general form of the action and our
results from this point on are not sensitive to the exact
shape of the confining potential. Above the classical tran-
sition point $\delta\nu = 0$, the transverse mode becomes un-
stable. This corresponds to the formation of the zigzag
structure. To stabilize the system we keep the quartic
term φ^4. Contrary to the claims of Ref. [12], above the
transition the classical soft mode is gapped.

Quantum fluctuations affect both the position and the
nature of the phase transition. To determine their effect,
it is helpful to fermionize the problem. To this end we
rediscretize the coordinate x and consider a set of par-
ticles moving in a double-well potential $-\lambda\varphi_j^2 + \varphi_j^4$ with
nearest-neighbor interaction $(\varphi_j - \varphi_{j+1})^2$ between them.
At sufficiently large λ each particle is almost completely
localized in one of the minima, and its position can be
described by a spin operator, $\varphi_j = \pm\sqrt{\lambda/2} = \sqrt{\lambda/2}\sigma_j^z$. In
terms of these pseudospin variables the Hamiltonian con-

tains two terms: $-t\sum_j \sigma_j^x$ describing tunneling between the
two minima of the double-well potential and $-\nu\sum_j \sigma_j^z \sigma_{j+1}^z$
accounting for the nearest-neighbor interactions. Rotating
$\sigma^x \to -\sigma^z$ and applying the Jordan-Wigner transforma-
tion, one obtains the Hamiltonian

$$\mathcal{H}_f = \sum_j [2ta_j^\dagger a_j - \nu(a_j^\dagger - a_j)(a_{j+1}^\dagger + a_{j+1})]. \tag{4}$$

Since the number of fermions is not conserved, the
Hamiltonian (4) should be diagonalized by performing a
Bogoliubov transformation. As a result one easily finds
that the excitation spectrum of the Hamiltonian (4) has a
gap Δ that vanishes when $t = \nu$. We identify this point
with the phase transition from the one-dimensional state of
the wire at $t > \nu$ when all the fermionic states in the
Hamiltonian (4) are empty, to the quasi-one-dimensional
state at $\nu > t$, in which fermionic states describing the
transverse degrees of freedom in the wire are filled, but
possess a spectral gap. Near the transition the gap behaves
linearly, $\Delta = 2|\nu - t|$.

In experiments with quantum wires, the transition from a
one-dimensional to a quasi-one-dimensional state is ob-
served when the chemical potential μ of electrons is tuned
by applying a gate voltage. The parameters t and ν of the
Hamiltonian (4) are expected to be nonsingular functions
of μ. The transition occurs at the critical value μ_c, defined
as a solution of the equation $t(\mu) = \nu(\mu)$. The gap in the
excitation spectrum is then linear in the distance from the
transition,

$$\Delta \propto |\mu - \mu_c|. \tag{5}$$

To better understand the nature of this transition, it is
helpful to consider the well-known mapping between
phase transitions in d-dimensional quantum systems and
$(d + 1)$-dimensional classical models [14]. In particular,
the phase transition in the one-dimensional quantum model
(3) is equivalent to that in the two-dimensional classical
Ising model [15]. In this mapping the gap Δ becomes the
inverse correlation length r_c^{-1} of the Ising model, and the
scaling $r_c \propto |T - T_c|^{-1}$, well-known from the exact solu-
tions, is equivalent to Eq. (5). The relation between these
phase transitions can be made more explicit by noticing
that our Hamiltonian (4) essentially coincides with the
transfer matrix [16] of the Ising model near the transition
point.

In the discussion leading to the result (5), the interac-
tions in the quantum wire were assumed to be very strong.
To explore the fate of the gap as the interaction strength is
reduced, we now turn to the case of weak interactions. In
this case the transition to the quasi-one-dimensional state
occurs when electrons start populating the second subband
of transverse quantization in the wire. The essential phys-
ics of the problem is captured by the model of interacting
electrons that may occupy two subbands. The low-energy
properties of the system are described by four interaction
constants. The three constants, g_1, g_2, and g_x, correspond

to density-density interactions in the first subband, the second one, and between the two subbands, respectively. The fourth coupling constant g_t accounts for the possibility of transfer of pairs of electrons between the subbands, Fig. 1(a).

It is well known that in one-dimensional systems density-density couplings renormalize the velocities of the acoustic low-energy excitations, but do not lead to the emergence of spectral gaps [17]. On the other hand, the coupling g_t creates and destroys pairs of electrons in each subband and thus can, in principle, lead to a BCS-like gap in the spectrum [18,19]. Since the coupling constants in weakly interacting one-dimensional electron systems acquire logarithmic renormalizations at low energies [17], the existence of a gap is determined by the scaling of g_t.

The renormalization group equations for the four coupling constants have been derived in Ref. [18]. As the bandwidth of the problem is scaled from D_0 down to D, the renormalization of the coupling constants can be found by solving the system of two coupled equations

$$y'_t = y y_t, \qquad y' = y_t^2. \qquad (6)$$

Here the derivatives are with respect to $\xi = \ln(D_0/D)$,

$$y_t = \frac{g_t}{\pi\hbar}\sqrt{\frac{(v_{F1} + v_{F2})^2 + 4v_{F1}v_{F2}}{2v_{F1}v_{F2}(v_{F1} + v_{F2})^2}},$$

$$y = -\frac{1}{2\pi\hbar}\left(\frac{g_1}{v_{F1}} + \frac{g_2}{v_{F2}} - \frac{4g_x}{v_{F1} + v_{F2}}\right),$$

v_{F1} and v_{F2} are the Fermi velocities in the two subbands.

The renormalization group flow corresponding to the Eqs. (6) is shown in Fig. 1(b). To find the initial values of y_t and y we compute the coupling constants in first order in the interaction strength. Assuming that the Coulomb interactions between electrons are screened by a gate at distance d, in the limit of low electron density in the second subband we find with logarithmic accuracy $g_1^{(0)} = g_x^{(0)} = 2e^2 \ln(k_{F1}d)$ and $g_2^{(0)} \sim e^2(k_{F2}d)^2 \ln(1/k_{F2}d)$. It is important to note that $g_2^{(0)}/v_{F2}$ vanishes when approaching the transition. This is a consequence of the Pauli principle. When the average distance between electrons is large, interactions between them are effectively local. Then, as
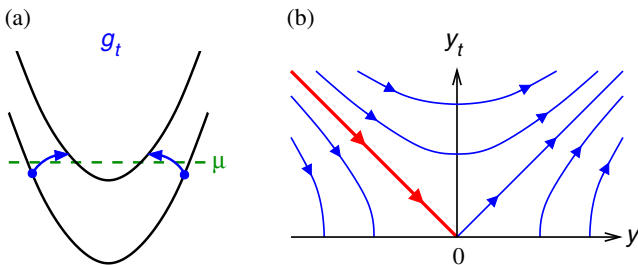

FIG. 1 (color online).   (a) The scattering processes transferring pairs of particles between the two subbands. (b) The flow diagram for the renormalization group (6).

identical fermions never occupy the same place, electrons essentially do not interact. From these estimates we conclude that $y^{(0)}$ is positive, $y^{(0)} \simeq (3e^2/\pi\hbar v_{F1}) \ln(k_{F1}d)$, and according to the flow diagram Fig. 1(b), the interaction constant g_t scales to infinity. Consequently, the system develops a spectral gap. Our result differs from the one obtained in Ref. [18], where no gap was found at $v_{F2} \to 0$ because of the assumption $g_t^{(0)} = g_1^{(0)} = g_2^{(0)} = g_x^{(0)}$. This choice of the initial conditions is not appropriate in our case.

To find the value of the gap, we estimate $g_t^{(0)}$ near the transition as $g_t^{(0)} \sim e^2 k_{F2}/k_{F1}$ and obtain

$$\Delta \propto (\mu - \mu_c)^\alpha. \qquad (7)$$

Thus the gap in the spectrum of transverse excitations of the wire exists not only when the interactions are strong, but also when they are weak. Unlike the case of strong interactions (5), at weak coupling the power-law dependence (8) has a very large exponent $\alpha = (4y^{(0)})^{-1} \gg 1$.

Based on these findings, namely, the existence of a gap at both weak and strong interactions, we expect that the system supports only one gapless excitation mode in the vicinity of the transition at any interaction strength. To gain further insight into the evolution of the transition between the two limiting cases, we derive the effective Hamiltonian of the system at arbitrary interaction strength. Since the interactions between electrons in the lower subband are no longer weak and only their properties near the Fermi level are important, it is convenient to use the bosonization approach [17]. On the other hand, as we discussed, near the transition interactions between electrons in the second subband are negligible, $g_2 \to 0$. Furthermore, the curvature of their spectrum is important in this regime, so the description in terms of fermionic operators is more appropriate. The nonvanishing density-density interactions can still be described by the constants g_1 and g_x, although their values may no longer be computed in first-order perturbation theory. Under these conditions the Hamiltonian has the form

$$\mathcal{H} = \frac{\hbar v_{F1}}{2\pi}\int dx\left((\partial\theta)^2 + \frac{(\partial\phi)^2}{K^2}\right) - \frac{\hbar^2}{2m}\int dx\,\psi^\dagger\partial^2\psi$$
$$+ \gamma_t\int dx\{[(\partial\psi)\psi - \psi\partial\psi]e^{2i\kappa\theta(x)} + \text{H.c.}\}. \qquad (8)$$

Here the bosonic fields $\phi(x)$ and $\theta(x)$ describe the density excitations in the first subband, $K = (1 + g_1/\pi\hbar v_{F1})^{-1/2}$ is the respective Luttinger-liquid parameter, ψ is the electron destruction operator for the second subband, the constant $\gamma_t \sim e^2$, and $\kappa = 1 - K^2 g_x/\pi\hbar v_{F1}$. In deriving Eq. (8) we performed a unitary transformation [20] which removed the density-density coupling between the two subbands and changed the phase factor $e^{2i\theta}$ in the last term to $e^{2i\kappa\theta}$.

The Hamiltonian (8) interpolates between the limits of weak and strong interactions. In the weak coupling limit
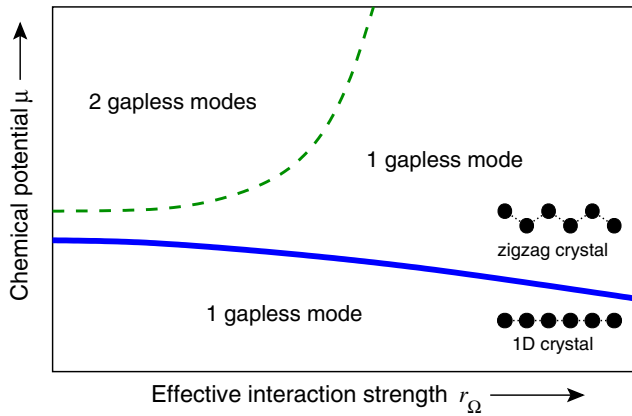
FIG. 2 (color online). Phase diagram of the electronic system in a quantum wire. The effective interaction strength $r_\Omega \equiv r_0/a_B$ can be tuned by varying the confining potential. In the vicinity of the transition to a quasi-one-dimensional state (the solid line) the system supports only one gapless excitation mode at any interaction strength. The state with two gapless excitation modes (above the dashed line) is expected only at relatively weak interactions.

$\kappa \to 1$, and a simple scaling analysis recovers the renormalization group Eqs. (6). At strong interactions the problem of evaluating the coupling constants g_1 and g_x is nontrivial, but in the regime $e^2/\hbar v_{F1} \ll 1 \ll (e^2/\hbar v_{F1}) \times \ln(k_{F1}d)$ one can still use our earlier estimates $g_1 = g_x = 2e^2 \ln(k_{F1}d)$ and conclude that $\kappa \to 0$. Interestingly, in this case the bosonic and fermionic parts of the Hamiltonian (8) decouple, with the latter becoming equivalent to Eq. (4).

One can use the Hamiltonian (8) to discuss the evolution of the gap with varying interaction strength. In the limit of strong interactions, when $\kappa = 0$, the magnitude of the pairing term scales to zero near the transition as k_{F2}, i.e., slower than the Fermi energy $E_{F2} \propto k_{F2}^2$. In this regime, the gap equals the Fermi energy, $\Delta = E_{F2}$ cf. Eq. (5). At strong but finite interactions the pairing term suffers additional power-law suppression at $k_{F2} \to 0$ because of the factor $e^{2i\kappa\theta}$. However, as long as it scales slower than the Fermi energy, the magnitude of the gap remains $\Delta = E_{F2}$. At weaker interactions, when κ exceeds a certain critical value, the pairing term scales to zero faster than the Fermi energy. In this regime the gap develops in a small vicinity of the Fermi points, and its dependence on chemical potential is given by a nonuniversal power-law (7) with exponent $\alpha > 1$. A more detailed theory of the transition at intermediate interaction strengths will be reported elsewhere [21].

Our results are summarized in the phase diagram Fig. 2. The electron system in a quantum wire remains one-dimensional and has a single acoustic excitation branch until the chemical potential reaches a certain critical value μ_c (solid line). At the critical point there is a second gapless mode, and the system can no longer be viewed as one-dimensional. At $\mu > \mu_c$ the second mode develops a gap $\Delta \propto (\mu - \mu_c)^\alpha$ with exponent $\alpha = 1$ at strong inter-

actions, but very large α at weak coupling. At weak interactions, as the chemical potential is increased further, the residual interactions g_2 grow, and the gap disappears (dashed line in Fig. 2). This happens at a small but finite value of the electron density $\sim(k_F d^2)^{-1}$ in the second subband. Thus even at vanishing interactions the solid and dashed lines do not merge, i.e., as long as the interactions are not strictly zero, in a small region of μ above the transition the second mode is gapped, albeit with exponentially small Δ. We see no physical reason for the gap to disappear at strong coupling. In experiments, the presence of a gap will affect the temperature dependence of the conductance which is expected to show activated behavior even above the transition into the quasi-one-dimensional state. The doubling of the zero-temperature conductance (from e^2/h to $2e^2/h$ for spinless electrons) occurs at the dashed line in Fig. 2.

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