Devil’s staircase of incompressible electron states in a nanotube

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It is shown that a periodic potential applied to a nanotube can lock electrons into incompressible states. Depending on whether electrons are weakly or tightly bound to the potential, excitation gaps open up either due to the Bragg diffraction enhanced by the Tomonaga – Luttinger correlations, or via pinning of the Wigner crystal. Incompressible states can be detected in a Thouless pump setup, in which a slowly moving periodic potential induces quantized current, with a possibility to pump on average a fraction of an electron per cycle as a result of interactions.

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A carbon nanotube (NT) is a strongly interacting electron system known to be a host of many-body effects [1], including Luttinger liquid behavior [2]. At half-filling the NT is effectively dilute, and a crossover from the liquid to the 1d Wigner crystal [3] is expected [4].

Here we suggest that an external periodic potential can be a probe of both crystallization and Luttinger correlations. We show that incompressible electron states arise when the electron number density \( \bar{\rho} \) (relative to half-filling) is commensurate with the potential period \( \lambda_{\text{ext}} \):

\[
\bar{\rho} = \frac{m_{\text{tot}}}{\lambda_{\text{ext}}} , \quad m_{\text{tot}} = 4m .
\] (1)

In Eq. (1), \( m \) is the number of the NT electrons of each of the four polarizations [5] per period. To calculate excitation gaps we generalize the Pokrovsky–Talapov theory [6] for the case of the four coupled fermion modes.

In the absence of interactions, Bragg diffraction on the potential opens minigaps at integer density (1), \( |m| = 1, 2, \ldots [7] \). Interactions profoundly change the spectrum, yielding a devil’s staircase of incompressible states at rational \( m = p/q \). In such a state, the NT electron system is locked by the potential into a \( q\lambda_{\text{ext}} \)-periodic structure. If detected, e.g. in a Thouless pump setup [7], corresponding minigaps would provide a direct probe of interactions, with a possibility to map the devil’s staircase by pumping at fractions of the base frequency.

One-dimensional interacting electrons are conventionally described by the Tomonaga - Luttinger liquid [2]. This hydrodynamic approach is valid in a small momentum shell near the Fermi points, with excitations extended over the whole system. Adequate description of crystallization and commensurability requires including the curvature of the electronic dispersion that becomes important at low density. The curvature can yield crystallization or commensuration by coupling charge and spin modes and by introducing a length scale into an otherwise scale-invariant Gaussian theory. In this work we treat both electron interactions and the curvature of the dispersion non-perturbatively by making use of the relativistic Dirac spectrum of a half–filled nanotube. Curvature is controlled by the Dirac gap and is bosonized exactly by virtue of the massive Thirring - sine-Gordon duality. [8, 9] This enables us to study incompressible states both in the limit of a narrow–gap Luttinger liquid and in that of the locked Wigner crystal.

Our course of action is to introduce the bosonized description for the NT electrons, develop the phase soliton method and find excitation gaps from the renormalized sine–Gordon action, draw the phase diagram in the semi-classical limit, and comment on the experimental means to detect incompressible states.

The model. — Nanotube electrons in the forward scattering approximation [10] are described by the four flavors of Dirac fermions \( \psi_\alpha = (\psi_\alpha^R, \psi_\alpha^L)^T, \alpha = 1 \ldots 4 \), whose interaction is written in terms of the smooth envelope \( \rho(x) = \sum_{\alpha=1}^4 \psi_\alpha^+(x)\psi_\alpha(x) \) of the total charge density. The second-quantized Hamiltonian \( \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{bs}} + \mathcal{H}_{\text{ext}} \), where \( \mathcal{H}_0 \) is the massless Dirac Hamiltonian

\[
\mathcal{H}_0 = -i\hbar v \int \sum_{\alpha=1}^4 \psi_\alpha^+ \sigma_3 \partial_x \psi_\alpha dx + \frac{1}{2} \sum_k \rho_{-k} V(k) \rho_k
\] (2)

with the Coulomb interaction \( V(k) = \frac{2e^2}{\pi \xi} \ln [1 + (ka)^{-2}] \) for a tube of radius \( a \) placed on a substrate with the dielectric constant \( \xi \). The curvature of the electron dispersion controlled by the gap \( 2\Delta_0 \) at half-filling introduces backscattering at each NT Dirac point:

\[
\mathcal{H}_{\text{bs}} = \Delta_0 \int \sum_{\alpha=1}^4 \psi_\alpha^+ \sigma_1 \psi_\alpha dx .
\] (3)

We emphasize that the backscattering \( \Delta_0 \) is not the usual interaction-induced \( V(2k_F) \) term (which is undetectably small in metallic NTs), but rather is present at the single-particle level [5, 11]: Depending on the tube chirality, the bare gap \( \Delta_0 \) can be in the range \( \Delta_0 \lesssim 10 \text{meV} \) to \( \sim 0.5 \text{eV} \); it can also be controlled by the parallel magnetic field [12]. Adding the periodic potential \( U(x) \) and the chemical potential \( \mu \) [\( \mu = 0 \) at half-filling] results in

\[
\mathcal{H}_{\text{ext}} = \int dx \rho(x) \{ U(x) - \mu \} ,
\] (4)

\[
U(x) = A \cos k_{\text{ext}} x , \quad k_{\text{ext}} = \frac{2\pi}{\lambda_{\text{ext}}} .
\] (5)

Qualitatively, our findings will be valid for any realistic potential which justifies the simplest choice (5): typically,
Bosonization of the nanotube electrons $\psi_\alpha = \frac{1}{\sqrt{2\pi}} e^{i\theta_\alpha}$ is exact even in the presence of (3). It maps the problem of the four interacting Dirac fermion modes onto the sine-Gordon model of the four coupled bose fields $\Theta_\alpha$. We rotate [4, 7] to the basis of the charge mode $\theta^0$ and three neutral modes $\theta^a$, in which case the charge density $\rho(x) = \frac{2}{\pi} \partial_x \theta^0$, and the Gaussian action (bosonized $H_0$) is diagonal $[\hbar = v = 1]$:

$$\mathcal{L}_0 = \frac{1}{2\pi} \int dx \left( (\partial_x \theta^0)^2 - K (\partial_x \theta^0)^2 + \sum_{a=1}^3 (\partial_x \theta^a)^2 \right).$$

The slow momentum dependence of the charge stiffness $K_k = 1 + 4\nu V(k)$, $\nu^{-1} = \pi \hbar v$, is irrelevant, and we take it as constant $K \equiv K_{k=1}/\hbar$, $l_{ch}$ being the size of the charged-mode soliton (described below). Assuming $l_{ch} \sim l_\theta$, with the screening length $l_\theta \sim 1 \mu m$, and using $e^2/\hbar v \approx 2.7$, one estimates $K \approx 40$ for the stand-alone tube; $K \approx 10$ if the tube is placed on a substrate with dielectric constant $\varepsilon \approx 10$. The logarithmic behavior of $V(k)$ underlies the fact that the Coulomb interaction $V(x) \propto 1/|x|$ is essentially zero in one dimension, $\frac{1}{2} \int dxdx' \rho(x)V(x-x')\rho(x') \approx \frac{\hbar^2}{4\pi} \int dx K(\partial_x \theta^0)^2$.

The nonlinear part of the sine-Gordon Lagrangian [coming from $H_{bs}$] reads [4, 7, 13]

$$\mathcal{L}_{bs} = - \int dx g_0 \mathcal{F}(\theta^0 + 2\mu k_{ext} x - 2\bar{A} \sin k_{ext} x, \theta^a),$$

$$\mathcal{F}(\theta^0, \theta^a) = \cos \theta^0 \cdot \prod_{a=1}^3 \cos \theta^a + \sin \theta^0 \cdot \prod_{a=1}^3 \sin \theta^a,$$

where $g_0 = 4\Delta_0/\pi D a^2$, and $D \approx \hbar v/\alpha$ is the 1d bandwidth. In Eq. (7) we included the coupling (4) to external fields by shifting the charge mode $\theta^0 \rightarrow \theta^0 - \frac{2\pi e}{\hbar \nu} \int_0^x K^{-1}(U-\mu) dx'$, with $\bar{\mu} \equiv \mu/(K_{\theta^0})$, $\bar{A} \equiv A/(K_{\theta^0})$, $\epsilon_0 \equiv \hbar k_{ext} v$.

In what follows, it is useful to first describe elementary excitations of the stand-alone tube, $U \equiv 0$. As shown by Levitov and Tsvelik [4], in the bosonized language adding one electron corresponds to a composite soliton of both the charge and the flavor modes. In such a composite object, the charge mode changes by $\pi/(2a)$ (adding unit charge) over the length $l_{ch}$, whereas the neutral sector adds a particular SU(4) flavor to the electron by means of the solitons of $\theta^a$ “switching” by $\pm \pi/2$ on a shorter scale $l_{fl} \sim K^{-1/2} l_{ch}$, right in the middle of the charge soliton. The composite soliton is a unit charge configuration of the minimal energy, obtained by optimizing the action $\mathcal{L}_0 + \mathcal{L}_{bs}$ in the limit of large Coulomb repulsion $K \gg 1$. Technically, such an optimization results in the soft neutral modes $\theta^a$ adjusting to create the effective potential $\mathcal{F}(\theta^0) = \min_{\theta^a} \mathcal{F}(\theta^a, \theta^0) \sim \cos 4\theta^0$ for the stiff charge mode $\theta^0$.

In the absence of external potential, $U \equiv 0$, the system $\mathcal{L}_0 + \mathcal{L}_{bs}$ describes the Wigner crystal - Luttinger liquid crossover. In particular, raising the chemical potential from half-filling [band insulator, or the “Dirac vacuum”] to just above the charge gap produces the train of weakly overlapping composite solitons described above [$\rho_{\theta} < 1$, “Wigner crystal”], in which overlapping charge solitons maintain a quasi-long-range order. Further increase of $\mu$ leads to strongly overlapping solitons rendering the nonlinear term (7) irrelevant [\rho_{\theta} > 1, Luttinger liquid]. We emphasize that the crystal - liquid crossover occurs due to the finite soliton size $l_\theta \propto \Delta_0^{-1}$ that scales inversely with the curvature of the dispersion. Curvature is also responsible for binding flavor to charge through the term (7). The $U \equiv 0$ system is compressible [4].

Periodic potential locks electrons into incompressible states. Technically, the term (7) becomes relevant whenever the density $2\bar{\mu} = \bar{m}$ [Eq. (1)] is integer [7]. When $m$ is a simple fraction, $2\bar{\mu} = p/q$, to identify incompressible states one utilizes the phase soliton method [6]. We generalize it for the case of the four nanotube modes by expanding in powers of the coupling $g_0$ as $\theta^a = \hat{\theta}^a + g_0 \theta^{(1)} + ... + g_0^j \theta^{(n)} + ...$, $j = 0, a$, and finding the effective Lagrangian $\mathcal{L}_m[\theta^0, \theta^a]$ for the phase modes $\theta^0, \theta^a$ constant in the commensurate phase, whereas an excitation is a composite phase soliton, in which the phase fields $\theta^0(x), \theta^a(x)$ describe a slow deformation of the regular commensurate configuration. Excitation gap is given by the energy of the composite soliton, renormalized by quantum fluctuations.

We note that it is the curvature $\propto \Delta_0$ that yields incompressible states. Same is true for the non-interacting electrons: When $\Delta_0 = 0$, the external potential is gauged away from the Hamiltonian $-i\hbar v \sigma_3 \partial_x U(x)$.

The composite phase soliton is a result of optimization of the corresponding effective action $\mathcal{L}_m[\theta^0, \theta^a]$ (examples of which are given below). This problem will be similar to the $U \equiv 0$ case described above: When interaction is strong, $K \gg 1$, the neutral phase modes $\theta^a$ adjust [on the scale $l_{fl}$] to create an effective potential for the charged phase mode $\theta^0$. The crucial difference from the former case is that this optimization will qualitatively depend on whether the system is in the regime of the Luttinger liquid or in that of the Wigner crystal. In this sense, periodic potential naturally distinguishes between the opposite sides of the crystal - liquid crossover, by bringing about the additional length scale, its period $\lambda_{ext}$. Technically, the saddle point of $\mathcal{L}_m$ will depend on whether the neutral modes are adiabatic or fast on the length scale on which the effective potential (7) changes appreciably. Below we consider both cases separately.

Bragg diffraction in a four-flavor Luttinger liquid.— In the adiabatic limit $l_{fl} \gg \lambda_{ext}$ of extended flavor excitations, exchange is important: The system (correlated over many $\lambda_{ext}$) “knows” that it is comprised of particles of the four different flavors. This limit is connected to the non-interacting case, where particles repel only due to the Pauli principle. For integer density $m$, averag-
\[ \Delta_m \equiv 2 \Delta_0 J_m (2 \hat{A}) \]
Fermi approximation \( \rho(x) \approx \rho_{TF}(x) \propto U(x) \) estimates the interaction energy inside each half-period (“quantum dot”) as \( \frac{e^2}{\hbar} \int dx dx' \frac{\rho_{TF}(x)\rho_{TF}(x')}{|x-x'|} \approx \frac{n^2 e^2}{2C_1} \), where the “dot capacitance” \( C_1 \approx \frac{2\pi m}{\hbar^2} \). In this limit, all the hexagon domains of the phase diagram become identical with the width \( e^2/C_1 \). Remarkably, this period asymptotically follows from Eq. (11) with \( A' \approx \frac{e^2}{\hbar} \). A near-by \( K = K_1/\lambda_{ext} \approx K = -1 \), using the Bessel function zeroes \( 2\hat{A}_{n_{tot}}^{(n)} \approx \frac{3\pi}{4} + \frac{\pi n}{2} + \pi n, n = \min\{n_e, n_h\} \). The borders between the domains correspond to the incompressible states with fractional \( n_e \) and \( n_h \) (not shown).

Quantized current.— The devil’s staircase can be mapped in the Thouless pump setup [7]. With the Fermi level in the gap, a slowly moving wave \( U(x-st) \) with the frequency \( f = s/\lambda_{ext} \) will generate the quantized current \( j = m_{tot}ef \). The moving potential can be created by gating, optical methods, or acoustic field. Estimated gap values \( \Delta_m \) in the meV range ensure adiabaticity leading to current quantization and possible metrological applications. Novel incompressible states with fractional \( m \) would correspond to the current quantized in the fractions of \( 4ef \), as illustrated in Fig. 1. Current changes sign at half-filling due to the Dirac symmetry.

Conclusions.— We demonstrated that coupling to a periodic potential results in the devil’s staircase of incompressible electron states. Excitation gaps are found in the limit of the narrow-gap Luttinger liquid and in that of the Wigner crystal, by selecting the saddle point of the nonlinear action of the four bosonic modes. When the Coulomb interaction dominates, the system behaves as a single fermion mode with renormalized mass and velocity. Control over the NT gap, the screening length, and the parameters of the potential makes this setup a unique probe of the Luttinger liquid - Wigner crystal crossover and of commensuration effects in 1d. Novel effect of adiabatic pumping at fractions of base frequency is linked to the interaction-induced incompressible states. The effective single-mode description could also rationalize recent manifestations of Wigner crystallization in transport, such as the \( e^2/h \) steps in conductance [15].

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