Quantum criticality in a Mott pn-junction in an armchair carbon nanotube

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In an armchair carbon nanotube pn junction the p- and n- regions are separated by a region of a Mott insulator, which can backscatter electrons only in pairs. We predict a quantum-critical behavior in such a pn junction. Depending on the junction’s built-in electric field \( E \), its conductance \( G \) scales either to zero or to the ideal value \( G = 4e^2/h \) as the temperature \( T \) is lowered. The two types of the \( G(T) \) dependence indicate the existence, at some special value of \( E \), of an intermediate quantum critical point with a finite conductance \( G < 4e^2/h \). This makes the pn junction drastically different from a simple barrier in a Luttinger liquid.

Transport measurements in carbon nanotube (CNT) devices reveal strongly correlated behavior of conduction electrons. Experiments on tunneling into single-wall CNT [1,2] or across a barrier interrupting a CNT [4] demonstrated a power law bias- and temperature-dependence of the current, consistent with a gapless excitation spectrum and Luttinger correlations of the electron liquid. Recent experiments [5] showed that armchair CNTs develop a gap in the spectrum of charge excitations at zero doping. The gap formation could be attributed to the electron Umklapp processes [5,6], which back-scatter pairs of electrons. These processes drive armchair CNTs into the Mott-insulating state. In contrast, undoped semiconducting CNTs are simple band insulators. Although Mott and band insulators are qualitatively different, no clear experimental signature of that dichotomy has been observed in CNTs.

In this Letter we predict that the difference should manifest itself in the conduction of a pn junction formed by bipolar doping of a CNT. In contrast to a simple “band” pn junction, in which the barrier between the p- and n- regions is formed by a band insulator, a “Mott” pn junction formed in a pristine armchair CNT does not back-scatter single electrons. However, the Umklapp backscattering of pairs of electrons remains effective near its center. In short junctions these processes are irrelevant and do not alter the perfect zero-temperature conductance \( (G = 4e^2/h) \). In longer junctions, Umklapp processes bring about the Mott-insulator state and drive the zero-temperature conductance to zero. The gap formation could be attributed to the electron Umklapp processes [4,5], which back-scatter pairs of electrons. These processes drive armchair CNTs into the Mott-insulating state. In contrast, undoped semiconducting CNTs are simple band insulators.

We consider a single pn-junction that is formed by a static potential \( U(x) \) imposed by two gates, as in Fig. 1(b). In the p- and n- regions \( U(x) \) saturates to \( \pm U_0 \). The electron wave functions in the intersecting bands have opposite parity and do not break the symmetry between the A and B sublattices [7]. We assume that \( U(x) \) is smooth on the interatomic scale and does not make detailed predictions for the \( G(T, E) \) dependence in the vicinity of the quantum phase transition.

FIG. 1: (a) Electron spectrum near the Dirac points \( \alpha = \pm 1 \) (+ or − indicates parity). (b) Near \( x = 0 \) the gate potential is \( U(x) \approx -eEx \) and saturates to \( \pm U_0 \) in the p- and n- regions. (c) Schematic picture of the conductance dependence on \( E \) at different temperatures. The \( G(E) \) curves at different temperatures intersect at the fixed point and increase monotonically with \( E \). The step in \( G(E) \) at \( T = 0 \), indicates a quantum phase transition. (d) RG flow for the conductance.

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mode velocities are absent, and we may write the noninteracting part of the electron Hamiltonian as
\[
H_0 = \sum_{\alpha, \sigma} \int dx \psi_{\alpha \sigma}^+(x) [-i \varepsilon \partial_x + U(x)] \psi_{\alpha \sigma}(x).
\]
Here \(\varepsilon \approx 8 \times 10^5\) m/s is the Fermi velocity, \(\alpha = \pm\) is the valley index, \(\sigma = \pm\) labels left and right movers, and \(\sigma\) the electron spin.

We assume that the number of unit cells \(N\) around the circumference of an \((N, N)\) armchair interaction CNT is large. To zeroth order in \(1/N\) the Coulomb interaction of electron-electron (e-e) backscattering is absent. The forward scattering part of the e-e interactions is,
\[
V_f = \frac{V(0)}{2} \int dx n(x); \quad n(x) = \sum_{\alpha, \sigma} \psi_{\alpha \sigma}^+(x) \psi_{\alpha \sigma}(x).
\]
Here \(\varepsilon \approx 2e^2 \ln(d/R)\) is the forward scattering matrix element (we assume that the Coulomb interaction is screened by the gate at a distance \(d\) from the CNT).

The gate potential \(U(x)\) results in a position-dependent doping density characterized by the Fermi wave vector \(k_F(x) \sim -U(x)/\varepsilon\). We can bosonize the electron operators by the standard procedure\[9\]
\[
\psi_{\alpha \sigma}(x) = \frac{F_{\alpha \sigma}}{\sqrt{2 \pi \xi}} e^{i [\int \kappa_0(x') dx' + \Phi_{\alpha \sigma}(x)]} e^{i \Theta_{\alpha \sigma}(x)}.
\]
Here \(\xi \sim R\) is the short distance cutoff, \(F_{\alpha \sigma}\) are Klein factors. The bosonic fields \(\Phi\) and \(\Theta\) obey the standard commutation relations\[9\]\[
[\Phi_{\alpha \sigma}(x), \Theta_{\alpha' \sigma'}(x')] = -i \pi \delta_{\alpha \alpha'} \delta_{\sigma \sigma'} \delta(x - x').
\]
In the bosonic representation the electron density is\[9\]
\[
u(x) = 4k_F(x)/\pi - \sum_{\alpha, \sigma} \partial_x \Phi_{\alpha \sigma}(x)/\pi \quad \text{and the forward scattering part of the Hamiltonian} \quad H_f \equiv H_0 + V_f \quad \text{reduces to the same form as in a uniform CNTs}[10].
\]
\[
H_f = \int \frac{dx}{2\pi} \sum_j u_j \left[ K_j (\partial_x \Theta_j)^2 + (\partial_x \Phi_j)^2 / K_j \right].
\]
Here \(j = c\pm, s\pm\) labels charge \((c)\) and spin \((s)\) modes that are symmetric \((+\)\) or antisymmetric \((-\)\) in the valley index \(\alpha\). They are related to the fields \(\Phi_{\alpha \sigma}\) by \(\Phi_{\alpha \sigma} = (\Phi_{\alpha + c} + \alpha \Phi_{\alpha - c} + \sigma \Phi_{\alpha + s} + \sigma \Phi_{\alpha - s})/2\). Only the \(c+\) mode carries charge and the other three are neutral. The mode velocities are \(u_j = v_F/K_j\), where the Luttinger parameters are \(K_{c+} = 1/\sqrt{1 + 4v_F^2/\pi v_F} \ll 1\) and \(K_j = 1\) for the neutral modes.

Backscattering interactions are small in \(1/N\)\[8\], and may be treated as perturbations to the Hamiltonian\[2]. Some of them are relevant and qualitatively change the low energy physics. The most relevant backscattering interaction corresponds to the so-called Umklapp processes, which scatter two right-movers into left-moving states or vice-versa\[4\][10]. In the presence of doping the Umklapp Hamiltonian can be written as\[8\]
\[
H_U = -\int \frac{dx}{2\pi \xi^2} \cos\left(2\Phi_{c+}(x) - 4 \int_0^x k_F(y) dy \right) \times \\
\{g_3 \cos[2\Theta_{c-}(x)] + (g_3 - g_1) \cos[2\Phi_{c+}(x)] \}
\]
\[
g_1 \cos[2\Phi_{c-}(x)] - \cos[2\Phi_{c+}(x)] \}.
\]
Here the coupling constants \(g_1\) and \(g_3\) are of order \(e^2/\pi\) and \(g_3 > g_1\). The low energy electron Hamiltonian of the pn-junction is given by the sum of Eqs.\[8\] and \(\ref{eq:4}\),
\[
H = H_f + H_U.
\]
The position-dependent Fermi vector \(k_F(x)\) in Eq.\[3\] saturates to constant values \(\pm k_0\) in the n- and p- regions whereas near \(x = 0\) it has a linear dependence of \(x\),
\[
k_F(x) = -x/L_E^\perp.
\]
The length scale \(L_E\) is defined by the built-in electric field \(E\) controlled by the gate voltages, \(L_E \sim \sqrt{\varepsilon/\pi E}\).

Relating the current operator to charge field as \(j = -2e\partial_t \Phi_{c+}(x = 0, t)/\pi\) and using the Kubo formula we can express the device conductance as\[8\]
\[
G = i \frac{8e^2}{\pi \hbar} \lim_{\omega \to 0} \omega \mathcal{G}_\omega(0, 0).
\]
Here \(\mathcal{G}_\omega(x, x')\) is the retarded Green’s function of the charge field, \(\mathcal{G}_\omega(x, x') = -i \int_0^\infty dt e^{i\omega t} \langle \hat{\mathcal{G}}_{c+}(x, t, \Phi_{c+}(x', 0)) \rangle\).

In the absence of Umklapp interactions evaluation of the Green’s function is straightforward and gives
\[
\mathcal{G}_\omega^0(x, x') = -i \pi (K_{c+}/2\omega_+) e^{i\omega_+|x-x'|/u_{c+}},
\]
where \(\omega_+ = \omega + i\eta\). When substituting this expression into Eq.\[8\] it should be born in mind that the dc conductance is controlled by the leads, where LL effects are absent. Thus the Luttinger parameter should be set to unity, \(K_{c+} \to 1\)\[11\], yielding \(G_0 = 4e^2/h\).

The Umklapp processes degrade electric current by backscattering pairs of electrons and thus decrease the device conductance. They are most effective near the zero doping point \(x = 0\) and strongly suppressed deep in the p- and n- regions. At low temperatures, \(T \ll v_Fk_0\), the Umklapp backscattering in the p- and n- regions result in exponentially small \(\sim \exp(-2v_Fk_0/T)\) resistivity. We assume that the length of the p- and n- regions is not sufficient to compensate for this exponential smallness and neglect this contribution. In this approximation backscattering arises from the spatial region \(|x| \lesssim T/\varepsilon E\), where \(|k_F(x)| \lesssim T/\varepsilon E\). At \(T \ll U_0\) the spatial dependence of \(k_F(x)\) in this region is linear. Therefore the pn-junction may be modeled by the Hamiltonian\[4\] with \(k_F(x)\) given by Eq.\[8\] in the entire space.
Spatial localization of backscattering enables us to express Green’s function of the charge mode as

\[ G_\omega(0,0) = G_\omega^0(0) + G_\omega^0(0) \int_{-\infty}^{\infty} dx dx' T_\omega(x,x') G_\omega^0(0). \]  

(8)

Here \( T_\omega(x,x') \) is the part of the T-matrix that corresponds to scattering of a plasmon into a single plasmon. Using Wick’s theorem (c.f. Appendix A of Ref. [12]) one can show that it can be expressed as

\[ T_\omega(x,x') = -i \int_0^\infty dt e^{i \omega t} \langle [\partial_\theta \mathcal{H}_U(x,t), \partial_\theta \mathcal{H}_U(x',0)] \rangle + \delta(x - x') \langle \partial_\theta^2 \mathcal{H}_U(x) \rangle, \]

(9)

where \( \mathcal{H}_U(x,t) \) is the Umklapp Hamiltonian density and \( \partial_\theta \) denotes a partial derivative with respect to \( \Phi \).

In the low frequency limit needed for evaluating the dc conductance the unperturbed Green’s functions \( G_\omega^0 \) in Eq. (8) are given by Eq. (7) with \( K_\omega \)

\[ K \]

value, 4\( L \), because of localization of backscattering \( \ll \) contrast to a

The T-matrix properties are dominated by the fluctuations of bosonic modes with frequencies on the order of the temperature \( T \) and characteristic spatial scale of \( L_T \approx v_F / T \). Provided the device length is longer than \( L_T \) the T-matrix needs to be evaluated using the Hamiltonian \( \mathcal{H}_U \) with the values of the Luttinger parameters corresponding to the device interior.

The energy gap \( \Delta \sim (v_F / \xi)(g_3/v_F)^{1-K_{c+}} \)

induced by the Umklapp interaction in a uniform CNT at zero
doping defines an additional characteristic length scale, \( \zeta = v_F / \Delta \). Backscattering at the pn-junction is weak for \( L_E \ll \zeta \) and strong for \( L_E \gg \zeta \).

For \( L_E \ll \zeta \) the correction to the ideal conductance may be expanded in perturbation series in \( H_U \), Eq. (9).

Using Eqs. (10), (9) we get to second order in \( H_U \), \( \delta G^{(2)} = -c(2\pi T \xi / u_{c+})^{2K_{c+}}(L_E / \xi)^2(3g_1^2 - 2g_1g_3 + 2g_3^2) / v_F^2 \)

where \( c = (e^2 / h)B(K_{c+} + 1, K_{c+} + 1) / 2\pi \), with \( B(x, y) \) being the Euler Beta function. This result may be rewritten as

\[ \delta G^{(2)} \sim (e^2 / h) (L_E / \zeta)^2 (T / \Delta)^{2K_{c+}}. \]

It vanishes at \( T \rightarrow 0 \), which corresponds to irrelevance of point-like Umklapp scattering in the renormalization group (RG) sense.

Although higher order terms in perturbation theory are smaller in powers of \( L_E / \zeta \) they have different temperature dependence. In the fourth order correction to the ideal conductance the most relevant term is \( \delta G^{(4)} \sim -c(e^2 / h)(L_E / \zeta)^4 (T / \Delta)^{8K_{c+} - 2}. \)

This result can also be obtained using the following RG considerations. Because of localization of backscattering to the the region of size \( |x| \leq L_E \) at low temperatures, \( T \ll v_F / L_E \), the pn-junction acts as a point scatterer. In contrast to a potential point scatter \[ \xi \] the point-scatter can only scatter pairs of electrons. The Umklapp scattering may be described by an effective “impurity” Hamiltonian \( \mathcal{H}_I \sim L_E \mathcal{H}_2(0) \). Upon reduction of the energy band width, \( \lambda_0 \sim v_F / \xi \rightarrow \Lambda = \lambda_0 e^{-1} \), new operators are generated in the effective Hamiltonian of the barrier. They have the form of higher powers of \( \mathcal{H}_2 \). The most relevant of those is \( \mathcal{H}_4 \sim (4\Phi_{\text{ext}}(0)) \), with the scaling dimension \( 4K_{c+} - 1 \). The correction \( \delta G^{(4)} \) can be obtained by the lowest order perturbation theory in \( \mathcal{H}_4 \), \( \delta G^{(4)} \sim (e^2 / h) \int dt \langle [\mathcal{H}_4(t), \mathcal{H}_2(0)] \rangle \propto T^{8K_{c+} - 2}. \)

For \( K_{c+} < 1 / 4 \) the \( \mathcal{H}_4 \) is relevant and \( \delta G^{(4)} \) diverges at zero temperature. The RG fixed point (FP) at perfect transmission is unstable, and the system flows to strong backscattering even at \( L_E \ll \zeta \). We show below that the strong backscattering FP is stable. The expected RG flow is as shown in Fig. (d). It corresponds to vanishing zero temperature conductance. We note that the temperature dependence of conductance is nonmonotonic. In the regime of applicability of perturbation theory \( \delta G = -a(L_E / \zeta)^2 (T / \Delta)^{2K_{c+}} - b(L_E / \zeta)^4 (T / \Delta)^{8K_{c+} - 2} \)

where \( a \) and \( b \) are constants on the order of \( e^2 / h \). The maximum conductance is reached at \( T \sim \Delta (L_E / \zeta)^{1/(1-3K_{c+})} \).

Because of the large value of the interaction constant, \( e^2 / v_F \approx 2.7 \) and the sensitivity of the forward scattering matrix element \( V(0) \) to screening by the gates both cases \( K_{c+} < 1 / 4 \) and \( K_{c+} > 1 / 4 \) may be realized.

For \( K_{c+} > 1 / 4 \) all backscattering operators generated in the process of renormalization are irrelevant. Therefore the FP at perfect transmission is stable for weak backscattering, \( L_E \ll \zeta \). At the same time, the analysis below shows that a perfect reflection fixed point is stable at \( K_{c+} < 1 \). This indicates the existence at \( 1 / 4 < K_{c+} < 1 \) of a quantum phase transition in the conductance of pn-junction, controlled by the ratio \( L_E / \zeta \).

At strong backscattering, \( L_E \gg \zeta \), the pn-junction may be viewed as two semi-infinite Luttinger liquids separated by a strong barrier where the bosonic fields are pinned to one of the classical minima of the Umklapp Hamiltonian. The minima form a periodic lattice in the four-dimensional space \( \Phi = \pi n_j / 2 \), with \( n_j \) are integers, which are either all even or all odd. Charge transport between the p- and n-regions proceeds via tunneling between different points in the lattice [14]. The tunneling operator corresponding to the shift \( \{ n_j \} \rightarrow \{ n_j + \delta n_j \} \) is

\[ \exp(i \sum_j [\theta_j(x_1) - \theta_j(x_2)] [\delta n_j / 2]) \]

where \( x_1 \) and \( x_2 \) label the points just to the left and to the right of the barrier. Its scaling dimension is \( 1 - \sum_j (\delta n_j)^2 / (4K_{c+}) \). The operators that transfer charge across the junction must have nonzero \( \delta n_{c+} \). For \( K_{c+} < 1 \) all of them are irrelevant, and thus the zero temperature conductance vanishes.

The stable FPs at perfect transmission and reflection for \( 1 / 4 < K_{c+} < 1 \) must be separated by an unstable FP with an intermediate value of zero temperature conductance. The pn-junction can be tunned to this FP by adjusting the parameter \( L_E \). The dependence of conductance on \( L_E \) at low temperature is schematically pre-
sented in Fig. 1(c). The critical conductance and critical exponents at the intermediate fixed point depend on the values of the Luttinger parameters \( K_j \).

To analyze the intermediate FP near \( K_{c+} = 1/4 \) we note that only two of the operators generated in the course of renormalization have scaling dimensions that are reasonably small: \( H_4 \) and \( H_U \) (respective scaling dimensions \( 4K_{c+} - 1 \) and \( K_{c+} \)). All other operators are strongly irrelevant. The proximity of the values of \( K_{c+} \) corresponding to marginality of \( H_U \) and \( H_4 \) (\( K_{c+} = 0 \), and \( K_{c+} = 1/4 \)) enables one to use a kind of \( \epsilon \)-expansion in which both \( \epsilon = K_{c+} \) and \( \epsilon_4 = K_{c+} - 1/4 \) are assumed small. In this case the intermediate FP is perturbatively accessible. Writing the effective pinning Hamiltonian as \( H_{eff} = \Lambda r_4 \cos(4\Phi_4 + \cos(2\Phi_4)\sum_a r_a \cos(2\phi_a)) \), where \( r_4, r_a \) are dimensionless amplitudes and \( a \) labels the neutral modes, we obtain the RG equations to leading order in \( \epsilon, \epsilon_4 \),

\[
d r_r a = -\epsilon a + r a r_4, \quad (11a)
\]

\[
d r_r a = -4\epsilon_4 r_4 + \sum a r_a^2/4, \quad (11b)
\]

where \( d_i = d/dl \). The intermediate FP exists for \( \epsilon_4 > 0 \) and is located at \( r_4 = \epsilon \), \( \epsilon_4 = 16\epsilon_4 \epsilon \). The FP conductance can be found by using lowest order perturbation theory with FP values of the reflection amplitudes \([13] \), \( G^* = 4(\epsilon^2/h)(1 - \epsilon_4 - \epsilon^2/32\epsilon_4) \). The presence of the \( \epsilon_4 \) in the denominator in the last term signals that Eq. (11) is valid provided \( \epsilon_4 \gg \epsilon^2 \). Near the FP the conductance behaves as \( G(T) - G^* \sim -\epsilon^2/h(1 - L_E/L_{E}^*) T/\xi(T/E) \), where \( \lambda = -2\epsilon_4 + 2\sqrt{\epsilon_4^2 + 2\epsilon_4} \). A similar analysis in the limiting case of \( 1 - K_{c+} = \eta \to 0 \), gives the intermediate FP conductance \( G^* \propto \eta^2 \). Interpolation between these two limiting cases gives the RG flow shown in Fig. 1(d).

The above picture is modified if single-electron backscattering is present. In a symmetric armchair CNT it can be caused by a magnetic field \( B \) applied along the CNT axis or by the electron-phonon (ep) interactions. The corresponding backscattering Hamiltonian may be written as \([15] [17] \)

\[
\delta H = -i \int dx \sum_{\alpha \sigma} \hat{\psi}_{\alpha \sigma}(x) \hat{\psi}_{-\alpha \sigma} r[\alpha \Delta_u(x) + \Delta_B], \quad (12)
\]

where \( \Delta_B \) and \( \Delta_u \) are respectively the gaps induced in the single particle spectrum by the magnetic field, \( \Delta_B = (\pi/2)cBv_F R \), and by the lattice deformation. At low temperatures only the twist acoustic (TA) phonons are important and \( \Delta_u(x) = g_T \partial_x u(x) \), where \( u(x) \) is the TA mode displacement and \( g_T \sim 1/\sqrt{N} \ll 1 \) is the corresponding coupling constant. As in the case of two-particle processes, single electron backscattering is effective only in the vicinity of the pn-junction, \( |x| \lesssim L_E \). The zero-transmission FP is stable with respect to single electron backscattering.

For \( L_E \ll \zeta \) and at small \( B \) and \( g_T \) the stability of the FP at perfect transmission with respect to single particle backscattering may be examined by perturbation theory. Bosonizing the fermion operators in Eq. (12) as in Eq. (1) we find the lowest order correction \( \delta G \sim -(\epsilon^2/h)[(L_E/\zeta)^2(f_2/p_2)^2(\xi(T/v_F)^{1+K_{c+}}/2 + (L_E \Delta_B/v_F)^2(\nu_F T/E)(K_{c+} - 1/2)]. \quad (12) \) Here \( \rho \) is the mass per unit length of the CNT and \( s_F \) is the speed of sound for the TA mode \([16] \). The temperature dependence of the two terms here shows the stability of the perfect transmission FP with respect to the ep backscattering and its instability with respect to \( B \neq 0 \).

Combining the stability analysis of the perfect transmission and perfect reflection FPs we conclude that the intermediate FP is not destroyed by the ep interactions. However application of a magnetic field drives the zero temperature conductance of the junction to zero. This reveals that magnetoresistance of a CNT pn-junction \([18] \) is strongly enhanced by the Luttinger liquid effects.

In conclusion, the Mott-insulating state of an armchair CNT should manifest itself in the dependence of the pn junction conductance \( G \) on the temperature \( T \) and built-in electric field \( E \). In a broad range of parameters, the \( G(T, E) \) dependence is controlled by a \( T = 0 \) quantum phase transition occurring at some value of \( E = E^* \). The critical behavior of \( G(T, E) \) is controlled by an unstable fixed point with conductance \( G^* < 4\epsilon^2/h \). That suggests the possibility of the scaling analysis of experimental data used in investigations of quantum phase transitions \([19] \).

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