Impurity pinning in transport through 1D Mott-Hubbard and spin gap insulators.

V.V. Ponomarenko* and N. Nagaosa
Department of Applied Physics, University of Tokyo, Bunkyo-ku, Tokyo 113, Japan
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A low energy crossover \( \Gamma \) induced by Fermi liquid reservoirs in transport through a 1D Mott-Hubbard insulator of finite length \( L \) is examined in the presence of impurity pinning. Under the assumption that the Hubbard gap \( 2M \) is large enough: \( M > T_L \equiv v_c/L \) (\( v_c \): charge velocity in the wire) and the impurity backscattering rate \( \Gamma_1 \ll T_L \), the conductance vs. voltage/temperature displays a zero-energy resonance. Transport through a spin gapped 1D system is also described availing of duality between the backscattered current of this system and the direct current of the Mott-Hubbard insulator.

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Recent developments in the nano-fabrication technique have allowed to produce relatively clean one channel wires of \( 1−10 \mu m \) length. In these wires, 1D Tomonaga-Luttinger Liquid (TLL) behavior \( \Gamma \) was observed in transport measurements \( \Gamma \). Then it has been suggested that the correlated insulating behavior may be tuned with this setup \( \Gamma \). This behavior of the 1D electron systems is expected \( \Gamma \) at half-filling where any Umklapp scattering has to open a Hubbard gap \( 2M \) in the charge mode spectrum of the infinite wire if the forward scattering is repulsive. Earlier consideration \( \Gamma \) predicted crossover from Fermi liquid to that of a Mott-Hubbard insulator in the one channel wire of long enough length: \( M > T_L \equiv v_c/L \) (\( v_c \): charge velocity in the wire). Charge in this insulator is carried by soliton excitations of the condensate emerging in the charge mode. This insulator, which is probably the easiest for the experimental observation, features two marginal quantities \( \Gamma \): charge of the soliton is unchanged \( e \) (\( e = \hbar = 1 \) below) and the exponent \( 1/2 \) characterizing the electron-soliton transition brings about similarity with the free electron tunneling through a resonant level.

In this paper we investigate the effect of impurity backscattering of low rate \( \Gamma_1 \ll M \) on the above crossover. For low energy following Schmid \( \Gamma \) the problem is mapped through a Duality Transform onto the model of a point scatterer with pseudospin imbedded in TLL. It is solved exactly by fermionization. The result shows that the impurity enlarges the width of a zero energy resonance in the conductance up to \( \Gamma_1 + \Gamma_2 \) where the exponentially small \( \Gamma_2 \) \( \Gamma_2 \approx \sqrt{T_L M e^{-2M/T_L}} \) is the rate of tunneling of the condensate phase. The linear bias conductance at zero temperature \( G = \frac{1}{\hbar e (\Gamma_1 + \Gamma_2)} \) reveals an exponential enhancement of the amplitude of the impurity potential \( \sqrt{\Gamma_1/\Gamma_2} \) by the condensate tunneling. This suppression of the resonant conductance does not affect the saturation of the current at \( J = \Gamma_2 \) above the crossover as far as \( \Gamma_1 + \Gamma_2 \ll T_L \). Finally, the result is addressed to the case when the gap opens in the spin mode of the wire. It occurs if the effective interaction between electrons inside the wire is attractive \( \Gamma \). Although it is not expected for the semiconductor nanostructure, it has been observed in quasi 1D organics \( \Gamma \). The current backscattering in this system coincides with the direct one of the Mott-Hubbard insulator multiplied by a factor \( \frac{\Gamma_1}{\Gamma_2} \), where \( \Gamma_1 \) has the same meaning for this system as \( \Gamma_1 \) above. So, the backscattering current is zero in the absence of impurities, and the current is maximum \( V/\pi \). Impurity appearance gives rise to backscattering together with simultaneous tunneling between the spin mode vacua of the wire. The conductance is suppressed below a crossover energy and recovers above it. It results in a constant shift \( \Delta J = -\Gamma_1 \) of the current at high voltage.

Transport through a 1D channel wire confined between two leads could be modeled by a 1D system of electrons whose pairwise interaction is local and switched off outside the finite length of the wire. Applying bosonization and spin-charge separation we can describe the charge and spin density fluctuations \( \rho_b(x, t) = \left< \phi_b(x, t) \right>/\sqrt{2\pi} \), \( b = c, s \), respectively, with (charge and spin) bosonic fields \( \phi_{c,s} \). Without impurities their Lagrangian symmetrical under the spin rotation reads

\[
\mathcal{L} = \int dx \sum_{b=c,s} \frac{v_b(x)}{2g_b} \left\{ \frac{1}{v_F} \left( \frac{\partial \phi_b(t, x)}{\sqrt{4\pi}} \right)^2 - \left( \frac{\partial_c \phi_b(t, x)}{\sqrt{4\pi}} \right)^2 \right\} - E_b^2 U_b \frac{\varphi(x)}{\pi v_F} \cos \left( \frac{2\mu_b}{v_F} x + \sqrt{2} \phi_c(t, x) \right)
\]

where \( \varphi(x) = \theta(x)\theta(L - x) \) specifies one channel wire of the length \( L \) adiabatically attached to the leads \( x > L, x < 0 \), and \( v_F(E_F) \) denotes the Fermi velocity (energy) in the channel. The parameter \( \mu_c \equiv \mu \) varies the chemical potential inside the wire from its zero value at half-filling and \( \mu_s = 0 \). The constants of the forward
scattering differ inside the wire $g_b(x) = g_b$ for $x \in [0, L]$ from those in the leads $g_b(x) = 1$, and an Umklapp scattering (backscattering) of the strength $U_{c,s}(U_s)$ is introduced inside the wire. The velocities $v_{c,s}(x)$ change from $v_F$ outside the wire to some constants $v_{c,s}$ inside it. We can eliminate them rescaling the spacial coordinate $x_{old}$ in the charge and spin Lagrangians of (1) into $x_{new} \equiv \int_0^{x_{old}} dy/v_{c,s}(y)$. As a result, the new coordinate will have an inverse energy dimension and the length of the wire becomes different for the charge mode $L \rightarrow 1/T_L$ and spin mode $L \rightarrow 1/T'_L$. Applying renormalization-group results of the uniform sin-Gordon model at energies larger than $T_L$ or $T'_L$ we come to the renormalized coordinates in (2). For the repulsive interaction initially $g_s > 1 > g_c$, the constant $U_s$ of backscattering flows to zero and $g_s$ to 1, bringing the spin mode into the regime of the free TLL. The constant $U_c$ of Umklapp process increases, reaching the free fermion value $M$ from $\text{Umklapp process}$ increases, reaching the free fermion value $M$ from $\text{Umklapp process}$ increases, reaching the free fermion value $M$ from $\text{Umklapp process}$ increases, reaching the free fermion value $M$ from $\text{Umklapp process}$ increases, reaching the free fermion value $M$.

For the attractive interaction initially $g_s < 1 < g_c$, both constants $U_{c,s}$ flow vice versa resulting in the spin gap insulator and TLL of some $g_c > 1$ in the charge mode. Both cases of the interaction remain to some extent symmetrically conjugated under the spin-charge exchange even after accounting for a weak backscattering on a point impurity potential inside the wire $0 < x_0 < L$:

$$L_{\text{imp}} = -\frac{2V_{\text{imp}}}{\pi \alpha} \cos(\phi_c(t, x) + \varphi_0) \cos(\phi_s(t, x_0) / \sqrt{2})$$

where $x_{c,s} = x_0 / v_{c,s}$, $\varphi_0 \equiv \varphi + \mu x_c$ includes a phase of the scatterer $\varphi$. The amplitude of the potential $V_{\text{imp}}$ specifies transmittance coefficient $\tilde{\alpha}_s$ as $1 / (1 + V_{\text{imp}}^2)$, and $\alpha \simeq 1 / E_F$ is momentum cut-off assumed to be determined by the Fermi energy. Below we will first elaborate the case of the Mott-Hubbard insulator adjusting results to the transport through the spin gap insulator at the end.

**Duality Transform** - An effective model for energies lower than some cut-off $D'$ specified below may be read off following Schmid from the expression for the partition function $Z$ associated to the Lagrangian plus. Without impurities the spin and charge modes are decoupled. After integrating out $\phi_c$ in the reservoirs the charge mode contribution into $Z$ describes rare tunneling between neighbor degenerate vacua of the massive charge mode in the wire characterized by the quantized values of $\sqrt{2} \phi_c(\tau, x) + 2 \mu x = M \sin \omega_x (\mu < M)$ with the pre-factor $P$ and the energy cut-off $D'$ proportional to $T_L$ on approaching the perturbative regime $T_L \sim M$. The calculation by instanton techniques has corrected $P = C \times \sqrt{D'/\sin^3 \omega x T_L}!^3$ with the constant $C$ of the order of 1. The parameter $D'$ is a high-energy cut-off to the long-time asymptotics of the kink-kink interaction: $F(\tau) = \ln \left( \sqrt{\tau^2 + 1 / D'^2} \right)$ created by the reservoirs. It varies with $\mu < D' \sim \sqrt{M T_L}$ at $\mu = 0$ to $D' \simeq (M/\mu) T_L$ if $\mu > T_L$. A crucial modification to this consideration produced by the impurity under the assumption $E_F V_{\text{imp}} \ll M$ ensues from the shift of the $m$-vacuum. Since it is equal to $(-1)^m \frac{2V_{\text{imp}}}{\pi \alpha} \cos \phi \cos(\phi / \sqrt{2})$ the neighbor vacua become non-degenerate. This can be accounted for by assigning opposite values of the pseudospin variable $\sigma = \pm 1$ to the neighbor vacua which are the eigenvalues of the third component of the Pauli matrix $\sigma_3$. The energy splitting becomes an operator $\sigma_3 2V_{\text{imp}} / \pi \alpha \cos \phi \cos(\phi / \sqrt{2})$ acting on the pseudospins, and every (anti-)instanton tunneling rotates a $\sigma_3$-value into its opposite with the Pauli matrix $\sigma_1$. The partial function then can be written as

$$Z \propto \sum_{N=0}^{\infty} \sum_{\alpha_j=\pm} \int D\phi \frac{e^{-S_0[\phi]}}{N!} T_{\tau, \sigma} \left\{ \int dt \prod_{i=1}^{N} P e^{-s_0 / \tau L \sigma_1(t_i)} \right\} \times \exp \left( \sum_{i,j} \frac{\alpha_i \alpha_j}{2} F(\tau_i - \tau_j) + \frac{2 \cos \phi V_{\text{imp}}}{\pi \alpha} \right) \right) \left( \int d \tau \sigma_3(\tau) \cos \left( \frac{\phi / \sqrt{2}}{\sqrt{2}} \right) \right)$$

Here $S_0[\phi] = \int_0^\beta d\tau \int dx \left( (\partial_\tau \phi_s(\tau, x))^2 + (\partial_\tau \phi_s(\tau, x))^2 / (8\pi) \right)$ is the free TLL Euclidean action. All $\tau$-integrals run from 0 to inverse temperature $\beta = 1 / T$ and $\sum_j a_j = 0$. To have all $\sigma_1, \sigma_3$-matrices time-ordered under the sign $T$, we attributed each of them to a corresponding time $\tau$ assuming that their time evolu-

\[ \text{tation is trivial. Noticing that the interaction } F \text{ coincides with the pair correlator of some bosonic field } \theta_c \text{ whose evolution is described with the free TLL action } S_0[\theta_c], \text{ we re-write (3) ascribing a factor } \exp(\mp \theta_c(\tau_j, 0) / \sqrt{2}) \text{ to the } \tau_j \text{ (anti-)instanton, respectively:} \]

\[ \int d \tau \sigma_3(\tau) \cos \left( \frac{\phi / \sqrt{2}}{\sqrt{2}} \right) \]
\[ Z \propto \text{Tr}_V \left\{ \int D\phi_s D\theta_s e^{\mathcal{L}} - \mathcal{S}_0[\phi_s] - \mathcal{S}_0[\theta_s] + 2 \int d\tau [Pe^{-\frac{\pi}{2} \sigma_1(\tau) \cos(\frac{\phi_s(\tau,0)}{\sqrt{2}})} + \cos \varphi V_{\text{imp}} \sigma_3(\tau) \cos(\frac{\phi_s(\tau,x_s)}{\sqrt{2}})] \right\} \]

(4)

It is easy to recognize a standard Hamiltonian form

\[ \mathcal{H} = \mathcal{H}_0[\phi_s(x)] + \mathcal{H}_0[\theta_s(x)] - 2Pe^{-\sigma_0/T_L} \sigma_1 \cos(\theta_s(0)/\sqrt{2}) - \frac{2V_{\text{imp}}}{\pi} \cos(\varphi) \sigma_3 \cos(\frac{\phi_s(x_s)}{\sqrt{2}}) \]

(5)

Here \( \phi_s(x) \) and \( \theta_s(x) \) are Schrödinger’s bosonic operators related to the variables \( \phi_s(\tau,x) \) and \( \theta_s(\tau,x) \) of the functional integration in (4). The operator \( \mathcal{H}_0[\phi_s(x)] \) (\( \mathcal{H}_0[\theta_s(x)] \), \( \mathcal{H}_0[\phi_s(x)] \) \( \mathcal{H}_0[\theta_s(x)] \)), a function of the field \( \phi_s(x) \) \( \theta_s(x) \) and its conjugate is a free TLL Hamiltonian \( \langle g = 1 \rangle \) corresponding to the free TLL action \( \mathcal{S}_0[\phi_s] \) \( \mathcal{S}_0[\theta_s] \) in (4), respectively. The Dual model specified by (4) is equivalent to the initial one (3) at low energy. It relates to a Point Scatterer with internal degree of freedom in TLL. Fortunately, this in general rather complicated model may be solved easily through fermionization in our particular case. This simplification stems from the marginal behavior of the Mott-Hubbard insulator: the charge of the transport carriers does not change on passing from the low energies to the higher ones despite the nature of the carriers does.

Fermionization - From the commutation relations and hermiticity, the Pauli matrices can be written as \( \sigma_\alpha = (-1)^{\alpha+1} \sum_\beta \gamma e^{\alpha,\beta} \xi_\beta \xi_\gamma \) with Majorana fermions \( \xi_1,2,3 \) and antisymmetrical tensor \( \epsilon : \epsilon^{123} = 1 \). Since the interaction in (4) is point-like localized and its evolution involves only the appropriate time-dependent correlators,

\[ \mathcal{L}_F = i\xi \partial_t \psi_c(t) + \sum_{a,c,s} \int dx \psi_c^\dagger(\partial_t + \partial_x) \psi_s - \sqrt{\Gamma_1} [\psi_c^\dagger(0,t) \epsilon e^{-iVt} + h.c.] - \sqrt{\Gamma_2} [\psi_c^\dagger(0,t) \epsilon e^{-iVt} + h.c.] \]

(6)

where the rate of impurity scattering is \( \Gamma_1 = \frac{2e_E}{\pi} (\cos(\varphi) V_{\text{imp}})^2 \) and the rate of the instanton tunneling is \( \Gamma_2 = 2\pi C^2 \sqrt{T_L M} \sin^2 \varphi e^{-2m/T_L} \). The current flowing through the channel is \( J = -\frac{\partial \mathcal{L}_F}{\partial \theta_c} = -i\sqrt{\Gamma_2} \psi_c^\dagger(0,t) \epsilon e^{-iVt} - h.c.] \). Its calculation with the non-equilibrium Lagrangian (3) needs avail of the Keldysh technique. Transforming voltage into the non-zero chemical potential of the fermions equal to \(-V\), we can write in standard notations (4):

\[ J = 2\sqrt{\Gamma_2} \int \frac{d\omega}{2\pi} \text{Re} G_{\psi_c}(\omega) \geq \Gamma_2 \int \frac{d\omega}{2\pi} \text{Im} [2 \times (1 - f(\frac{\omega + V}{T}) G_\xi^{\uparrow}(\omega) + G_\xi^{\downarrow}(\omega)) ] \]

(7)

where \( f \) is the Fermi distribution function. To find the Green functions \( G_\xi^{\uparrow}(\omega) \) \( G_\xi^{\downarrow}(\omega) \) of the Majorana field, its free Green functions: \( g_\xi^{\uparrow,A}(\omega) = 2/((\omega + i0)) \), \( g_\xi^{\downarrow,A} = \pm 2\pi i \delta(\omega) \) are substituted into the appropriate Dyson equations (4):

\[ G_\xi^{\uparrow}(\omega) = g_\xi^{\uparrow,A}(\omega) + \Sigma_\xi^{\uparrow}(\omega) G_\xi^{\uparrow}(\omega) \]

\[ G_\xi^{\downarrow}(\omega) = g_\xi^{\downarrow,A}(\omega) + \Sigma_\xi^{\downarrow}(\omega) G_\xi^{\downarrow}(\omega) \]

(8)

where \( \Sigma_\xi^{\uparrow,A} \) stands for \( \Sigma_\xi^{\uparrow,A} = \mp i(\Gamma_1 + \Gamma_2) \), \( \Sigma_\xi^{\downarrow,A} = -i(2(2 + \sum_j I(\omega \pm V)/T)) + 2(1 - f(\omega/T)) \). Their substitution into (3) and into (4), subsequently, results in the current:

\[ J = 2\Gamma_2 [\Gamma_1 + \Gamma_2] \int \frac{d\omega}{\pi} f(\omega/2T) - f(\omega/2T) \]

(9)

which is the current passing through a resonant level of the half-width \( 2(\Gamma_1 + \Gamma_2) \) and suppressed by the factor \( \Gamma_2/(\Gamma_1 + \Gamma_2) \). The typical features of this current can be
illustrated with its zero temperature behavior versus voltage and the linear bias conductance $G$ versus temperature, respectively:

$$ J = \frac{2\Gamma_2}{\pi} \arctan \left( \frac{V}{2(\Gamma_1 + \Gamma_2)} \right) $$

$$ G = \frac{\Gamma_2}{\pi^2 T} \psi' \left( \frac{1}{2} + \frac{\Gamma_1 + \Gamma_2}{\pi T} \right) $$ (11)

where $\psi'(x)$ is the derivative of the digamma function, $\psi'(1/2) = \pi^2/2$, and the high temperature asymptotics of $G$ is $\Gamma_2/(2T)$. The zero-temperature conductance $G \rightarrow \frac{\pi \Gamma_2}{(\Gamma_1 + \Gamma_2)}$ is the function of $\Gamma_1/\Gamma_2 \propto (\cos \varphi V_{imp}^{\alpha}/T_L)^2 E_F/\sqrt{T_L M \sin^3 \varphi}$. Comparison with the initial transmittance of the impurity scatterer shows that $\sqrt{\Gamma_1/\Gamma_2}$ may be conceived as a renormalization of the initial amplitude $V_{imp}$ by the instanton exponent and a power factor of the TLL for $g = 1/2$.

**Spin gap insulator** - In this case the chemical potential of the spin mode always lies in the center of a gap $2M$. Meanwhile the charge mode is inhomogeneous TLL with the constant $g_c \equiv g > 1$ ($g_c = 1$) inside (outside) the wire. Under Duality Transform applied to the massive spin mode the partition function $Z'$ takes the form of Eq.(11) with the following modifications. The field $\phi_s(\theta_s)$ is changed by $\phi_c(\theta_s)$, respectively, and $x_s$ by $x_c$. The factor cos $\varphi$ disappears, as $\varphi$ is accumulated by $\phi_c$. The amplitude of the instanton tunneling between the spin mode vacua becomes $P e^{-M/T_L}$, where a new pre-factor $P$ and cut-off $D^*$ are specified by the same expressions which were written for $P$ and $D'$, respectively, after substitution of $T_L$ instead of $T_c$ into them.

The action for the $\phi_c$ field is inhomogeneous: $S[\phi_c] = \int_0^B d\tau \int dx \{ (\partial_r \phi_c(\tau, x) + (\partial_x \phi_c(\tau, x)) \} / (8 g_c(x) \pi)$. To proceed in line with the above scheme of calculation, we have to first integrate out the quick modes of the $\phi_c$ field whose energies are larger than $T_L$. Unless $v_c/v_s$ becomes essentially small at $g \gg 1$, these energies lie much higher than the expected crossover. Therefore, we can integrate neglecting the weak tunneling between the spin mode vacua. In the lowest order in $V_{imp}^2$, variation of the cut-off from $E_F$ to $T_L$ results in multiplication of $V_{imp}^2$ by a factor $\langle E_F/T_L \rangle^{2g} F(x_c T_L)$ where $F(x, T_L)$ accounts for the interference produced by the inhomogeneity of the forward scattering. This function may be extracted from the long-time asymptotics of $\langle \phi_c(x, t) e^{-i\phi_c(x, 0)} \rangle$ calculated separately with $S[\phi_c]$ as:

$$ F^2(z) = \text{const} \left( z^2 + \gamma^2 \right)^{g}\prod_{m=1}^{\infty} \left( (m + 2)^2 + \gamma^2 \right)^{2g m^{2m+1}} \approx \text{const} \times \left( (z^2 + \gamma^2)/(1 - z^2 + \gamma^2) \right)^{g^2}, \quad \gamma = T_L/E_F $$

Here the rate of the instanton tunneling $\Gamma_2' = 2\pi C^2 \sqrt{T_L M} e^{-2M/T_L}$ has an manifest similarity with $\Gamma_2$ and the rate of impurity scattering $\Gamma_1 = \frac{2\pi C^2}{\sqrt{T_L M}} e^{-2M/T_L} F(x_c T_L) V_{imp}^2$ acquires an additional factor $(E_F/T_L)^{2g} F(x_c T_L)$, as $g_c > 1$. Creation and annihilation of the fermion of the charge mode in the fermionized model describes a change of chirality of one quasiparticle inside the wire. Therefore, the term proportional to $\sqrt{\Gamma_1}$ in (12) leads to the backscattering current: $J_{osc} = -\frac{\partial \mathcal{L}_F}{\partial (\psi^{+}_c)} = -i \sqrt{\Gamma_1} \psi^{+}_c (0, t) \xi(t) e^{-i\mathcal{E} t} - h.c.]$ equal to minus deviation of the direct current from its maximum $\mathcal{V}/\pi$ value. The new Lagrangian (12) and the current $J_{osc}$ transform into the old Lagrangian (9) and the current $J$, respectively, on changing $\Gamma_1, \Gamma_2$ by $\Gamma_2', \Gamma_1'$. Hence the average value of $J_{osc}$ may be extracted from (12) in the same way. In particular, the linear bias conductance: $G = (1 - \frac{\Gamma_1'}{\Gamma_2'}) \psi'(1/2 + \{ \Gamma_1' + \Gamma_2' \})/(\pi T)$) is strongly suppressed at $T = 0$ as $G = \frac{\Gamma_2'}{\Gamma_1' + \Gamma_2'}$. Similarly to the Mott-Hubbard case it shows that the initial amplitude of the potential $V_{imp}$ renormalizes to $\sqrt{\Gamma_1'/\Gamma_2'} \times V_{imp} e^{M/T_L} \sqrt{E_F/E_F/T_L}^{1-g} F(x_c)/\sqrt{T_L M}$ at low energy. Above the crossover temperature $2(\Gamma_1 + \Gamma_2')$ the conductance recovers as $\frac{1}{\pi} \left( 1 - \frac{\Gamma_1'}{\Gamma_2'} \right)$. The backscattering current related to (10) results in the constant shift of the direct current $J = \mathcal{V}/\pi - \Gamma_1'$ above the voltage crossover $2(\Gamma_1' + \Gamma_2')$.

Finally, we have shown that a zero-energy resonance in transport through a 1D Mott-Hubbard insulator of finite length predicted [9] for the clean wire stands weak impurity pinning while the rate of the impurity backscattering $\Gamma_1$ is small $\Gamma_1 \ll T_L$. We have also described how opening a gap in the spin mode suppresses the charge transport.

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* On leave of absence from A.F.Ioffe Physical Technical Institute, 194021, St. Petersburg, Russia.

Present address: Department of Physics and Astronomy, SUNY at Stony Brook, NY 11794, USA.
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