Conductance of a Mott Quantum Wire

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We consider transport through a one-dimensional conductor subject to an external periodic potential and connected to non-interacting leads (a “Mott quantum wire”). For the case of a strong periodic potential, the conductance is shown to jump from zero, for the chemical potential lying within the Mott-Hubbard gap, to the non-interacting value of $2e^2/h$, as soon as the chemical potential crosses the gap edge. This behavior is strikingly different from that of an optical conductivity, which varies continuously with the carrier concentration. For the case of a weak potential, the perturbative correction to the conductance due to Umklapp scattering is absent away from half-filling.

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It has long been understood that the result of a transport measurement depends on the measurement procedure [1]. The most famous example is perhaps a ballistic one-dimensional (1D) wire. The real part of its conductivity has a familiar Drude peak at $\omega = 0$, indicating an obvious fact that an ideal system exhibits no resistance to the stationary current flow. On the other hand, the same wire being attached to the reservoirs exhibits a finite (two-probe) conductance of $2e^2/h$. The importance of the measurement procedure has been emphasized in recent work [2–4], which have shown that the conductance of a Luttinger-liquid wire attached to the reservoirs via non-interacting leads remains at its non-interacting value of $2e^2/h$, regardless of the interactions in the wire, although the conductivity of an infinite wire is indeed renormalized by the interactions.

In this work, we focus our attention on transport through another system whose properties are generally believed to be strongly affected by the interactions, i.e., on a 1D conductor subject to an external periodic potential. In such a system, Umklapp scattering of electrons leads to an opening of the Mott-Hubbard gap, so that the system is an insulator at half-filling. Away from half-filling some conduction occurs. Almost all we know about transport through such a system is valid for a bulk sample (except for very recent studies [5–7]), whose conductivity is assumed to be measured in a contactless way, e.g., via electromagnetic losses. The main question we are asking in this work is: how does a (doped) Mott insulator conduct when being attached to non-interacting leads?

For the sake of concreteness, the system we have in mind will be taken as a quantum wire subject to a periodic gate potential (cf. Fig. 1a), similar to that fabricated in the experiments [4,5]. For brevity, we shall refer to such a system as to a “Mott quantum wire”. In what follows, we consider both the cases of strong and weak periodic potential (compared to the Fermi energy in the wire). Our main finding is that as long as a Mott quantum wire is conducting, it is an ideal conductor. This conclusion is qualified as follows. i) In the case of a strong periodic potential, the wire is an insulator whenever the chemical potential lies within the Mott-Hubbard gap, regardless of the measurement procedure. However, as the chemical potential crosses the gap edge, the conductance jumps from zero to its non-interacting value, $2e^2/h$. (In what follows, we will put $\hbar = 1$ everywhere except for the results for the conductances.) ii) If the system is not at half-filling, the case of a weak periodic potential can be treated via the perturbation theory, which shows that the $dc$ conductance of the wire is not affected by Umklapp scattering.

(i) Strong periodic potential. In this case a wire is effectively split into individual “sites” (dots) connected via tunneling of electrons. We assume that there is about one electron per site on average, i.e., the system is close to half-filling. In the presence of Umklapp scattering, a Mott-Hubbard gap opens up at $k = \pm \pi/2a$, where $a$ is the period of the potential. We begin by considering an infinite wire without leads. This situation is best described by the tight-binding model of a Hubbard type

$$H = -\frac{t}{2} \sum_{s,n} (\psi_s^\dagger(n) \psi_s(n+1) + \psi_{s+1}^\dagger(n+1) \psi_s(n)) -\mu \sum_{s,n} \psi_s^\dagger(n) \psi_s(n) + g \sum_{n} \psi_{s+1}^\dagger(n) \psi_s^\dagger(n) \psi_s(n).$$

(1)

Linearizing the spectrum around $\cos(k_F a) = -\mu/t$, expanding the fermion operators in right and left movers, and taking the continuum limit, we arrive at the following bosonized Hamiltonian for the charge degrees of freedom

$$H = \frac{1}{2} \int dx \left[v_F (\partial_x \theta)^2 + (v_F + ga/\pi) (\partial_x \phi)^2\right]$$

$$-\frac{g}{a \pi^2} \cos(\sqrt{8\pi} \phi + q_0 x) + 2gn [\frac{2}{\sqrt{\pi}} \partial_x \phi],$$

(2)

where $q_0 = 4k_F - 2\pi/a$, $n = \frac{1}{2} \sum_s <\psi_s^\dagger(n) \psi_s(n)>$ is an average number of carriers per site, and $v_F = ta \sin(k_F a)$. Shifting the $\phi$ field to remove the $q_0 x$ term under the cosine shifts the chemical potential: $\mu \rightarrow \tilde{\mu} = gn - (v_F + ga/\pi)(k_F - \pi/2a)$. To treat this Hamiltonian in the strong coupling limit $g \gg v_F$, we map it onto a system of spinless fermions [4,5]. Introducing new boson fields
\[ \varphi = \sqrt{2} \phi \theta = \theta \rho / \sqrt{2}, \] which preserve commutation relations, we re-write the Hamiltonian (3) in terms of new right- (left-) moving spinless fermions \( \psi_+ (\psi_-) \)

\[ H = \int dx \left( v \psi_+^\dagger (-i \partial_x) \psi_+ + \psi_-^\dagger (i \partial_x) \psi_- : + \bar{\mu} \psi_+^\dagger \psi_+ + \psi_-^\dagger \psi_- : + \frac{g}{\pi} \alpha \left( \psi_+^\dagger \psi_- + \psi_-^\dagger \psi_+ \right) + g_{res} \psi_+^\dagger \psi_+ : \psi_-^\dagger \psi_- : \right), \] (3)

where \( v = \frac{\sqrt{2}}{2} v_F + \frac{g}{\pi}, g_{res} = \frac{1}{2} (g a - 3 \pi v_F), \) \( \alpha \) is the short-distance cut-off, and left-moving fermions were unitarily transformed \( \psi_- \rightarrow i \psi_-, \psi_+^\dagger \rightarrow -i \psi_-^\dagger \). The last term represents the residual interaction between fermions. The chain of transformations \( \phi \rightarrow \phi \rightarrow \psi_\pm \) describes a change from the charge density wave description to the charge soliton one. Under this transformation, the density of charge fluctuations becomes

\[ \rho(x) = \frac{\sqrt{2}}{2} \partial_x \phi \rho = \frac{1}{2} \partial_x \varphi' = \sum_{s=\pm} : \psi_s^\dagger \psi_s : \] and the current \( j(x) = -v_F \sqrt{2} \partial_x \phi \rho = 2 v_F : \psi_+^\dagger \psi_- + \psi_-^\dagger \psi_+ : \).

Following Schulz [2], we diagonalize the quadratic part of (3) and find two bands of excitations with dispersion \( \omega \bar{c}_{\pm} = \bar{\mu} \pm \sqrt{v^2 \bar{c}^2 + \bar{g}^2}, \) where \( \bar{g} = \frac{g}{\pi \rho} \) is the Mott-Hubbard gap. If \( \bar{\mu} \) crosses the top of the lower band, then the density of carriers (holes) is \( \nu = \sqrt{\nu^2 - \bar{g}^2 / (\pi v)} \) for \( \bar{\mu} > \bar{g}, \) and zero otherwise. Close to half-filling, we again linearize the spectrum around the hole Fermi points \( k_c = \pm \nu / \pi \) and represent the low-energy charge excitations in terms of new right- (left-) moving fields \( \beta_1(\beta_2) \) with momenta close to \( k_c \). In doing that, one finds that the residual interaction term renormalizes to \( g_{res} (\frac{v k_c}{\bar{\mu}})^2 \int dx : \beta_1^\dagger \beta_1 \beta_2^\dagger \beta_2 : \), whereas the part

\[ H_0 = \int dx \frac{v^2 k_c}{\bar{\mu}} \left( \beta_1^\dagger (i \partial_x) \beta_1 + \beta_2^\dagger (i \partial_x) \beta_2 \right) \] (4)

describes free propagation with the renormalized velocity \( \bar{v} = \frac{v k_c}{\bar{\mu}} = v \sqrt{1 - \bar{g}^2 / (\pi v \bar{\mu})} \). As half-filling is approached, \( k_c \rightarrow 0, \) the residual interaction vanishes faster than the renormalized velocity due to the additional power of \( k_c, \) and thus can be neglected altogether. The bosonization of free Hamiltonian (4) is straightforward, and we find for the low-energy action

\[ S_0 = \frac{1}{2} \int dt \int dx \frac{1}{\bar{v}} (\partial_t \bar{\varphi})^2 - \bar{v} (\partial_x \bar{\varphi})^2, \] (5)

while the charge density becomes \( \rho(x) = \partial_x \bar{\varphi} / \sqrt{\bar{v}} \) and the current \( j(x) = -2 v_F \sqrt{1 - \bar{g}^2 / (\pi v \bar{\mu})} \partial_x \theta / \sqrt{\bar{v}}. \) The continuity equation \( \partial_t \rho(x) + \partial_x j(x) = 0 \) then leads to \( \nu = 2 v_F. \) The non-local conductivity \( \sigma(\omega, q) \) can now be calculated with the help of either fermionic [Eq. (3)] or bosonic [Eq. (4)] formalisms. Both approaches give for the optical conductivity \( \sigma(\omega, 0) = 4 \pi e^2 v^2 F \delta(\omega) / \bar{\mu} \) [5]. Notice that the Drude weight goes to zero linearly with the density of carriers. On the other hand, the conductance \( G \) (defined as the ratio of the current to the voltage which is applied to a finite segment of otherwise uniform wire) is related to the static conductivity \( \sigma(0, q) \), which in our case takes the form \( \sigma(0, q) = e^2 \delta(q) \theta (\bar{\mu} - \bar{g}) / 2 \pi. \) Correspondingly, \( G = (e^2 / h) \theta (\bar{\mu} - \bar{g}) \), which for \( \bar{\mu} > \bar{g} \) coincides with the conductance of noninteracting spinless electrons (in agreement with \( K_F \rightarrow 1 / 2 \) for \( \nu \rightarrow 0 \) [1]) and drops abruptly to zero in the insulating phase, when \( K_F = 0. \) To be more precise, we have to recall that the continuum approximation works only when the average distance between the carriers \( 1 / \nu \) is smaller than the wire length \( L; \) thus a narrow region, in which \( \bar{\mu} \) is so close to \( \bar{g} \) that \( \nu L \leq 1, \) has to be excluded.

To describe a finite Mott wire connected to a non-interacting leads we use the approach due to Safi and Schulz [2, 4]. The action of charge modes in the leads is that of a free boson field \( \varphi_\rho \) with velocity \( v_F, \) and thus can be obtained from action (3) by a simple substitution \( \bar{v} \rightarrow v_F, \bar{\varphi} \rightarrow \varphi_\rho. \) Observe now that we can describe the charge dynamics in the whole system by a single equation

\[ \frac{1}{v(x)} \partial_t^2 \chi - \partial_x (v(x) \partial_x \chi) = 0, \] (6)

where \( v(x) = v_F, \chi = \varphi_\rho \) in the leads, and \( v(x) = \bar{v}, \chi = \bar{\varphi} \) in the wire. With this identification we have \( \rho(x) = \frac{\sqrt{2}}{2} \partial_x \chi \) and \( j(x) = -\sqrt{2} \partial_t \chi \) throughout the system, where \( z = \sqrt{2} \) in the leads and \( z = 1 \) in the wire. Let us consider now a transmission of a boson wave from the lead to the wire [4], corresponding to a transmission of a single charge:

\[ \chi_{lead} = e^{i(\nu x - \omega_\nu t)} - R e^{-i(\nu x + \omega_\nu t)} \]

\[ \chi_{wire} = T e^{i(q' z - \omega_{q'} t)}. \]

(7)

The density reflection coefficient \( R = \partial_\nu \chi_{lead} / \partial_\nu \chi_{lead} \) where \( r (l) \) refers to right (left) moving excitations. Current continuity \( j(-0) = j(+0) \) gives \( \sqrt{2} (1 - R) = T, \) whereas the condition \( v_F \partial_x \chi(-0) = \bar{v} \partial_x \chi(+0) \) gives \( T = 1 + R, \) where we have also used the energy conservation \( \omega_\nu = \omega_{q'}, \) and thus \( R = \frac{\sqrt{2} - 1}{\sqrt{2} + 1}. \) Analogous consideration for the wave traveling from the wire to the lead shows that its reflection coefficient is equal to \(-R. \) The system lead-wire-lead can now be modeled as two semi-transparent mirrors, the sign of the reflection coefficient depending on whether the wave is coming from the wire or the lead [3, 4]. Summing over multiple reflections, we obtain the total charge transmitted through the system

\[ Q_{trans} = (1 - R^2) \sum_{n=0}^{\infty} R^{2n} = 1, \] whereas the reflected charge is \( Q_{refl} = R - (1 - R^2) \sum_{n=0}^{\infty} R^{2n+1} = 0. \) Thus we have perfect transmission and \( G = \frac{2}{\pi^2}. \) This result is valid as long as there are carriers in the wire, i.e., away from half-filling. At half-filling, when there are no propagating excitations in the wire, the reflection coefficient is equal to 1 and the conductance goes to zero (we
which open at $k = \pi/2l_0$, become $g - \bar{g}$.

As the basis is formed by the Bloch states, which has to be used

Note that we are no longer constrained by the half-filling

periodic potential can be found via the non-degenerate

long enough wires). Summarizing,

$$
G = \frac{2e^2}{h} \theta(\bar{g} - g).
$$

where $q_0 = G_0 - 4k_F$ and $K$ characterizes the strength of

interactions. Eq. (14) is generalized to the inhomogeneous case

(b), which implies that the external periodic potential is applied to the quantum wire ($|x| \leq L/2$), which is described by the set of constants $\{v_2, K, g\}$. Noninteracting leads with $\{v_1 = v_F, K_1 = 1, g = 0\}$ are attached

adiabatically to the both ends of the wire.

The conductivity is related to the retarded Green's function of the field $\varphi_\rho$ via the Kubo formula [15]:

$$
\sigma(x, y, \omega) = \frac{-ie^2\omega}{\pi} G_R(x, y, \omega).
$$

To the second order in $g_U$, one has

$$
\delta G_R(x, y, \omega) = 4\pi \int dz_1 dz_2 \frac{g^2_0(x)}{\alpha^2} \cos(q_0(x_1 - x_2))
\times G_R(x_1, \omega) (G_R(x_2, y, \omega) F_R(x_1, x_2, \omega)
- G_R(x_1, y, \omega) F_R(x_2, x_2, 0)).
$$

Here the retarded function $F_R(x_1, x_2, \omega) = \int_0^\infty dt e^{i\omega t} \text{Im} F_M(x_1, x_2, it - 0)$ is related to the imaginary-time correlator of $\cos(\sqrt{8\pi} \varphi_\rho)$ [13]:

$$
F_M(x_1, x_2, \tau) = \text{exp} \left\{ -8\pi \int_0^\infty \frac{d\bar{\omega}}{2\pi} \left( G_M(x_1, x_1, \bar{\omega})
+ G_M(x_2, x_2, \bar{\omega}) - 2G_M(x_1, x_2, \bar{\omega}) \cos(\bar{\omega}\tau) \right) \right\}
$$

Let us start with the case of a uniform wire $[K(x), v(x) = \text{const} \forall x]$ subject to a weak periodic potential applied to a finite segment of length $L$, i.e., $g_U(x) = 0$ for $|x| > L/2$. We concentrate on the limiting cases of “high” and “low” frequencies, i.e., when $\omega_L \equiv L\omega/v \gg 1 (\ll 1)$, respectively, and assume that $\omega \ll v q_0$. The difference between these two cases comes about from the integration over the center-of-mass coordinate of the pair $(x_1, x_2)$. Carrying out this integration, we obtain

$$
\delta G_R(x, y, \omega) = \frac{2\pi g^2_0 K^2}{\alpha^2 \omega^2} \int_0^\infty ds \cos(q_0 s) F(s),
$$

where $s = (x_1 - x_2)/2$ and
\[ \mathcal{F}(s) = \begin{cases} P(0)F_R(s, 0) - P(s)F_R(s, \omega); & \omega_L \gg 1; \\ \theta(L - s)(L - s)|F_R(s, 0) - F_R(s, \omega)|; & \omega_L \ll 1. \end{cases} \]

Here \( P(s) = \sum_{j=\pm}(\frac{t_f}{\omega})^{2j} + |x - y + js|e^{i\omega|x-y+js|/\nu} \) and \( F_R(s, \omega) = \sin 2\pi \int_{|s|/\nu}^{\infty} \text{d}te^{i\omega t} \left( \frac{t_f^2}{t_f^2 + \pi^2} \right)^{2K} \), where \( t_f^{-1} \sim E_F \) is the high-frequency cut-off. Finally, relating the conductivity to the current \( I(x, \omega) = \int_{-L/2}^{L/2} \text{d}y\sigma(x, y)E(y) \omega \) and defining the conductance as \( G(\omega) = I(L/2, \omega)/V(\omega) \), we find the correction to the conductance \( \delta G(\omega) = -(e^2\gamma^2/\nu^2) \times \gamma(\omega) \), where

\[ \gamma(\omega) = \begin{cases} C_\text{>} \cos(\omega L)(q_0^2)^{4K-4}; & \omega_L \gg 1; \\ C_\text{<} \frac{1 - \cos(q_0 L)}{(q_0^2)^{4K-2}}; & \omega_L \ll 1, \end{cases} \]

where \( C_\text{>} = \frac{2^{2-1-K}(2K - 1)\sin(2\pi K)}{(2K - 1)K^2} \) and \( C_\text{<} = \frac{2\pi}{\Gamma(4K)} \). The high-frequency result could have been obtained by assuming that the periodic potential is applied over infinite length (as in, e.g., Ref. 3, i.e. it is a “bulk” result. The low-frequency limit shows a remarkable feature: away for half-filling, the correction to the conductance of a finite-length wire is absent. Indeed, for \( q_0L \gg 1 \), where our results are only valid, \( q_0^{-2}(1 - \cos(q_0L)) \rightarrow \pi L^2\delta(q_0L)/2 \), i.e., the periodic potential does not affect the conductance for \( q_0 \neq 0 \).

We now return to the original problem of interest: a quantum wire of length \( L \) with parameters \( \{K_2, v_2, g_2\} \) connected to the leads with parameters \( \{K_1, v_1, 0\} \). In the high-frequency limit, the correlation function \( F_R \) reduces to its short-time and short-distance asymptotic form, which coincides with that of a uniform wire with parameters \( K_2, v_2 \). Therefore, the result is given by the top line in Eq. (14) with \( K \rightarrow K_2, v \rightarrow v_2 \). In the low-frequency limit, the \( t \)–integration is determined by the asymptotics of \( F_R \) at \( t \sim 1/\omega \gg t_L = L/v_2 \). Using an explicit form of \( G_M \) for an inhomogeneous Luttinger liquid 3, one can see that for such long times the time dependence of \( F_R \) is determined by the leads: \( F_R(t) \sim (t_f/t_L)^{4K_2}\text{Im} \{t_L (i - \omega t_L)^{4K_1}\} \). Concentrating on the case of noninteracting leads (\( K_1 = 1 \)), we find

\[ \delta G(\omega) = -\frac{\pi^2}{3} \frac{c^2}{h} \frac{\gamma}{v_2} \left( \frac{\alpha}{2L} \right)^{4K_2-4} \delta(q_0L)(\omega L)^2. \]

Thus away from half-filling, there is no perturbative correction to the conductance due to a weak periodical modulation of the quantum wire connected to the leads (cf. also Ref. 10). This result is a perturbative analog of the result (8) from the previous section.

Absence of the conductance correction in the perturbation theory can be understood as follows. For \( \omega \ll \nu/L \), boson field \( \varphi_\rho \) varies slowly on the scale of \( L \) and hence the cosine-term in (10) can be approximated as \( g_\omega \cos(\sqrt{\pi}\varphi_\rho(0, \tau)) \int_{-L/2}^{L/2} \text{d}x \cos(q_0x) \simeq \pi gL\delta(q_0L)(\nu/L)^2 \), from which it is clear that this perturbation is effective only at half-filling. It can be shown that both \( 1/K(x) \) and \( 1/v(x) \) acquire singular corrections proportional to \( \delta(x) \), i.e., their local values at \( x = 0 \) tend to infinity. The scaling dimension of the \( \cos(\sqrt{\pi}\varphi_\rho(0, \tau)) \) operator with \( K \) and \( v \) vanishing at \( x = 0 \) is equal to zero. Thus this operator is relevant and requires a non-perturbative treatment which was carried out in the previous section.

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