

# Quantum Wire Hybridized with a Single-Level Impurity

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We have studied low-temperature properties of interacting electrons in a one-dimensional quantum wire (Luttinger liquid) side-hybridized with a single-level impurity. The hybridization induces a back-scattering of electrons in the wire which strongly affects its low energy properties. Using a one-loop renormalization group approach valid for a weak electron-electron interaction, we have calculated a transmission coefficient through the wire,  $\mathcal{T}(\varepsilon)$ , and a local density of states,  $\nu(\varepsilon)$  at low energies  $\varepsilon$ . In particular, we have found that the antiresonance in  $\mathcal{T}(\varepsilon)$  has a generalized Breit-Wigner shape with the effective width  $\Gamma(\varepsilon)$  which diverges at the Fermi level.

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Low-temperature physics of one-dimensional (1D) electron systems (quantum wires or nanotubes) is strongly affected by electron-electron interactions. Electrons in such a system form a Luttinger liquid (LL) [1] characterized by power-law decay of various correlation functions [2, 3]. This characteristic feature of the LL has been established via conductance measurements and a scanning tunnelling microscopy (STM) both in carbon nanotubes [4] and semiconductor quantum wires [5].

Inserting a potential impurity or a weak link (e.g., a tunnel barrier) into the LL results in the power-law suppression of a local density of states (LDoS) at the impurity site [6] and thus to suppression of the conductance at low temperatures  $T$ ,  $x$ -ray edge singularity, etc. [6, 7, 8]. If the barrier interrupting the LL (e.g., a quantum dot coupled to two LL leads) carries a discrete localized state, its hybridization with extended states leads to a sharp resonant transmission [9] described by a generalized Breit-Wigner formula with the energy-dependent effective width vanishing at the Fermi level at  $T = 0$ .

Transmission and tunnelling measurements in the presence of controlled defects have been performed in both quantum wires [5] and carbon nanotubes for various defect geometries [10]. In this paper we consider how the low- $T$  electron properties of a 1D wire are affected by the hybridization with a discrete localized level in a geometry where an impurity or a quantum dot (QD) carrying such a level is side-coupled to the wire.

When such an impurity is hybridized with a 1D Fermi gas, the resonant level broadens to acquire a Lorentzian shape centered at  $\varepsilon_0$  of the width  $\Gamma_0 = \pi\nu_0|t_0|^2$  ( $\nu_0$  is the DoS in the absence of the impurity and  $t_0$  is the tunneling amplitude). We assume that there is only one level close to the Fermi level  $\varepsilon_F$ , while the level spacing,  $\delta$ , on the impurity is large,  $\delta \gg \Gamma_0, T$ . For a QD we further assume that it is in the peak of the Coulomb blockade. Then the electron LDoS of the Fermi gas in the vicinity of the impurity ( $x = 0$ ) acquires a resonant dip,

$$\frac{\nu_0(\varepsilon)}{\nu_0} = \mathcal{T}_0(\varepsilon) = \frac{(\varepsilon - \varepsilon_0)^2}{(\varepsilon - \varepsilon_0)^2 + \Gamma_0^2}, \quad (1)$$

where all energies are counted from  $\varepsilon_F$ . This describes an *antiresonant* structure of the transmission coefficient  $\mathcal{T}_0(\varepsilon)$ . In contrast to the resonant tunneling, it is the reflection coefficient  $\mathcal{R}_0(\varepsilon) = 1 - \mathcal{T}_0(\varepsilon)$  which has in this case the Breit-Wigner form, reaching the perfect reflection,  $\mathcal{R}_0(\varepsilon_0) = 1$ , at the resonance,  $\varepsilon = \varepsilon_0$ .

As usual in the LL theory, even a weak electron-electron interaction drastically changes both the LDoS near the impurity and the transmission coefficient. We will show that the transmission coefficient is given by

$$\mathcal{T}(\varepsilon) = \frac{(\varepsilon - \varepsilon_0)^2}{(\varepsilon - \varepsilon_0)^2 + \Gamma^2(\varepsilon)}, \quad (2)$$

while the LDoS of conduction electrons near the impurity ( $x = 0$ ), is given by

$$\frac{\nu(\varepsilon)}{\nu_0} = \frac{\Gamma(\varepsilon)}{\Gamma_0} \frac{(\varepsilon - \varepsilon_0)^2}{(\varepsilon - \varepsilon_0)^2 + \Gamma^2(\varepsilon)}, \quad (3)$$

and the resonant level takes the shape

$$\nu_d(\varepsilon) = \frac{1}{\pi} \frac{\Gamma(\varepsilon)}{(\varepsilon - \varepsilon_0)^2 + \Gamma^2(\varepsilon)}. \quad (4)$$

The effective level width  $\Gamma(\varepsilon)$  in Eqs. (2)–(4) diverges in the low-energy limit  $|\varepsilon| \rightarrow 0$ ,

$$\Gamma(\varepsilon) = \Gamma_0 [(\Gamma_0^2 + \varepsilon_0^2)^{1/2} / |\varepsilon|]^\alpha, \quad (5)$$

and saturates at  $\Gamma_0$  for  $\varepsilon \gtrsim \max(\varepsilon_0, \Gamma_0)$ . Here the electron-electron interaction parameter  $\alpha \equiv 1/g - 1$  is assumed to be small,  $\alpha \ll 1$ , where  $g \equiv v/v_F$  is the Luttinger parameter,  $v$  ( $v_F$ ) is the renormalized (bare) Fermi velocity. The divergence in Eq. (5) is cut by temperature  $T$ . For  $T \rightarrow 0$ , Eqs. (2) and (3) have a double-dip structure with  $\mathcal{T}$  and  $\nu$  vanishing both at  $\varepsilon = \varepsilon_0$  and at  $\varepsilon = 0$ .

The antiresonance described by Eq. (2) differs drastically from the resonance in the transmission through a barrier [9] where (for a symmetric double-barrier)  $\mathcal{T} = 1$  at  $\varepsilon = \varepsilon_0$ , with the resonance width *vanishing* at  $\varepsilon \rightarrow 0$ . On the contrary, the width of the antiresonance,  $\Gamma(\varepsilon)$  in Eq. (5), *diverges* at  $\varepsilon \rightarrow 0$ . Furthermore, the intuitively expected generalization of the Fermi-gas relation

between the level width and LDoS, i.e.  $\Gamma(\varepsilon) = \pi\nu(\varepsilon)|t_0|^2$ , fails at low energies for the weak-interaction limit. Just the opposite, in this limit  $\Gamma(\varepsilon) \propto \nu^{-1}(\varepsilon)$  at  $\varepsilon \rightarrow 0$  while the direct proportionality  $\Gamma(\varepsilon) \propto \nu(\varepsilon)$  is restored off the resonance, at  $|\varepsilon - \varepsilon_0| \gg \Gamma(\varepsilon)$  in Eqs. (2)–(4).

The seemingly counter-intuitive relation  $\Gamma(\varepsilon) \propto \nu^{-1}(\varepsilon)$  at  $\varepsilon \rightarrow 0$  follows from the mapping to the case of the potential impurity: the hybridized impurity reduces to the former in the limit  $\varepsilon \ll \varepsilon_0$ ,  $\Gamma(\varepsilon)$ . Then both the transmission coefficient and the LDoS should vanish at the Fermi level,  $\mathcal{T}(\varepsilon) \propto \nu^2(\varepsilon) \propto \varepsilon^{2\alpha}$  as in [6, 7]. As it is seen from Eqs. (2) and (3), such a behavior is ensured by the divergence in Eq. (5). Accordingly, the  $T$ -dependence of the conductance becomes  $[\varepsilon_0/\Gamma(T)]^2 \propto \varepsilon_0^2 T^{2\alpha}$ .

Such a mapping does not work for the strong electron-electron interaction in the LL. Indeed, let us start with the hybridized level off the resonance with the Fermi level,  $\Gamma_0 \ll \varepsilon_0$ . In this weak hybridization limit the level effective width is found perturbatively in  $\Gamma_0/\varepsilon_0$ :

$$\Gamma(\varepsilon) = \pi\nu_{\text{bulk}}(\varepsilon)|t_0|^2 \propto \varepsilon^\gamma, \quad \gamma \equiv (1-g)^2/2g \quad (6)$$

Here  $\nu_{\text{bulk}}(\varepsilon)$  is the electron DoS in the pure LL system. For  $\gamma > 1$ , the width of the Breit-Wigner peak is  $\Gamma(\varepsilon_0)$  and the effective perturbation parameter  $\Gamma(\varepsilon_0)/\varepsilon_0$  remains small and vanishes when the peak approaches the Fermi level ( $\varepsilon_0 \rightarrow 0$ ). Thus Eq. (6) is self-consistent when  $\gamma > 1$ . In this regime the side-hybridized impurity becomes irrelevant, similar to the case of the nanowire T-junction [11], and the zero- $T$  conductance through the LL should remain ideal as in the pure LL [12].

So, in contrast to the potential impurity case, there are two distinct regimes: the hybridized impurity makes no impact on the low-energy properties of the strongly interacting LL, while ‘cuts in two’ (at  $\varepsilon \rightarrow 0$ ) a 1D wire with the weak interaction which we now consider.

We start with the Hamiltonian describing a single impurity level hybridized with the LL:

$$H = H_{LL} + t_0\psi^\dagger(0)d + \bar{t}_0d^\dagger\psi(0) + \varepsilon_0d^\dagger d. \quad (7)$$

Here  $H_{LL}$  is the standard Luttinger Hamiltonian of interacting spinless electrons in 1D. The LL creation and annihilation operators are split into the superposition of those for right-moving ( $r$ ) and left-moving ( $\ell$ ) electrons,  $\psi(x) = \psi_r(x)e^{ik_F x} + \psi_\ell(x)e^{-ik_F x}$ , while  $d^\dagger$ ,  $d$  are the operators for the impurity level. In what follows we consider the spinless (spin-polarized) case. A spinful case can be different, as for a very large dot side-attached to the LL [13], but this is beyond the scope of the current Letter.

The Green functions for non-interacting *hybridized* conduction electrons and for  $d$  electrons are given by

$$\begin{aligned} \hat{G}_0(x, x'; \varepsilon) &= \hat{g}(x - x'; \varepsilon) + iv_F \hat{G}(x; \varepsilon) \hat{T}_0(\varepsilon) \hat{g}(-x'; \varepsilon), \\ \mathcal{G}_0^R(\varepsilon) &= [\varepsilon - \varepsilon_0 + i\Gamma_0]^{-1}. \end{aligned} \quad (8)$$

In the Keldysh technique [15] used here both  $\hat{G}$  and  $\hat{\mathcal{G}}$  are matrices in the Keldysh space;  $\hat{G}$  is also a matrix in the

$r$ - $\ell$  space; the retarded component of the Green function of (non-hybridized) conduction electrons is given by

$$\hat{g}^R(x; \varepsilon) = -\frac{i}{v_F} \hat{\theta}_x e^{i\frac{\varepsilon}{v_F}|x|}, \quad \hat{\theta}_x = \begin{pmatrix} \theta(x) & 0 \\ 0 & \theta(-x) \end{pmatrix},$$

where  $\hat{\theta}_x$  is a matrix in the  $r$ - $\ell$  space, with  $\theta(x)$  being the step-function. Here the  $T$ -matrix is related to the scattering matrix  $S$  by  $T \equiv S - I$ . The bare  $\hat{T}$ -matrix is  $\hat{T}_0^R(\varepsilon) = r_0(\varepsilon)[\hat{1} + \hat{\sigma}_x]$ , where  $\hat{\sigma}_x$  is the Pauli matrix and  $r_0(\varepsilon)$  and  $t_0(\varepsilon)$  are the bare reflection and transmission amplitudes,  $r_0(\varepsilon) = t_0(\varepsilon) - 1 = -i\Gamma_0(\varepsilon - \varepsilon_0 + i\Gamma_0)^{-1}$ .

The interaction corrections to  $\hat{G}$  and  $\hat{\mathcal{G}}$  can be expressed via the appropriate self-energies. The self-energy of the conduction electrons has the form

$$\hat{\Sigma}(x) = i\alpha v_F \int d\varepsilon' [\hat{G}_0^<(x, x'; \varepsilon) - \hat{g}_\varepsilon^<(0)], \quad (9)$$

where the  $\hat{G}^<$  component of the Keldysh Green function is related to the retarded and advanced components via

$$\hat{G}_0^<(x, x'; \varepsilon) = -n_F(\varepsilon) [\hat{G}_0^R(x, x'; \varepsilon) - \hat{G}_0^A(x, x'; \varepsilon)],$$

and  $n_F(\varepsilon)$  is the Fermi distribution function. The interaction parameter  $\alpha$  is given by  $\alpha = [V(0) - V(2k_F)]/(2\pi v_F)$ , with  $V(0)$  and  $V(2k_F)$  being the Fourier transforms of the electron-electron interaction potential  $V(x)$  in the forward- and back-scattering channel. Substituting the expression for  $\hat{G}_0^<$  into Eq. (9) we find the self-energy of the conduction electrons in the linear in  $\alpha$  order:

$$\hat{\Sigma}(x) = -\alpha \hat{\theta}_x \hat{\sigma}_x \int d\varepsilon' n_F(\varepsilon') r_0(\varepsilon') e^{i\frac{2\varepsilon'}{v_F}|x|} + \text{h.c.}$$

The first-order correction to the Green function of the conduction electrons is then given by

$$\delta\hat{G}^R(x, x'; \varepsilon) = \int dx_1 \hat{G}_0^R(x, x_1; \varepsilon) \hat{\Sigma}(x_1) \hat{G}_0^R(x_1, x'; \varepsilon) \quad (10)$$

and is graphically represented in Fig. 1a. Now the correction to the  $\mathcal{T}(\varepsilon)$  is found from the asymptotic expressions

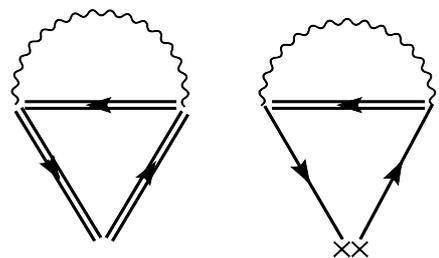


FIG. 1: The lowest-order Fock-type corrections: (a) the LDoS of the conduction electrons; (b) the  $d$ -electron self-energy (the appropriate Hartree corrections are not shown). Diagram (a) with open ends would represent  $\delta\hat{G}(x, x'; \varepsilon)$ . Single and double lines correspond to the Green functions  $\hat{g}$  and  $\hat{G}_0$ ; crosses to the tunneling amplitudes  $t_0$ ; wavy lines to the interaction.

$\hat{G}^R(x, x' \rightarrow \pm\infty)$  which are related to the T-matrix in the same way as  $\hat{G}_0$  to  $T_0$ , Eq. (8):

$$\delta\hat{T}(\varepsilon) = -\frac{\alpha}{2} \left[ \hat{S}_0(\varepsilon)\hat{\sigma}_x\hat{S}_0(\varepsilon)\bar{\mathcal{L}}_0(\varepsilon) - \hat{\sigma}_x\mathcal{L}_0(\varepsilon) \right] \quad (11)$$

where

$$\mathcal{L}_0(\varepsilon) = \int_{-\infty}^{+\infty} \frac{n_F(\varepsilon') d\varepsilon'}{\varepsilon - \varepsilon'} r_0(\varepsilon') \simeq r_0(\varepsilon) \ln \frac{\varepsilon_0 - i\Gamma_0}{\max(\varepsilon, T)}. \quad (12)$$

From Eq. (11) we find the corrections to  $r_0$  and  $t_0$ :

$$\delta t = -\alpha r_0 t_0 \bar{\mathcal{L}}_0, \quad \delta r = -\frac{\alpha}{2} [(r_0^2 + t_0^2) \bar{\mathcal{L}}_0 - \mathcal{L}_0]. \quad (13)$$

We focus further considerations on the strong-hybridization case,  $\varepsilon_0 \ll \Gamma_0$ , as in the opposite case an impact of the resonant impurity on the LDoS takes place only in a very narrow region  $\varepsilon \lesssim \Gamma_0(\Gamma_0/\varepsilon_0)^{1/\alpha}$ .

The divergence at  $(\varepsilon, T) \rightarrow 0$  in Eq. (12) necessitates a resummation of the main logarithmic corrections in all orders which is performed in the weak-interaction limit within the standard renormalization group (RG) approach. The appropriate scheme was elaborated in Ref. [7] and used also for dealing with a resonant scatterer inside the LL [9]. A crucial difference comes in the present case from the *anti-resonant* character of the scatterer which means that the reflection amplitude,  $r_0(\varepsilon)$ , vanishes at the energies higher than  $\Gamma_0$ . Hence, there are no two different regimes present in the resonant case [9] (the low-energy one with  $\varepsilon \lesssim \Gamma_0$  and the high-energy one, with  $\varepsilon$  between  $\Gamma_0$  and the bandwidth) but only the low-energy one where generic integro-differential RG equations become ordinary differential equations.

Following the same line of reasoning as in [7, 9] we integrate out the energy window  $[\Gamma_0/\lambda, \Gamma_0]$  with  $\lambda$  being a running cut-off. The RG flows start at  $\lambda = 1$ , with the initial conditions  $\mathcal{T} = \mathcal{T}_0$ ,  $\Sigma_d^R = -i\Gamma_0$ , and stop at  $\lambda = \Gamma_0/|\varepsilon|$ . The corresponding RG equations for the scattering amplitudes take the standard form:

$$\frac{d \ln t(\varepsilon, \lambda)}{d \ln \lambda} = -\alpha \mathcal{R}, \quad \frac{d \ln r(\varepsilon, \lambda)}{d \ln \lambda} = \alpha \mathcal{T}. \quad (14)$$

The solution to Eq. (14) gives the transmission coefficient  $\mathcal{T}(\varepsilon) = |t(\varepsilon)|^2$ , Eq. (2). Note that if one changed the initial conditions in Eq. (14) from the antiresonance to the resonance (when it is  $\mathcal{T}_0$  rather than  $\mathcal{R}_0$  has the Breit-Wigner form), then the solution to these equations would coincide with that obtained for the symmetric double-barrier [9], but with the high-energy cutoff at  $\Gamma_0$ .

The correction to the self-energy  $\Sigma_{d0}^R$  of the impurity Green function is represented in Fig. 1b and has the form:

$$\delta\Sigma_d^R(\varepsilon) = -\alpha \Sigma_{d0}^R \bar{\mathcal{L}}(\varepsilon) \quad (15)$$

Then in a similar way one derives from the perturbative expression (15) the RG equation for  $\Sigma_d$ :

$$\frac{d \ln \Sigma_d^R(\varepsilon, \lambda)}{d \ln \lambda} = \alpha \quad (16)$$

Such a ‘‘poor man’’ RG approach can be justified through the use of a functional bosonization technique in the form suggested in [14]. In contrast to the standard operator bosonization, it is suitable for making the weak interaction expansion. In this framework, one can integrate out the conduction electrons degrees of freedom for  $\alpha \ll 1$ . The RG analysis of the effective d-electron action confirms the validity of the RG equation (16). Solving this equation results in the following energy dependence of the  $d$  electron level width:

$$\Sigma_d^R(\varepsilon) = -i\Gamma_0(\Gamma_0/|\varepsilon|)^\alpha \equiv -i\Gamma(\varepsilon), \quad (17)$$

where  $\Gamma(\varepsilon)$  is given by Eq.(5). The impurity DoS around the resonant level is then  $\nu_d(\varepsilon) = -(1/\pi)\text{Im}[\varepsilon - \varepsilon_0 - \Sigma_d^R]^{-1}$ , which results in Eq. (4).

To find the LDoS of the LL electrons in the vicinity of the impurity we use the exact relationship between the impurity Green function,  $\mathcal{G}^R(\varepsilon) = [\varepsilon - \varepsilon_0 - \Sigma_d^R(\varepsilon)]^{-1}$ , and the local Green function,  $G^R(\varepsilon)$ , of the LL electrons,

$$\mathcal{G}^R(\varepsilon) = \mathcal{G}_{00}^R(\varepsilon) + \mathcal{G}_{00}^R(\varepsilon)|t|^2 G^R(\varepsilon)\mathcal{G}_{00}^R(\varepsilon), \quad (18)$$

where  $G^R(\varepsilon) = \sum_{\eta, \eta'} G_{\eta\eta'}^R(0, 0; \varepsilon)$  with  $\eta, \eta' = r, \ell$  and  $\mathcal{G}_{00}^R(\varepsilon) = (\varepsilon - \varepsilon_0 + i0)^{-1}$ . Using this identity one can prove the exact relationship between the LDoS of the LL electrons at  $x = 0$ ,  $\nu(\varepsilon) = -(1/\pi)\text{Im}G^R(\varepsilon)$ , and the impurity DoS  $\nu_d(\varepsilon)$ :

$$(\varepsilon - \varepsilon_0)^2 \nu_d(\varepsilon) = |t|^2 \nu(\varepsilon). \quad (19)$$

Together with Eq. (4) this identity leads to the expression (3) for the LDoS of the conduction electrons at  $x = 0$ . It shows a double-dip at  $\varepsilon = \varepsilon_0$  and  $\varepsilon = 0$  in  $\nu(\varepsilon)$  which can be observed for  $T \lesssim \varepsilon_0, \Gamma_0 e^{-1/\alpha}$ .

The RG equations (14), (16) are valid only in the region  $|\varepsilon|, \varepsilon_0 \ll \Gamma_0$  (where the expansion in  $\alpha$  contains logarithmic divergences) while outside this region the interaction corrections are non-singular. Therefore, Eqs. (3) and (4) could be considered as possible interpolation formulae which are asymptotically exact both for low energies (the RG regime) and for high energies (the Fermi gas limit).

Now we briefly address the problem of the resonant-level occupation,  $n(\varepsilon_0)$ . This problem has first been studied for the resonant level side-hybridized with a *chiral* LL [16], and later [17] for the level in a QD connecting two *non-chiral* LL's. The present case of the level side-hybridized with a *non-chiral* LL differs from that in [16] by the back-scattering induced change in the LDoS, Eq. (3). However, in the weak-interaction limit  $\nu_d(\varepsilon)$ , Eq. (4) substantially deviates from the Lorentzian only in a small region,  $\varepsilon \lesssim \Gamma_0 e^{-1/\alpha}$ . Thus  $n(\varepsilon_0)$  differs only by a small correction from that for the Fermi gas,  $n(\varepsilon_0) = 1/2 - (1/\pi) \arctan(\varepsilon_0/\Gamma_0)$ . In the strong interaction limit,  $\Gamma(\varepsilon)$  in  $\nu_d(\varepsilon)$  is given by Eq. (6) for  $\gamma > 1$ . Then  $\nu_d(\varepsilon)$  is sharply peaked around  $\varepsilon_0$  with the width  $\Gamma(\varepsilon_0) \ll \varepsilon_0$  at  $\varepsilon_0 \rightarrow 0$ . This leads to the expression for

$n(\varepsilon_0)$  like for the Fermi gas above, but with  $\Gamma_0 \mapsto \Gamma(\varepsilon_0)$ . Since  $|\varepsilon_0|/\Gamma(\varepsilon_0) \rightarrow \infty$  at  $\varepsilon_0 \rightarrow 0$ , the occupation  $n(\varepsilon_0)$  has the Fermi jump at  $\varepsilon_0 = 0$ . This is in agreement with the explanation after Eq. (6) that the  $d$ -level remains off the resonance with the Fermi level in the wire at  $\varepsilon_0 \rightarrow 0$ .

Low- $T$  resonant transport in the geometry similar to that considered in this Letter (a QD side-coupled to a single-channel quantum wire) has already been experimentally investigated [18]. To detect Luttinger features described here further transport and STM measurements are required similar to those performed in [5].

To conclude, we have studied low- $T$  properties of the non-chiral LL hybridized with a side-attached impurity carrying a single resonant level. The results for the transmission through the LL and the electron LDoS in the LL and on the impurity are given by Eqs. (2)–(6). The antiresonance in the transmission coefficient has a double-dip described by the generalized Breit-Wigner formula with the effective width  $\Gamma(\varepsilon)$  that diverges at the Fermi level ( $\varepsilon \rightarrow 0$ ) in the weak interaction limit, Eq. (5), while vanishes for the strong electron-electron interaction, Eq. (6). This is in a striking contrast to the known results for the resonant transmission through a (symmetric) double-barrier, where the width of the peak always vanishes at the Fermi level [9]. Furthermore, in the vicinity of the Fermi level, the intuitively expected relation  $\Gamma(\varepsilon) \propto \nu(\varepsilon)$  holds only for the strong interaction, with  $\nu(\varepsilon)$  being the intrinsic DoS in the LL. For the weak interaction the inverse proportionality takes place,  $\Gamma(\varepsilon) \propto \nu^{-1}(\varepsilon)$ , with  $\nu(\varepsilon)$  being LDoS modified by the impurity, Eq. (3) and (5). Such a behavior of  $\Gamma(\varepsilon)$  indicates the existence of a quantum phase transition in the interaction strength: the side-attached impurity does not affect low- $T$  properties of the LL with the strong electron-electron interaction, while results in the zero conductance and LDoS at the Fermi level for the weak interaction.

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