Interacting resonant level coupled to a Luttinger liquid: Population vs. density of states

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Abstract

We consider the problem of a single level quantum dot coupled to the edge of a one-dimensional Luttinger liquid wire by both a hopping term and electron-electron interactions. Using bosonization and Coulomb gas mapping of the Anderson-Yuval type we show that thermodynamic properties of the level, in particular, its occupation, depend on the various interactions in the system only through a single quantity — the corresponding Fermi edge singularity exponent. However, dynamical properties, such as the level density of states, depend in a different way on each type of interaction. Hence, we can construct different models, with and without interactions in the wire, with equal Fermi edge singularity exponents, which have identical population curves, although they originate from very different level densities of states. The latter may either be regular or show a power-law suppression or enhancement at the Fermi energy. These predictions are verified to a high degree of accuracy using the density matrix renormalization group algorithm to calculate the dot occupation, and classical Monte Carlo simulations on the corresponding Coulomb gas model to extract the level density of states.

Key words: Luttinger liquid, Quantum dots, Impurity Levels, Coulomb gas

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1. Introduction

The behavior of low-dimensional electronic systems has been in the focus of many experimental and theoretical studies in recent years. Such systems are important both because of the fundamental interest in the strongly correlated physics they exhibit, as well as their role as the building blocks for creating nano-scale devices. The one-dimensional case is a particularly interesting one. When no symmetry is spontaneously broken and the one-dimensional system is metallic, its low energy dynamics is described by the Luttinger liquid (LL) theory [1]. The latter offers one of the clearest realizations of non Fermi liquid physics. These systems have been experimentally realized in a variety of ways, including narrow quantum wires in semiconducting heterostructures, metallic nanowires, and carbon nanotubes. A closely related concept is that of chiral LLs, which describe the physics of edge states in the fractional quantum Hall effect [2]. A natural question which arises is the effect of impurities on these systems, either naturally occurring or artificially introduced (e.g., quantum dots and anti-dots). While this topic has been investigated for some time, most of the previous works are restricted to the study of transport properties [1–5], while other phenomena have been only occasionally considered [6–13].

In this paper we investigate one of the simplest systems of this kind, namely a single level attached to the
end of a LL (or, equivalently, a level in the vicinity of a chiral LL). We include short-range interactions between the charge of the level and the charges in its neighborhood in the wire. Although transport properties are, of course, not relevant here, many other phenomena can be investigated. In this paper we compare thermodynamic properties, in particular, the level population (which can be measured by placing a quantum point contact in the vicinity of the level), to dynamic properties, such as the level density of states (LDOS; this can be probed by tunnel spectroscopy). In section 2 we demonstrate, using the Anderson-Yuval approach, that while thermodynamic properties are universal, and are affected by the various interactions only through a single parameter (identified as the Fermi edge singularity exponent), dynamic properties are sensitive to the specific physics of the different interaction types. Based on this analysis, in section 3 we construct different systems, some LLs and some not, which are tested numerically to have the same dependence of the population on the level energy, although their LDoSs (of which the population is an integral) are very different. These results are discussed and summarized in section 4.

2. Model and Coulomb gas analysis

The system described in the Introduction can be modeled by the Hamiltonian $H = H_w + H_l + H_{lw}$. The first term is the wire Hamiltonian, described by the standard Tomonaga-Luttinger model. In bosonized form, it is given by [1]:

$$H_w = \frac{\nu}{2\pi} \int_0^\infty \left\{ \frac{1}{g} [\nabla \theta(x)]^2 + g [\nabla \phi(x)]^2 \right\} dx,$$

(1)

where the bosonic fields $\theta(x)$ and $\phi(x)$ obey the commutation relation $[\theta(x), \phi(y)] = i\pi \Theta(x-y)$, and the boundary condition $\theta(0) = 0$. Here $g$ and $\nu$ are the usual interaction parameter and excitation velocity, respectively, and $\Theta(x)$ is Heaviside’s step function. The second term of the full Hamiltonian describes the level: $H_l = \varepsilon_0 d^\dagger d$, where $d^\dagger (d)$ is the level creation (annihilation) operator and $\varepsilon_0$ is its energy. Finally, the level and the wire are coupled by:

$$H_{lw} = - \left[ T_w d^\dagger \psi(0) + H.c. \right] +$$

$$U_{lw} \left( d^d - \frac{1}{2} \right) : \psi(0)\psi(0) :. $$

(2)

The first part of $H_{lw}$ describes the level-wire hopping, parametrized by a tunneling matrix element $T_w$, while the second part, in which the colons denote normal ordering, is a local level-wire interaction of strength $U_{lw}$. The electronic annihilation operator at the wire’s edge is given by $\psi(0) = \chi e^{i\phi(0)}/\sqrt{2\pi a}$, using Majorana Fermi operators $\chi$ and a short distance cutoff (e.g., a lattice spacing) $a$.

Following Anderson and Yuval’s method [14], any quantity of interest is expanded to all orders in $T_w$. This results in a series of correlation functions, which are calculated for $T_w = 0$ [15,16]. Because of the level-wire interaction, there is a potential at the edge of the wire which flips between $\pm U_{lw}$ when each hopping occurs, i.e., we have a sequence of Fermi edge singularity events [17].

Let us first discuss the thermodynamic properties of the model, e.g.: the level population (to be denoted by $n_{level}$), entropy and the specific heat. These can be expressed through the partition function $Z$ of the model and its derivative with respect to the parameters of the system, such as the level energy $\varepsilon_0$ and the temperature $T$. In the Anderson-Yuval approach, the partition function acquires the form of a grand canonical partition function of a classical system of particles (hopping events) residing on the imaginary time axis of the original quantum model (i.e., on a circle whose circumference is the inverse of the temperature $T$ of the level-wire system). We assign to a particle corresponding to hopping of an electron from the level to the wire a positive charge, and to a particle describing the reverse process a negative charge. Thus, the charges must be alternating in sign, and their total number has to be even. Denoting the position of the $i$th particle by $\tau_i$ and the sign of the charge of the first one by $s$, we obtain:

$$Z = \sum_{\substack{N=0 \atop s=\pm 1}}^{\infty} \left( \frac{\Gamma_0 \xi_0}{\pi} \right)^N \int_0^{1/T} \frac{d\tau_2}{\xi_0} \int_0^{\tau_2 - \xi_0} \frac{d\tau_3}{\xi_0} \cdots \int_0^{\tau_2 - \xi_0} \frac{d\tau_3}{\xi_0} \exp \left[ -H_{CG}(\{\tau_i\}, s) \right],$$

(3)
so that the particles have a fugacity $\sqrt{\Gamma_0} / \pi$, where $\xi_0$ is a short time (ultraviolet) cutoff and $\Gamma_0$ is the level width (an expression for which is given below). The Hamiltonian of the classical system reads:

$$H_{CG}(\{\tau_i\}, s) = \alpha_{FES} \sum_{i<j=1}^{2N} (-1)^{i+j} \ln \left\{ \frac{\pi T \xi_0}{\sin[\pi T (\tau_j - \tau_i)]} \right\} + \frac{e_0}{T} \left\{ \frac{1}{2} - s \left[ T \sum_{i=1}^{2N} (-1)^i \tau_i - \frac{1}{2} \right] \right\}.$$  

The first part of this expression describes an interaction between the particles, which is similar in form to the electrostatic interaction between charged rods, giving Eqs. (3-4) the name “Coulomb gas expansion”. The (absolute value of the) charge of each particle is $\tau_i$.

The second part of this expression describes the imaginary time ordering operator. The value, however, varies at half filling due to particle-hole symmetry, which is the case in our numerical calculations.

Up to now, the values of $\alpha_{FES}$ and $\Gamma_0$ have not been specified. When there are no intra-wire interactions (i.e., $g = 1$), we have the usual interacting resonant level model, in which case $\alpha_{FES} = (1 - \frac{\pi}{2} \delta)^2$, and $\Gamma_0 = \pi |T_{iw}|^2 \rho_0 \cos(\delta)$, where $\delta$ is the phase shift of the electron on the surface of the wire due to the level-wise interaction, and $\rho_0$ is the density of states in the wire edge at the Fermi energy $[17,18]$. For an interacting wire ($g \neq 1$) the situation is somewhat more complicated. Since there is no backscattering in this problem, calculations using bosonization [1] yield $\alpha_{FES} = (1 - g \delta_0^2 / \pi \nu_0)^2 / g$, and $\Gamma_0 = \pi |T_{iw}|^2 \rho_0$. Comparing these expressions with the previous ones in the limit of $g = 1$ (noninteracting wire), we see that the results of bosonization replace the phase shift $\delta$ by its first Born approximation value. Thus, the values of $\alpha_{FES}$ and $\Gamma_0$ in any particular systems are renormalized by irrelevant terms not appearing in the Tomonaga-Luttinger Hamiltonian (1). It is natural to expect that, taking these effects into account, for a general model we would get $\alpha_{FES} = \frac{1}{g} \left( 1 - \frac{2g}{\pi} \delta_{eff} \right)^2$, for some effective phase shift $\delta_{eff} \in [-\pi/2, \pi/2]$, so that $\Gamma_0$ will be given by $\pi |T_{iw}|^2 \nu_0 \cos(\delta_{eff})$. This can be shown to be valid for models in which $\alpha_{FES}$ can be exactly evaluated [13]. Finally, it should be noted that in general $\epsilon_0$ is also modified by a term representing the difference in the total energy of the wire caused by the potential applied on it by an empty or a filled level. This correction can also be related to the phase shifts. Its value, however, vanishes at half filling due to particle-hole symmetry, which is the case in our numerical calculations.

Let us now turn to the LDoS, which we shall denote by $\rho_{level}(\omega)$. This quantity is equal (up to a factor of $1/\pi$) to the imaginary part of the level retarded Green function, which in turn can be obtained by analytic continuation from the corresponding Matsubara Green function in the upper complex frequency plane [19]. In the imaginary time domain the Matsubara Green function is defined by $G_i(\tau) \equiv -\frac{1}{Z} \sum_{\sigma} \text{Tr} \{ T_\tau e^{-\nu_0 / \pi} a(\tau) a^\dagger(0) \}$, where $T_\tau$ is the imaginary time ordering operator. The numerator of this expression can be given a Coulomb-gas representation, which has the same form as Eqs. (3-4) with two additional charges of sizes $\pm (\sqrt{\gamma} / \pi |T_{iw}|^2)$, inserted at $\tau$ and at the origin, respectively. These charges correspond to the level creation and annihilation operators appearing in the definition of the Green function.

From the above results we can immediately see an interesting distinction between the Coulomb-gas expression for the partition function and that for the LDoS: The former contains only three parameters: $\Gamma_0$, $\epsilon_0$, and $\alpha_{FES}$, while the latter explicitly depends on $g$ too. As both the interactions in the wire and the level-wire interactions affect the partition function mainly through a single combination — the Fermi edge singularity exponent $\alpha_{FES}$, thermodynamics cannot be used to distinguish between the different interaction types. In other words, one can construct very different models, whose interactions differ in strength and even in sign, which will have the same thermodynamic properties, provided $\Gamma_0$, $\epsilon_0$, and $\alpha_{FES}$ are indeed the same. On the other hand the LDoS, which depends explicitly on $g$, can be used to disentangle the effects of intra-wire and level-wire interaction, and will thus behave...
Fig. 1. (Color online) DMRG results for the level population as a function of its energy, for three different models denoted by the three different symbol types. The curves on which the symbols reside (which serve as a guide to the eye) correspond to the various $\alpha_{\text{FES}}$ values (the larger $\alpha_{\text{FES}}$ the narrower the curve and vice versa). See the text for further details.

differently for these different systems. In fact, it can be expected that at low energies the LDoS should behave like the tunneling density of states near the end of a LL, i.e., it will vary as $[\max(\omega, T, v/L)]^{1/g-1}$ [1].

Thus, it exhibits a power law, which depends only on the LL parameter $g$ and not on $\alpha_{\text{FES}}$, i.e., on the interactions in the wire but not on the level-wire coupling. These considerations thus give rise to a quite surprising possibility: In spite of the fact that the level population is the integral of the LDoS times the Fermi-Dirac distribution function, a LL system (i.e., a system with nearest-neighbor interactions. In this case, the wire and level-wire Hamiltonians are given by:

$$H_w = \sum_{i=1}^{N-1} \left(-t c_i^\dagger c_{i+1} + \text{H.c.}\right) +$$

$$U \left( c_i^\dagger c_i - \frac{1}{2} \right) \left( c_{i+1}^\dagger c_{i+1} - \frac{1}{2} \right),$$

$$(5)$$

$$H_{lw} = -\left(t_{lw} c_i^\dagger d + \text{H.c.}\right) +$$

$$U_{lw} \left(d^\dagger d - \frac{1}{2}\right) \left(c_i^\dagger c_i - \frac{1}{2}\right),$$

$$(6)$$

where $c_i^\dagger$ ($c_i$) is a creation (annihilation) operator for an electron at the wire’s $i$’th site, $t$ and $U$ are the nearest-neighbor hopping and interaction strengths along the chain, and $t_{lw}, U_{lw}$ denote the corresponding quantities in the level-wire coupling term. The latter are related to the parameters of the continuum level-wire coupling Hamiltonian (2) by $T_{lw} = t_{lw} \sqrt{a}$, and $U_{lw} = U_{lw} a$, $a$ being the lattice spacing. Using boundary conformal field theory arguments and the Bethe ansatz, it can be shown that for this model [13]:

3. Numerical results

In this section we show numerical data confirming the results of the previous section, i.e., that the level population is universal (equal for different models), although the LDoS is not.

To find the level occupation we have performed density matrix renormalization group (DMRG) [20] calculations on a particular realization of a LL wire represented by a half-filled $N$-site tight binding chain with nearest neighbor interactions. In this case, the wire and

Fig. 2. (Color online) Monte Carlo results for the LDoS as a function of frequency, measured from the Fermi energy for three different models, all with $\alpha_{\text{FES}} = 2/3$, $\epsilon_0/T_0 = 0.7$, and $T/T_0 = 0.04$. The three curves correspond to three different values of $g$, as indicated in the legend. Inset: temperature dependence of the LDoS at the Fermi energy (symbols), together with the expected power-low behavior (line). See the text for further details.
\[ \alpha_{\text{FES}} = \frac{1}{g} \left[ 1 - \frac{2g}{\pi} \tan^{-1} \left( \frac{U_{lw}}{\sqrt{(2t)^2 - U^2}} \right) \right]^2, \quad (7) \]

where \( g = \pi / [2 \cos^{-1}(-U/2t)] \).

In Fig. 1 we show the level population as a function of its energy. The different curves correspond to different \( \alpha_{\text{FES}} \) values. On each such curve there are symbols of three types, denoting DMRG data in three different systems: (i) \( U = 0 \) but \( U_{lw} \neq 0 \); (ii) \( U \neq 0 \) but \( U_{lw} = 0 \); (iii) both \( U \neq 0 \) and \( U_{lw} \neq 0 \). The interactions in the three three models were chosen so as to give equal \( \alpha_{\text{FES}} \) values, as denoted in the figure’s legend [For model (c) we used \( U = \pm 0.5t \), with sign opposite to that of model (b)]. In all cases we have kept \( \Gamma_0 = 10^{-4}t \) (by choosing \( t_{lw} \) appropriately), and \( N = 100v/t \). A block size of 256 was used. From the results one can clearly see that the population is indeed universal, and is equal for different models provided \( \alpha_{\text{FES}} \) is the same, although the interaction strengths are different in magnitude and sign for the three cases.

From the data of Fig. 1 we observe that the population vs. level energy curves become wider as \( \alpha_{\text{FES}} \) becomes smaller and vice-versa. Our previous results show that smaller \( \alpha_{\text{FES}} \) implies either \( g > 1 \) (i.e., attractive interactions in the wire) or \( U_{lw} > 0 \). This could be understood since both options should enhance the effective level-wire hopping, and thus lead to a wider population curve. Indeed, for \( g > 1 \) it is well known that the local density of states at the edge of a LL (or at the middle of a chiral LL) is enhanced at the Fermi energy [1], so level-wire hopping becomes effectively stronger. Similarly, \( U_{lw} > 0 \) also facilitates larger tunneling by the Mahan exciton effect [17]; due to the level-wire repulsion, when the level is empty the site at the wire’s end tends to be occupied and vice versa; hence, it helps the electrons overcome the limitations on hopping induced by the Pauli principle. In the same way we can understand why larger \( \alpha_{\text{FES}} \) will cause narrower population curves.

To find the LDoS we used classical Monte-Carlo calculations to compute the imaginary-time Green function from its Coulomb gas representation. The results were then Fourier transformed into Matsubara frequency domain, and analytically continued to obtain the retarded Green function using the Padé approximant technique [21]. The results are shown in Fig. 2. The three curves have parameters which are approximately equal to those of the three models represented by the widest curve of Fig. 1. We immediately see that, although the populations are, to a very high accuracy, equal in the three models, since \( \alpha_{\text{FES}} = 2/3 \) for all of them (actually, the Coulomb gas representation would predict exactly identical occupations), the LDoS are markedly different, having a maximum, a minimum, or no special feature near the Fermi energy for \( g > 1 \), \( g < 1 \), and \( g = 1 \), respectively. In the inset we demonstrate that the LDoS at the Fermi energy has a power-law dependence on temperature for all three cases, with the expected power of \( 1/g - 1 \).

4. Conclusions

To conclude, we have shown, both analytically and numerically, that the thermodynamics of a level coupled to the edge of a LL is universal, depending on only a few parameters. Thus, thermodynamic quantities (in particular — the level occupation) of a level coupled to a LL can be equal to the corresponding quantities in other systems which are Fermi-liquids. This occurs although thermodynamic quantities are determined by dynamic properties which are not universal. In this work we have concentrated on the level occupation, which is determined by the LDoS. The latter exhibits a power law behavior at low frequency with a power directly related to LL parameters, which cannot be reproduced by a Fermi-liquid. Yet, this LL-specific power law does not reflect itself in a LL-specific \( n_{\text{level}}(\varepsilon_0) \) dependence. Thus, thermodynamics of quantum impurities may not help to expose LL physics. Nevertheless, our results imply that interesting phenomena in such systems may be studied on equivalent models with non-interacting wires, which are much easier to approach, both analytically and numerically (using, e.g., Wilson’s numerical renormalization group [22]).

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