Finite Size Analysis of Luttinger Liquids with a Source of $2k_f$ Scattering

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Numerical analysis of the spectrum of large finite size Luttinger liquids ($g < 1$) in the presence of a single source of $2k_f$ scattering has been made possible thanks to an effective integration of high degrees of freedom. Presence of irrelevant operators and their manifestation in transport are issues treated independently. We confirm the existence of two irrelevant operators: particle hopping and charge oscillations, with regions of dominance separated by $g = 1/2$. Temperature dependence of conductance is shown to be controlled by hopping alone, giving $G \sim T^{2/g-2}$. Frequency dependence is affected by both operators, giving $G \sim \omega^{2/g-2}$ for $g > 1/2$, and $G \sim \omega^2$ for $g < 1/2$.

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The search for metallic non-Fermi liquid behavior, motivated by normal state properties of high $T_c$ superconductors [1], has renewed the interest in one-dimensional (1d) interacting system. Interactions endow particles in 1d with properties that are qualitatively different from the quasi-particle Fermi liquid picture, requiring a new description under the name of Luttinger liquids (LL) [2]. Transport is severely affected and, for instance, the conductance of a perfect channel passes from being universal to depend on the interaction strength [3]. More striking is the effect of even a single impurity: depending on the host conductance, the imperfection can either transmit or reflect perfectly [3]. Although there have been great advances in the nanofabrication of 1d structures [4], the realization that edge states of quantum Hall effect liquids are chiral LL [5] has opened new perspectives to this field. Now it seems possible to give experimental reality [6] to idealizations such as a single source of $2k_f$ scattering in an otherwise perfect LL.

A LL in the presence of a localized source of $2k_f$ scattering is described by [2,3]

$$H = \int dx \left( \frac{1}{2} (\pi g \Pi(x))^2 + \frac{1}{\pi g} (\partial_x \theta)^2 - u \delta(x) \cos(2\theta) \right)$$

(1)

where $\theta$ and $\Pi$ are canonical conjugate fields related to charge and current respectively, $g$ is the conductance in the absence of perturbation, and the impurity scattering is given by the last cosine term. For $g < 1$ (repulsive case) the perturbation is relevant [4,5], effectively splitting the system into two parts, with the phase at the impurity location, $\theta_o = \theta(x = 0)$, pinned in any of the equivalent minima of the cosine term. The pinning of $\theta_o$ blocks transport driving the conductance to zero [6]. At low energy, $\theta_o$ owes its residual dynamics to hopping processes between cosine minima (particle transport across the junction). This hopping is an irrelevant perturbation with scaling dimension $1/g$, giving the current-current correlator at the junction the imaginary time ($\tau$) dependence $\tau^{-2/g}$. Standard scaling for Kubo formula would then provide the following temperature ($T$) or frequency ($\omega$) dependence to the conductance: $G \sim \eta^{2/g-2}$, with $\eta = \omega$ or $T$, as Kane and Fisher (KF) have shown [3].

Based on the Self-Consistent Harmonic Approximation (SCHA) [8,9], which substitutes the effect of the cosine in Eq. 1 by a quadratic term $\alpha \theta_o^2$, Guinea et al. [10] have qualified this picture. They claim that, in addition to the hopping between minima, the SCHA suggests the existence of another irrelevant perturbation of dimension 2, describing oscillations of $\theta_o$ around its pinned value and providing the junction with a capacitance. (A density-density coupling between both sides of the already split system would be an equivalent description.) This new irrelevant operator (dominant for $g < 1/2$) would give rise to a $g$-independent $\tau^{-4}$ contribution to the junction current-current correlation. Scaling then dictates a $\omega^2$ dependence for the conductance, replacing the KF result $\omega^{2/g-2}$ when $g < 1/2$.

The case for this new operator seems strong. Based on a perturbative analysis, Chamon et al. [11] have found evidence for the $\tau^{-4}$ dependence of the current-current correlator for $g < 1/2$. The same authors [12] have been forced to invoke the presence of a density-density coupling to understand features of the noise spectrum, and Tsvelik [13] has deduced the existence of a capacitance from Bethe ansatz techniques. On the other hand, the same scaling that gives the $\omega^2$ law for the dynamic conductance would predict a $T^2$ temperature dependence for the static conductance replacing the KF prediction for $g < 1/2$. Unfortunately this last result contradicts the exact solution found for $g = 1/3$ from Bethe ansatz techniques [14], which is in agreement with the KF analysis $G \sim T^{2/g-2}$. This confronts us with a puzzling situation.

Naive scaling is not guaranteed to work, and to settle the problem described above one would like to separate the following two issues: (i) presence of irrelevant operators (nature, dimension, and region of dominance), and (ii) their manifestation in physical properties. With this in mind, we have adopted a finite size approach in this paper. The idea is well known: solving $H$ in a finite size $L$ amounts to probing the system with a energy scale set by $1/L$. The low energy spectrum of the (scaled) Hamiltonian $LH$ becomes scale invariant in the limit $L = \infty$ (fixed point). The
presence of irrelevant operators and their scaling dimensions can be read off from the $L$ dependence of the approach to the fixed point.

Unfortunately, this simple idea faces severe implementation problems. The number of degrees of freedom grows gigantically with size, and there is no real chance of solving exactly a finite system of even modest size. One should resort to approximations that keep a manageable number of states while ensuring that they truly describe the low energy sector of interest. In our case, the use of the SCHA as an intermediate step will help us handle this problem in a transparent and reliable way, as we will see.

It is well known that, under the guise of a variational approach, the SCHA performs a perturbative renormalization\textsuperscript{[10]}: replacement of the cosine term in Eq. (1) by a self-consistent $\alpha \theta_0^2$ provides the following dependence: $\alpha \sim u^{1/(1-g)}$. This behavior is precisely what would have been obtained for the running coupling $u$ upon integration of its renormalization group (RG) flow up to the point where $u$ equals the cut-off energy, signalling the end of the perturbative regime. Thus, the low energy states of the SCHA have a built-in effect of the high energy modes. Although the SCHA flows to the same fixed point expected for the original problem ($\theta_o$ is also pinned), it loses memory of the discrete (global) translational invariance ($\theta \rightarrow \theta + n\pi$) of $H$. It is clear that the SCHA can pin $\theta_o$ at any of the translation-equivalent minima, suggesting the following procedure: replicate the SCHA states for each well, and use these states as a basis for the diagonalization of the original Hamiltonian.

The steps in the precise implementation of this idea are the following. (i) The Hamiltonian $H$ is regularized in a linear chain of $L$ sites with periodic boundary conditions, the cosine perturbation affecting only one lattice site. (ii) The SCHA is performed for every $L$, providing a basis which is replicated at every equivalent well. (iii) The regularized Hamiltonian is scaled, $h(L) = H L/\pi$, and diagonalized in the replicated SCHA basis, keeping a fixed number of states ($\sim 100$) per well and taking advantage of the $\theta$ translational symmetry.

It is important to stress that the \textit{true} Hamiltonian is diagonalized in a restricted basis provided by the SCHA as an intermediate step. The effective integration of high modes implied by the SCHA will prove crucial for the success of this approach. Matrix elements and overlaps pose no severe computational problem owing to the harmonic nature of the basis. The calculation has all the ingredients of tight-binding structure problem, and the spectrum adopts the form of energy ($\epsilon$) versus \textit{crystalline} momentum ($q$), associated with the (discrete) $\theta$-periodicity. $\theta$ being charge, $q$ can be identified with flux piercing the ring, enabling transport properties to be read off from $\epsilon(q)$\textsuperscript{[15]}.

We have performed calculations following the above described procedure for values of $g$ in the interval $1/3 \leq g < 1$, with lattice sizes in the range $100 < L < 10^7$, and values of $u$ bounded by $u < 10^{-1}$ (much less than the energy cut-off). The number of states per $\theta_o$ well is 100, having checked that doubling this number produces no significant changes. The first important point to remark is the $(u, L)$ dependence of the spectrum of the scaled $h(L)$ through the combination $u^{1/(1-g)} L$, allowing us to measure the effect of the perturbation by the following scaling variable:

$$\tilde{u}(u, L) = u (2/L)^{g-1}$$

Trading $1/L$ for temperature, this is the same scaling variable found by KF\textsuperscript{[3]} to describe their conductance results. This scaling is a consequence of the RG flow for the relevant coupling $u$. In our scheme, this property comes through the mentioned dependence $\alpha \sim u^{1/(1-g)}$ of the SCHA, emphasizing again its implicit integration of high degrees of freedom.

Representative results for the spectrum are shown in Fig. 1, where the two lower bands $\epsilon_{1,2}(q)$ of $h(L)$ for $g = 0.4$ are plotted for increasing values of $\tilde{u}$. (Similar results are obtained for all values of $g$.) The spectrum evolves smoothly from the fixed point $\tilde{u} = 0^+$\textsuperscript{[10]} to that of $\tilde{u} \rightarrow \infty$, where (flat band) energies and degeneracies are, of course, those of a broken chain. Although our interest is the approach to this last fixed point, the analysis of the departure point $\tilde{u} \sim 0$ provides a critical test of our treatment. In the left panel of Fig. 1 we have superimposed the exact result for the (folded) parabola of current-carrying states of a perfect LL with our results. The agreement is perfect, and one should emphasize that the scheme of our calculation is the same for all values of $\tilde{u}$. That means, in the solid-state language, that we are reproducing the free particle dispersion starting out of a tight-binding basis. Following this parabola upwards in energy, discrepancies between exact and calculated results appear, due to the limited basis employed (this happens around $\epsilon \sim 5$ in the present case). This provides us with a quantitative measure of the validity of our results.

All calculations presented here are for energies within this $(\tilde{u} = 0)$ confidence limit, even though it is clear that this energy window will widens with increasing $\tilde{u}$. A further point to notice in the small $\tilde{u}$ limit is that the \textit{Bragg} gap, $\delta \epsilon_B \equiv \epsilon_2(\pi) - \epsilon_1(\pi)$, opens with a dependence $\delta \epsilon_B \sim \tilde{u} \sim L^{1-g}$. This is the expected perturbative behavior for the $2k_F$ perturbation of a LL, which grows with scaling dimension $g$. This agreement in the nominally worse situation for a scheme based on a tight-binding approach, gives us confidence in the quality of our approach.

Now we study irrelevant operators. The most conspicuous effect in the approach to the $\tilde{u} = \infty$ fixed point is the lack of band dispersion. This reflects the vanishing particle hopping across the junction (tunnel between $\theta_o$ minima).
We characterize this residual hopping by the dispersion of the lowest band, and present its $L$ dependence in Fig. 2 (left panel). For all values of $g$ it shows the dependence

$$\delta \epsilon_1 \equiv (\epsilon_1(\pi) - \epsilon_1(0)) \sim L^{1-1/g},$$

(3)
corresponding to a scaling dimension $1/g$, in agreement with Eq. (5), where only the operator responsible for band dispersion can appear.

Let us now consider other clear feature of the spectrum in Fig. 1: the approach of the second band to its asymptotic value at the Brillouin zone center, $\delta \epsilon_2 \equiv (1 - \epsilon_2(0))$. Its $L$ dependence is plotted in Fig. 2 (right panel) and summarized as follows:

$$\delta \epsilon_2 \equiv |1 - \epsilon_2(0)| \sim \begin{cases} L^{1-1/g} & (1/2 < g < 1) \\ L^{-1} & (g < 1/2) \end{cases}$$

(4)

If tunnel between wells were the only irrelevant operator, then we would always have the first result of Eq. (3). This is certainly what happens for $g > 1/2$, while for $g < 1/2$ the behavior obtained is precisely that expected from the presence of an operator with scaling dimension 2 describing fluctuations of the pinned phase $\theta_o$, as explained before. These results confirm the picture for two irrelevant operators described at the beginning, with the value $g = 1/2$ marking the boundary between regions of dominance.

Now we study the consequences for transport properties, beginning with the temperature dependence of the static conductance. Although we cannot calculate the conductance of the infinite system as a function of $T$, we can circumvent this problem by defining a running temperature for each size, $T = 2/L$, so that the energy scale for a given size is also the temperature. We define the conductance for each size-temperature according to

$$\tilde{G}(u, L, T = 2/L) = \pi^2 < \partial^2_q \epsilon > T,$$

(5)

where its well known expression as a thermal average $(< >_T)$ of the second derivative of energy versus flux has been used [13].

Although the $\tilde{G}$ so calculated is not the true (infinite size) conductance as a function of $T$, it is clear that it will be a universal function of the scaling variable $\tilde{u}$ [Eq. (5)], with the same scaling dependences. Results for $\tilde{G}(\tilde{u})$ are plotted in Fig. 3 (left panel) for $g = 0.4$. Notice the correct limit $\tilde{G}(\tilde{u} \rightarrow 0) \rightarrow g$, and a smooth crossover to the asymptotic behavior $\tilde{G}(\tilde{u} \rightarrow \infty) \rightarrow \tilde{u}^{-2/9}$. This limit implies (remember $T = 2/L$) that $\tilde{G} \sim T^{2/9-2}$, in agreement with the KF result. Similar results have been obtained for all values of $g$, at both sides of $g = 1/2$. This should not surprise in view of Eq. (3), where only the operator responsible for band dispersion can appear.

Now we study the dynamic conductance, that is, the $\omega$ dependence of the (real) part of $G$ (zero temperature). Placing a time dependent voltage (represented by a vector potential) right at the junction adds a term to the Hamiltonian

$$\delta \epsilon_2 \equiv \epsilon_2(0) \sim \begin{cases} L^{1-1/g} & (1/2 < g < 1) \\ L^{-1} & (g < 1/2) \end{cases}$$

(4)

Placing a time dependent voltage (represented by a vector potential) right at the junction adds a term to the Hamiltonian

$$H' = a\tilde{u}^2 \epsilon,$$

where $a$ is a suitable constant of order one [12]. This term does not change the energy dispersion, but does add a transition frequency, whereupon the conductance changes from

$$G_{\omega}(\tilde{u}) \sim \omega^{2-g/2}$$

(4)

for $1/2 < g < 1$, to

$$G_{\omega}(\tilde{u}) \sim \omega^2$$

(4)

for $g < 1/2$. Once again, these results are in agreement with the picture presented in the introduction, meaning that both irrelevant operators contribute to $G(\omega)$. For $g > 1/2$ hopping dominates and one obtains the KF result. For $g < 1/2$ oscillations of the pinned $\theta_o$ dominate, and $G(\omega)$ reflects the capacitance interpretation of this irrelevant perturbation. It is interesting to notice that a simplified analytical treatment that keeps only the two lowest states per well, shows that the oscillator strength comes from two contributions. One performs the transition for the states of the same well ($\theta_o \rightarrow \theta_o \pm \pi$), and only depends on the hopping irrelevant operator. This difference would help explain why the capacitance operator does not show up in the static conductance: its contribution to the oscillator strength is through transitions conserving $\theta_o$ (charge).
In summary, we have studied the low energy properties of a LL in the presence of $2k_f$ scattering in the repulsive regime $g < 1$. The numerical analysis of the spectrum for very large sizes has been made possible thanks to the use of the SCHA as an intermediate step that effectively integrates high energy states. Accuracy has been tested in the nominally worst case of small $u$. Presence of irrelevant operators and their manifestation in transport are two issues treated independently. We confirm the existence of two irrelevant operators, with $g = 1/2$ as the boundary between their regions of dominance. One represents particle hopping, and has dimension $1/g$. The other describes charge oscillations around the pinned value, and has dimension $2$. Temperature dependence of the static conductance has been shown to be controlled by the hopping operator alone, giving $G \sim T^{2-g-2}$ for all values of $g$. Frequency dependence is affected by both operators, giving $G \sim \omega^\eta$, with $\eta = (2/g - 2)$ for $g > 1/2$, and $\eta = 2$ for $g < 1/2$. Conceptual simplicity, tested numerical accuracy, and versatility in handling different aspects make this approach a promising tool for other quantum impurity problems.

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FIG. 1. Two lowest bands $\epsilon_{1,2}(q)$ of the scaled hamiltonian $h(L) = HL/\pi$ with $g = 0.4$ for four increasing values of the scaled perturbation [Eq.(2)] $\tilde{u} = 0^+, 0.72, 1.63$ and 34.9 (left to right). The continuous line of left panel is the exact result of a perfect LL.

FIG. 2. Left panel: $\ln(\delta \epsilon_1)$ [Eq.(3)] versus $\ln(L/\pi)$ for $g = 0.7, 0.55, 1/2, 0.4$, and $1/3$ (top to bottom). Continuous lines are asymptotic behavior [Eq.(3)]. Right panel: as in left panel for $\ln(\delta \epsilon_2)$ [Eq.(4)] with $g = 0.7, 0.55, 1/3, 0.4$, and $1/2$ (top to bottom).

FIG. 3. Left panel: $\ln(\tilde{G})$ [Eq.(5)] versus $\ln(\tilde{u})$ [Eq. (2)] for $g = 0.4$ with results for 200 $(u, L)$ points collapsed onto a single scaling curve. Continuous line is the asymptotic behavior $\sim \tilde{u}^{-2/g}$. Arrow marks the exact limit for $\tilde{u} = 0$. Right panel: $\ln(f_{12})$ [Eq.(7)] versus $\ln(L/\pi)$ for $g = 0.7, 0.55, 1/2, 1/3$, and 0.4 (top to bottom). Continuous lines are asymptotic behavior [Eqs.(7)].
