Numerical Renormalization Group at Marginal Spectral Density: Application to Tunneling in Luttinger Liquids

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Many quantum mechanical problems (such as dissipative phase fluctuations in metallic and superconducting nanocircuits or impurity scattering in Luttinger liquids) involve a continuum of bosonic modes with a marginal spectral density diverging as the inverse of energy. We construct a numerical renormalization group in this singular case, with a manageable violation of scale separation at high energy, capturing reliably the low energy physics. The method is demonstrated by a nonperturbative solution over several energy decades for the dynamical conductance of a Luttinger liquid with a single static defect.

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The bosonic description of fermionic systems, possibly subject to strong interactions, has a long history, ranging from phase fluctuations in superconducting circuits [1,2] following Josephson's initial ideas to quantum transport in metallic grains [3] and in strongly correlated materials near the Mott transition [4]. Here the phase Φ conjugate to the electron charge is the relevant physical variable to understand the interplay of tunneling and Coulomb blockade. Another striking example concerns one-dimensional electronic wires, the so-called Luttinger liquids (LLs), where noninteracting plasmon modes provide a faithful representation of electronic density fluctuations in the bosonization language [5–7]. Quite remarkably, all these different physical problems share similar features, because one can describe the electrons by an exponential phase factor $e^{i\Phi}$, so that the nature of the phase dynamics determines the underlying physics. Randomization of $e^{i\Phi}$ occurs, for instance, in the presence of strong Coulomb blockade, leading to electronic localization [3,4]. In contrast, the phase locks itself in the case of easy fluctuations of the electron charge characterizing dissipationless supercurrent [1] or Fermi liquid states [4]. The intermediate situation of soft (algebraic) phase decay leads to the well-known non-Fermi liquid features of a LL [5–7].

In most cases, greater complexity arises due to the coupling of the bosonic mode Φ to static disorder or dynamical defects, such as discrete Andreev levels [8,9] in superconducting weak links [10] or magnetic Kondo impurities in metallic junctions [11,12] and interacting wires [13,14]. By focusing the discussion on the case of impurity effects in LLs, but keeping this more general framework in mind, many technical and physical questions are still open to date, both in the original fermionic formulation and in the bosonic version of the problem. In the fermionic viewpoint, the difficulty is to handle simultaneously strong interactions within 1D wires with the presence of exponentially small energy scales arising from the impurity [11,15]. The density matrix renormalization group [16] can tackle correlated wires but only on a linear energy scale, which does not allow us to really extract critical exponents [17]; the numerical renormalization group (NRG) [18,19] can, however, deal with impurity physics on an exponential energy range but only for uncorrelated Fermi liquids. A method that could incorporate both virtues would therefore be quite useful, which is the goal of this Letter.

By using the bosonic language, the description of interacting electrons by noninteracting bosons helps tremendously, but difficulties still arise. Apart from perturbative analysis (or fine-tuning of the model parameters to allow an exact solution) [5–7], the analytical bosonization technique offers limited information on quantum impurity problems, because the physics crosses over from weak to strong coupling, for instance, due to Kondo screening. Actually, all this complexity is already encoded by a static defect in LLs, which drives the conductance from e^2/h to zero on an energy scale that can be exponentially small in the backscattering amplitude, a problem that has triggered substantial work, based on approximate analytical methods [15,17,20–23] or numerical techniques on a linear energy scale, such as density matrix renormalization group and quantum Monte Carlo calculations [2,17,24].

The idea we henceforth present is to use recent developments of the bosonic NRG [25–27] in order to tackle numerically the phase fluctuation problem in a broad range of parameters, with possible extensions to dynamical defects. This, however, faces an immediate and seemingly intractable difficulty. Quite common to the Josephson effect in a dissipative environment [9], to quantum tunneling in resistive circuits [12,28–30], or to tunneling into LLs [12,15,17,20–23] is the marginal form of the bare local bosonic spectrum, given by the correlation function $\mathcal{G}^0_\Phi(i\omega) = 2\pi/|\omega|$ at an imaginary frequency. The key step in the NRG procedure is the scale separation that results from a logarithmic discretization of the energy band $\omega_n = \omega_c \Lambda^{-n}$, with $1 < \Lambda$. A generalized power-law density of states (with exponent $s \geq -1$ and high energy cutoff ω_c) of the form $J(\omega) = 2\pi\omega_c^{-1-s}\omega^s\Theta(\omega_c - \omega)$

can be considered for both fermionic [31] and bosonic models [25–27], providing the following coupling strength of the states at energy ω_n:

$$\gamma_n^2 = \int_{\omega_{n+1}}^{\omega_n} d\omega J(\omega) = 2\pi \frac{1-\Lambda^{-(s+1)}}{s+1}\Lambda^{-n(s+1)}. \quad (1)$$

For all $s > -1$, the couplings γ_n^2 decay exponentially with n, which allows an iterative diagonalization of the problem: The possibility of building progressively the Hilbert space from high to low energies is the reason behind the huge success of NRG to solve quantum impurity problems in a linear numerical effort [18,19]. However, the marginal case $s = -1$ is special in the sense that the couplings $\gamma_n^2 = 2\pi \log(\Lambda)$ do not decay anymore, invalidating clearly the whole scheme. We stress that we are considering quantum impurity Hamiltonians that depend explicitly on the phase factor $e^{i\Phi}$ and not on the spatial derivative of the bosonic mode, $\partial_x\Phi$. This latter case, which arises, for instance, in the so-called Ohmic spin-boson model [25], corresponds to the much simpler situation of the linear spectrum ($s = 1$) of the field $\partial_x\Phi$ and can be easily handled by the bosonic NRG.

This complete violation of scale separation for the marginal case $s = -1$ seems to disqualify our proposed extension of the NRG. However, a free electron wire with a constant density of states (described by the standard fermionic NRG at $s = 0$) is equivalent to a free bosonic bath with $s = -1$ due to the bosonization mapping, so that one may believe that the marginal situation could be tackled by using some clever variant of the bosonic NRG. In order to move forward, let us investigate with greater detail the problem of tunneling in LLs. The fermionic Hamiltonian reads in terms of second quantized left- and right-moving electron modes $\psi_{L,R}^\dagger(x)$ at linear position x in the wire (omitting the electron spin for simplicity)

$$H = \int dx[iv_F\psi_L^\dagger\partial_x\psi_L - iv_F\psi_R^\dagger\partial_x\psi_R + g_2\psi_R^\dagger\psi_R\psi_L^\dagger\psi_L] - V_{\rm bs}[\psi_R^\dagger\psi_L + \psi_L^\dagger\psi_R]_{|x=0}, \quad (2)$$

where v_F is the Fermi velocity, g_2 the short-range Coulomb repulsion between left- and right-moving electrons, and $V_{\rm bs}$ the impurity backward scattering amplitude at the $x = 0$ location of the defect (forward impurity scattering and g_4 interaction within a given Fermi point do not affect the physics and were discarded). The presence of the interaction term g_2 clearly prevents a direct fermionic NRG solution of the model, which requires Fermi liquid leads. Yet, one can use the exact bosonization mapping [5–7] to reexpress the electronic variables in terms of noninteracting collective charge density excitations $\Phi(x)$ and conjugate field $\Pi(x)$. After standard manipulations [5–7,15] one obtains

$$H = \int \frac{dx}{8\pi}\{[\Pi(x)]^2 + [\partial_x\Phi(x)]^2\} - v_\star^\star\cos[\sqrt{K}\Phi(x=0)]_\star^\star, \quad (3)$$

where normal ordering of the cosine operator, which will be crucial for the rigorous formulation of the NRG algorithm, has been emphasized. We have also introduced a small backscattering energy scale $v \propto V_{\rm bs}$ and the important Luttinger liquid parameter $K = [(1-g_2)/(1+g_2)]^{1/2} \leq 1$, into which all interaction effects have been encapsulated.

Let us now present how the bosonic NRG [25] can be tailored to address the impurity model (3), which has the form of a boundary sine-Gordon Hamiltonian. The derivation of the "star" NRG follows the usual procedure [19,25] by considering the equivalent energy representation in terms of a continuum of canonical bosons $a_\epsilon^\dagger$:

$$H = \int_0^{\omega_c} d\epsilon\epsilon a_\epsilon^\dagger a_\epsilon - v_\star^\star\cos[\sqrt{K}\Phi]_\star^\star, \quad (4)$$

$$\Phi \equiv \Phi(x=0) = \sqrt{2}\int_0^{\omega_c} d\epsilon \frac{a_\epsilon^\dagger + a_\epsilon}{\sqrt{\epsilon}}. \quad (5)$$

The bosonic fields are then decomposed in Fourier modes ($p \in \mathbb{Z}$, $n \in \mathbb{N}$) on each interval $\omega_{n+1} < \epsilon < \omega_n$ of width $d_n = (1-\Lambda^{-1})\Lambda^{-n}$:

$$a_\epsilon^\dagger = \sum_{n,p} \frac{e^{i2\pi p\epsilon/d_n}}{\sqrt{d_n}} a_{n,p}^\dagger. \quad (6)$$

The first NRG approximation consists in neglecting all $p \neq 0$ modes, keeping only the operators $a_n^\dagger \equiv a_{n,0}^\dagger$ (this step becomes exact in the $\Lambda \to 1$ limit [19]). This leads to the star Hamiltonian:

$$H_S = \sum_{n=0}^{+\infty} \xi_n a_n^\dagger a_n - v_\star^\star\cos\left[\sqrt{K}\sum_{n=0}^{+\infty}\frac{\gamma_n}{\sqrt{\pi}}(a_n^\dagger + a_n)\right]_\star^\star \quad (7)$$

with the "impurity" coupling strength already given in Eq. (1) by $\gamma_n^2 = 2\pi\log(\Lambda)$ in the marginal case $s = -1$. The typical energy ξ_n in each shell is defined by

$$\xi_n = \frac{1}{\gamma_n^2}\int_{\omega_{n+1}}^{\omega_n} d\omega\omega J(\omega) = \frac{1-\Lambda^{-1}}{\log(\Lambda)}\omega_c\Lambda^{-n}. \quad (8)$$

As a benchmark of the discretization for the marginal case $s = -1$, one can easily compute from (7) the resulting approximation for the original Green's function:

$$\mathcal{G}_{\Phi,\Lambda}^0(i\omega) = \frac{4}{1-\Lambda^{-1}}\sum_{n=0}^{+\infty}\frac{\omega_c\Lambda^{-n}}{\omega^2 + [\frac{1-\Lambda^{-1}}{\log(\Lambda)}]^2\omega_c^2\Lambda^{-2n}}, \quad (9)$$

which can be checked to converge exponentially fast at $\omega \ll \omega_c$ to the exact result $\mathcal{G}_\Phi^0(i\omega) = \frac{2\pi}{|\omega|}$ even for $\Lambda = 2$ (we keep this standard value from now on). However, despite the clear exponential decay of the energies

(8), the nondecreasing value of the couplings γ_n implies a violation of scale separation on *all* shells and prevents the solution by iterative diagonalization of Hamiltonian (7).

The first key idea in successfully constructing the marginal bosonic NRG is to assume that the energy spectrum is also bounded from *below*:

$$J(\omega) = \frac{2\pi}{\omega}\Theta(\omega_c - \omega)\Theta(\omega - \omega_{\min}). \tag{10}$$

Clearly, both the energies ϵ_n and the couplings γ_n are not modified by this choice (γ_n still do not decay), and they are just cut off for $n > n_{\min}$, with $\omega_{\min} = \omega_c \Lambda^{-n_{\min}}$, so that nothing seems gained naively. We can, however, try to pursue with the second step of the standard NRG procedure, which amounts to the exact mapping on the Wilson chain [19,25]. This simple tridiagonalization procedure of Hamiltonian (7) leads to the following "chain" form in terms of new canonical bosons $b_n^\dagger$:

$$H_C = \sum_{n=0}^{+\infty}[\epsilon_n b_n^\dagger b_n + t_n(b_n^\dagger b_{n+1} + \text{H.c.})] - v \overset{\star}{_\star}\cos[\alpha(b_0^\dagger + b_0)]\overset{\star}{_\star} \tag{11}$$

with $\alpha = \sqrt{2K\log(\omega_c/\omega_{\min})}$. Clearly, the impurity part of the chain Hamiltonian (11) breaks down for $\omega_{\min} \to 0$, owing to the divergence of α, but one can check numerically that the construction is valid for nonzero $\omega_{\min}$. The on-site energies ϵ_n and hoppings t_n of the Wilson chain can indeed be obtained by numerical tridiagonalization of Eq. (7). For the value $\omega_{\min} = 10^{-5}$ of the lower cutoff, these are plotted together with the star parameters in Fig. 1. The exponential decay of *both* chain parameters ϵ_n and t_n that we discover here is clearly a remarkable surprise that enables the extension of the NRG to the marginal situation $s = -1$. This crucial feature comes at a small price, seen by the first increase of the chain parameters from site $n = 0$ to site $n = 1$. Thus the maximal violation of scale separation in the star NRG presents a small remanence in the chain NRG, limited only to the first shell. Interestingly, the initial jump of the parameters is just proportional to $\log(\omega_c/\omega_{\min})$, so that the lower cutoff $\omega_{\min}$ can be decreased on exponential scales without paying a huge numerical cost.

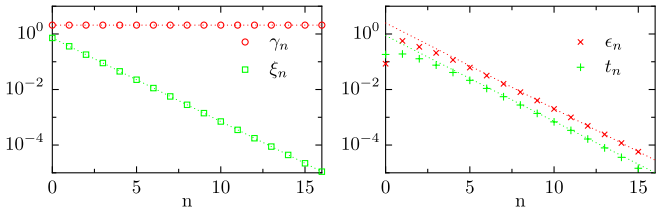

FIG. 1 (color online). Left panel: Parameters ξ_n and γ_n of the star NRG as a function of n for $0 \le n \le n_{\min} = 16$; the coupling γ_n does not decay and violates scale separation on *all* shells. Right panel: Parameters ϵ_n and t_n of the chain NRG; scale separation is broken only on the first shell, as seen by the initial increase of both parameters, before further exponential decay (shown by dotted lines as guides to the eye).

A last difficulty due to the unusual form of the impurity Hamiltonian (11) must be addressed. In the standard NRG [19,25], only linear to quadrilinear operators are present in the Hamiltonian. However, the central role played by the phase factor $e^{i\Phi}$ leads to a cosine term at the impurity site, hence an operator of infinite order which according to bosonization [7] must be normal ordered. The required operator $\mathcal{O} = \overset{\star}{_\star}\cos[\alpha(b_0^\dagger + b_0)]\overset{\star}{_\star} = \cos(\alpha b_0^\dagger)\cos(\alpha b_0) - \sin(\alpha b_0^\dagger)\sin(\alpha b_0)$ can be decomposed onto Fock states $|m\rangle$ of the bosonic creation operator $b_0^\dagger$:

$$\langle m|\mathcal{O}|p\rangle = \sqrt{m!p!}\,\text{Re}\sum_{k=0}^{\text{Min}(m,p)}\frac{(i\alpha)^{m+p-2k}}{(m-k)!(p-k)!k!}. \tag{12}$$

The construction of the impurity term in (11) proceeds by a truncation of the infinite Fock space on the initial Wilson site limited to states with an occupation number less than a given N_0 and use of the matrix elements (12). Typically, $N_0 = 150$ ensures a good representation of the Hamiltonian. Each further site $n > 0$ of the chain is described by a basis of N_b states [25] (we take $N_b = 12$ here). At increasing n, the growing size of the total Hilbert space becomes rapidly unmanageable, and a truncation to N_{trunc} states is necessary as usual [19]. We used $N_{\text{trunc}} = 800$ in all our computations, and $\omega_c = 1$ was set as the energy unit.

In contrast to more complex extensions of impurity models with dynamical degrees of freedom (such as the Kondo model in a Luttinger liquid [13,14]), the present impurity problem benefits from several known limits that allow us to benchmark our numerics. For instance, there exists an exact solution for the dynamical conductance [5–7,15] (in units of e^2/h) at $K = 1/2$:

$$G^{\text{exact}}(\omega) = \frac{K\omega}{2\pi}\,\text{Re}[\mathcal{G}_\Phi(\omega)] = \frac{1}{2} - \frac{\Omega}{2\omega}\arctan\left(\frac{\omega}{\Omega}\right), \tag{13}$$

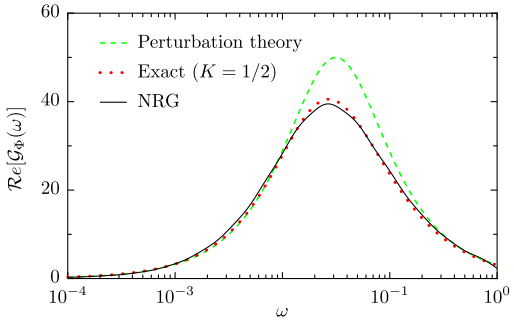

FIG. 2 (color online). Bosonic correlation function $[\text{Re}\mathcal{G}_\Phi(\omega)]$ at real frequency ω for the LL parameter $K = 1/2$ comparing (bottom to top) the NRG to the exact result (13) and to the strong and weak interaction perturbation theory given, respectively, by (14) and (15) (these two expressions are by accident equivalent for $K = 1/2$ but nonetheless not exact).

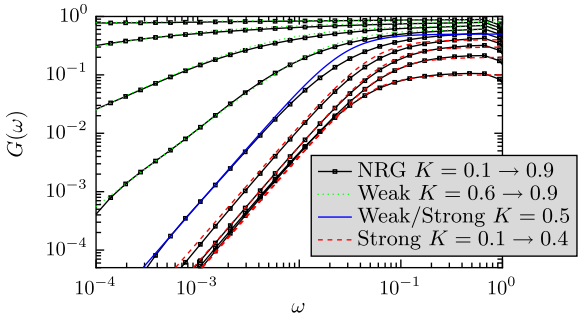

FIG. 3 (color online). Dynamical conductance $G(\omega)$ in units of e^2/h for nine values of the LL parameter K between 0.1 and 0.9, as obtained by the NRG (symbols, bottom to top). Comparison is made for $K \leq 0.5$ to the strong interaction and for $K \geq 0.5$ to the weak interaction limits.

where $\Omega = e^{\gamma} v^2$, with Euler's constant γ, is the crossover energy at which the impurity cuts the chain (for $K = 1/2$). Perturbation theory works also at strong interaction $K \ll 1$, in which case the self-consistent harmonic approximation applies [20]:

$$G^{\text{strong}}(\omega) = \frac{1}{2} \frac{\omega^2}{\omega^2 + (\Omega^\star)^2} \tag{14}$$

with $\Omega^\star = 2\pi K v^{1/(1-K)}$ the crossover scale. Finally, the limit of weak interaction $1 - K \ll 1$ is also known from several approaches [5,6,15,17,21–23]:

$$G^{\text{weak}}(\omega) = \frac{K \omega^{(2/K)-2}}{\omega^{(2/K)-2} + (\Omega^\star)^{(2/K)-2}}. \tag{15}$$

Figure 2 compares our NRG data for $K = 1/2$ with the exact solution and perturbation theory, which shows the excellent convergence of the NRG and the sizable discrepancies of both perturbative expansions. More systematic analysis for various K values in Fig. 3 demonstrates the progressive departure of the perturbative results from the numerics. The ability of the marginal bosonic NRG to describe nonperturbatively universal transport features with *high accuracy* should thus make it a precious tool to test scaling behavior of impurity physics in LLs.

In conclusion, we have established an extension of the NRG to deal with the marginal situation of a density of states diverging as the inverse of energy. The potentially most promising applications of the NRG at marginal coupling concern the physics of dynamical impurities coupled to phase fluctuations, a large class of physical problems where no alternative analytical or numerical techniques exist to date. This development could allow us to address many currently open issues, such as nonequilibrium transport with strong correlations (using a mapping onto equilibrium q-oscillator models [32]), Kondo physics in Luttinger liquids [12–14], and Ohmic dissipation in Andreev level qubits [8–10].

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