

Nonequilibrium Functional Renormalization Group for Interacting Quantum Systems

Severin G. Jakobs,¹ Volker Meden,² and Herbert Schoeller¹

¹*Institut für Theoretische Physik A, RWTH Aachen, D-52056 Aachen, Germany*

²*Institut für Theoretische Physik, Universität Göttingen, D-37077 Göttingen, Germany*

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We propose a nonequilibrium version of functional renormalization within the Keldysh formalism by introducing a complex-valued flow parameter in the Fermi or Bose functions of each reservoir. Our cutoff scheme provides a unified approach to equilibrium and nonequilibrium situations. We apply it to nonequilibrium transport through an interacting quantum wire coupled to two reservoirs and show that the nonequilibrium occupation induces new power law exponents for the conductance.

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Introduction.—Relevant energy scales of interacting quantum many-body systems are typically spread over several orders of magnitude. Conventional perturbative approaches to such systems which treat all energy scales at once often fail, especially in low dimensions where they typically lead to divergences at low energies (see, e.g., Ref. [1]). A successful approach to these systems is given by renormalization group (RG) schemes, which are based on the idea of treating energy scales successively from high to low [1,2]. A broadly applicable example is the functional RG (FRG). In this approach an infrared cutoff is introduced in the bare propagator and an exact infinite hierarchy of flow equations for Green or vertex functions is derived [3]. This method benefits from various advantages: (i) it is not restricted to field theories but can directly be applied to microscopic models; (ii) the physics on all energy scales can be studied, not only the low energy asymptotics; (iii) it provides a systematic scheme for approximations allowing for the study of systems with many interacting degrees of freedom (“large” systems). In thermal equilibrium the FRG has been used successfully for the study of microscopic models of correlated fermions in 0, 1, and 2 dimensions [4,5]. In particular the FRG scheme for the one-particle irreducible vertex functions [6–8] has the advantage that the self-energy is fed back nonperturbatively into the FRG flow, which is essential for 0 and 1 dimensional systems [4].

The FRG is usually formulated within the equilibrium imaginary time Matsubara formalism. A generalization to the real time Keldysh approach is highly desirable as it makes nonequilibrium systems treatable and does not require an elaborate analytic continuation of the Green functions (GFs). RG methods developed so far in the framework of Keldysh formalism [9,10] are restricted to systems with only a few interacting degrees of freedom. Wegner’s flow equation method provides an alternative “RG-like” approach to nonequilibrium, but up to now was also only used for small systems [11]. Recent attempts to develop RG schemes within Keldysh formalism (for the steady state) by using a *real* frequency or momentum cutoff in the free propagator [12–14] are promising but face

many severe technical problems. In this Letter we propose a fundamentally new approach by introducing an *imaginary* frequency cutoff in the Fermi or Bose functions of the reservoirs, which are coupled to the quantum system under consideration. If reservoir r is characterized by temperature T_r and chemical potential μ_r , we introduce a multi-dimensional (or complex-valued) flow parameter $\Lambda = (\{\Lambda_r\}_r, \lambda)$ by the replacement

$$\begin{aligned} f_r(\omega) &= \frac{1}{e^{(\omega - \mu_r)/T_r} \pm 1} \\ &= T_r \sum_{\omega_n^r} \frac{e^{i\omega_n^r 0^+}}{i\omega_n^r - \omega + \mu_r} \\ \rightarrow f_r^{\Lambda, \Lambda_r}(\omega) &= T_r \sum_{\omega_n^r} \frac{\Theta(|\omega_n^r| - \lambda) e^{i\omega_n^r 0^+}}{i\omega_n^r - \omega + \Lambda_r}, \end{aligned} \quad (1)$$

with $\omega_n^r = (2n + 1)\pi T_r$ or $\omega_n^r = 2n\pi T_r$ denoting the Matsubara frequencies for fermions or bosons, respectively. The imaginary component λ of the flow parameter corresponds to the imaginary frequency cutoff used in Matsubara formalism FRG. For a simple truncation scheme we show [see Eq. (3)] that this cutoff results in the identical flow equation as found by the Matsubara FRG in the special case of equilibrium. For Fermions, λ regularizes infrared divergences by broadening the step in the Fermi function in a way comparable to an augmented temperature $T \sim \lambda$. Therefore the flow generated by λ is quite similar to the temperature-flow scheme known from equilibrium [15]. The real components Λ_r of the flow parameter correspond to the chemical potentials of the reservoirs and allow for a continuous interpolation between equilibrium and nonequilibrium, generalizing the known temperature-flow scheme to a voltage-flow scheme for nonequilibrium problems.

Applying our scheme to quantum transport through a wire coupled to reservoirs, we show that the nonequilibrium distribution can change the power law exponent of the local density of states leading to novel exponents in the conductance. This exemplifies that nonequilibrium can even modify the *scaling behavior*, whereas recently discussed decoherence effects induced by relaxation pro-

cesses associated with the finite current lead to an additional cutoff of the RG flow [16].

Model and cutoff scheme.—We consider an interacting quantum system with Hamiltonian $H_S = H_S^{(0)} + V$, where $H_S^{(0)} = \sum_l \epsilon_l c_l^\dagger c_l$ is quadratic in the field operators (including arbitrary impurity configurations) and V denotes the interaction. This system is coupled to several noninteracting reservoirs (labeled by the index r) described by $H_{\text{res}} = \sum_r H_{\text{res}}^r = \sum_{kr} \epsilon_{kr} a_{kr}^\dagger a_{kr}$, which are in a grandcanonical distribution with (possibly different) temperatures T_r and chemical potentials μ_r . The coupling between H_S and H_{res} can involve an arbitrary number of system or reservoir field operators, in order to describe particle and energy exchange or nonlinear couplings. Although our general formalism is applicable to all these cases, for simplicity we restrict ourselves in this Letter to the special case of one kind of fermionic or bosonic particle which can tunnel between the reservoirs and the quantum system, described by the tunneling Hamiltonian $H_T = \sum_{klr} t_{kl}^\dagger a_{kr}^\dagger c_l + \text{H.c.}$ We assume interactions that conserve particle number and consider only the nonequilibrium steady state limit where time-translational invariance holds. Given $H = H_S^{(0)} + H_{\text{res}} + H_T + V$ and expanding in H_T and V , one can apply standard quantum field theoretical diagrammatic approaches in imaginary (Matsubara formalism) or real (Keldysh formalism) times to calculate all (non)equilibrium GFs from which physical observables like, e.g., charge, spin, or heat currents can be deduced.

The FRG within Matsubara formalism is based on introducing an infrared cutoff Λ in the free one-particle GF $g_{\text{eq},l}(i\omega_n) = 1/(i\omega_n - \epsilon_l + \mu)$ of the quantum system. A choice often used in 0 and 1 dimension [4] is to cut off the imaginary Matsubara frequencies via $g_{\text{eq}}^\Lambda(i\omega_n) = \Theta(|\omega_n| - \Lambda)g_{\text{eq}}(i\omega_n)$. In the nonequilibrium case, a natural adaptation to Keldysh formalism is a frequency cutoff in the free Keldysh GF of the quantum system via $g^\Lambda(\omega) = \Theta(|\omega| - \Lambda)g(\omega)$. Here g consists of the four components $g^c, g^<, g^>, g^{\bar{c}}$ or the three independent components $g^{\text{Ret}}, g^<, g^{\text{Av}}$. While this approach was used to study transport properties of interacting systems in nonequilibrium [12,13], it suffers from certain drawbacks when the truncation schemes developed in equilibrium [4] are applied: First the causality relation $\Sigma^c + \Sigma^{\bar{c}} = \Sigma^< + \Sigma^>$ of the self-energy is violated. Second, it was found that for stronger interactions singularities in the flow equations are induced making them numerically difficult to tackle [13]. Third, the FRG flow along the real axis has to pass the poles of the free resolvent making a numerical treatment very expensive for large systems with many discrete single-particle states [12]. The first (and possibly also the second) problem can be circumvented by choosing a cutoff in momentum instead of frequency space [14]. This provides a meaningful approach for homogeneous (bulk) materials, but not for the structured, mesoscopic systems we are mainly interested in. In such setups momentum is not a

good quantum number. We note that the third problem is present for all cutoff schemes on the real frequency or momentum axis.

For these reasons, we propose the use of a complex-valued flow parameter with imaginary part λ cutting off the Matsubara poles of the Fermi or Bose functions of the reservoirs and real parts Λ_r describing flowing chemical potentials, as defined by Eq. (1). It is essential to implement the cutoff in the distribution functions of the reservoirs and not in the initial distribution function of the system because the former determine the nonequilibrium occupation of the system in the steady state whereas the latter does not affect the steady state at all. The distribution functions of the reservoirs appear diagrammatically in the free lesser GF of reservoir r , given by $g_r^<(\omega) = \mp f_r(\omega) \times (g_r^{\text{Ret}} - g_r^{\text{Av}})(\omega)$ with $g_{kr}^{\text{Ret/Av}}(\omega) = 1/(\omega - \epsilon_{kr} \pm i\eta)$. As the insertion of the cutoff is merely a manipulation of the particle distribution, the causality relation is not violated.

A typical starting point of the FRG flow will be at $\lambda = \infty$ (with arbitrary Λ_r) which yields $f_r^\Lambda \equiv 0$ corresponding to an empty system with known properties. In particular any possible infrared divergence will be regularized at this point. The FRG flow stops at $(\{\Lambda_r = \mu_r\}_r, \lambda = 0)$, fully restoring all distribution functions. The path along which the FRG flows through the $(\{\Lambda_r\}_r, \lambda)$ space can be chosen in an arbitrary way without affecting the result at the end of the flow as long as the infinite hierarchy of equations is treated exactly. In the common case of truncations however, different paths may lead to different approximations for the vertex functions. Particular paths are defined by letting first flow λ to 0 while keeping the Λ_r constant and in a second step adjusting the Λ_r to μ_r . In the model discussed at the end of this Letter we find that the numerical solution is most stable if one sets $\Lambda_r = \mu_r$ right from the beginning.

Derivation of the flow equations.—The flow equations for the irreducible vertex functions can be derived by a simple diagrammatic procedure [12] in contrast to the formalism based on generating functionals [13]. The k -particle vertex function γ_k is defined as the sum of all one-particle irreducible diagrams with k amputated incoming lines and k amputated outgoing lines. An example is the self-energy $\Sigma \equiv \gamma_1$. A diagram D_k contributing to γ_k consists of vertices representing the interaction V , which are connected by directed lines representing the reservoir dressed GF $\mathcal{G}^\Lambda = [g^{-1} - \Sigma_{\text{res}}^\Lambda]^{-1}$ of the system. The lines depend on Λ via the reservoir self-energy $\Sigma_{\text{res}}^\Lambda = \sum_r \Sigma_r^\Lambda$, with $\Sigma_r^\Lambda(\omega) = (t^r)^\dagger g_r^\Lambda(\omega) t^r$ (in matrix notation) where the free propagator g_r^Λ of the reservoir contains f_r^Λ in its $<$ component. An irreducible diagram $D_k = D_k^\Lambda$ depends on Λ via its internal lines \mathcal{G}^Λ , which enter its value multiplicatively. Consequently the derivative $\partial_\Lambda D_k^\Lambda$ is given by product rule as a sum over all diagrams D_k^Λ which are identical to D_k^Λ except for having one differentiated GF $\partial_\Lambda \mathcal{G}^\Lambda$ among its lines. We represent $\partial_\Lambda \mathcal{G}^\Lambda$ diagrammatically by a crossed-out line. In order to determine

$\partial_\Lambda \gamma_k^\Lambda = \sum \partial_\Lambda D_k^\Lambda$ we thus have to calculate the sum off all diagrams D_k^Λ which result from crossing out any line in any diagram D_k^Λ contributing to γ_k^Λ .

Imagine amputating temporarily the crossed-out line from a diagram D_k^Λ . As D_k^Λ was irreducible, the remaining part is still connected and of such structure that it becomes irreducible when the crossed-out line is reinstalled. This structure is given by a chain of irreducible subdiagrams connected by single lines, which becomes a closed ring when the crossed-out line is reinstalled. Indeed, except for multiplicity (which cancels certain symmetry prefactors), the diagrams D_k^Λ are exactly all possible rings of irreducible subdiagrams closed by a crossed-out line. For an example see Fig. 1(a). In order to determine $\partial_\Lambda \gamma_k^\Lambda = \sum D_k^\Lambda$ let us first add up all diagrams D_k^Λ , which have identical ring structure and differ only in the form of the irreducible subdiagrams. The summation of all possible subdiagrams then yields vertex functions connected to a ring; see Fig. 1(b). By further summation of rings of vertex functions, which are identical except for self-energy insertions, we obtain full GFs $G^\Lambda = \mathcal{G}^\Lambda + \mathcal{G}^\Lambda \Sigma^\Lambda \mathcal{G}^\Lambda + \dots$ connecting the vertex functions and one propagator $S^\Lambda = \mathcal{G}^\Lambda \mathcal{G}^{\Lambda-1} [\partial_\Lambda \mathcal{G}^\Lambda] \mathcal{G}^{\Lambda-1} \mathcal{G}^\Lambda$ closing the ring; compare Fig. 1(c) (where the resulting ring contains only one vertex function).

Concluding, $\frac{\partial}{\partial \Lambda} \gamma_k^\Lambda(\nu'_1 \dots \nu'_k | \nu_1 \dots \nu_k)$ (with incoming indices ν_1, \dots, ν_k and outgoing indices ν'_1, \dots, ν'_k , where ν stand for frequency, state, and contour index) is determined as follows: Draw all rings consisting of vertex functions $\gamma_2^\Lambda, \gamma_3^\Lambda, \dots, \gamma_{k+1}^\Lambda$, which have the external indices ν'_1, \dots, ν_k all in all, and which are connected to rings by full propagator lines and exactly one full crossed-out propagator representing S^Λ . Evaluate these diagrams as usual, treating the vertex functions as normal vertices. Because of the special ring structure and the distinguished position of the crossed-out line there is no need for prefactors corresponding to symmetries or equivalent lines.

S^Λ has vanishing retarded and advanced components but nonzero lesser-component $S^{\Lambda, <} = G^{\Lambda, \text{Ret}}(\partial_\Lambda \Sigma_{\text{res}}^{\Lambda, <}) G^{\Lambda, \text{Av}}$ with $\partial_\Lambda \Sigma_{\text{res}}^{\Lambda, <} = \pm i \sum_r (\partial_\Lambda f_r^\Lambda) \Gamma_r$ and $\Gamma_r = i(\Sigma_r^{\text{Ret}} - \Sigma_r^{\text{Av}})$. In the λ direction due to

$$\frac{\partial}{\partial \lambda} f_r^\Lambda(\omega) = -T_r \sum_{\omega_n} \frac{\delta(|\omega_n^r| - \lambda)}{i\omega_n^r - \omega + \Lambda_r}, \quad (2)$$

at most one Matsubara frequency contributes to S^Λ . This

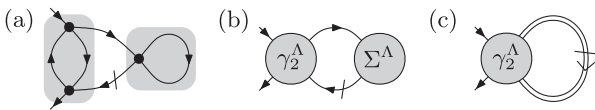


FIG. 1. (a) A diagram D_1^Λ contributing to $\partial_\Lambda \Sigma^\Lambda \equiv \partial_\Lambda \gamma_1^\Lambda$. The one-particle irreducible subdiagrams connected to a ring are marked by gray underlays. (b) When adding up all rings with the same structure, the subdiagrams sum to vertex functions. (c) Resumming the self-energy insertions yields the propagator S^Λ .

feature largely reduces the computational effort for a numerical evaluation of the flow along the λ direction and is the reason for calling S^Λ the single scale propagator in the Matsubara FRG. The flow along the Λ_r directions benefits from a similar advantage if the T_r are small. Consider, e.g., the case $\lambda = 0$. Then $\partial_{\Lambda_r} f_r^\Lambda(\omega)|_{\lambda=0} = -\partial_\omega f_r(\omega)|_{\mu_r=\Lambda_r}$ as a function of energy has a peak at $\omega = \Lambda_r$ of width $\sim T_r$. Frequency integration has to be carried out only around this peak, reducing the computational effort.

According to the diagrammatic rules formulated above, the single contribution to the flow of the self-energy $\partial_\Lambda \Sigma^\Lambda$ stems from the diagram in Fig. 1(c) yielding

$$\frac{\partial}{\partial \Lambda} \Sigma_{\nu'\nu}^\Lambda = \mp \frac{i}{2\pi} \sum_{\nu_1, \nu'_1} \gamma_2^\Lambda(\nu', \nu'_1 | \nu, \nu_1) S_{\nu_1 \nu'_1}^\Lambda. \quad (3)$$

In the special case of equilibrium and neglecting the renormalization of the two-particle vertex, it is straightforward to show that this RG equation is identical to the one of the Matsubara FRG [17,18].

Quantum wire with contact barriers.—As an application of our method we discuss nonequilibrium steady state transport through an interacting quantum wire (Luttinger liquid, LL), end-contacted through tunnel barriers to two noninteracting reservoirs. In equilibrium strong barriers induce slowly decaying (\sim inverse distance) oscillatory effective potentials of range proportional to the thermal length $\frac{v_F}{T}$ in the LL, which lead to a one-particle spectral weight that goes as $\rho(\omega) \sim \max\{|\omega - \mu|, T\}^{\alpha_B}$ close to the barrier [19]. The boundary exponent is given by $\alpha_B = \frac{1}{K} - 1$, where the LL parameter K depends on the strength of the interaction and the filling. For a long wire contacted via high tunnel barriers by noninteracting leads this induces a power law for the linear conductance $G \sim T^{\alpha_B}$ [18]. We show that finite bias voltage and asymmetric coupling to the leads give rise to two different exponents. We use a tight-binding model for the noninteracting part $H_0 = H_S^{(0)} + H_{\text{res}} + H_T$

$$H_0 = - \sum_{\substack{j \in \mathbb{Z} \\ j \neq 0, N}} c_{j+1}^\dagger c_j - \tau_L c_1^\dagger c_0 - \tau_R c_{N+1}^\dagger c_N + \text{H.c.} \quad (4)$$

and take $V = U \sum_{j=1}^{N-1} \rho_j \rho_{j+1}$ for the interaction, with $\rho_j = c_j^\dagger c_j - \frac{1}{2}$. The semi-infinite noninteracting parts $j < 1$ and $j > N$ of the chain represent the left (L) and right (R) reservoir. We choose $\Lambda_{L,R} \equiv \mu_{L,R}$ and let λ flow from ∞ to 0. With $f^{\lambda=\infty} \equiv 0$ the flow of the interacting part of the self-energy starts at $\Sigma_{ij}^{\lambda=\infty, \text{Ret}} = 0$. We truncate the hierarchy of flow equations by setting $\gamma_2^\Lambda \simeq \gamma_2^{\lambda=\infty} = \bar{v}$, an approximation which was used successfully in equilibrium [17] and is justified if the interaction is sufficiently small to neglect the inelastic processes it generates. In equilibrium our truncated flow equation is identical to that of the Matsubara FRG and hence known to produce results which agree qualitatively to those obtained by other methods for interactions such that $1/2 < K \leq 1$. Quantitative agree-

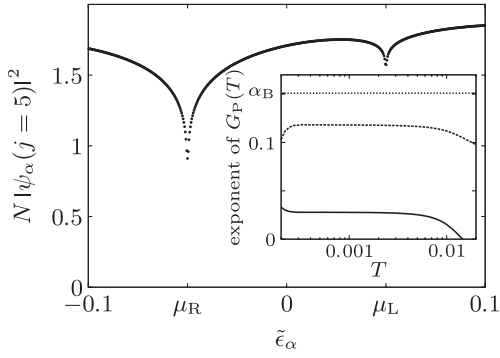


FIG. 2. Suppression of the one-particle wave function as function of energy near the boundary (at site 5) at $T = 10^{-4}$. Inset: Exponent of the conductance through a probe lead weakly coupled to site 5 as function of T for $\mu_P = \mu_L = 0.05$ (solid line) and $\mu_P = \mu_R = -0.05$ (dashed line). Using the same truncation scheme in equilibrium ($\mu_L = \mu_R = 0$), the functional RG yields the boundary exponent $\alpha_B \approx 0.151$ (dotted line). $N = 20\,000$, $U = 0.5$, $\tau_L = 0.075$, $\tau_R = 0.15$.

ment is achieved for $|1 - K| \ll 1$. In particular, the scaling exponent comes out correctly in leading order in U [17,18]. For small tunneling $\tau_r \ll 1$, the flow equation is given by

$$\frac{\partial \Sigma_{ij}^{\lambda, \text{Ret}}}{\partial \lambda} = - \sum_{r, \omega_n^r} T_r \frac{\Gamma_r}{\Gamma} \delta(|\omega_n^r| - \lambda) \bar{v}_{ik,jl} G_{lk}(i\omega_n^r + \mu_r) \quad (5)$$

with $\Gamma = \Gamma_L + \Gamma_R$, $\Gamma_L = \Gamma_L(E)_{11}$, and $\Gamma_R = \Gamma_R(E)_{NN}$ [the energy dependence of $\Gamma(E)$ can be neglected near the Fermi levels of the reservoirs]. Thus the contribution of each reservoir is weighted by Γ_r , arising from the fact that the noninteracting occupation of states in the wire is given by $[\Gamma_L f_L(\epsilon) + \Gamma_R f_R(\epsilon)]/\Gamma$. During the FRG flow, each reservoir contribution generates oscillations of the effective potential which influence the other's formation via back coupling through Eq. (5). This mutual influence can be neglected for small interaction leading to two independent oscillations with period given by the Fermi wavelength and amplitude proportional to Γ_r of the corresponding reservoir. We define in the single-particle subspace an effective Hamiltonian of the quantum wire by $h_{\text{eff}} = H_S^{(0)} + \Sigma^{\lambda=0, \text{Ret}}$ with eigenfunctions ψ_α and eigenvalues $\tilde{\epsilon}_\alpha$. The area of the discrete peak at energy $E \sim \tilde{\epsilon}_\alpha$ of the local spectral density $\rho(E)_{jj}$ at site j is proportional to $|\psi_\alpha(j)|^2$, which scales as $\max\{|\tilde{\epsilon}_\alpha - \mu_L|, T_L\}^{\alpha_L} \times \max\{|\tilde{\epsilon}_\alpha - \mu_R|, T_R\}^{\alpha_R}$ if j is close to the boundary [20], where $\alpha_r = \alpha_B(\mu_r)\Gamma_r/\Gamma$; see Fig. 2. Experimentally, this can be tested by attaching weakly a probe lead with chemical potential μ_P to the wire near the left or right boundary at position j_P . Using the Landauer-Büttiker formula we obtain for $\Gamma_P \ll \Gamma_L, \Gamma_R$ and T_P larger than the level spacing that the conductance in the third lead is given by

$$G_P = e \frac{\partial I_P}{\partial \mu_P} = -e^2 \Gamma_P \sum_\alpha |\psi_\alpha(j_P)|^2 f_P'(\tilde{\epsilon}_\alpha). \quad (6)$$

Thus the conductance G_P scales as T^{α_r} for $\mu_P = \mu_r$, with

$r = L, R$, as shown in the inset of Fig. 2. To obtain this result we used a particular path in the complex “cutoff space.” The exponents remain unchanged if a different path is chosen. Similar results were obtained applying bosonization to an effective field theory [21].

Summary.—We have shown that the FRG can be generalized in a natural and numerically efficient and stable way to study nonequilibrium transport through interacting systems by introducing a complex flow parameter to the distribution function of each reservoir. We explained how the flow equations of the FRG can be understood in terms of diagrams and set up diagrammatic rules to determine the flow equations. We applied our method to a microscopic model for steady state transport through an end-contacted, interacting quantum wire and found that nonequilibrium changes the scaling exponents by making them dependant on the height of the contact barriers.

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