Exploring excited eigenstates of many-body systems using the functional renormalization group

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We introduce approximate, functional renormalization group based schemes to obtain correlation functions in pure excited eigenstates of large fermionic many-body systems at arbitrary energies. The algorithms are thoroughly benchmarked and their strengths and shortcomings are documented using a one-dimensional interacting tight-binding chain as a prototypical testbed. We study two ‘toy applications’ from the world of Luttinger liquid physics: the survival of power laws in lowly-excited states as well as the spectral function of high-energy ‘block’ excitations which feature several single-particle Fermi edges.

I. INTRODUCTION

The complexity of diagonalizing the Hamiltonian or solving the time-dependent Schrödinger equation of interacting quantum problems grows exponentially with the number of particles involved. Over the last decades, a plethora of techniques were developed to study the physics of many-body systems which are in thermal equilibrium (most importantly in the ground state) as well as the out-of-equilibrium dynamics induced by pre-defined initial states. In contrast, far less attention was devoted to devising methods which can access pure excited eigenstates at arbitrary energies. While some progress has been made recently (which was partly triggered by the newly-emerging field of many-body localization,1,2 a phenomenon that cannot be investigated via thermal ensembles), a ‘golden standard’ approach has yet to be discovered. Exact diagonalization is restricted to small systems. Proposals how to obtain a matrix product representation of excited states are limited to one dimension and work only if the area law holds (i.e., in localized phases).3–7 Analytical approaches8 such as the Bethe ansatz can only be used for integrable models. Hence, it is desirable to develop additional pure state techniques which feature their own, unique set of strengths and shortcomings.

In this paper, we introduce several, functional renormalization group (FRG) based algorithms to compute correlation functions in pure excited states of fermionic many-body systems. The FRG extends standard Feynman perturbation theory by incorporating an RG idea on the level of Green’s functions.9,10 The method was first set up in thermal equilibrium (i.e., on the Matsubara axis) where it was used to study, e.g., instabilities in 2d systems11–13 or the properties of quantum dots and wires.14–17 Later on, the FRG was extended to Keldysh space and problems out of equilibrium were tackled18–24 (see also Refs. 25–28 for other developments). The key drawback of the method is the need to truncate its hierarchy of flow equations; thereafter, all results are only controlled up to a certain (usually first or second) order in the two-particle interaction while still including a RG resummation of higher-order contributions. Thus, their validity needs to be assessed carefully on a case-by-case basis. On the upside, the FRG can be used to access large systems and is not a low-entanglement framework. Thus, an approximate, FRG-based description of correlation functions in pure excited states would complement more accurate predictions obtained, e.g., via exact diagonalization. It is the goal of this work to develop and test such a ‘xFRG’ approach.

One way to obtain a pure eigenstate of a generic Hamiltonian is to analytically determine an excited state of a noninteracting system and to then switch on interactions adiabatically. We illustrate how to simplify the real-time Keldysh FRG of Ref. 21 under the assumption of adiabaticity in order to efficiently implement this protocol (this method will be called xFRG-t-Γ). Thereafter, a new RG cutoff scheme is devised which is specifically tailored to the adiabatic nature of the problem (xFRG-t-ρ). We briefly discuss how to obtain an eigenstate directly (i.e., without resorting to the time evolution protocol) via a coupling to a non-thermal bath (xFRG-ω).

After developing the different xFRG schemes and deriving the corresponding flow equations (Sec. III), we carry out several algorithmic tests and document the limitations and promises of our approach (Sec. IV). Thereafter, two ‘toy applications’ from the world of one-dimensional Luttinger liquid physics are presented: the survival of power laws in lowly-excited states as well as the spectral function of high-energy ‘block’ excitations which feature multiple Fermi edges (Sec. V). We include an overview of the FRG approach to both equilibrium and nonequilibrium problems and introduce several improvements to these methods (Sec. II), which form the basis for the new developments presented in this paper.
II. REVISITING MATSUBARA AND KELDYSH FRG

In this section we will first introduce the models discussed in this paper as well as the notion of Green’s functions. We then review the FRG formalism in Mastubara and Keldysh space which allow one to tackle equilibrium and time-dependent scenarios, respectively. The xFRG builds upon these concepts, and its derivation in Sec. III will employ many of the relations that we discuss here. We also present several algorithmic improvements that cannot be found in the existing literature.

A. Model

We set up the FRG for general fermionic, particle-number conserving Hamiltonians with single- and two-particle contributions:

\[ H = H^0 + H^{\text{int}} \]

\[ H^0 = \sum_{i,j} h_{i,j}^0 c_i^\dagger c_j \]

\[ H^{\text{int}} = \frac{1}{4} \sum_{i,j,k,l} u_{i,j,k,l} c_i^\dagger c_j^\dagger c_l c_k, \]

where \( c_i^{(t)} \) are the fermionic annihilation (creation) operators and \( i \) denotes the single-particle index. \( H^0 \) is the quadratic part of the Hamiltonian while \( H^{\text{int}} \) constitutes the two-particle interaction. The single-particle matrix representation of \( H^0 \) is denoted by \( h^0 \).

As an application, we will later on study one-dimensional tight-binding chains with \( N \) sites. We will therefore frequently discuss how the final FRG flow equations can be solved efficiently for such models.

B. Green’s functions

1. Definitions

An efficient way to describe nonequilibrium systems is the Keldysh formalism. Therein, the real-time single-particle correlation functions are defined as

\[ [G^{\text{ret}}(t,t')]_{i,j} = -i\theta(t - t') \langle c_i(t)c_j(t') \rangle_{\rho_0} \]

\[ G^{\text{adv}}(t,t') = [G^{\text{ret}}(t',t)]^\dagger \]

\[ [G^{<}(t,t')]_{i,j} = -i \langle c_j(t')c_i(t) \rangle_{\rho_0} \]

\[ G^{>}(t,t') = -[G^{<}(t',t)]^\dagger \]

\[ G^{K}(t,t') = G^{<}(t,t') + G^{>}(t,t') \]

and are referred to as retarded, advanced, lesser, greater and Keldysh Green’s function. The initial density matrix is given by

\[ \rho_0 = \frac{1}{Z} \exp(-K), \quad Z = \text{Tr} \left[ \exp(-K) \right] \]

\[ K = \sum_{i,j} \bar{K}_{i,j} c_i^\dagger c_j, \quad \langle c_i^\dagger c_j \rangle_{\rho_0} =: \bar{n}_{j,i} = \left( \frac{1}{e^{\epsilon_i/\theta} + 1} \right)_{i,j}, \]

and \( \langle \ldots \rangle_{\rho_0} = \text{Tr} \left( \rho_0 \ldots \right) \) denotes the corresponding expectation value. The time arguments are to be understood in the Heisenberg picture, and \([A,B]_-\) refers to the commutator.

2. The noninteracting case

If the system is described by a time-independent, noninteracting Hamiltonian \( H^0 \), obtaining the Green’s functions is straightforward. In the basis where \( H^0 \) (but not necessarily \( \rho_0 \)) is diagonal,

\[ H^0 = \sum_k c_k^\dagger c_k, \]

one finds

\[ [G^{\text{ret}}_0(t,t')]_{k,k'} = -i\theta(t - t')e^{-i\epsilon_k(t-t')}\delta_{k,k'} \]

\[ [G^{<}_0(t,t')]_{k,k'} = i e^{-i\epsilon_k t'} \langle c_k^\dagger c_k \rangle_{\rho_0} e^{i\epsilon_k t} \]

which transformed to the original basis yields

\[ G^{\text{ret}}_0(t,t') = -i\theta(t - t')e^{-i\epsilon_k(t-t')} \]

\[ [G^{<}_0(t,t')]_{i,j} = i e^{-i\epsilon_k t'} \langle c_j^\dagger c_i \rangle_{\rho_0} e^{i\epsilon_k t'} \]

\[ \Rightarrow G^{K}_0(t,t') = -i G^{\text{ret}}_0(t,0) (1 - 2\bar{n}) G^{\text{adv}}_0(0, t'). \]

Here and in the following, matrix multiplications are implied in expressions such as \( G^{\text{ret}}_0(t,0) n G^{\text{adv}}_0(0, t') \).

If \( H^0 \) and \( \rho_0 \) commute (which is true, e.g., for a thermal state), the lesser and Keldysh Green’s functions take a more recognizable form:

\[ [H^0, \rho_0]_- = 0 \Rightarrow G^{<}_0(t,t') = ie^{-i\epsilon_k(t-t')}\bar{n}, \]

\[ G^{K}_0(t,t') = -ie^{-i\epsilon_k(t-t')} (1 - 2\bar{n}). \]

(3)

Analogously to Eq. (2), the case of a time-dependent noninteracting Hamiltonian can be treated:

\[ G^{\text{ret}}_0(t,t') = -i\theta(t - t’) T e^{-i \int_0^{t'} dt' h_k(t')} \]

\[ G^{<}_0(t,t') = i G^{\text{ret}}_0(t,0) n G^{\text{adv}}_0(0, t) \]

\[ G^{K}_0(t,t') = -i G^{\text{ret}}_0(t,0) (1 - 2\bar{n}) G^{\text{adv}}_0(0, t'). \]
The two-particle interaction is taken into account via a self-energy. The connection between the noninteracting and interacting Green’s function is given by a Dyson equation:

\[ G(t, t') = G_0(t, t') + \int_0^\infty dt_1 dt_2 G_0(t, t_1) \Sigma(t_1, t_2) G(t_2, t') \]

where we employed Eq. (4). We will later on show that a leading-order FRG scheme yields self-energies which are time-local and have a vanishing Keldysh component:

\[ \Sigma^R(t, t') = 0, \quad \Sigma^T(t, t') = -\Sigma^R(t) \delta(t - t'), \]

which renders it particularly simple to evaluate Eq. (6):

\[
G^R(t, t') = -i \theta(t - t') e^{-i \int_{t'}^t dt [K^R(t') + \Sigma^R(t')]} G^R(t, 0) \]

Hence, \( h^0 + \Sigma^R \) takes the role of an effective Hamiltonian. Furthermore, the following group property holds in this situation:\(^{21}\)

\[ T e^{i(\int_{t'}^t dt [\hat{H} + \Sigma^R(t)])} T e^{i(\int_{t'}^t dt [\hat{H} + \Sigma^R(t)])} = e^{-i \int_{t'}^t dt [\hat{H} + \Sigma^R(t)]} G^R(t, t') \]

that will allow for a major simplification of the FRG flow equations.

4. Green’s functions: steady state and equilibrium

If the system reaches a steady state, all correlation functions in this state only depend on the time differences. Thus, one can define the Fourier transform as

\[
G^R(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega(t-t')} G^R(t-t') = [G^\text{adv}(\omega)]^\dagger
\]

\[
G^K(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega(t-t')} G^K(t-t') = -[G^K(\omega)]^\dagger,
\]

where we send the initial time to \(-\infty\). In the noninteracting, time-independent case, the retarded Green’s function takes the standard form

\[
G^R_0(\omega) = \frac{1}{\omega - h^0 + i0^+}.
\]

In a thermal state (where \( \rho_0 \) is not necessarily of the form of Eq. (1)),

\[
\rho_0 = e^{-\beta H}/\text{Tr} \left( e^{-\beta H} \right),
\]

the fluctuation-dissipation theorem (FDT) holds:

\[
G^K(\omega) = [1 - 2n_F(\omega)] \left[ G^R(\omega) - G^\text{adv}(\omega) \right]
\]

with the Fermi distribution \( n_F \)

\[
1 - 2n_F(\omega) = \tanh \left( (\omega - \mu)/\beta \right)
\]

at inverse temperature \( \beta \) and chemical potential \( \mu \). Hence, all single-particle correlation functions can be extracted from \( G^R \).

The Dyson equation (see Eq. (6)) in a steady state reads

\[
G^R(\omega) = G^R_0(\omega) + G^R_0(\omega) \Sigma^R(\omega) G^R(\omega)
\]

\[
G^K(\omega) = G^R(\omega) \left[ G^R_0(\omega) \Sigma^R(\omega) G^R(\omega) \right]^{-1} + \Sigma^K(\omega) G^\text{adv}(\omega)
\]

\[
= G^R(\omega) \Sigma^K(\omega) G^\text{adv}(\omega),
\]

where in the second line of the last equation decay processes are assumed to lead to a fading memory of the initial density \( \rho_0 \) in Eq. (6).

5. Analytic continuation

We now elaborate how to obtain the real-time Keldysh Green’s function of an effectively noninteracting, time-independent system efficiently using an analytic continuation; this will be important for later applications. Using the inverse Fourier transform, we find

\[
G^K(t, t) = \frac{1}{2\pi} \int d\omega \left[ 1 - 2n_F(\omega) \right] \left[ G^R_0(\omega) - G^\text{adv}_0(\omega) \right].
\]

The time label \( t \) in equilibrium is arbitrary; we keep it to differentiate between time- and frequency-space. This expression can be recast as a contour integral,

\[
G^K_0(t, t) = \frac{1}{2\pi} \int dz e^{i\omega_0 t} \left[ 1 - 2n_F(z) \right] G^\text{eq}(z),
\]

where we introduced the equilibrium Green’s function:

\[
G^\text{eq}(z) = \frac{1}{\frac{z}{z - h^0}}
\]
⇒ \( G^{\text{ret}}(\omega) = G^{\text{eq}}(\omega + i0^+) \), \( G^{\text{adv}}(\omega) = G^{\text{eq}}(\omega - i0^+) \).

The contours \( \gamma_\pm \) are schematically shown in Fig. 1: the convergence factor is chosen differently in the upper and lower half of the complex plane to ensure decay in the respective regions.

The integrand of Eq. (11) has poles in the complex plane which are located at the eigenenergies of the Hamiltonian as well as at the fermionic Matsubara frequencies \( i\omega_n \in i\frac{2\pi}{\beta}(\mathbb{Z} + \frac{1}{2}) + \mu \); the latter originate from the Fermi distribution. Using the residue theorem, the contour can be deformed as depicted in Fig. 1. Due to the choice of the convergence factors, there are no contributions from the parts of the contour at infinite distance. This yields

\[
G_0^K(t, t) = \frac{2i}{\beta} \sum \alpha \, e^{-|\omega|\beta} G_0^{\text{eq}}(i\omega_n + \mu) \tag{12}
\]

and in the limit of \( T \rightarrow 0 \)

\[
G_0^K(t, t) = \frac{i}{\pi} \int d\omega e^{-|\omega|\beta} G_0^{\text{eq}}(i\omega + \mu) = \frac{i}{\pi} \lim_{A \rightarrow \infty} \int_{-A}^{A} d\omega e^{\text{eq}}(i\omega + \mu). \tag{13}
\]

One can show that for tight-binding models of linear dimension \( N \), the diagonal and first off-diagonal components of this expression can be evaluated in \( \mathcal{O}(N) \) operations.\textsuperscript{14,29} This will be important for later applications where we want to study Luttinger liquid power-laws for \( N \gg 1 \).

\[ G_0 \rightarrow G_0^A, \]

which is chosen such that all vertex functions at the initial value of the cutoff parameter \( \Lambda \) are easy to evaluate and the physical Green’s function is restored at its final value. The FRG formalism yields an infinite set of differential equations which can be solved after a truncation. In this context, we restrict ourselves to the lowest order approximation, which only consists of a single equation of the schematic form:

\[
\partial_\Lambda \Sigma^A = u S^A
\]

\[
S^A = \partial^A \Sigma^A := -G^A \left[ \partial_\Lambda \left( G_0^A \right)^{-1} \right] G^A. \tag{14}
\]

\( S^A \) is referred to as single-scale propagator, which in the case that the cutoff enters as a self-energy (see, e.g. Sec. II E, II F) simplifies to

\[
S^A = G^A \left( \partial_\Lambda \Sigma^A_{\text{cut}} \right) G^A. \tag{15}
\]

The precise form of Eq. (14) varies depending on the context and will be specified further in the later sections, where we also add the necessary indecies and contractions. This scheme includes all contributions of first order as well as some terms of arbitrarily high order and regularizes infrared divergences.

\[ \text{D. Matsubara FRG} \]

The simplest way to introduce a infrared regularization in Matsubara frequency space (i.e., in equilibrium) is a sharp cutoff\textsuperscript{18}

\[
G_0^A(i\omega) = G_0(i\omega) \theta(|\omega| - \Lambda)
\]

\[
S^A(i\omega) = [\delta(\omega - \Lambda) + \delta(\omega + \Lambda)] G_0^A(i\omega) \tag{16}
\]

which results in the following flow equation for the self-energy:

\[
\partial_\Lambda \Sigma^A_{i,j} = -\frac{1}{2\pi} \sum_{k,l} \sum_{\omega = \pm \Lambda} u_{i,k,j,l} \left( \frac{1}{i\omega - h_0 - \Sigma^A} \right)_{i,k}, \tag{17}
\]

where \( \Lambda \) is integrated from \( \infty \) to 0. If one removes the feedback of the self-energy on the right-hand side of this equation, one obtains standard perturbation theory. This illustrates that the FRG enhances perturbation theory by including a self-energy feedback; an integral is turned into a differential equation that treats different energy-scales successively in an RG sense.

\[ \text{E. Keldysh FRG} \]

We will now briefly present the FRG framework in Keldysh space for steady states since this will serve as
the basis for a generalization to excited states later. On
the Keldysh axis, we employ a auxiliary reservoir cutoff
scheme which is implemented by introducing a wide-band
bath that couples to every single-particle degree of
freedom of the system with a strength $\Lambda$. Such a reservoir
(which itself is in equilibrium) can be taken into account
using a self-energy of the form

$$
\Sigma_{\text{cut}}^\Lambda(\omega) = -i \Lambda \n_{\text{cut}}(\omega) [\Sigma_{\text{cut}}^\Lambda(\omega) - \Sigma_{\text{cut}}^{\text{adv}}(\omega)]
$$

(18)

where $\n_{\text{cut}}(\omega)$ is its Fermi function and the second equa-
tion is enforced by the fluctuation-dissipation theorem.
Thus, the reservoir-dressed Green’s function is given by

$$
G_{\text{cut}}^\Lambda(\omega) = \frac{1}{G_0^\Lambda(\omega)^{-1} + i \Lambda \n_{\text{cut}}(\omega) - \Sigma_{\text{cut}}^\Lambda(\omega)}
$$

and one can show (compare the retarded and Keldysh component of Eq. (15)) that

$$
S_{\text{cut}}^\Lambda(\omega) = \partial^\Lambda_t G_{\text{cut}}^\Lambda(\omega) = -i G_{\text{cut}}^\Lambda(\omega) G_{\text{cut}}^\Lambda(\omega)
$$

$$
S_{K}^\Lambda(\omega) = \partial^\Lambda_t G_{K}^\Lambda(\omega)
$$

$$
= S_{\text{cut}}^\Lambda(\omega) \left[ \Sigma_{\text{cut}}^\Lambda(\omega) + \Sigma_{K}^\Lambda(\omega) \right] G_{\text{adv}}^\Lambda(\omega)
$$

$$
+ G_{\text{cut}}^\Lambda(\omega) \left[ \Sigma_{\text{cut}}^\Lambda(\omega) + \Sigma_{K}^\Lambda(\omega) \right] S_{\text{adv}}^\Lambda(\omega)
$$

$$
+ G_{\text{cut}}^\Lambda(\omega) \left[ \partial^\Lambda_t \Sigma_{\text{cut}}^\Lambda(\omega) \right] G_{\text{adv}}^\Lambda(\omega)
$$

(19)

$$
\partial^\Lambda_t \Sigma_{i,j}^{\text{ret},\Lambda} = -\frac{i}{4\pi} \sum_{k,l} u_{i,k,j,l} \int d\omega \left[ S_{\text{cut}}^\Lambda(\omega) \right]_{l,k}
$$

$$
\text{FDT} = \frac{i}{4\pi} \sum_{k,l} u_{i,k,j,l} \int d\omega \text{sgn}(\omega)
$$

$$
\left[ \partial^\Lambda_t G_{\text{cut}}^\Lambda(\omega) - \partial^\Lambda_t G_{\text{adv}}^\Lambda(\omega) \right]_{l,k}
$$

$$
= -\frac{i}{4\pi} \sum_{k,l} u_{i,k,j,l} \int d\omega \text{sgn}(\omega)
$$

$$
\left[ i \partial^\Lambda_t G_{\text{cut}}^\Lambda(\omega) + i \partial^\Lambda_t G_{\text{adv}}^\Lambda(\omega) \right]_{l,k}
$$

$$
= -\frac{i}{4\pi} \sum_{k,l} u_{i,k,j,l} \left[ G_{\text{cut}}^\Lambda(0) + G_{\text{adv}}^\Lambda(0) \right]_{l,k}
$$

F. Time-dependent FRG

A time-dependent formulation of the FRG which em-

Note that the Keldysh FRG was first developed for

the FRG flow equations truncated to leading order are
given by (a detailed derivation of this can be found in

Ref. 21):

$$
\partial^\Lambda_t \Sigma_{i,j}^{\text{ret},\Lambda}(t, t') = i \delta(t - t') \sum_{k,l} \left[ S_{i,j}^{K}(t, t) \right]_{l,k} u_{i,k,j,l}(t)
$$

$$
\partial^\Lambda_t \Sigma_{i,j}^{K}(t, t')
$$

$$
= i \delta(t - t') \sum_{k,l} \left( S_{i,j}^{\text{ret},\Lambda} + S_{i,j}^{\text{adv},\Lambda} \right)_{l,k}(t, t) u_{i,k,j,l}(t)
$$

(21)
with the single-scale propagator (see Eq. (15))

$$S^{\text{ret},A}(t,t') = \int dt_1 dt_2 G^{\text{ret},A}(t,t_1) \left[ \partial_\Lambda \Sigma^{\text{cut}}_{\text{ret},A}(t_1,t_2) \right] G^{\text{ret},A}(t_2,t')$$

and

$$S^{K,A}(t,t') = \int dt_1 dt_2 \left\{ G^{\text{ret},A}(t,t_1) \left[ \partial_\Lambda \Sigma^{\text{cut}}_{\text{ret},A}(t_1,t_2) \right] G^{\text{ret},A}(t_2,t') + G^{\text{ret},A}(t,t_1) \left[ \partial_\Lambda \Sigma^{\text{cut}}_{\text{ret},A}(t_1,t_2) \right] G^{\text{ret},A}(t_2,t') + G^{K,A}(t,t_1) \left[ \partial_\Lambda \Sigma^{\text{cut}}_{\text{cut},A}(t_1,t_2) \right] G^{\text{cut},A}(t_2,t') \right\},$$

(22)

where $G^A$ refers to the full Green’s function obtained via Eq. (6). Due to the infinite temperature of the auxiliary reservoir, the cutoff $\Sigma^{\text{cut}}_{\text{cut}}$ used here has a vanishing Keldysh component (see Eq. (20)). The above equation then takes the form

$$S^{\text{ret},A}(t,t') = -i \int dt_1 G^{\text{ret},A}(t,t_1) G^{\text{ret},A}(t_1,t')$$

$$\Rightarrow S^{K,A}(t,t') = \partial_\Lambda \left[ G^{\text{ret},A}(t,0)(1 - 2\bar{n})G^{\text{adv},A}(0,t') \right]$$

$$+ G^{\text{ret},A}(t,0)(1 - 2\bar{n})G^{\text{adv},A}(0,t')$$

$$+ G^{\text{ret},A}(t,0)(1 - 2\bar{n})S^{\text{adv},A}(0,t').$$

(23)

Thus, in this scheme, the Keldysh self-energy does not flow:

$$\partial_\Lambda \Sigma^{K,A}(t,t') = 0$$

$$\partial_\Lambda \Sigma^{\text{ret},A}_{i,j}(t,t') = i\delta(t - t') \sum_{k,l} \left[ S^{K,A}(t,t) \right]_{i,k} u_{i,k,j,l}(t)$$

The initial conditions correspond to the self-energy contribution of the thermalized system at infinite temperature:

$$\Sigma^{K,A=\infty}(t,t') = 0$$

$$\Sigma^{\text{ret},A=\infty}_{i,j}(t,t') = \frac{1}{2} \delta(t - t') \sum_{k,l} u_{i,k,j,l}(t).$$

Hence, the Keldysh self-energy remains zero throughout the flow and the retarded self-energy is time-local. This type of self-energy has been discussed in Eq. (7) and Eq. (8).

Due to the time-local structure of the self-energy, the group property presented in Eq. (8) holds and the single-scale propagator of Eq. (23) can be simplified further:

$$G^{\text{ret},A}(t,t') = (t - t')G^{\text{ret},A}(t,t')$$

$$S^{K,A}(t,t') = (t + t')G^{K,A}(t,t'),$$

resulting in the final form of the flow equations:

$$\partial_\Lambda \Sigma^{K,A}(t,t') = 0$$

$$\partial_\Lambda \Sigma^{\text{ret},A}_{i,j}(t,t') = 2i t \delta(t - t') \sum_{k,l} \left[ G^{K,A}(t,t) \right]_{i,k} u_{i,k,j,l}(t).$$

(24)

One can show that the causality relation is conserved within this FRG scheme. By virtue of group property (see Eq. (8)) $G^{K,A}$ can be computed sequentially:

$$G^{K,A}(t + \Delta, t + \Delta)$$

$$= -i G^{\text{ret},A}(t + \Delta, 0)(1 - 2\bar{n})G^{\text{adv},A}(0, t + \Delta)$$

Eq. (24)

$$E^{\text{eq}} = -i G^{\text{ret},A}(t + \Delta, t)G^{\text{ret},A}(t, 0)(1 - 2\bar{n})$$

$$G^{\text{adv},A}(0, t)G^{\text{adv},A}(t, t + \Delta)$$

$$= G^{\text{ret},A}(t + \Delta, t)G^{K,A}(t, t)G^{\text{adv},A}(t, t + \Delta).$$

Thus, the computationally most expensive part in this scheme is the time evolution (i.e., calculating and applying $G^{\text{ret}/\text{adv},A}$). In the case of a tight-binding chain, one can make use of a Trotter decomposition of the (in this case tri-diagonal) effective Hamiltonian to speed up the numerics: For a tri-diagonal matrix $M$ we define the block diagonal matrices $M^A$ and $M^B$ as

$$M_{i,i} = a_i \quad M_{i,i+1} = \begin{cases} b_i & \text{if } i \text{ even} \\ b_{i+1} & \text{if } i \text{ odd} \end{cases}$$

$$M^B = M - M^A$$

such that $M = M^A + M^B$. The Baker-Campbell-Hausdorff formula then yields

$$e^M = e^\frac{M^A}{2} e^\frac{M^B}{2} + O\left(\|M\|^3\right)$$

$$\lim_{N \to \infty} \prod_{i=1}^N e^\frac{M^A}{2N} e^\frac{M^B}{2N} e^\frac{M^A}{2N} = \frac{M^A}{2N} \frac{M^B}{2N} \frac{M^A}{2N}.$$ 

Hence, the error is controlled by the size of $\|M/N\|$, where $\| \cdot \|$ denotes the matrix norm. For the applications considered later (i.e., one-dimensional tight-binding models), it is straightforward to reach convergence.

As the exponential function is easily evaluated for this kind of block diagonal matrices, the above provides a computationally efficient way to calculate the retarded and Keldysh Green’s function. For large time intervals the most expensive part is to compute the sparse-dense-product $G^{\text{ret}}(t + \Delta,t)G^{K}(t,t)G^{\text{adv}}(t, t + \Delta)$, as $G^K(t,t)$ will generally be dense for large times, even if the initial $\bar{n}$ is sparse.

### III. EXCITED STATE FRG

We now introduce three ways to obtain correlation functions in excited eigenstates of an interacting Hamiltonian using the FRG.

The first two are based on an adiabatic time-evolution: The system is first prepared in an excited eigenstate of the noninteracting system and the interaction is then adiabatically turned on. This process is approximated using the functional renormalization group in real-time Keldysh space.
The third method employs the stationary-state Keldysh FRG of Sec. II E; excited states are targeted via a generalization of the reservoir cutoff scheme known from equilibrium.

A. xFRG-$t$-$\Gamma$: Adiabatic time-evolution in Keldysh space with a reservoir cutoff

1. Time-space formulation

The goal is to use the time-dependent FRG described in Sec. II F to approximate the evolution of an excited eigenstate of the noninteracting system when interactions are switched on adiabatically. Since the self-energy is time-local in this scheme,

$$h(t) := h^0 + \Sigma^\text{ret}(t)$$

takes the place of an effective single-particle Hamiltonian. We suppress the $A$-dependence to keep the expressions more readable and introduce the notation

$$h(t) |\Psi_i(t)\rangle = \epsilon_i(t) |\Psi_i(t)\rangle$$

$$h(t) \in \mathbb{C}^{N \times N}, \ |\Psi_i(t)\rangle \in \mathbb{C}^N$$

$$\epsilon_i(t) < \epsilon_j(t) \quad \forall i < j$$

$$|\epsilon_i(t) - \epsilon_j(t)| > \Delta \quad \forall i,j,t,$$

where $\epsilon_i(t)$ and $|\Psi_i(t)\rangle$ denote the instantaneous single-particle eigenvalues and eigenstates of the matrix $h(t)$. $\Delta$ is an arbitrary, non-zero gap that ensures the absence of level crossings. The initial density matrix associated with a pure many-body eigenstate of the noninteracting, initial Hamiltonian is characterized by a sequence of occupations $n_i$ of the single-particle eigenstates $|\Psi_i(0)\rangle$ of $h^0$:

$$\tilde{n}(t = 0) = \sum_i n_i |\Psi_i(0)\rangle \langle \Psi_i(0)|, \ n_i \in \{0,1\}. \quad (25)$$

If the rate of change of the effective Hamiltonian $h(t)$ is slow enough, the time evolution of this matrix is given by

$$\tilde{n}(t) = \sum_i n_i |\Psi_i(t)\rangle \langle \Psi_i(t)|$$

(26)

with the same sequence of $n_i$.

We can now further simplify the time-dependent FRG flow equations in the adiabatic limit. Using Eq. (7), the Keldysh Green’s function can be written as

$$G^K_{A}(t,t) = -ie^{-2\Lambda t} \left[ 1 - 2G^{\text{ret},A=0}(t,0)\tilde{n}(t = 0)G^{\text{adv},A=0}(0,t) \right]$$

$$= -ie^{-2\Lambda t} \left[ 1 - 2\tilde{n}(t) \right],$$

(27)

where we note that the time evolution in the third line is performed in absence of the auxiliary reservoir. Thus, the levels are discrete and the considerations of Eq. (26) apply. $\tilde{n}^\Lambda$ only implicitly depends on $\Lambda$ (the eigenstates will change with the flow). Under these circumstances, the flow equation (24) can be rewritten conveniently by the following change of variables:

$$\xi = e^{-2\Lambda t} \Rightarrow \partial_\Lambda f(\Lambda) \left( \partial_\xi f(\Lambda(\xi)) \right)$$

$$\partial_\Lambda = -2\xi \partial_\xi.$$

The final differential equations read:

$$\frac{d \Sigma^\text{ret}_{i,j}(t, t')}{dt} = \frac{i}{2} \delta(t - t') \sum_{k,l} \left[ G^K_{0i,k'}(t, t) \right]_{l,k} u_{i,k,j,l}(t)$$

$$\tilde{G}^K_{\xi}(\xi) = -i \left[ 1 - 2\tilde{n}^\xi(t) \right]$$

$$\tilde{n}^\xi(t) = \sum_i n_i |\Psi_i(t)\rangle \langle \Psi_i(t)|,$$

(28)

where $\xi$ is to be integrated from 0 to 1. Note that this flow equation is simpler than Eq. (24), since it is to be evaluated only at a single fixed time and interaction.

2. Generalizing the fluctuation-dissipation theorem

We will now show how Eq. (28) can be evaluated efficiently without the need to fully diagonalize $h(t)$. To this end, we first generalize the fluctuation-dissipation theorem to nonthermal steady states in (effectively) non-interacting systems. Such states are characterized by a density matrix that commutes with the single-particle Hamiltonian:

$$[h^0, \tilde{n}] = 0.$$

Under this condition there is a common eigenbasis of $h^0$ and $\tilde{n}$ in which Eq. (3) immediately leads to

$$\left[ G^K_{0i,k'}(\omega) \right]_{k,k'} = i(1 - 2\tilde{n}_{k,k'}) \delta(\omega - \epsilon_k) \delta_{k,k'}$$

$$= (1 - 2\tilde{n}_{k,k'}) \left[ G^{\text{ret}}_{0}(\omega) - G^{\text{adv}}_{0}(\omega) \right]_{k,k} \delta_{k,k'},$$

If we now assume that $\tilde{n}^\Lambda_{k,k'}$ is already uniquely defined by its energy (which is true, e.g., when the spectrum of $h^0$ is not degenerate), one can introduce a scalar distribution function

$$\tilde{n}^\Lambda_{k,k'} = n(\epsilon_k)$$

such that

$$\left[ G^K_{0i,k'}(\omega) \right]_{k,k'} = [1 - 2n(\omega)] \left[ G^{\text{ret}}_{0}(\omega) - G^{\text{adv}}_{0}(\omega) \right]_{k,k} \delta_{k,k'},$$

or in the original basis:

$$G^K_{0i,k'} = [1 - 2n(\omega)] \left[ G^{\text{ret}}_{0}(\omega) - G^{\text{adv}}_{0}(\omega) \right].$$
This is a direct generalization of the fluctuation-dissipation theorem given in Eq. (10).

Next, we generalize Eq. (13). From now on, we focus on the most relevant case which is a state characterized by the distribution function

\[ n(\omega) = \sum_i \sigma_i \theta(\omega_i - \omega), \quad \sigma_i \in \{\pm 1\} \tag{29} \]

where successive \( \sigma_i \) need to have opposite sign

\[ \sigma_i = -\sigma_{i+1} \]

in order to obtain a physical density. This object is analogous to the \( n_i \) of the previous section (see Eq. (25)) and describes the sequence of occupied and unoccupied single-particle eigenstates. Using a deformation of the integration contour, we obtain

\[ G^K_0(t, t) = \sum_j \frac{i \tilde{\sigma}_j}{\pi} \int d\omega e^{-|\omega|^2} G^\sigma_0(i\omega + \omega_j). \tag{30} \]

3. Frequency-space formulation

It is now clear that Eq. (28) can be evaluated without the need to fully diagonalize \( h(t) \). Namely, the analytic continuation discussed in Sec. II.B.4 immediately yields

\[ G^{K, \xi}(t, t) = \sum_{n_i \neq n_{i+1}} \frac{i \tilde{\sigma}_i}{\pi} \int d\omega e^{-|\omega|^2} \frac{1}{i\omega + \tilde{\omega}_i(t) - h^0 - \Sigma^{ret, \xi}(t)} \]

where we have introduced

\[ \tilde{\sigma}_i = n_i - n_{i+1} \]

\[ \tilde{\omega}_i(t) = \frac{\epsilon_i(t) + \epsilon_{i+1}(t)}{2} \]

in analogy to Eq. (29). The \( \epsilon_i(t) \) in this expression are the eigenvalues of the effective single-particle Hamiltonian \( h(t) = h^0 + \Sigma^{ret, \xi}(t) \). Hence, Eq. (28) can be evaluated in \( \mathcal{O}(N) \) operations for tight-binding models (which we will discuss in Sec. IV-V) using Eq. (31).

However, the functional form of Eq. (31) also hints towards a problem: in every step the Green’s function is integrated over all imaginary frequencies. This is structurally different from the ground-state flow equation (compare Eq. (16)) and will be investigated more closely in Sec. IV.C.

The algorithm presented in this section can also be applied to the ground-state but will not necessarily give the same results due to the truncation of the flow equations and difference in cutoff. Hence, comparing the results for the ground-state provides a nontrivial check that will be discussed in Sec. IV.C.

B. xFRG-\( t_{\rho_1,2} \): Adiabatic time-evolution in Keldysh space with an initial-configuration cutoff

We now introduce a second approach which is also based on an adiabatic time-evolution. We still use Keldysh space FRG but develop a specialized cutoff for the case that the initial state is an excited eigenstate.

The cutoff in the free Green’s functions is introduced by choosing an initial density matrix that depends on \( \Lambda \). The causality relation is conserved by construction and one can work in the Keldysh basis. Thus, the cutoff can be introduced on the level of the initial Keldysh Green’s function (compare Eq. (30)):

\[ G^{K, \Lambda}(0, 0) = G^{K, \Lambda}_0(0, 0) = -i(1 - 2\bar{n}^\Lambda) \]

\[ := \sum_{n_i \neq n_{i+1}} \frac{i \tilde{\sigma}_i}{\pi} \int_{-\infty}^{\Lambda} \int_{\Lambda}^{\infty} d\omega e^{-|\omega|^2} \frac{1}{i\omega + \tilde{\omega}_i(0) - h^0} \]

while the time evolution is still given by Eq. (7). By construction, \( [h^0, \bar{n}^\Lambda] = 0 \), and thus the time-evolved Keldysh Green’s function \( G^K(t, t) \) can be computed purely from \( h^0 + \Sigma(t) \) (compare Sec. III.A). The free retarded and advanced Green’s functions do not acquire a cutoff in this scheme. The initial condition at \( \Lambda = \infty \) is simply the \( T = \infty \) state while for \( \Lambda = 0 \) one retrieves the physical density. The time-evolved single-scale propagator in the instantaneous eigenbasis takes the form

\[ \text{xFRG-}t_{\rho_1} : \]

\[ S^{K, \Lambda}(t, t) = \partial_t^A G^{K, \Lambda}(t, t) \]

\[ = \sum_k \sum_{n_i \neq n_{i+1}} \sum_{\omega = \pm \Lambda} \frac{i \tilde{\sigma}_i}{\pi} |\psi_k(t)\rangle \langle \psi_k(t)| \frac{1}{i\omega + \tilde{\omega}_i(0) - \epsilon_k(0)} S^{\text{ret,} \Lambda}(t, t) = 0, \]

\[ \tag{32} \]

which together with Eq. (21) constitutes the flow equation. As in the previous scheme, the vanishing retarded component of the single-scale propagator leads to a vanishing flow of the Keldysh self-energy. To calculate the Keldysh component of the single-scale propagator, in general one has to diagonalize the effective Hamiltonian at time \( t \) to obtain the instantaneous eigenstates, which is costly for large systems. A physical approximation can be made by replacing

\[ \frac{1}{i\omega + \tilde{\omega}_i(0) - \epsilon_k(0)} \rightarrow \frac{1}{i\omega + \tilde{\omega}_i(t) - \epsilon_k(t)}. \]

This approximation ensures that the correct number of levels is above and below \( \tilde{\omega}_i(t) \) and only deviates from an exact treatment of Eq. (32) in higher orders of the interaction since \( \tilde{\omega}_i(0) - \tilde{\omega}_i(t) \in \mathcal{O}(U) \), \( \epsilon_k(0) - \epsilon_k(t) \in \mathcal{O}(U) \). Using this approximation, \( S^{K, \Lambda} \) takes the more convenient form

\[ S^{K, \Lambda}(t, t) \approx \sum_{n_i \neq n_{i+1}} \sum_{\omega = \pm \Lambda} \frac{\tilde{\sigma}_i}{\pi} G^{eq, \Lambda}(i\omega + \tilde{\omega}_i(t)). \]
The resulting flow equation reads:

\( \text{xFRG-} t\text{-}\rho_2: \)

\[
\partial_t \Sigma^\text{ret,}\Lambda_{n,j}(t, t') = -\frac{1}{2\pi} \sum_{k,l} \sum_n \sum_{n', \omega = \pm \Lambda} \sigma_n u_{n,k,j,l} \left[ \frac{1}{i\omega + \omega'_n(t) - h^0 - \Sigma^\text{ret,}\Lambda(t)} \right]_{l,k} \delta(t - t'),
\]

which can be evaluated (for tight-binding chains) in \( \mathcal{O}(N) \) operations.

C. xFRG-\( \omega \): Steady-state Keldysh FRG with a non-thermal reservoir cutoff

We now devise a third way of obtaining an effective noninteracting description of an excited eigenstate for an interacting model which is not based on an adiabatic time-evolution but instead employs the steady-state Keldysh formalism of Sec. II E. The system is assumed to be in the steady-state induced by a reservoir. As before, this reservoir is used as the cutoff, but it is now no longer in equilibrium but instead chosen to be in a non-thermal, pure state described by the distribution function

\[
n(\omega) = \sum_i \sigma_i \theta(\omega_i - \omega).
\]

At the beginning of the flow where the coupling \( \Lambda \) to the reservoir is strong, all levels are infinitely broadened and thus half-filled and uncorrelated (i.e., described by a \( T = \infty \) state). For small couplings (i.e., at the end of the flow), the energy-scales of the physical Hamiltonian dominate and the distribution function governing the steady state becomes equal to the one of the reservoir. Hence, one recovers the physical system featuring a non-thermal distribution function.

This cutoff procedure leads to a flow equation of the form (see Eq. (19))

\( \text{xFRG-} \omega: \)

\[
\partial_t \Sigma^\text{ret,}\Lambda_{i,j}(t, t') = -\frac{1}{2\pi} \sum_{k,l} \sum_n \sum_{n', \omega = \pm \Lambda} \sigma_n u_{n,k,j,l} \left[ G^\text{ret,}\Lambda(\omega_n) + G^\text{adv,}\Lambda(\omega_n') \right]_{l,k} \delta(t - t'),
\]

which is remarkably similar to the one found in the previous section (see Eq. (33)) and even coincides, if the relevant parts of the spectrum are invariant when lowering the cutoff. In general, however, the effective single-particle spectrum will change during the flow. By definition of the cutoff scheme, at no point the particle number is fixed, only the occupation in energy space. The actual number of particles in the final system cannot be fixed beforehand.

IV. COMPARISON OF THE DIFFERENT SCHEMES

In this section, we perform various tests to explore the range of validity of the different xFRG schemes. Due to the first order truncation, results are guaranteed to agree only to linear order in \( U \). All higher orders are uncontrolled and may differ.

A. Tight-binding Hamiltonian

For the rest of this paper, we focus on a tight-binding model:

\[
H^\text{th} = H^\text{hop} + H^\text{int} + H^\text{ph}
\]

\[
H^\text{hop} = \sum_{i=1}^{N-1} c^\dagger_i c_{i+1} + \text{h.c.}
\]

\[
H^\text{int} = U \sum_{i=1}^{N-1} c^\dagger_i c_{i+1} c^\dagger_{i+1} c_i
\]

\[
H^\text{ph} = -\frac{U}{2} (c_1^\dagger c_1 + c_N^\dagger c_N) - U \sum_{i=2}^{N-1} c_i^\dagger c_i,
\]

where the single-particle index enumerates the Wannier basis states. Here, \( H^\text{ph} \) is introduced to enforce particle-hole symmetry. We use the hopping amplitude between adjacent sites as the energy-scale.

In the thermodynamic limit, the model described by Eq. (34) is gapless for \( U < 2 \) and thus its low-energy physics is governed by the Luttinger liquid fixed point.\(^{33}\) The Luttinger parameter is known from Bethe ansatz calculations and at half filling reads

\[
K^\frac{1}{2} = \frac{1}{\frac{\pi}{2} \arccos \left( -\frac{U}{2} \right)} = 1 - \frac{U}{\pi} + \mathcal{O}(U^2).
\]

For other fillings, the expressions take more involved forms, but for the scope of this paper only the first order expansion is needed at quarter- and three-quarter filling:

\[
K_i^\frac{1}{2} = 1 - \frac{U}{\pi \sqrt{2}} + \mathcal{O}(U^2) = K^\frac{1}{2}.
\]

B. Comparison of the excited state schemes

Here, we compare the results of the xFRG-\( t\text{-}\Gamma \) with those obtained from explicit time evolution using the tFRG of Sec. II F. By construction, in the adiabatic limit and if no gaps close during the time-evolution, these results need to agree. We prepare the system in
a highly excited eigenstate of the noninteracting system with \( N = 80 \) sites (illustrated in the upper right inset of Fig. 5). The interaction is ramped up smoothly from \( U = 0 \) to \( U_{\text{final}} = 0.5 \) in an increasingly long time span of length \( t_{\text{final}} \):

\[
\frac{U(t)}{U_{\text{final}}} = \begin{cases} 
0 & t < 0.1 t_{\text{final}} \\
\sin^2 \left( \frac{t-0.1 t_{\text{final}}}{0.09 t_{\text{final}}} \right) & 0.1 t_{\text{final}} \leq t < 0.9 t_{\text{final}} \\
1 & 0.9 t_{\text{final}} \leq t
\end{cases}
\]

where the initial and final region of constant interaction were used to gauge the adiabaticity and control the error acquired by the time-evolution due to the Trotter decomposition. The mean deviation in occupation numbers in the final state is shown in Fig. 2. The difference between the results decreases with increasing \( t_{\text{final}} \). The saturation at large \( t_{\text{final}} \) can be explained by numerical inaccuracies in the integration and time evolution.

The bottom left inset of Fig. 2 shows the average difference in occupations obtained by the xFRG-\( t-\Gamma \), xFRG-\( t-p_1 \) and xFRG-\( t-p_2 \) methods. The pairwise difference is quadratic in the interaction, as expected. Even though the xFRG-\( t-p_2 \) and xFRG-\( t-p_1 \) do also differ in quadratic order, their deviation is small compared to the difference between the xFRG-\( t-p_{1,2} \) and the xFRG-\( t-\Gamma \). For this reason, we will not discuss the xFRG-\( t-p_1 \) method in the rest of this paper and instead focus on the computationally cheaper xFRG-\( t-p_2 \).

Obtaining a specific sequence of \( n_i \) within the xFRG-\( \omega \) scheme is computationally more demanding: One can use the noninteracting eigenenergies to make an initial guess for the distribution function \( n(\omega) \) in energy-space, but this guess has to be iteratively refined since the effective single-particle spectrum is deformed during the flow and the final effective Hamiltonian depends on the \( n_i \). For this reason, the xFRG-\( \omega \) is not included in this comparison.

C. Comparison with ground-state FRG

Another important test for the different xFRG-techniques is to compare them to the ground-state FRG of Sec. II D. As different cutoffs are used and the hierarchy of flow equations is truncated, only agreement to first order is guaranteed.

To study this in detail, we compute the spectral function

\[
A_1(\omega) = -\frac{1}{\pi} \text{Im} \left[ G_{\text{ret}}(\omega)_{1,1} \right].
\]

Luttinger liquid theory in the ground-state predicts that for frequencies around the Fermi edge, a power-law suppression occurs at the boundary of our tight-binding chain:

\[
A_1(\omega) \sim \omega^{K-1}.
\]

The exponent has a nontrivial linear contribution, rendering this spectral function an ideal testbed for the different xFRG methods.

For definiteness, we discuss the half filled ground-state. In this case, the auxiliary reservoir used in xFRG-\( \omega \) is just in its ground-state. As discussed in Sec. II E, a reservoir cutoff where the auxiliary reservoir is in its ground-state yields the same flow equations as the Matsubara FRG and will thus not be discussed independently.

Furthermore, also the approximate xFRG-\( t-\rho_2 \) scheme (see Sec. III B) yields the same flow equations as the Matsubara FRG: in the ground-state, there is only one jump in the sequence of occupations of eigenstates (at \( N/2 \)). Due to particle-hole symmetry, \( \epsilon_i = \epsilon_{N-i} \) and thus \( \tilde{\omega}_{N/2}(t) = 0 \). Therefore, Eq. (33) is identical to Eq. (17). In contrast, the xFRG-\( t-\Gamma \) leads to different flow equations and will now be discussed alongside the xFRG-\( t-\rho_2 \).

The logarithmic derivative (see Fig. 3) shows that the xFRG-\( t-\rho_2 \) indeed yields a power-law suppression of the boundary spectral function. In contrast, the \( T = \infty \) reservoir cutoff used in the xFRG-\( t-\Gamma \) fails at this task. This is plausible since the infinite temperature reservoir does not provide a proper low-energy cutoff in the adiabatic limit; all energy scales enter in every step of the calculation (see Eq. (31)).

A similar analysis can be performed for other fillings, where the flow equations of the xFRG-\( t-\rho_2 \) differ from
be interested in the excitation-energy density defined as $(E - E_{GS})/N$.

### B. Friedel Oscillations

We first investigate the Friedel oscillations that emerge around boundaries. A finite tight-binding chain will display oscillations in the density profile (i.e., the occupation numbers) at the ends (or near any other impurity) at zero temperature and if particle-hole symmetry is broken. We restrict ourselves to the case of a clean, finite chain and set $H^p = 0$ (see Eq. (34)) to break particle-hole symmetry explicitly. Luttinger liquid physics predicts that

$$\left| \langle c_i^+ c_i \rangle - \frac{1}{2} \right| \sim i^{-K}.$$  

This power law can be obtained via a ground-state FRG calculation, and the linear correction to the non-interacting exponent can be computed from a leading-order scheme.\footnote{See Ref. \cite{footnote1} for further details.}

We now employ our xFRG framework to explore the effects of finite excitation energies and try to draw analogues with the thermal case: At finite temperatures, the algebraic decay is cut off on a length-scale proportional to $1/T$. We investigate whether Friedel oscillations persist in excited eigenstates and if their energy provides a cutoff in a similar fashion as temperature does in the thermal case. Since for small $T$ and a linearized dispersion at the Fermi-edge one has

$$E_T - E_0 \sim T^2,$$

we expect the Friedel oscillations be be cut off on a scale proportional to $1/\sqrt{E - E_{GS}}$.

As the xFRG algorithms scale linear in the number of changes in the sequence $n_i$ (compare Eqs. (31) and (33)), the computational cost can be kept low by fixing the number of single-particle excitations (by choosing a constant $\tilde{\beta}$) while varying the system size. This way, the algorithm scales linearly in the square root of the inverse energy density in the initial state.

The resulting occupation numbers are presented in the left panel of Fig. 4 for various states at different excitation-energy densities relative to the ground-state. To objectively measure the deviations from the ground-state Friedel oscillations, we define a cutoff scale

$$i^*_{\alpha} = \min \left\{ i \left| |n_i^{gs} - n_i^{ex}| > \alpha \right| \right\}$$

such that $i^*_{\alpha}$ gives the first site where the relative error compared to the Friedel oscillations of the ground-state exceeds $\alpha$. This scale is plotted in Fig. 4 as a function of the excitation energy density for various eigenstates and systems of different lengths. The line is a power-law fit resulting in

![Spectral function at the edge of a tight-binding chain](image)}
which is reasonably close to the thermal expectation of $-1/2$. This result does not depend on the chosen $\beta$ or the cutoff used. We thus conclude that Friedel oscillations survive to finite energy-densities and that the excitation energy simply provides an infrared cutoff.

Due to the shortcomings of xFRG-$t$-$\Gamma$ discussed in Sec. IV as well as the numerical effort in evaluating the xFRG-$t$-$\rho_1$ and xFRG-$\omega$, we solely employ the xFRG-$t$-$\rho_2$ from now on.

C. Conductance

Another prominent feature of Luttinger liquids is that any local impurity can completely suppress particle transport. Finite temperatures counteract this effect and yield a conductance that scales as a power-law in $T$.\textsuperscript{34}

In order to obtain the conductance, one would typically use the Meir-Wingreen formula\textsuperscript{35} on a system that is coupled to two reservoirs which differ by a finite bias voltage. However, even if the system is initially prepared in an excited eigenstate, the coupling to the reservoirs would eventually always lead to thermalization. Thus, the Meir-Wingreen approach to the steady-state conductance does not yield any non-trivial insights about excited eigenstates.

We now devise a heuristic formula to model transport properties of excited states on intermediate time scales. To this end, let us first revisit the thermal conductance of a system in presence of two leads coupled to the first and last site:\textsuperscript{35}

$$G = -4\pi^2 t^2_{L,R} \int \rho_L(\omega) \rho_R(\omega) f'(\omega) \left| [G^\text{ret}(\omega)]_{1,N} \right|^2 d\omega$$

where the second line assumes the bandwidth of the reservoirs to be much larger than the bandwidth of the system. $t_{L,R}$ denotes the hopping to the respective baths, $\Gamma_{R/L}$ is the hybridization between the system and the baths, $\rho_{L/R}$ is the density of states, and $f(\omega)$ is the Fermi function. $G^\text{ret}$ is computed in the presence of the reservoirs. However, one can see that $G^\text{ret}$ is still sharply peaked if the hybridization $\Gamma_{R/L}$ is small. Thus, if the temperature is larger than the typical level-spacing $B/N$ and the hybridization is small,

$$\frac{\Gamma}{N} \ll \frac{B}{N} \ll T,$$

one can calculate the integral explicitly for an effectively noninteracting system:

$$G = \sum_k -4\pi \Gamma f'(\omega_k) \frac{|U_{k,1} U_{k,N}|^2}{U_{k,1}^2 + U_{k,N}^2},$$

where

$$h = U \text{diag}(\omega_1, \ldots, \omega_N) U^T,$$

and $\Gamma_L = \Gamma_R = \Gamma$.

This expression measures the overlap of the eigenvectors at the Fermi edge with the ends of the system, which is reasonably close to a naive understanding of ‘conductance’. The limit described by Eq. (37) does not only allow us to obtain the conductance without evaluating numerical integrals but also has an additional advantage: If the coupling is weak, the self-energy can be obtained
using a decoupled system which is in a well-defined eigenstate, and the algorithms presented above can be directly employed. For an excited state, we thus concentrate on calculating

$$\frac{\tilde{G}^T}{\Gamma} = \sum_k -4\pi f'_T(\omega_k)|U_{k,1}U_{k,N}|^2 \frac{\omega_k}{\omega_k^2 + U_{k,N}^2},$$

(38)

which on intermediate timescales might capture the same physical phenomenon as the conductance at finite temperature. However, for the reasons outlined above this observable cannot be directly interpreted as a physical conductance. The physical current will include additional terms that contribute to equilibrating the system. For large enough systems, however, this current, when symmetrized, will only weakly depend on the chemical potential difference and thus for weak couplings one could expect to find an intermediate time regime where the quantity defined in Eq. (38) corresponds to the (symmetrized) linear conductance across the system weakly coupled to two reservoirs at temperature $T$. We again emphasize that this is a purely heuristic approach.

While the reservoir temperature $T$ in the above expression is a free parameter, it is intuitive that it needs to be large enough to excite many levels to avoid finite-size effects but at the same time small enough compared to the excitations in order not to overshadow the effects of the finite excitation energy. Furthermore, the precise choice should be irrelevant for this discussion to be meaningful. We now examine Eq. (38) in two cases.

1. Weak tunnel contacts at the ends of the system

We first discuss a clean system where the weak coupling to the reservoirs creates two strong impurities at the ends of the chain. As discussed in Ref. 15, the conductance in the thermal case scales as

$$G \sim T^{\frac{1}{2} - \alpha_{2-imp}}.$$

The conductance in excited eigenstates is shown in Fig. 5, and is consistent with a power-law of the form

$$G \sim \left(\sqrt{|E - E_{GS}|} \right)^{\alpha_{2-imp}}$$

where the $\alpha$s for different interactions (presented in Table 1) are in good agreement with the thermal expectation.

To ensure that neither the varying system sizes nor the energy-dependent reservoir temperature influence the observed power-law, the same calculation was repeated for a system of constant size using a constant temperature while varying $\tilde{\beta}$. Even though limited to a smaller range of energies, these calculations are consistent with the results shown in Fig. 5. Furthermore, the data does not show any systematic dependence on the reservoir temperature.

![Figure 5](image-url)

**FIG. 5.** Intermediate-time heuristic ‘conductance’ in excited eigenstates of a clean tight-binding chain weakly coupled to two reservoirs. The different colors represent different interactions while the symbols represent two different reservoir temperatures: $T = \sqrt{|E - E_{gs}|}/N$ (circles) and $T' = 2T$ (squares). The system size varies between $N = 4 \cdot 10^2$ to $N \approx 4 \cdot 10^4$ while $\tilde{\beta} = 0.05$ is kept constant. The lines are power-law fits.

| $U$ | $\alpha_{2-imp}$ | $\alpha_{3-imp}$ | $\alpha_{bath}$ |
|-----|-----------------|-----------------|-----------------|
| 0.25 | 0.076           | 0.074           | 0.080           |
| 0.5  | 0.146           | 0.145           | 0.161           |
| 1.0  | 0.279           | 0.332           | 0.333           |

**TABLE I.** Exponents extracted from the fits shown in Fig. 5 and 7 as well as the expectations from the Bethe-ansatz solution in the thermal system.

The effect of excitations can also be understood in terms of the individual $|U_{k,1}U_{k,N}|^2$ (compare Eq. (38)) depicted in Fig. 6. They illustrate that excitations constitute the leading contribution to the conductance for a wide range of reservoir temperatures while finite-size effects are expected to be relevant only for very low temperatures.

2. Additional impurity within the Luttinger liquid

We now turn to the more complex case where an additional impurity is placed within the tight-binding chain. As has been studied in detail in Ref. 31, the exponent in this case depends on the position of the impurity due to interference effects. If the impurity divides the chain in two parts of incommensurate lengths, an effective phase averaging takes place. This results in $G \sim \sqrt{G_1G_2G_3}$, where $G_i$ are the conductances for the individual barriers. Ref. 15 already reported that the conductance through impurities at the boundary from a Fermi liquid to a Luttinger liquid scales like

$$G_{1,3} \sim T^{-\left(\frac{1}{2} - 1\right)}.$$

For an impurity between two Luttinger liquids, one has

$$G_2 \sim T^{-2\left(\frac{\beta}{1}\right)}.$$ 

Therefore, the overall conductance is predicted to scale as

$$\Rightarrow G \sim T^{-2\left(\frac{\beta}{1}\right)}$$

which was confirmed in Ref. 31 for thermal states. The incommensurate position of the center impurity leads to an erratic behavior of the retarded Green’s function, introducing significantly more noise than in the case with only two impurities. To illustrate this issue, Fig. 6 shows a scatter plot of the overlap from one end of the system to the other for all eigenstates of the effective single-particle Hamiltonian. Even at relatively high energy densities the ground-state and the excited state appear very similar due to the high level of noise. In the case where the chain is divided in a simple fraction the exponent is, however, unchanged compared to the previous section and will thus not be investigated further.

To ensure incommensurability, we chose the lengths as successive Fibonacci numbers, which are coprime and their ratio converges toward an irrational number. The resulting conductances are depicted in Fig. 7. While it is hard to decide whether the curves actually follow a power-law, they are at least consistent with this expectation. The exponents can be extracted via a fit of the form

$$G \sim \left(\sqrt{E - E_{gs}}\right)^{2\alpha_{3\text{-imp}}}$$

and the resulting $\alpha_{3\text{-imp}}$ are presented in Table I. States with energy density above 0.1 were neglected as they show effects of the band curvature.

D. Block excitations

So far, we have analyzed generic excitations which leave the general step-shape of the function $n(\omega)$ unchanged and just alter it in a small region around the Fermi-edge where the (free) dispersion is nearly linear. As all observables in a Luttinger liquid are governed by the Hamiltonian at low energies, it is not surprising that the results are similar to those of thermal states. There is, however, a different set of excited states which are highly non-generic and different from thermal states, and thus we have no intuition for their physics. As an example, we consider a state where a whole block of fermions is excited to a higher energy region. In the simplest, most symmetric case this is modelled by

$$n_i = \begin{cases} 
1 & 1 \leq i \leq \frac{1}{3}N \\
0 & \frac{1}{3}N < i \leq \frac{1}{2}N \\
1 & \frac{1}{2}N < i \leq \frac{2}{3}N \\
0 & \frac{2}{3}N < i \leq N 
\end{cases}$$

(39)

which in contrast to the ground-state has three sharp, distinct edges in the distribution function. To investigate the physics in this state, we again study the spectral function at the boundary (compare Sec. IV C). Results are shown in the first panel of Fig. 8, where one can identify several points of non-analytic behavior. The logarithmic derivatives around these points are plotted in Fig. 10 and indicate the existence of power-laws. The spectral function around the center divergence seems to scale as

$$A_{\text{block}}(\omega) \sim |\omega|^{-\frac{4}{3}}$$
while the outer cusps are described by

\[ A_{\text{block}}(\omega - \omega_0^{1/3}) \sim \left| \omega - \omega_0^{1/3} \right|^{\frac{U/\pi}{1/2}}. \]

The rest of this section is devoted to understanding this result in terms of known Luttinger liquid physics. To this end, the center panel of Fig. 8 shows the spectral function in the quarter filled ground-state; the three-quarter filled case is the same but mirrored. Both show two cusps, one at the Fermi energy and a second one at the energy associated with \( \pi - k_F \). The first cusp is the one well studied in the literature while the second cusp is the result of umklapp scattering: the long-ranged potential, acquired by the Friedel oscillations, allows for processes with wave vector \( 2k_F \), which is either close to the Fermi surface or an umklapp term higher up in the spectrum (compare Fig. 9). Each of these is described by a power-law

\[ A(\omega - \omega_0)^{1/K} \sim \left| \omega - \omega_0 \right|^{1/K-1}. \]

\( K \) has to be calculated using the dispersion at the corresponding position in the spectrum (i.e., at quarter and three-quarter filling), and to first order the exponent is given by \( U/\pi \sqrt{2} \) (compare Eq. (36)).

Next, we discuss the inverted half filled ground-state (right panel of Fig. 8) which can still be obtained from the ground-state algorithm by using a negative temperature, or equivalently by analyzing the ground-state of \(-H\). As the sign of the hopping is arbitrary, we are thus just inspecting the ground-state of a tight-binding chain with attractive interactions; to leading order, the corresponding exponent is just \(-U/\pi\).
The left panel of Fig. 8 can now be understood as a superposition of the effects associated with the different jumps in the distribution function: The first and third discontinuity are located at the Fermi energy of a quarter- and three-quarter filled system, respectively. Their contributions coincide and (in the present approximation scheme) the exponents just add up to

\[ 2 \left( \frac{1}{K_{q}} - 1 \right) = \frac{U}{\pi \sqrt{2}} + O(U^2) = 2 \left( \frac{1}{K_{q}^2} - 1 \right). \]

The divergence in the center is described purely by the inverted ground-state.

Hence, the phenomenology of the very highly excited, non-generic case of a block-excitation can (at least to leading order) be interpreted in terms of ground-state Luttinger liquid physics.

VI. SUMMARY AND OUTLOOK

In this paper, we have shown how correlation functions in pure excited states of many-body systems can be obtained within the realm of the functional renormalization group; the key idea is to start out with a Slater determinant and to slowly switch on interactions. To this end, we simplified existing real-time Keldysh FRG flow equations for the special case of adiabaticity (xFRG-t-G) and also devised a novel cutoff scheme which is specifically tailored to this problem (xFRG-t-\rho). Due to the approximate nature of the method, the xFRG results do not necessarily agree with those of standard equilibrium FRG when targeting the ground state, which thus provides a nontrivial testing ground. Importantly, only the xFRG-t-\rho manages to reproduce the power-law suppression of the spectral function at the boundary of a Luttinger liquid; the xFRG-t-G fails at this task.

We subsequently employed the xFRG to study two toy problems. First, we demonstrated that Luttinger liquid power law behavior survives in lowly-excited pure states whose energy serves as an infrared cutoff. Second, we determined the spectral function of highly-excited, non-generic block excitations featuring multiple Fermi edges and illustrated that the system is effectively governed by a superposition of several Luttinger liquids.

The key drawback of the xFRG is its approximate character. Even though the underlying RG idea entails an infinite resummation of Feynman diagrams, all results presented in this paper are only guaranteed by be correct up to leading order in the interaction. The strengths of the xFRG are that it is not bound by the growth of entanglement and that large systems of up to 10^6 sites (in one dimension) can be treated easily.

Future directions include an extension of the xFRG flow equations to second order (which is possible but a major endeavour) as well as an application to many-body localized, topological systems.

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While there are fast algorithms to obtain the full spectrum of a tri-diagonal matrix in $O(N \ln N)$ operations\(^{37}\), it is sufficient in this context to compute the eigenvalues at the aforementioned changes in the $n_i$. This can be done using specialized algorithms like LAPACK’s dstemr/dstegr subroutines; in addition to many other features, these include an implementation of the algorithm presented in Ref. 38, which provides orthogonal eigenvectors and eigenvalues at arbitrary positions in the spectrum to working precision in $O(N)$ operations.

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