Interaction Quench in the Hubbard Model

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Motivated by recent experiments in ultracold atomic gases that explore the nonequilibrium dynamics of interacting quantum many-body systems, we investigate the opposite limit of Landau's Fermi-liquid paradigm: We study a Hubbard model with a sudden interaction quench, that is, the interaction is switched on at time $t = 0$. Using the flow equation method, we are able to study the real time dynamics for weak interaction U in a systematic expansion and find three clearly separated time regimes: (i) An initial buildup of correlations where the quasiparticles are formed. (ii) An intermediate quasi−steady regime resembling a zero temperature Fermi liquid with a nonequilibrium quasiparticle distribution function. (iii) The long-time limit described by a quantum Boltzmann equation leading to thermalization of the momentum distribution function with a temperature $T \propto U$.

The investigation of interacting quantum many-particle systems in nonequilibrium has recently attracted a lot of attention. A simple way to excite a system from its ground state is an interaction quench, a sudden switch of parameters in the Hamiltonian. The time evolution of the initial state is then generated by the quenched Hamiltonian, for which the initial state is generically not an eigenstate. Recent experiments have implemented quenches of ultracold atoms loaded on optical lattices and observed remarkable subsequent dynamics described as iterated ''collapse and revival'' of the initial superfluid phase [1,2]. Yet their theoretical description remains a challenge since many well-established equilibrium theoretical methods fail in nonequilibrium. From a theoretical point of view, the long-time limit poses particularly intriguing questions: Will an interacting closed quantum system prepared in some generic initial state equilibrate, that is behave like the equilibrium system with some nonzero temperature after waiting sufficiently long? In nonlinear classical systems similar questions have been addressed in a multitude of publications since the seminal work by Fermi, Pasta, and Ulam [3]. Nonequilibration has been linked to integrability since an integrable system is constrained by an infinite number of conservation laws.

However, much less is known about quantum systems. Since a pure state remains a pure state under unitary time evolution, the concept of thermalization is only meaningful for suitable observables. First theoretical results have shown that observables may approach limiting values or exhibit persistent oscillations which, even when time averaged, do not match with equilibrium properties [4,5]. A proposition by Rigol *et al.* [6] gave a statistical description for the stationary state of an integrable system in terms of a generalized Gibbs ensemble. Conditions for the applicability or nonapplicability of this scenario have been clarified in [7], and specific results have been obtained for the Luttinger model [8], hard core bosons in one dimension [9,10], and the infinite dimensional Falicov-Kimball model

[11]. While the concept of a generalized statistical ensemble proved helpful even for a less restrictive set of constraints [12], the role of integrability has been questioned by further numerical works: Breaking the integrability of spinless fermions on a 1D lattice has not altered relaxation to a nonthermal state [12]. Similarly, for the nonintegrable 1D Bose-Hubbard model signatures of thermalization could only be found for a limited regime of quenches, while others seemed to drive the system to nonthermal stationary states [13]. Exact results have been obtained for the opposite case of quenches from the Mott phase to the noninteracting Hamiltonian and show relaxation of local observables to a nonequilibrium steady state [14].

Motivated by these questions, we study an interaction quench in a Fermi liquid in $d > 1$ spatial dimensions, that is, we suddenly switch on the interaction at time $t = 0$. This is the extreme opposite limit of Landau's adiabatic switching on procedure, where one finds the celebrated one-to-one mapping between physical electrons and quasiparticles. In the sudden quench scenario, the system is prepared as the zero temperature ground state of the noninteracting Fermi gas at times $t < 0$, and then, for $t \geq 0$, subject to the time evolution with respect to the interacting Hamiltonian. We find three regimes of the time evolution, which are well separated for weak interaction: an initial quasiparticle formation regime, followed by a quasi−steady intermediate regime resembling a zero temperature Fermi-liquid, and a long-time thermalization regime where the momentum distribution function equilibrates. Concretely, we investigate the fermionic Hubbard model at half filling described by the following Hamiltonian (Fermi energy $\epsilon_F \equiv 0$)

$$H(t) = \sum_{k\sigma=\uparrow,\downarrow} \epsilon_k :c_{k\sigma}^\dagger c_{k\sigma}: + \Theta(t)U\sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) \tag{1}$$

and work out the time-dependent momentum distribution functions $N_k(t)$. Notice that this system is clearly non-integrable for $d > 1$ and one therefore expects generic behavior. Most of our results are obtained in the limit of high dimensions [15], but the calculation also applies to finite dimensions with the same conclusions up to quantitative details.

We study the above real time evolution problem by using the approach introduced in [16]. One solves the Heisenberg equations of motion for the operators that one is interested in by performing a unitary transformation to an (approximate) eigenbasis of the interacting Hamiltonian. There one can easily work out the time evolution and then transform back to the original basis where the initial state is specified. In this manner one induces a solution of the Heisenberg equations of motion for an operator in the original basis but without secular terms, which are usually a major problem in other approximation schemes [17]. Figure 1 gives a sketch of our approach. Notice that the same general idea was recently also used by Cazalilla to study the behavior of the exactly solvable one-dimensional Luttinger model subject to a quench [8].

Since our model is nonintegrable, we implement the above diagonalizing transformation by the flow equation method [18,19], which permits a systematic controlled expansion for many equilibrium and nonequilibrium quantum many-body problems [19]. One uses a continuous sequence of infinitesimal unitary transformations parametrized by a parameter B with dimension (energy)$^{-2}$ that connects the eigenbasis of the free Hamiltonian ($B = 0$) with the energy diagonal basis of the interacting Hamiltonian ($B = \infty$). Each infinitesimal step of the unitary transformation is defined by the canonical generator $\eta(B) = [H_0(B), H_{\mathrm{int}}(B)]$, where $H_0(B)$ is the diagonal and $H_{\mathrm{int}}(B)$ the interacting part of the Hamiltonian. This generator $\eta(B)$ has the required property of making $H(B)$ increasingly energy diagonal for $B \to \infty$ [18]. All operators $\mathcal{O}(B)$ (including the Hamiltonian itself) flow according to the differential equation $\partial \mathcal{O}(B)/\partial B = [\eta(B), \mathcal{O}(B)]$. Higher order terms generated by the commutator are truncated after normal ordering (denoted by : :), and the flow equations decompose into a set of ordinary differential
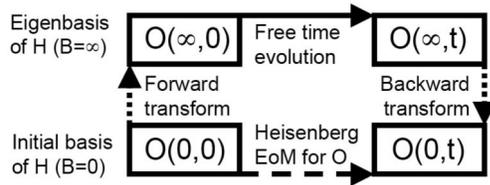

FIG. 1. The Heisenberg equation of motion for an observable O is solved by transforming to the $B = \infty$ eigenbasis of the interacting Hamiltonian H (forward transformation), where the time evolution can be computed easily. Time evolution introduces phase shifts, and therefore the form of the observable in the initial basis $B = 0$ (after a backward transformation) changes as a function of time.

equations resembling scaling equations in a renormalization approach. However, contrary to conventional renormalization schemes which reduce the size of the effective Hilbert space, the flow equation approach retains the full Hilbert space, which makes it particularly appropriate for nonequilibrium problems (for more details, see [19]).

Flow equations for the Hubbard model.—First we work out the diagonalizing flow equation transformation for the Hubbard Hamiltonian. The expansion parameter is the (small) interaction U and normal ordering is with respect to the zero temperature Fermi-Dirac distribution:

$$H(B) = \sum_{k\sigma=\uparrow,\downarrow} \epsilon_k :c^\dagger_{k\sigma}c_{k\sigma}: + \sum_{p'pq'q} U_{p'pq'q}(B):c^\dagger_{p'\uparrow}c_{p\uparrow}c^\dagger_{q'\downarrow}c_{q\downarrow}:$$
$$(2)$$

with $U_{p'pq'q}(B = 0) = U$. The flow of the one-particle energies and the generation of higher normal-ordered terms in the Hamiltonian can be neglected since we are interested in results in second order in U. The flow of the interaction is to leading order given by $U_{p'pq'q}(B) = U \exp(-B\Delta^2_{p'pq'q})$ with an energy difference $\Delta_{p'pq'q} \overset{\mathrm{def}}{=} \epsilon_{p'} - \epsilon_p + \epsilon_{q'} - \epsilon_q$.

Next we work out the flow equation transformation for the number operator $\mathcal{N}_{k\uparrow}(B) = \mathcal{C}^\dagger_{k\uparrow}(B)\mathcal{C}_{k\uparrow}(B)$, which can be obtained from the transformation of a single creation operator $\mathcal{C}^\dagger_{k\uparrow}(B)$. Under the sequence of unitary transformations the operator changes its form to describe dressing by electron-hole pairs. A truncated ansatz reads

$$\mathcal{C}^\dagger_{k\uparrow}(B) = h_k(B)c^\dagger_{k\uparrow} + \sum_{p'q'p} M^k_{p'q'p}(B)\delta^{k+p}_{p'+q'}:c^\dagger_{p'\uparrow}c^\dagger_{q'\downarrow}c_{p\downarrow}:.$$
$$(3)$$

We introduce the zero temperature momentum distribution function of a free Fermi gas n_k and define $n_k^- \overset{\mathrm{def}}{=} 1 - n_k$ and a phase space factor $Q_{p'pq'}[n] \overset{\mathrm{def}}{=} n_{p'}^- n_{q'}^- n_p + n_{p'} n_{q'} n_p^-$. The flow equations for the creation operator are

$$\frac{\partial h_k(B)}{\partial B} = U \sum_{p'q'p} M^k_{p'q'p}(B)\Delta_{kp'pq'}e^{-B\Delta^2_{kp'pq'}}Q_{p'pq'}[n]$$

$$\frac{\partial M^k_{p'q'p}(B)}{\partial B} = h_k(B)U\Delta_{p'pq'k}e^{-B\Delta^2_{p'pq'k}}. \qquad (4)$$

Here and in the ansatz (3) we have only taken into account the terms that are required to describe the momentum distribution function up to second order in U. The initial conditions for the above transformation of $\mathcal{C}^\dagger_{k\uparrow}$ are $h_k(0) = 1$ and $M^k_{p'q'p}(0) = 0$ [i.e., $\mathcal{C}^\dagger_{k\uparrow}(B = 0) = c^\dagger_{k\uparrow}$], and we denote the asymptotic values from the solution of (4) by $h_k(B = \infty, t = 0)$ and $M^k_{p'q'p}(B = \infty, t = 0)$. Time evolution according to Fig. 1 yields $h_k(B = \infty, t) = h_k(B = \infty, t = 0)e^{-i\epsilon_k t}$ and $M^k_{p'q'p}(B = \infty, t) = M^k_{p'q'p}(B = \infty, t = 0)e^{-i(\epsilon_{p'}+\epsilon_{q'}-\epsilon_p)t}$, which are then input as the initial

conditions of the system of equations (4) at $B = \infty$.
Integrating back to $B = 0$ gives the time evolved creation
operator in the original basis, and it is straightforward to
evaluate the time-dependent momentum distribution func-
tion with respect to the initial Fermi gas state [20].

Nonequilibrium momentum distribution function.—One
finds the following time-dependent additional term to the
distribution n_k of the free Fermi gas in $O(U^2)$:

$$\Delta N_k^{\mathrm{NEQ}}(t) = N_k^{\mathrm{NEQ}}(t) - n_k$$

$$= -4U^2 \int_{-\infty}^{\infty} dE \, \frac{\sin^2(\frac{(\epsilon_k - E)t}{2})}{(\epsilon_k - E)^2} J_k(E; n). \quad (5)$$

The phase space factor $J_k(E; n)$ resembles the quasiparticle
collision integral of a quantum Boltzmann equation:

$$J_k(E; n) = \sum_{p'q'p} \delta_{p+k}^{p'+q'} \delta_{\epsilon_p + E}^{\epsilon_{p'} + \epsilon_{q'}} [n_k n_p n_{p'}^- n_{q'}^- - n_k^- n_p^- n_{p'} n_{q'}].$$

For computational convenience we use the limit of infinite
dimensions, specifically a Gaussian density of states
$\rho(\epsilon) = \exp[-(\epsilon/t^*)^2/2]/\sqrt{2\pi}t^*$ [15]. In the sequel $\rho_F = \rho(\epsilon = 0)$ denotes the density of states at the Fermi level.
Results from a numerical evaluation of the above scheme
for three time steps are presented in Fig. 2.

Equilibrium momentum distribution function.—
Equations (4) can also be used to evaluate the equilibrium
distribution function, which will later be important for
comparison. In fact, the asymptotic value $h_{k_F}(B = \infty)$ at
the Fermi energy is directly related to the quasiparticle
residue (Z factor), $Z^{\mathrm{EQU}} = [h_{k_F}(B = \infty)]^2$ [19]. It is easy
to solve (4) analytically at the Fermi energy for zero
temperature in $O(U^2)$, and one finds for momenta k infini-
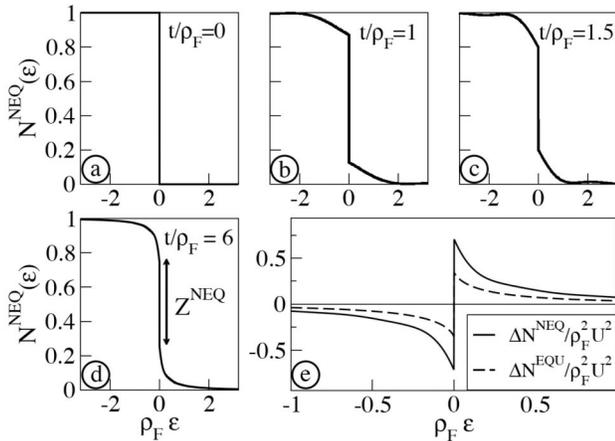tesimally above or below the Fermi surface

FIG. 2. (a)–(d) Time evolution of $N^{\mathrm{NEQ}}(\epsilon)$ plotted around the
Fermi energy for $\rho_F U = 0.6$. A fast reduction of the disconti-
nuity and $1/t$ oscillations can be observed. The arrow in
(d) indicates the size of the quasiparticle residue in the quasi–
steady regime. In (e) the universal curves for $\Delta N_k = N_k - n_k$
are given for both equilibrium and for the nonequilibrium quasi–
steady state in the weak-coupling limit.

$$\Delta N_k^{\mathrm{EQU}} = -U^2 \int_{-\infty}^{\infty} dE \, \frac{J_k(E; n)}{(\epsilon_k - E)^2} \quad (6)$$

consistent with a conventional perturbative evaluation.

Short-time correlation buildup.—The numerical evalu-
ation of the momentum distribution function depicted in
Fig. 2 shows the initial buildup of a correlated state from
the Fermi gas. For times $0 < t \lesssim \rho_F^{-1} U^{-2}$ one observes a
fast reduction of the Fermi surface discontinuity and $1/t$
oscillations in the momentum distribution function. This
short-time regime can be understood as the formation of
quasiparticles from the free electrons of the initial non-
interacting Fermi gas.

Intermediate quasi–steady regime.—For times t of or-
der $\rho_F^{-1} U^{-2}$ the sinusoidal time dependence in (5) gener-
ates an increasing localization in energy space, which
eventually becomes a δ function (Fermi's golden rule).
There are no further changes in the momentum distribution
function for times $t \gtrsim \rho_F^{-1} U^{-2}$ in the present order of the
calculation. For momenta k infinitesimally above or below
the Fermi surface one then finds from (5):

$$\Delta N_k^{\mathrm{NEQ}}(t \to \infty) = -4U^2 \int_{-\infty}^{\infty} dE \, \frac{1}{2} \frac{J_k(E; n)}{(\epsilon_k - E)^2} = 2\Delta N_k^{\mathrm{EQU}}$$

$$(7)$$

since $\sin^2$ in (5) yields a factor $1/2$ in the long-time limit.
In the quasi–steady state the momentum distribution func-
tion is therefore that of a zero temperature Fermi liquid.
However, from (7) one deduces that its Z factor is smaller
than in equilibrium, $1 - Z^{\mathrm{NEQ}} = 2(1 - Z^{\mathrm{EQU}})$. This factor
2 implies a quasiparticle distribution function in the vicin-
ity of the Fermi surface in the quasi–steady state equal to
the equilibrium distribution function of the physical elec-
trons, $N_k^{\mathrm{QP:NEQ}} = N_k^{\mathrm{EQU}}$, as opposed to its equilibrium
distribution, $N_k^{\mathrm{QP:EQU}} = \Theta(k_F - k)$.

Remarkably, Cazalilla's findings [8] for the interaction
quench in the Luttinger model mirror these features: the
critical exponent describing the asymptotic behavior of the
electronic Green's function differs from the equilibrium
result. As Cazalilla points out this corresponds to a non-
equilibrium distribution for the bosonic modes after bo-
sonization. A main difference between the Luttinger liquid
and the Fermi-liquid cases follows from the integrability of
the Luttinger liquid with an infinite number of conservation
laws, which make this regime stable for $t \to \infty$. For the
Fermi liquid, on the other hand, on shell interactions lead
to thermalization, as we will see next.

Thermalization.—The previous flow equation calcula-
tion of the real time dynamics contains all contributions to
the time evolution for times smaller than $\rho_F^{-3} U^{-4}$. For the
long-time dynamics one generally expects a quantum
Boltzmann equation (QBE) to be a valid description [21]

$$\frac{\partial N_k^{\mathrm{QP}}(t)}{\partial t} = -\rho_F U^2 J_k(E = \epsilon_k, N^{\mathrm{QP}}(t)). \quad (8)$$

Here the quasiparticle momentum distribution function

$N_k^{\mathrm{QP:NEQ}}$ derived above serves as the initial condition. Because $N_k^{\mathrm{QP:NEQ}}$ allows nonzero phase space for scattering processes in the vicinity of the Fermi surface [originating, ultimately, from the factor 2 in (7)], the initial quasiparticle distribution function starts to evolve on the time scale $t \propto \rho_F^{-3} U^{-4}$. This implies that the quasi–steady electron distribution function depicted in Fig. 2(d) starts to decay on this time scale, and one approaches a Fermi-Dirac distribution [being the only stable fixed point of (8)] with a nonzero temperature T.

The above scenario fits well into the picture of nonequilibrium field theories describing, e.g., the early Universe [17]. The excitation energy of the initial quantum state (the Fermi gas) with respect to the equilibrium ground state of (1) is $E_{\mathrm{ex}} = \alpha \rho_F U^2$ in the weak interaction limit with some lattice-dependent constant $\alpha > 0$. The short-time correlation buildup corresponds to prethermalization, where the kinetic and interaction energy in (1) flow from 0 to $E_{\mathrm{int}}^{\mathrm{NEQ}} = -2\alpha \rho_F U^2$ and $E_{\mathrm{kin}}^{\mathrm{NEQ}} = 2\alpha \rho_F U^2$. This follows immediately from the Feynman-Hellman theorem and the fact that the total energy remains zero for all times. $E_{\mathrm{int}}^{\mathrm{NEQ}}$ equals the equilibrium interaction energy, while $E_{\mathrm{kin}}^{\mathrm{NEQ}} = E_{\mathrm{kin}}^{\mathrm{EQU}} + E_{\mathrm{ex}}$. The kinetic and interaction energy then remain constant throughout the quasi–steady regime and the long-time limit, and therefore the system has *prethermalized* for these average quantities. In the thermalization regime the system redistributes its additional excitation energy E_{ex} in the kinetic energy over the different momenta and reaches a Fermi-Dirac distribution with temperature $T \propto U$.

Higher order flow equations.—Clearly, it would be desirable to derive (8) within the framework of the real time flow equation calculation. However, a calculation to order U^4 is beyond the scope of the present work. Still, one can identify a particular contribution in fourth order leading to a finite lifetime of order $\rho_F^{-3} U^{-4}$ for an electron at the Fermi surface, which is consistent with the dynamics implied by the QBE. The short-time evolution of the system for times smaller than $\rho_F^{-3} U^{-4}$ obtained from the full solution of the Heisenberg equations of motion therefore matches the long-time dynamics described by the QBE, and we have a consistent picture on all time scales. Another effect of the fourth order contributions is that the sharp Fermi edge of the quasi–steady state gets smeared out on an energy scale $\rho_F^3 U^4$, which, however, does not essentially modify our previous conclusions. Therefore, strictly speaking, the discontinuity of the momentum distribution function disappears immediately for $t > 0$, but this effect only becomes noticeable for times of order $\rho_F^{-3} U^{-4}$.

Conclusions.—We have discussed the real time evolution of the Hubbard model with a sudden interaction quench for a weak interaction U. Ultimately, the system completely thermalizes its excitation energy E_{ex} and

reaches a temperature $T \propto U$. This thermalization regime only sets in on the time scale $\rho_F^{-3} U^{-4}$. This follows from the observation that the short-time behavior up to times of order $\rho_F^{-1} U^{-2}$ amounts to quasiparticle formation with a momentum distribution function with a discontinuity at the Fermi energy. Therefore, a quasi–steady prethermalized state emerges for times $\rho_F^{-1} U^{-2} \lesssim t \lesssim \rho_F^{-3} U^{-4}$. Its momentum distribution function looks like a zero temperature Fermi liquid, but with the wrong quasiparticle residue with respect to the interacting ground state. It is this nonequilibrium quasiparticle residue that allows for phase space for scattering processes in a quantum Boltzmann equation description for times $t \gtrsim \rho_F^{-3} U^{-4}$, which then leads to thermalization of the momentum distribution function.

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