Lack of thermalization for integrability-breaking impurities

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Abstract – We investigate the effects of localized integrability-breaking perturbations on the large
times dynamics of thermodynamic one-dimensional quantum and classical systems. In particular,
we suddenly activate an impurity which breaks the integrability of an otherwise homogeneous
system. We focus on the large times dynamics and on the thermalization properties of the im-
purity, which is shown to have mere perturbative effects even at infinite times, thus preventing
thermalization. This is in clear contrast with homogeneous integrability-breaking terms, which
display the prethermalization paradigm and are expected to eventually cause thermalization, no
matter the weakness of the integrability-breaking term. Analytic quantitative results are obtained
in the case in which the bulk Hamiltonian is free and the impurity interacting.

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Introduction. – Recent experimental advances in the
cold atom’s world [1–15] caused an outburst of theoretical
efforts aimed to understand the out-of-equilibrium prop-
erties of closed many-body quantum systems. In partic-
ular, dimensional reduction and the extreme precision in
the coupling tunability gave access to the one-dimensional
world, allowing the experimental realization of several
playgrounds for theoretical physicists, such as integrable
models [16–18]. Integrable systems possess infinitely many
local conserved quantities, which deeply affect their out-
of-equilibrium features: after a homogeneous quantum
quench [19], local observables relax to a steady state which
is not described by the usual thermal ensemble. The infor-
mation encrypted in the conserved degrees of freedom is
retained up to infinite time and the Gibbs ensemble urges
a modification: this led to the construction of the Gen-
eralized Gibbs Ensemble (GGE) \( e^{-\sum_i \beta_i \hat{Q}_i} \) [20–32], where
all the relevant (quasi)local conserved charges \( \hat{Q}_i \) [33–47]
are taken into account. In view of the remarkable differ-
ence between non-integrable and integrable models, under-
standing the effect of integrability-breaking perturbations
is a central question, from both a theoretical and an exper-
imental point of view. In particular, what is the destiny
of a system with weakly broken integrability? The ho-
mogeneous case has been thoroughly investigated in the
last years and the so-called “prethermalization” [48–64]
paradigm has been identified. Local observables relax in
two steps: on a short time scale the system apparently
reaches a non-trivial GGE state, built on the integrable
part of the Hamiltonian. Subsequently, a slow drift to-
wards a final thermal ensemble is observed: such a picture
found experimental confirmation [65–68]. Crucially, the
magnitude of the integrability breaking term affects the
time scale on which the thermal ensemble is attained [48],
but does not spoil the dichotomy between integrable and
non-integrable systems. In contrast with the homogeneous
case, the effect of localized integrability-breaking terms
has not been systematically assessed so far. The activation
of a localized perturbation could seem a rather innocent
operation, but it has tremendous consequences on a frag-
ile property such as integrability [69,70]. More specifically,
we consider at time \( t < 0 \) an integrable Hamiltonian \( \hat{H}_I \),
the infinite system being initialized in a suitable homo-
genous GGE. For \( t \geq 0 \), we activate a localized perturbation
\( \hat{V}(x) \), which we refer to as “defect” or “impurity”
\[
\hat{H} = \hat{H}_I + \int_{-\Delta}^{\Delta} dx \hat{V}(x).
\]

Generalizing the modes of free systems, integrable
Hamiltonians are diagonalized in terms of multi-particle
states [16–18]. Because of the infinite set of constraints
due to the conserved charges, these quasiparticles neces-
sarily undergo only elastic pairwise scattering events. In
the thermodynamic limit, homogeneous GGEs are in a
one-to-one correspondence [40] with a set of root densi-
ties [18], which describe the density of quasiparticles with
inhomogeneous root density $\rho$. For simplicity, we restrict ourselves to the case of a single root density $\rho(k)$.

Although the impurity breaks the integrability of the system as a whole, far from the defect the system is locally described by an integrable Hamiltonian, with stable quasiparticle excitations. Therefore, in the spirit of the Generalized Hydrodynamics (GHD) [71,72] (see also refs. [73–88]), at large times and far from the defect the system locally relaxes to an inhomogeneous GGE [69,89–91]. The latter is fully determined by an inhomogeneous root density $\rho_{x,t}(k)$, with the appealing semiclassical interpretation of a local density of particles. Due to the ballistic spreading characteristic of integrable models, the propagating GGE only depends on the “ray” $\zeta = x/t$: such a state has been named Local Quasi-Stationary State (LQSS) [72]. In contrast, the limit $t \to \infty$ with finite $x$ is known as the Non-Equilibrium Stationary State (NESS) [69,92–94].

While localized impurities have been frequently studied in a whole variety of contexts (see, in particular, refs. [95,96] for integrability-breaking issues), the large times dynamics in the present framework has been analyzed only in free models and CFTs [89–91,93,97], being the defect free or CFT invariant, respectively (see, however, [69]). Instead, we eventually consider $V$ to be an integrability-breaking interaction.

From the semiclassical viewpoint, quasiparticles undergo non-elastic scattering events while crossing the defect’s region, leading immediately to the natural central question of the present work: how does the density root of the quasiparticles emerging from the defect look like? At large times, a finite subsystem encompassing the defect will relax to the NESS. Reasonably, the latter can be expected to be described by a GGE’s density matrix and, being the Hamiltonian the only conserved charge, it appears natural to revert to thermal states. Based on the insight gained in the homogeneous case, long transients can be imagined, but a thermal state should be eventually reached: in this case, the quasiparticles emerging from the defect look like? At large times, a finite subsystem encompassing the defect should be thermally distributed. However, preliminary numerical results go against this natural expectation [70].

In this work we study the thermalizing properties of integrability-breaking impurities. In contrast with the homogeneous case, we show how a weak integrability-breaking defect has poor mixing properties which ultimately prevent thermalization. We focus on a free theory in the bulk, but with an interacting defect: we build a perturbative expansion of the LQSS in the strength of the interaction, which is finite at any order. For technical reasons clarified later on, we focus on continuum models which are not suited for efficient numerical methods such as DMRG [98]. However, the same questions can be posed in classical models (see refs. [99,100] for the construction of GGE and GHD in classical integrable field theories), which allow for a numerical benchmark. We expect the same general conclusions to hold true also in truly interacting integrable models, in view of the following heuristic argument.

**Some heuristic considerations.** – It is widely accepted that standard time-dependent perturbation theory [101] is not suited to study the late-time physics of thermodynamically large homogeneous systems, making necessary to resort to other methods [48,102]. This is due to secular terms that grow unbounded in time: thermalization is intrinsically a non-perturbative effect. However, simple heuristic arguments point out the possible perturbative nature of the defect. We semiclassically regard the initial state as a gas of quasiparticles which, for $t > 0$, undergo inelastic scattering within the support of the perturbation. In the case of a homogeneous integrability-breaking term, a given quasiparticle takes part in a growing number of inelastic scatterings, piling up a cumulative effect which leads to secular terms. In contrast, in the impurity case, a traveling quasiparticle can undergo inelastic processes only on the defect’s support, where it typically spends a finite amount of time. Therefore, small inelastic scatterings cannot sum up to an appreciable contribution, suggesting the perturbative nature of the impurity. Moreover, it could be argued that in the low density limit only the few-body physics rules the dynamics on the defect. Few-body physics has weak thermalizing properties, see, e.g., ref. [103] for the two-particles case. Albeit physically sounding, these considerations remain on a heuristic ground and can be regarded as plausible as the previous reasoning, based on the conserved charges: in this perspective, a rigorous and well-controlled benchmark is needed.

**A specific model.** – In order to test our ideas, we consider a chain of harmonic oscillators

$$\hat{H}_I = \int_{-\infty}^{\infty} dx \frac{1}{2} \left\{ \hat{\Pi}^2(x) + [\partial_x \hat{\phi}(x)]^2 + m^2 \hat{\phi}^2(x) \right\},$$

(2)

where $\hat{\Pi}(x)$ and $\hat{\phi}(x)$ are conjugated fields $[\hat{\phi}(x), \hat{\Pi}(y)] = i\delta(x-y)$. Being $\hat{H}_I$ free, is of course also integrable. Generalizations to other free models, such as Galilean-invariant bosons and fermions (see the Supplementary Material Supplementarymaterial.pdf (SM)), are straightforward.

The integrability-breaking potential is chosen as a function of $\hat{\phi}(x)$, i.e., $\hat{V}(x) = V(\hat{\phi}(x))$. $\hat{H}_I$ is diagonalized in the Fourier space in terms of bosonic operators $\hat{a}(k), \hat{a}^\dagger(q) = \delta(k-q) [104]$ and the modes are readily interpreted as the quasiparticles with energy $E(k) = \sqrt{k^2 + m^2}$ and velocity $v(k) = \partial_k E(k)$. GGEs are simply gaussian ensembles in $a(k)$ [105–108] (and in the field $\phi$), with the root density being associated with the mode density $\langle a^\dagger(k) a(q) \rangle = \delta(k-q) \rho(k)$. Therefore, the two-point function computed on a GGE $\Gamma_{c\rightarrow r}(x-y) = \langle \hat{\phi}_c(x) \hat{\phi}_r(y) \rangle_{\text{GGE}}$ is

$$\Gamma_c(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\cos(E(k)t - kx)}{E(k)} \rho(k) + \frac{\cos(kx)}{2E(k)} e^{-iE(k)t}.$$

(3)
At large times, after the defect activation and far from it, the GHD prediction states that the two-point correlator has the same expression as above, provided we replace \( \rho(k) \rightarrow \rho_{x,t}(k) \) [71,72],

\[
\rho_{x,t}(k) = \rho(k) + \Theta(|v(k)| - |\zeta|) \Theta(v(k)\zeta)\delta \rho(k). \tag{4}
\]

Above, \( \Theta \) is the Heaviside Theta function and \( \zeta = x/t \). The interpretation is clear: for \( t > 0 \) a perturbation of the initial root density \( \delta \rho(k) \) ballistically propagates from the impurity, affecting only a finite interval of length \(|v(k)| \) on the right (left) of the defect for \( v(k) > 0 \) (\( v(k) < 0 \)). The computation of the emergent LQSS (see SM for details), confirms eq. (4) to describe also the time evolution functions in the defect region. The time needed to factor, we are going to show that \( \rho(k) \) + \( \delta \rho(k) \). In order to point out the poor thermalization properties of the defect, we are going to show that \( \delta \rho(k) \) can be made arbitrarily small, making the outgoing quasiparticles distribution close to \( \rho(k) \), which can be chosen to be far from thermal. In truly interacting integrable models, eq. (4) needs to be modified [71,72], but it retains the same physical meaning. It is convenient to proceed through the equation of motion in the Heisenberg picture

\[
\partial_t^2 \hat{\phi}_t(x) = \partial_x^2 \hat{\phi}_t(x) - m^2 \hat{\phi}_t(x) - : V'(\hat{\phi}_t(x)) :, \tag{5}
\]

which can be equivalently reformulated in an integral equation

\[
\hat{\phi}_t(x) = \hat{\psi}_t(x) - \int_{-\infty}^{\infty} d\tau \int_{-\Delta}^{\Delta} dy G_{t-\tau}(x-y) : V'(\hat{\phi}_\tau(y)) :. \tag{6}
\]

Above, \( \hat{\psi}_t(x) \) is the field operator evolved in absence of interaction \( \hat{\psi}_t(x) = e^{itB_t} \hat{\phi}_0(x)e^{-itB_t} \), \( V' \) is the derivative of \( V \) and \( G_{\tau} \) the free retarded Green function

\[
G_{\tau}(x) = \Theta(t) \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{ikx}}{E(k)} \sin(E(k)t). \tag{7}
\]

Normal ordering \( \langle : \rangle \) must be introduced to remove UV singularities [104] and it can be achieved inserting proper counterterms in the potential, or equivalently dropping the vacuum contribution in the normal ordered correlators. In this respect, \( \langle \hat{\psi}_t(x)\hat{\psi}_\tau(y) \rangle \) is defined as per eq. (3) dropping the \( \cos(kx)e^{-iE(k)t}/(2E(k)) \) term.

In the physical assumption that the defect’s region locally relaxes to a stationary state on a finite timescale, the emergent LQSS and NESS can be derived from eq. (6) and \( \delta \rho(k) \) (4) completely determined in terms of correlation functions in the defect region. The time needed to the defect in order to relax contributes only as a transient, thus ineffective in the infinite time limit. The lengthy, albeit simple, derivation is left to SM and we define

\[
A_{x,x'}(t) = \lim_{T \rightarrow \infty} \langle : V'(\hat{\phi}_{t+T}(x)) : V'(\hat{\phi}_{T}(x')) : \rangle, \tag{8}
\]

where the fields are computed within the defect support and the expectation values are taken with respect to the initial conditions. A second auxiliary function \( F_{x,x'}(t) \) naturally emerges in the derivation of the LQSS (see SM) and it is defined through the following convolution:

\[
\lim_{T \rightarrow \infty} \langle : V'(\hat{\phi}_{t+T}(y)) : \hat{\psi}_T(x') : \rangle = \int_{-\infty}^{\infty} d\tau \int_{-\Delta}^{\Delta} dy' \Gamma_{-\tau}(x' - y') F_{y,y'}(t - \tau). \tag{9}
\]

Above, \( \hat{\phi} \) is always supported on the defect, while no restriction is imposed on \( \hat{\psi} \). With these definitions, the large times emergence of the LQSS can be derived and the scattered root density \( \delta \rho(k) \) computed as (see SM)

\[
\delta \rho(k) = \frac{\Re(A_k) - (\rho(k) + 1)\Im(F_k^+)}{2E(k)|v(k)|} + \frac{\rho(k)\Im(F_k^-)}{2E(k)|v(k)|}. \tag{10}
\]

We are left with the issue of computing \( A_{x,x'}(t) \) and \( F_{x,x'}(t) \), which we now consider within perturbation theory. From now on, we focus on the simplest example of a \( \delta \)-like defect (i.e., in eq. (6) replace \( V' \rightarrow (2\Delta)^{-1}V' \) and take \( \Delta \rightarrow 0 \), but see SM for the finite interval case.

**The gaussian defect.** Any perturbative analysis is constructed starting from an exact solution. Therefore, we consider a Gaussian repulsive \( \delta \)-supported defect \( V(\phi) = \mu^2 \phi^2/2 \), which ultimately lays the foundation of the forthcoming perturbation theory in the truly interacting case. In eq. (6) we compute all the fields on the defect and obtain

\[
\hat{\phi}_0(0) = \hat{\psi}_0(0) - \mu^2 \int_{-\infty}^{\infty} d\tau G_{t-\tau}(0)\hat{\phi}_0(0). \tag{13}
\]

Since we are ultimately interested in the infinite time limit and assume relaxation on the top of the defect, we can extend the time-integration domain in the infinite past. Equation (13) is then reformulated in the Fourier space through the definition of \( g(\omega) = \int_{-\infty}^{\infty} d\tau e^{-i\omega\tau} G_{\tau}(0) \). From eq. (7) we get

\[
g(\omega) = \begin{cases} 
\text{sign}(\omega)/(2\sqrt{\omega^2 - m^2}), & |\omega| > m, \\
1/(2\sqrt{m^2 - \omega^2}), & |\omega| < m.
\end{cases} \tag{14}
\]
Equation (13) in the Fourier space states
\[
\hat{\Phi}(\omega) = \hat{\Psi}(\omega) - \mu^2 \hat{g}(\omega) \hat{\Phi}(\omega),
\]  
where $\hat{\Phi}, \hat{\Psi}$ are the Fourier transforms of the fields. In its simplicity, eq. (15) has a lot to teach: even though it can be easily solved
\[
\hat{\Phi}(\omega) = (1 + \mu^2 \hat{g}(\omega))^{-1} \hat{\Psi}(\omega),
\]  
it is worth blindly proceeding through a recursive solution, as we would have done considering $\mu^2$ in perturbation theory
\[
\hat{\Phi}(\omega) = \hat{\Psi}(\omega) - \mu^2 \hat{g}(\omega) \hat{\Phi}(\omega) + [\mu^2 \hat{g}(\omega)]^2 \hat{\Phi}(\omega) + \ldots.
\]  
This series is ill defined, since $g(\omega)$ is singular when $\omega = |m|$ (despite eq. (16) being regular): this encloses a clear physical meaning. Tracking back the singularity from eq. (14) to the definition of the Green function (7), it is evident that the singularities are due to the modes with $k = 0$, which are such that $E(k = 0) = m$ and $v(k = 0) = 0$. Singularities in the frequency space are translated into secular terms when read in time: as we previously commented, secular terms are due to quasiparticles that keep on interacting as time goes further. In the defect’s case, the only quasiparticles that can interact for arbitrary long times are those sat on the defect, i.e., having zero velocity, thus explaining the singularities in eq. (17). The unperturbed field $\hat{\Psi}$ satisfies the Wick theorem and the two-point function is computed on a GGE as per eq. (3); a straightforward use of eq. (16) allows to compute $A_k$ and $F_k^\pm$ and subsequently $\delta \rho(k)$,
\[
\delta \rho(k) = \mu^4 \, \frac{\rho(-k) - \rho(k)}{4E(k)^2 v^2(k) + \mu^4}.
\]  
The general structure of eq. (18) could have been forecast on general considerations. Being the model non-interacting, $\delta \rho(k)$ must be a function of the initial root density $\rho(k)$. Moreover, a free particle scattering on an external potential can be either transmitted or reflected, forcing $\delta \rho(k)$ to be a function only of $\rho(\pm k)$. Finally, the parity invariance of the dynamics and the conservation of the energy flux forces $\delta \rho(k) = S(k)(\rho(k) - \rho(-k))$ with $S(k)$ symmetric in $k \rightarrow -k$, which must be determined by actual computations, as we did.

The interacting defect. – We now turn on the interaction choosing $V(\phi) = \mu^2 \phi^2 / 2 + \lambda \phi^4 / 4!$, $\delta V$ being a truly interacting potential. An expansion around $\mu^2 = \lambda = 0$ is plagued with singularities, exactly as it happens in eq. (17). However, if we rather expand around the solution $\mu^2 > 0$, $\lambda = 0$, we are adding a repulsive potential on the defect, with the consequence that no quasiparticles with zero velocity can remain on the top of it. The perturbative expansion around $\mu^2 > 0$, $\lambda = 0$ is no longer singular. For definiteness, we focus on the explicit case
\[
\delta V(\phi) = \dot{\phi}^4 / 4!,
\]  
where the analogue of eq. (15) is readily recast as
\[
\hat{\Phi}(\omega) = \frac{1}{1 + \mu^2 \hat{g}(\omega)} \hat{\Psi}(\omega) - \frac{\lambda}{3!} \frac{\hat{g}(\omega)}{1 + \mu^2 \hat{g}(\omega)} \int \frac{d^3 \nu}{(2\pi)^2} \delta(\nu - \sum_{i=1}^{3} \nu_i) : \prod_{i=1}^{3} \hat{\Phi}(\nu_i) :.
\]  
A recursive solution of the above provides a $\lambda$-expansion around the solution $\mu^2 > 0$, $\lambda = 0$ (16). When compared with the perturbative expansion around $\mu^2 = 0$ (17), a recursive solution of eq. (19) replaces the propagator $g(\omega)$ with $g(\omega) / (1 + \mu^2 \hat{g}(\omega))$ which is no longer singular for $\mu^2 > 0$. Therefore, the perturbative series remains finite at any order and secular terms are absent (see SM). A systematic treatment of the perturbative expansion is left to SM: here we simply quote that the $O(\lambda^4)$ result can be obtained replacing $\mu^2 \rightarrow \mu^2 + \lambda \alpha$ in eq. (18), where
\[
\alpha = \int_0^\infty \frac{dk}{2\pi} \frac{2E(k)v^2(k)}{4\pi^2 E(k)} \frac{1}{\mu^2} (\rho(k) + \rho(-k)).
\]  
Our choice of considering a continuum model can be finally motivated: lattice systems have a bounded dispersion law, which leads to self-trapping and to the formation of bound states even in the case of repulsive potentials [109]. This
necessarily causes singularities in $g(\omega)/(1 + \mu^2 g(\omega))$ (associated with the bound states) that eventually plague the recursive solution of eq. (19) (see SM).

The classical case. – So far, we have focused on a quantum model, but the Hamiltonian (2) can be also regarded as a classical object, functional of the classical fields $\phi$ and $\Pi$. Interestingly, in the classical realm the perturbative series can be shown to be convergent for bounded interactions (see SM). Hereafter, we enlist the minor changes between the quantum and classical case. The GGE correlator (3) retains the same form even in the classical case, provided we drop the “$\cos(\k x)e^{-i\omega t}/(2E(k))$” contribution, which in the quantum case was due to the non-trivial commutator of the modes. The Green function (7) and the equation of motion (6) do not change, but the normal ordering is now absent. The definitions of the $A_{k,x}(t)$ and $F_{k,x}(t)$ functions, eq. (8) and eq. (9), remain the same (without normal ordering), while in the definition of $\delta \rho(k)$, eq. (10), we must replace $\rho(k) + 1 \rightarrow \rho(k)$. Incidentally, the classical and quantum results for the Gaussian defect (18) and the $O(\lambda)$ order in the interacting case (20) coincide. The LQSS prediction is tested against direct numerical simulations in fig. 1, finding excellent agreement, while in fig. 2 the main focus is the NESS limit.

Conclusions. – We considered the issue of suddenly activating an integrability-breaking localized perturbation, in an otherwise homogeneous integrable model. In contrast with the homogeneous case, which is intrinsically non-perturbative and eventually leads to thermalization, the localized impurity has less dramatic mixing properties being, at least in the example analyzed, relegated to perturbative effects. In the case where the bulk theory is free, our claim is supported by an order-by-order finite perturbative expansion constructed on top of a Gaussian repulsive defect. Several interesting questions are left to future investigations. First of all, non-perturbative effects are present in lattice systems, due to the phenomenon of self-trapping: however, in view of our heuristic considerations, small integrability-breaking defects are expected not to lead to thermalization, as numerically observed in [70]. Another interesting point concerns the defect’s size, whose growth could lead to a crossover in its thermalizing properties. We can expect that as the defect support is increased, the behavior of the integrability-breaking region becomes much closer to a thermodynamic system, which should thermalize due to integrability breaking.

Another interesting question concerns finite-size effects: rather than a truly infinite system, we could have considered, for example, periodic boundary conditions on a ring of length $L$. In this case, a single quasiparticle can interact several times with the impurity as it travels along the ring: in this case, following our heuristic argument, non-perturbative effects are expected to build up in the infinite-time limit, leading to a final thermalization. However, in the limit of large $L$, we can confide in a hydrodynamic approach generalizing eq. (4) for finite sizes and then study the relaxation to a thermal ensemble. While we save such an analysis for future studies, we can readily comment on the expected thermalization time scale $\tau_{\text{th}}$. Indeed, we expect it to be proportional to the number of times a quasiparticle undergoes a scattering event, i.e., $\propto L^{-3}$, weighted with the first perturbative order of $\delta \rho$ (10) which allows for non-trivial mixing among modes. As we commented, in the example we analyzed the first perturbative order simply renormalizes the mass (20) of the non-interacting result, which allows only to mix modes with opposite momenta (18). Instead, the next-to-leading order allows for non-trivial mixing, therefore we expect it can induce thermalization, leading to the estimation $\tau_{\text{th}} \propto 1/(\lambda^2 L)$. In general, quantitative results in truly interacting integrable models are surely a compelling quest.

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Fig. 2: Single-time realizations of the $\langle \phi^2 \rangle$ profile for $\lambda = 3$ (same parameters of fig. 1 are used). Panels (a)–(d): the evolving profile is compared with the $O(\lambda^2)$ analytical result (which already saturates the LQSS prediction, as depicted in fig. 1) for various times and at relatively small distances from the defect, emphasizing the NESS limit. For large times, local observables attain the NESS value predicted by eq. (4): corrections at finite distances from the impurity are observed, as expected. Panels (e), (f): larger distances and times are considered.
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