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Fluctuation-dissipation theorem in isolated quantum systems out of equilibrium

Ehsan Khatami[1], Guido Pupillo[2], Mark Srednicki[3] and Marcos Rigol[4]

[1]Department of Physics, University of California, Davis, California 95616, USA

[2]IPCMS (UMR 7504) and ISIS (UMR 7006), Université de Strasbourg and CNRS, Strasbourg, France

[3]Department of Physics, University of California, Santa Barbara, California 93106, USA

[4]Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA

E-mail: ekhatami@ucdavis.edu

Abstract. We study the validity of the fluctuation-dissipation theorem for an isolated quantum system of harmonically trapped dipolar molecules taken out of equilibrium by means of a quench, a sudden change in the Hamiltonian parameters. We find that the integrability of the system plays a crucial role in the validity of the fluctuation-dissipation theorem. Namely, the system thermalizes according to the eigenstate thermalization hypothesis and the theorem holds if the system is nonintegrable after the quench. However, it fails if the system is integrable, unless the initial state is an eigenstate of a nonintegrable Hamiltonian, in which case the system still thermalizes despite the eigenstate thermalization hypothesis failing to describe it.

1. Introduction

Non-equilibrium dynamics of isolated quantum many-body systems have attracted a great deal of attention in recent years, partly owing to the significant experimental advancements being made in the simulation of such systems by confining, and controlling the interactions of, ultracold atomic gazes. To generate non-equilibrium dynamics, these systems can be prepared in an initial state that is not an eigenstate of the Hamiltonian being simulated, a process called quenching. Among prominent experimental examples are the realization of "quantum Newton's cradle" using Bose gases confined in one-dimensional geometries [1], or their relaxation on a uniform lattice after being prepared in an initial state with alternating site densities [2].

Numerical studies have also played an important role in this regard by showing that, unlike generic nonintegrable systems, integrable systems do not thermalize after quench, and that observables after relaxation can be described by a generalized Gibbs ensemble, in which all constants of motion play a role similar to the temperature [3, 4]. In case of nonintegrable isolated systems, the thermalization can be understood via the eigenstate thermalization hypothesis (ETH) [5, 6, 4].

Recently, other questions related to the dynamics of these systems after quench have arisen, in particular, as related to the validity of the fluctuation-dissipation theorem (FDT). The FDT is an important theorem in statistical mechanics, which relates response functions to the dynamic correlations in the system. If a classical or quantum system at equilibrium experiences a small perturbation, FDT states that the perturbation dissipates in time in the same way as a random thermal or quantum fluctuation. The FDT is valid as long as the perturbation is in the linear response regime and that the system is in thermal equilibrium. However, the applicability of the theorem to systems out of equilibrium, especially to isolated quantum system taken far from equilibrium is much less clear.

Recent analytic studies have concluded that the FDT is not valid for integrable systems out of equilibrium as it does not lead to a unique definition for temperature [7, 8], and that for a subsystem of an infinite system, dynamics are described by the same ensemble that describes its static properties [9]. The validity of FDT for an entire isolated system, either integrable or generic nonintegrable, however, has been investigated only in a recent publication by us [10], where exact diagonalization has been used to study the properties of one-dimensional systems of hard-core bosons with dipolar interactions after quench. We have found that the FDT holds for the system out of equilibrium in two scenarios: (i) when the system after quench is nonintegrable, and (ii) when the initial state before the quench is an eigenstate of a nonintegrable Hamiltonian.

In this paper, we report new numerical results for the nonlocal observable of zero momentum occupation number and study the dynamics of correlation functions that allow us to determine the validity of the FDT at a higher temperature than in Ref. [10] to explore the role temperature may play. We start with the Hamiltonian for hard-core bosons with dipolar interaction trapped in a harmonic potential:

$$\hat{H} = -\sum_{j=1}^{L-1} \left(\hat{b}_j^\dagger \hat{b}_{j+1} + \text{H.c.} \right) + V \sum_{j<l} \frac{\hat{n}_j \hat{n}_l}{|j-l|^3} + g \sum_j x_j^2 \hat{n}_j, \tag{1}$$

where $\hat{b}_j^\dagger$ ($\hat{b}_j$) creates (annihilates) a hard-core boson ($\hat{b}_j^{\dagger 2} = \hat{b}_j^2 = 0$) at site j, and $\hat{n}_j = \hat{b}_j^\dagger \hat{b}_j$ is the number operator. The hopping amplitude is set to one as the unit of energy throughout this paper, V is the strength of the dipolar interaction, g is the strength of the confining potential, x_j the distance of site j from the center of the trap, and L the number of lattice sites. We always choose the total number of bosons to be $L/3$. Also $\hbar = k_B = 1$, and we use open boundary conditions. To reduce the computational burden, we work in the subspace with even parity under reflection. The systems described by the above Hamiltonian can be realized in experiments using gas of bosonic ground state molecules such as, LiCs with dipole moment ~ 5.6 Debye, confined longitudinally by a one-dimensional optical lattice.

We perform three different quenches:

(i) $\{V_{\text{ini}} = 0, g_{\text{ini}} = \gamma\} \rightarrow \{V_{\text{fin}} = 0, g_{\text{fin}} = \gamma/10\}$ (integrable to integrable),

(ii) $\{V_{\text{ini}} = 8, g_{\text{ini}} = \gamma\} \rightarrow \{V_{\text{fin}} = 0, g_{\text{fin}} = \gamma\}$ (nonintegrable to integrable), and

(iii) $\{V_{\text{ini}} = 8, g_{\text{ini}} = \gamma\} \rightarrow \{V_{\text{fin}} = 2, g_{\text{fin}} = \gamma\}$ (nonintegrable to nonintegrable).

in which γ is chosen such that $\gamma x_1^2 = \gamma x_L^2 = 4$. We fix the temperature to $T = 10$, in the sense that the initial state for different quenches, $|\phi_{\text{ini}}\rangle$, is selected such that the energy of the system $E_{\text{tot}} = \langle \phi_{\text{ini}} | \hat{H}_{\text{fin}} | \phi_{\text{ini}} \rangle$ after the quench (when the system is described by $\hat{H}_{\text{fin}}$) corresponds to the energy of the canonical ensemble, i.e., $E_{\text{tot}} = \text{Tr}\{e^{-\hat{H}_{\text{fin}}/T} \hat{H}_{\text{fin}}\}/\text{Tr}\{e^{-\hat{H}_{\text{fin}}/T}\}$ at $T = 10$.

Following the conventions used in Refs.[11, 10], we define three correlation functions. The first one is called the fluctuation correlation:

$$C_{\text{Fluc}}(t) \propto \sum_{\substack{\alpha\beta \\ \alpha\neq\beta}} |c_\alpha|^2 |c_\beta|^2 |O_{\alpha\beta}|^2 e^{i(E_\alpha - E_\beta)t}, \tag{2}$$

where E_α are eigenvalues of $\hat{H}_{\text{fin}}$, c_α are the overlap functions of the initial state and the eigenstates of the final Hamiltonian, and $O_{\alpha\beta}$ are the matrix elements of the observable $\hat{O}$. $C_{\text{Fluc}}(t)$ relates the expectation value of the observable at time $t + t'$ to its value at an earlier time t' (when a fluctuation is assumed to have taken place), i.e., $O_{t'+t} = C_{\text{Fluc}}(t)O_{t'}$. The second correlation function we study is

$$C_{\text{Diss}}(t) \propto \sum_{\substack{\alpha\beta \\ \alpha\neq\beta}} \frac{e^{-E_\alpha/T} - e^{-E_\beta/T}}{E_\beta - E_\alpha} |O_{\alpha\beta}|^2 e^{i(E_\alpha - E_\beta)t}, \tag{3}$$

which is calculated using Kubo's linear response formula [12, 11] assuming that a perturbation has been applied to the system at time $t = 0$. $C_{\text{Diss}}(t)$ relates the expectation value of the observable at time t to its
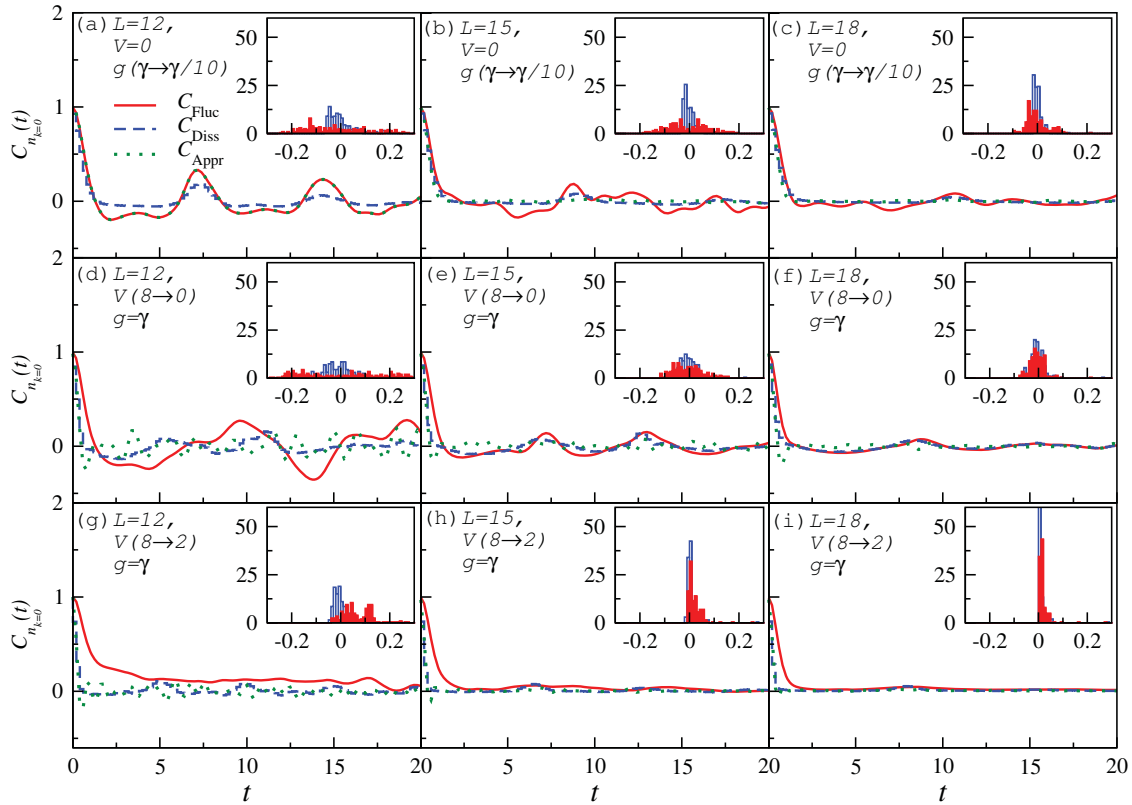
Figure 1. Correlation functions $C_{\text{Fluc}}(t)$, $C_{\text{Diss}}(t)$, and $C_{\text{Appr}}(t)$ when the observable is the zero momentum occupation number, $n_{k=0}$ vs time t at $T = 10$. Results are shown for the three quenches (i)-(iii) (from top to bottom, respectively), and three different sizes, $L = 12$, 15, and 18, (left to right). The insets show normalized histograms of $C_{\text{Fluc}}(t)$ (filled red bars) and $C_{\text{Diss}}(t)$ (empty blue bars) calculated for 200 data points between $t = 0$ and 40.

thermal value before the perturbation, i.e., $O_t = C_{\text{Diss}}(t)O_{\text{Thermal}}$. Finally, the third correlation function we calculate is

$$C_{\text{Appr}}(t) \propto \int_{-\infty}^{+\infty} d\omega |f(E,\omega)|^2 e^{i\omega t}, \tag{4}$$

which can be shown to be valid if the observables follow the form suggested by the ETH [11], namely, $O_{\alpha\beta} = \Omega(E)\delta_{\alpha\beta} + e^{-S(E)/2}f(E,\omega)R_{\alpha\beta}$, where $E \equiv \frac{1}{2}(E_\alpha + E_\beta)$, $\omega \equiv E_\alpha - E_\beta$, $S(E)$ is the thermodynamic entropy at energy E, $e^{S(E)} = E\sum_\alpha \delta(E - E_\alpha)$, $\Omega(E)$ and $f(E,\omega)$ are smooth functions of their arguments, and $R_{\alpha\beta}$ is a random variable. The proportionality constant for all three correlation functions are such that $C(0) = 1$. Note that $C_{\text{Fluc}}(t)$ depends explicitly on the choice of the initial state through the overlap functions, c_α, whereas $C_{\text{Diss}}(t)$ is a thermal quantity. If the system thermalizes after the quench and the ETH is valid, it can be shown that both of the above correlation functions reduce to $C_{\text{Appr}}(t)$. In the following, we study these functions over time for the three quenches described above and analyze how similar or different they are. If the agreement of the fluctuation and dissipation correlation functions over time improves by increasing the system size, we conclude that the FDT is valid for the non-equilibrium system under investigation. If they also agree with the $C_{\text{Appr}}(t)$, then the ETH form for the observables is a valid one.

We study three system sizes, $L = 12$, 15 and 18. Due to the large Hilbert space and the amount of computational expense arising from the need to compute and work with off-diagonal expectation values
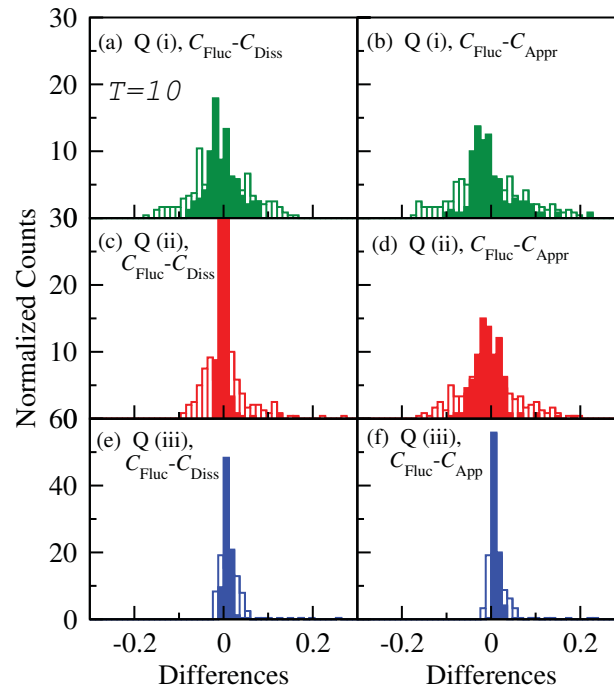
Figure 2. Normalized histograms of $C_{\text{Fluc}}(t) - C_{\text{Diss}}(t)$ (left panels) and $C_{\text{Fluc}}(t) - C_{\text{Appr}}(t)$ (right panels) for $n_{k=0}$, and for the three quenches (from top to bottom) and the two largest system sizes, calculated for 200 data points between $t = 0$ and 40. Empty bars are for $L = 15$, and filled bars are for $L = 18$.

of the observables, calculations for $L = 21$, which is the next size with one more particle, are currently unfeasible. Our computer program takes advantage of OpenMP parallelization for performing the sums in Eqs. (2) and (3).

In Fig. 2, we show these correlation functions for the nonlocal observable of zero momentum occupation number $n_{k=0}$. The system size increases in the panels from left to right and, from top to bottom, panels in different rows correspond to quenches (i) through (iii), respectively. In all cases, the correlation functions exhibit a fast drop from 1 followed by fluctuations over time. The time scale associated with the initial drop can be deduced from the width of the off-diagonal function $f(E_{\text{tot}}, \omega)$ as a function of ω. We also find that as the system size increases, the fluctuations in the correlation functions generally decreases. This is the case as the corresponding time scale is set by the average level spacing, which decreases exponentially by increasing the system size.

Those fluctuations are also suppressed in case of quench (iii) [Fig.1(g)-1(i)], due to the nonintegrable nature of the Hamiltonian. The magnitude of the fluctuations over time can be more carefully studied using histograms of the fluctuation and dissipation correlations, which are shown in the insets. As expected, we find that there is a qualitative different between the histograms in Fig. 1(c) and 1(f) and those in 1(i) for the largest system. For $L = 12$ finite-size effects prevent us from drawing such a distinction.

We also find that, at least for the two largest sizes, $C_{\text{Fluc}}(t)$ better agrees with $C_{\text{Diss}}(t)$ in case of quenches (ii) and (iii), in comparison to quench (i). This shows that, unlike for the integrable system after quench (i) from another integrable Hamiltonian, the FDT may be valid for the other two systems out of equilibrium. Namely, the nonintegrable system after quench (iii), and the integrable system after quench (ii), for which the initial state is an eigenstate of a nonintegrable Hamiltonian. $C_{\text{Appr}}(t)$ on the other hand, generally agrees with the other two correlation functions only in the case of quench (iii), and the agreement improves by increasing the system size. These observations are similar to those made in Ref. [10], based on results for a local observable (the density at the center of the trap), and at a lower
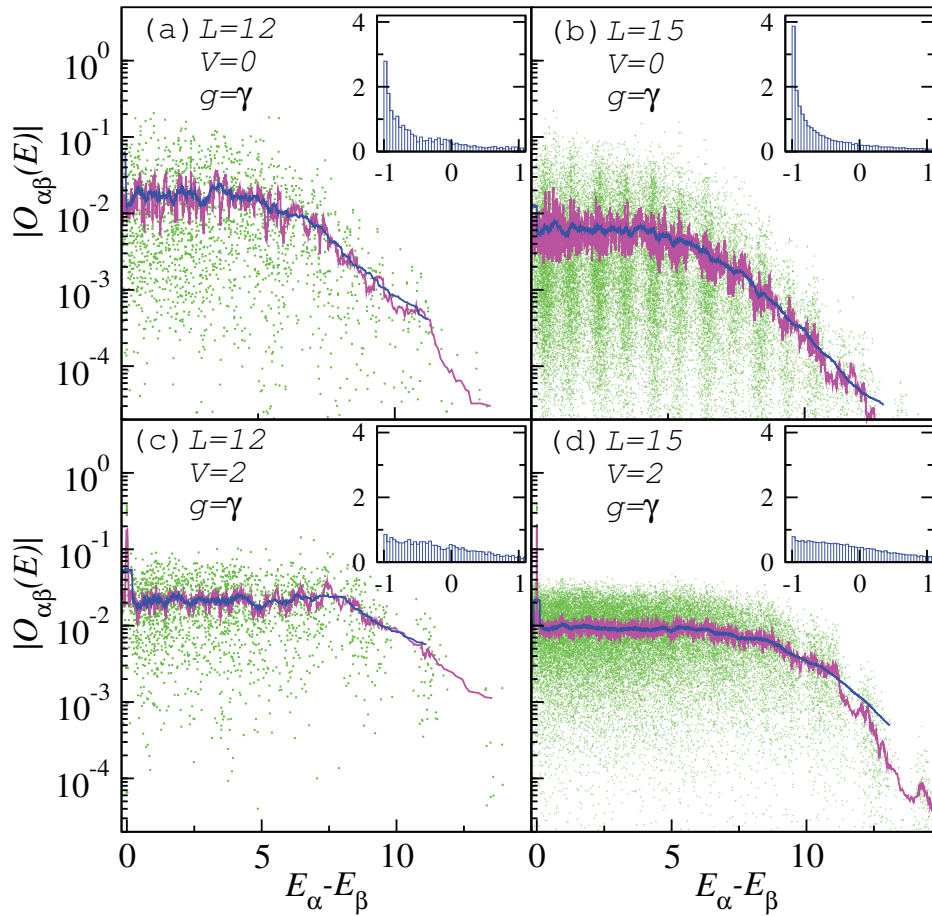
Figure 3. Absolute value of the off-diagonal matrix elements of $\hat{n}_{k=0}$ whose E falls within 0.1 of E_{tot} vs ω for $L = 12$ (left panels) and $L = 15$ (right panels). (a) and (b) correspond to the final Hamiltonian in quench (ii), and (c) and (d) correspond to the final Hamiltonian in quench (iii). Lines are running averages with subset lengths of 20 and 100 for $L = 12$, and 50 and 1000 for $L = 15$. We call the one with the larger subset length $f_{avg}(E, \omega)$. Insets show the histograms of the relative differences between the $n_{k=0}$ and f_{avg} The relative difference is defined as $(|O_{\alpha\beta}| - f_{avg})/f_{avg}$.

temperature of $T = 5$.

To better quantify these observations, in Fig. 2, we plot the normalized histograms of the differences between the fluctuation and dissipation, as well as the fluctuation and the approximate correlation functions for the two largest system sizes and for the three quenches. In case of quench (i), both the agreement between $C_{Fluc}(t)$ and $C_{Diss}(t)$, and between $C_{Fluc}(t)$ and $C_{Appr}(t)$ is poor as the histograms are relatively broad functions.

Quench (ii), however, shows a different trend [see Fig. 2(c) and 2(d)]. We find that the agreement between fluctuation and dissipation correlations improves as we increase L from 15 to 18, and in the same time, the agreement between the fluctuation and the approximate functions is not as significant. This suggests that in the thermodynamic limit, the integrable system out of equilibrium thermalizes, and the FDT is applicable, provided that the state before the quench corresponds to a nonintegrable Hamiltonian. Moreover, the thermalization has occurred in this case without the ETH being valid. These are consistent with recent suggestions for alternative approaches to thermalization of integrable systems [13]. The failure of ETH can be seen in Figs. 3(a) and 3(b), where the off-diagonal matrix elements of $n_{k=0}$ in the

energy eigenbasis do not exhibit a smooth function of the energy differences, ω, as predicted by the ETH form. The off-diagonal values fluctuate wildly with significantly large number of them having very small values. This trend is clearer for the larger system size of $L = 15$ in Fig. 3(b). Histograms of the relative differences of the off-diagonal values and a running average, shown in the insets, show a sharp feature at -1, indicating these large fluctuations.

For the nonintegrable system in case of quench (iii), we find that all three correlation functions mostly agree with each other over time, inferred from the sharp features of the histograms in Fig. 2(e) and 2(f) and that the agreement improves by increasing the size. This suggests that both the ETH and the FDT are valid for nonintegrable systems out of equilibrium. In fact, in Figs. 3(c) and 3(d), we see that the fluctuations in the off-diagonal elements of the observable are dramatically reduced from those in Figs. 3(a) and 3(b), resulting in a smoother function of ω, and offering more consistency with the ETH form. This is again reflected in the histograms, shown in the insets, which now have a more uniform functionality.

Acknowledgments

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