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Fluctuation-Dissipation Theorem in Isolated Quantum Dipolar Bosons After a Quench

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We examine the validity of fluctuation-dissipation relations in isolated quantum systems taken out of equilibrium by a sudden quench. We focus on the dynamics of trapped hard-core bosons in one-dimensional lattices with dipolar interactions whose strength is changed during the quench. We find indications that fluctuation-dissipation relations hold if the system is nonintegrable after the quench, as well as if it is integrable after the quench if the initial state is an equilibrium state of a nonintegrable Hamiltonian. On the other hand, we find indications that they fail if the system is integrable both before and after quenching.

The fluctuation-dissipation theorem (FDT) [1–3] is a fundamental relation in statistical mechanics which states that typical deviations from the equilibrium state caused by an external perturbation (within the linear response regime) dissipate in time in the same way as random fluctuations. The theorem applies to both classical and quantum systems as long as they are in thermal equilibrium. Fluctuation-dissipation relations are not, in general, satisfied for out-of-equilibrium systems, especially if the system is isolated. Studies of integrable models such as a Luttinger liquid [4] and the transverse Ising chain [5] have shown that the use of fluctuation-dissipation relations to define temperature leads to values of the temperature that depend on the momentum mode and/or the frequency being considered. More recently, Essler *et al.* [6] have shown that for a subsystem of an isolated infinite system, the basic form of the FDT holds, and that the same ensemble that describes the static properties also describes the dynamics.

The question of the applicability of the FDT to isolated quantum systems is particularly relevant to experiments with cold atomic gases [7, 8], whose dynamics is considered to be, to a good approximation, unitary [9]. In that context, the description of observables after relaxation (whenever relaxation to a time-independent value occurs) has been intensively explored in the recent literature [10]. This is because, for isolated quantum systems out of equilibrium, it is not apparent that thermalization can take place. For example, if the system is prepared in an initial pure state $|\phi_{\rm ini}\rangle$ that is not an eigenstate of the Hamiltonian $\hat{H}$ ($\hat{H}|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle$) (as in Ref. [9]), then the infinite-time average of the evolution of the observable $\hat{O}$ can be written as $\overline{\langle \hat{O}(t)\rangle} = \sum_\alpha |c_\alpha|^2 O_{\alpha\alpha} \equiv O_{\rm diag}$, where $c_\alpha = \langle\psi_\alpha|\phi_{\rm ini}\rangle$, $O_{\alpha\alpha} = \langle\psi_\alpha|\hat{O}|\psi_\alpha\rangle$, and we have assumed that the spectrum is nondegenerate. The outcome of the infinite-time average can be thought of as the prediction of a "diagonal" ensemble [11]. $O_{\rm diag}$ depends on the initial state through the c_α's (there is an exponentially large number of them) while the thermal predictions depend only on the total energy, $\langle\phi_{\rm ini}|\hat{H}|\phi_{\rm ini}\rangle$, i.e., they need not agree.

The lack of thermalization of some observables, in the specific case of quasi-one-dimensional geometries close to an integrable point, was seen in experiments [12], and, at integrability, confirmed in computational [13] and analytical [14] calculations. Away from integrability, computational studies have shown that few-body observables thermalize in general [11, 15–17], which can be understood in terms of the eigenstate thermalization hypothesis (ETH) [11, 18, 19]. We note that the nonintegrable systems studied computationally belong to two main classes of lattice models: (i) spin-polarized fermions, hard-core bosons, and spin models with short range (nearest and next nearest neighbor) interactions [11, 15, 16, 20], and (ii) the Bose-Hubbard model [17].

In this Letter, we go beyond these studies and report results that indicate that fluctuation-dissipation relations are also valid in generic isolated quantum systems after relaxation, while they fail at integrability. For that, we use exact diagonalization and study a third class of lattice models, hard-core bosons with dipolar interactions in one-dimension [21]. The latter are of special interest as they describe experiments with quantum gases of magnetic atoms trapped in optical lattices [22] as well as ground state polar molecules [23]. Rydberg-excited alkali atoms [24] and laser-cooled ions [25] may soon provide alternative realizations of correlated systems with dipolar interactions. The effect of having power-law decaying interactions in the dynamics and description of isolated quantum systems after relaxation is an important and open question that we address here.

The model Hamiltonian for those systems can be written as

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

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. J is the hopping amplitude, V the strength of the dipolar interaction, g 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 (the total number of bosons, p, is always chosen to be $p = L/3$). We set $J = 1$ (unit of energy throughout this paper), $\hbar = k_B = 1$, use open boundary conditions, and work in the subspace with even parity under reflection.

We focus on testing a fluctuation-dissipation relation after a quench for experimentally relevant observables, namely, site and momentum occupations (results for the density-density structure factor are presented in Ref. [26]). A scenario under which FDT holds in isolated systems out of equilibrium was put forward by one of us in Ref. [27]. There, it was shown that after a quantum or thermal fluctuation (assumed to occur at time t' [28], which was treated as a uniformly distributed random variable), it is overwhelmingly likely that $O_{t'\pm t} = C_{\text{Fluc}}(t)O_{t'}$, where $O_t = \langle\hat{O}(t)\rangle$ [29]. Formally, $C_{\text{Fluc}}(t)$ is related to the second moments of a probability distribution for O_t, $C_{\text{Fluc}}(t) = \overline{O_{t+t''}O_{t''}}/\overline{(O_{t''})^2}$, where infinite-time averages have been taken with respect to t''. Therefore, assuming that no degeneracies occur in the many-body spectrum or that they are unimportant, $C_{\text{Fluc}}(t)$ can be written as

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

where the proportionality constant is such that $C_{\text{Fluc}}(0) = 1$ [30]. The correlation function in Eq. (2) explicitly depends on the initial state through c_α.

Assuming that eigenstate thermalization occurs in the Hamiltonian of interest, the matrix elements of $\hat{O}$ in the energy eigenstate basis can be written as:

$$O_{\alpha\beta} = \Omega(E)\delta_{\alpha\beta} + e^{-S(E)/2} f(E,\omega) R_{\alpha\beta}, \qquad (3)$$

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 (e.g., with zero mean and unit variance). This is consistent with quantum chaos theory and is presumably valid for a wide range of circumstances [27, 31]. From Eq. (3), it follows straightforwardly that $C_{\text{Fluc}}(t) \sim C_{\text{Appr}}(t)$, where we have defined

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

and again, the proportionality constant is such that $C_{\text{Appr}}(0) = 1$ [32]. Therefore, we see that $C_{\text{Fluc}}(t)$ does not depend on the details of the initial state, in the same way that observables in the diagonal ensemble do not depend on such details.

We can then compare this result to how a typical deviation from thermal equilibrium (used to describe observables in the nonequilibrium system after relaxation) caused by an external perturbation "dissipates" in time. Assuming that the perturbation is small (linear response regime), and that it is applied at time $t = 0$, $C_{\text{Diss}}(t)$, defined via $O_t = C_{\text{Diss}}(t)O_{\text{Thermal}}$, can be calculated through Kubo's formula as [27, 33]

$$C_{\text{Diss}}(t) \propto \sum_{\substack{\alpha\beta \\ \alpha\neq\beta}} \frac{e^{-E_\alpha/T} - e^{-E_\beta/T}}{E_\beta - E_\alpha} |O_{\alpha\beta}|^2 e^{i(E_\alpha-E_\beta)t}, \qquad (5)$$

where again, we set $C_{\text{Diss}}(0) = 1$. Using Eq. (3), one finds that

$$C_{\text{Diss}}(t) \sim \int_{-\infty}^{+\infty} d\omega \frac{\sinh(\omega/2T)}{\omega} |f(E,\omega)|^2 e^{i\omega t} \sim C_{\text{Appr}}(t), \qquad (6)$$

where the last similarity is valid if the width of $f(E,\omega)$ [26] is of the order of, or smaller than, the temperature. The results in Eqs. (4) and (6) suggest that FDT holds in isolated quantum systems out of equilibrium under very general conditions.

In what follows, we study dipolar systems out of equilibrium and test whether their dynamics is consistent with the scenario above. This is a first step towards understanding the relevance of FDT, and of the specific scenario proposed in Ref. [27], to experiments with nonequilibrium ultracold quantum gases. The dynamics are studied after sudden quenches, for which the initial pure state $|\phi_{\text{ini}}\rangle$ is selected to be an eigenstate of (1) for $V = V_{\text{ini}}$ and $g = g_{\text{ini}}$ ($\hat{H}_{\text{ini}}$), and the evolution is studied under $\hat{H}_{\text{fin}}$ ($V = V_{\text{fin}}$ and $g = g_{\text{fin}}$), i. e., $|\phi(t)\rangle = e^{-i\hat{H}_{\text{fin}}t}|\phi_{\text{ini}}\rangle$. We consider the following three types of quenches: type (i) $\{V_{\text{ini}} = 0,\ g_{\text{ini}} = \gamma\}\to\{V_{\text{fin}} = 0,\ g_{\text{fin}} = \gamma/10\}$ (integrable to integrable), type (ii) $\{V_{\text{ini}} = 8,\ g_{\text{ini}} = \gamma\}\to\{V_{\text{fin}} = 0,\ g_{\text{fin}} = \gamma\}$ (nonintegrable to integrable), and type (iii) $\{V_{\text{ini}} = 8,\ g_{\text{ini}} = \gamma\}\to\{V_{\text{fin}} = 2,\ g_{\text{fin}} = \gamma\}$ (nonintegrable to nonintegrable). We choose γ such that $\gamma x_1^2 = \gamma x_L^2 = 4$, which ensures a (nearly) vanishing density at the edges of the lattice in the ground state. The initial state for different quenches, which need not be the ground state of $\hat{H}_{\text{ini}}$, is selected such that $E_{\text{tot}} = \langle\phi_{\text{ini}}|\hat{H}_{\text{fin}}|\phi_{\text{ini}}\rangle$ corresponds to the energy of a canonical ensemble with temperature $T = 5$, i. e., such that $E_{\text{tot}} = \text{Tr}\{e^{-\hat{H}_{\text{fin}}/T}\hat{H}_{\text{fin}}\}/\text{Tr}\{e^{-\hat{H}_{\text{fin}}/T}\}$.

In Fig. 1, we show results for $C_{\text{Fluc}}(t)$, $C_{\text{Diss}}(t)$, and $C_{\text{Appr}}(t)$ when the observable of interest is the occupation of the site in the center of the system $n_{j=L/2}$ (qualitatively similar results were obtained for other site occupations, for momenta occupations, and for the density-density structure factor [26]). The results are obtained for the three different quench types mentioned above and are shown for $L = 15$ and 18. For quench type (i), we find that none of the three correlation functions agree with each other and that the agreement does not improve with increasing L [see Figs. 1(a) and 1(b)]. There are also large time fluctuations, characteristic of the integrable nature of the final Hamiltonian [34]. We quantify these fluctuations by plotting the histograms of $C_{\text{Fluc}}(t)$ and $C_{\text{Diss}}(t)$ for an extended period of time in the insets. We find the histograms to be broad functions for quenches (i) and (ii) [Figs. 1(a)-1(d)].

Remarkably, in quenches type (ii) [Figs. 1(c) and 1(d)], which also have a final Hamiltonian that is integrable, $C_{\text{Fluc}}(t)$ and $C_{\text{Diss}}(t)$ are very similar to each other at each time and their differences decrease with increasing L. This indicates that the FDT holds. At the same time, we find differences between fluctuation/dissipation correlations and $C_{\text{Appr}}(t)$, indicating that the agreement between $C_{\text{Fluc}}(t)$ and $C_{\text{Diss}}(t)$ does not imply that Eq. (3) is valid. These observations can be understood if the initial state provides an unbiased sampling of the eigenstates of the final Hamiltonian. In that case, even though eigenstate thermalization does not occur, thermalization can take place [35] and this results in the applicability of FDT. In quenches type (ii), such an unbiased sampling occurs because of the nonintegrability of the initial Hamiltonian, whose eigenstates are random superpositions of eigenstates of the final integrable Hamiltonian with close energies [35].

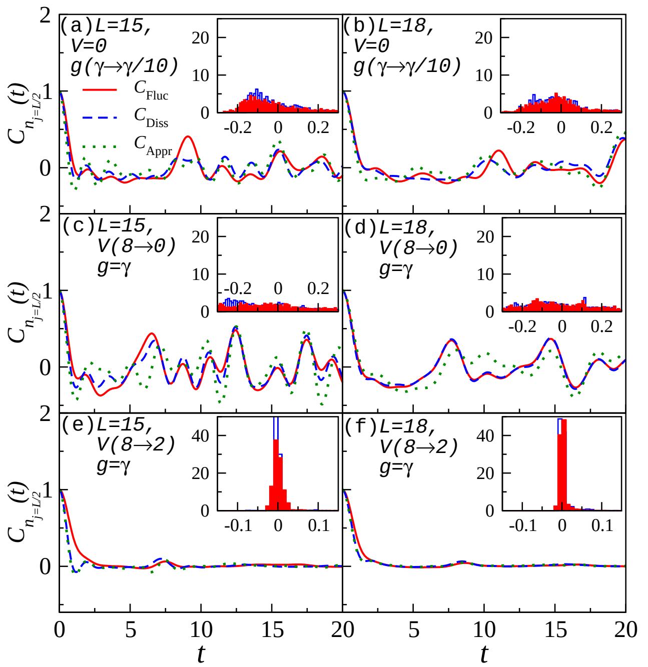

FIG. 1. Correlation functions, $C_{\rm Fluc}(t)$, $C_{\rm Diss}(t)$, and $C_{\rm Appr}(t)$ when the observable is $n_{j=L/2}$ vs time t. Results are shown for the three quenches (i)–(iii) (from top to bottom, respectively) explained in the text, and for $L = 15$ (left panels) and 18 (right panels). Results for $L = 12$ are presented in Ref. [26]. The insets show normalized histograms of $C_{\rm Fluc}(t)$ (red filled bars) and $C_{\rm Diss}(t)$ (blue empty bars) calculated for 2000 data points between $t = 0$ and 100.

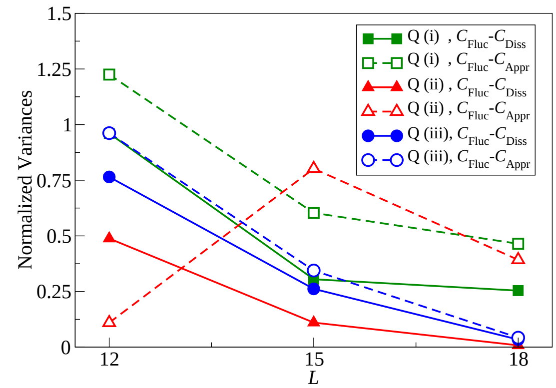

FIG. 2. Normalized variance of $C_{\rm Fluc}(t) - C_{\rm Diss}(t)$ and $C_{\rm Fluc}(t) - C_{\rm Appr}(t)$ vs the system size for the three quenches explained in the text [identified by Q (i), Q (ii), and Q (iii)], where the normalization factor is the average variance of the two functions for which the differences are calculated, e. g., $\text{Var}(C_{\rm Fluc} - C_{\rm Diss})/\frac{1}{2}[\text{Var}(C_{\rm Fluc}) + \text{Var}(C_{\rm Diss})]$. The observable is $n_{j=L/2}$. The variances are calculated for 2000 points between $t = 0$ and 100.

For quenches type (iii) [Figs. 1(e) and 1(f)], on the other hand, we find that not only $C_{\rm Fluc}(t)$ and $C_{\rm Diss}(t)$ are very close to each other, but also $C_{\rm Appr}(t)$ is very close to both of them, and that the differences between the three decrease with increasing L. Therefore, our results are consistent with the system exhibiting eigenstate thermalization [36], which means that the assumptions made in Eq. (3) are valid, and the applicability of the FDT follows. Furthermore, for quenches type (iii), one can see that time fluctuations are strongly suppressed when compared to those in quenches type (i) and type (ii) [better seen in the insets of Fig. 1(e)-(f)], which is a result of the nonintegrable nature of the final Hamiltonian [27, 37].

To quantify the differences between the three correlation functions and explore their dependence on the system size for each quench type, we calculate the normalized variances of $C_{\rm Fluc}(t) - C_{\rm Diss}(t)$ and $C_{\rm Fluc}(t) - C_{\rm Appr}(t)$. In Fig. 2, we show these quantities for the three quench types vs L. For quench type (i), the variances exhibit a tendency to saturate to a nonzero value as L increases, which indicates that $C_{\rm Fluc}(t)$ and $C_{\rm Diss}(t)$, as well as $C_{\rm Fluc}(t)$ and $C_{\rm Appr}(t)$, may remain different in the thermodynamic limit. This is consistent with the findings in Refs. [4, 5] where it was shown that in the thermodynamic limit, conventional fluctuation-dissipation relations with a unique temperature do not hold in integrable systems. For quench type (ii), we see that the variance of $C_{\rm Fluc}(t) - C_{\rm Diss}(t)$ decreases with increasing system size and becomes very small already for $L = 18$, indicating that $C_{\rm Fluc}(t)$ and $C_{\rm Diss}(t)$ possibly agree in the thermodynamic limit. The variance of $C_{\rm Fluc}(t) - C_{\rm Appr}(t)$, on the other hand, exhibits a more erratic behavior, and it is not apparent whether it vanishes for larger system sizes. For quench type (iii), the relative differences between $C_{\rm Fluc}(t)$, $C_{\rm Diss}(t)$, and $C_{\rm Appr}(t)$ exhibit a fast decline with increasing L, indicating that all three likely agree in the thermodynamic limit. These results strongly suggest that the FDT is applicable in the thermodynamic limit for quenches in which the final system is nonintegrable, as well as after quenches from nonintegrable to integrable systems, even though the ETH does not hold in the latter.

In order to gain an understanding of why FDT fails or applies depending on the nature of the final Hamiltonian, we explore to which extent Eq. (3) describes the behavior of the matrix elements of few-body observables in the nonintegrable case, and in which way it breaks down at integrability. In Fig. 3, we plot the off-diagonal elements of two observables, $n_{j=L/2}$, and the zero-momentum occupation number, $n_{k=0}$ vs the eigenenergy differences (ω) in a narrow energy window around $E = E_{\rm tot}$. Results are shown for matrix elements in the eigenstates of the final Hamiltonians in quenches type (ii) and type (iii) [38]. The off-diagonal matrix elements of both observables in the eigenstates of the integrable Hamiltonian [Fig. 3(a)-3(b)] exhibit a qualitatively different behavior from those in the nonintegrable one. In the integrable Hamiltonian, they exhibit extremely large fluctuations. In addition, a very large fraction of those elements (larger for $n_{j=L/2}$ than for $n_{k=0}$) have vanishing values. This makes any definition of a smooth function, $f(E,\omega)$, meaningless. Those results contrast the ones obtained in the nonintegrable case, where the fluctuations of the matrix elements have a different nature, and we do not find a large fraction of vanishing ones. To see that more clearly for $n_{k=0}$ (the better behaved of the two observables), in the insets of Fig. 3 we show the normal-

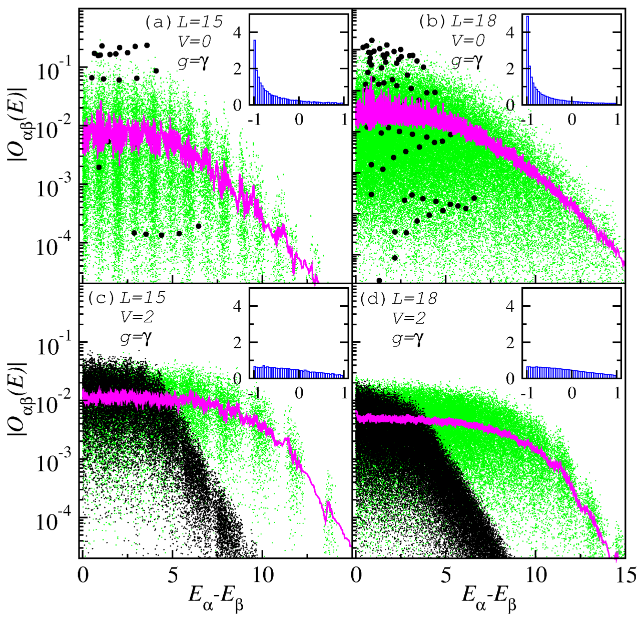

FIG. 3. Absolute value of the off-diagonal matrix elements of $\hat{n}_{j=L/2}$ and $\hat{n}_{k=0}$ in the eigenenergy basis, in a narrow energy window around $E = E_{\rm tot}$ (with a width of 0.1), vs the eigenenergy difference, $\omega = E_\alpha - E_\beta$. Results are shown for $L = 15$ (left panels) and $L = 18$ (right panels). (a)-(b) and (c)-(d) correspond to the final Hamiltonian in quenches (ii) and (iii), respectively. The green (light gray) symbols are the matrix elements of $\hat{n}_{k=0}$, and the black ones of $\hat{n}_{j=L/2}$. In (a)-(b), we have increased the size of the symbols for $n_{j=L/2}$ by a factor of 20 relative to those for $n_{k=0}$. To increase the resolution of the distribution of values in the case of $L = 18$, where a very large number of data points exists, we plot only 1 out of every 10 points for $n_{k=0}$ in (b), and for both observables in (d). Lines are running averages for $n_{k=0}$ with a subset length of 50 for $L = 15$ and 200 for $L = 18$. Insets show the histograms of the relative differences between the $n_{k=0}$ data and running averages ($f_{\rm avg}$) with subset sizes of 1000 for $L = 15$ and 10000 for $L = 18$. The relative difference is defined as $(|O_{\alpha\beta}| - f_{\rm avg})/f_{\rm avg}$.

ized histograms of the relative differences between the matrix elements for $n_{k=0}$ and a "smooth" function, defined as the running average of those elements over a large enough group of them (examples of the running averages are presented in the main panels). For the integrable system, we find that the histograms are not compatible with the uniform distribution postulated in Eq. (3), as a very sharp peak develops at -1 for both system sizes. That peak becomes sharper with increasing system size, reflecting an increasing fraction of vanishing off-diagonal matrix elements in those systems. For the nonintegrable Hamiltonian, on the other hand, the histograms are closer to a uniform distribution.

In summary, studying the dynamics of an experimentally relevant model of trapped hard-core bosons with dipolar interactions, we have found indications that the FDT is applicable to the properties of few-body observables in nonintegrable isolated quantum systems out of equilibrium, and that this follows from the ETH. Furthermore, we find indications that the FDT may also apply to integrable systems, for which the ETH is not valid, provided that the initial state before the quench is an equilibrium state (eigenstate) of a nonintegrable system.

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[29] By “overwhelmingly” we mean that the conditional probability distribution $P(O_{t'+t}|O_{t'})$ is a Gaussian centered at $C(t)O_{t'}$ whose width is proportional to δ/Δ, where Δ is the uncertainty in energy and δ is the level spacing [27]. It is expected that, in quenches in large systems, $\Delta \gg \delta$.
[30] We have subtracted a constant term containing the infinite-time average of O_t from this correlation function before normalization such that the infinite-time average of $C_{\rm Fluc}(t)$ is zero.
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