Memory effects in the Fermi-Pasta-Ulam Model

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Abstract

We study the intermediate scattering function of the Fermi-Pasta-Ulam Model by means of coarse-graining techniques derived via projection operator formalism as well as molecular dynamics simulations. For a strongly anharmonic interaction potential, the simulations show that the relaxation time of density correlations to their equilibrium value depends sensitively on the system’s temperature. We present a recursive method for an exact reconstruction of the time evolution of the function; its dynamics can be associated to a Generalized Langevin Equation, whose memory kernel is estimated with a cross analytical and numerical approach.

1 Introduction

The Fermi-Pasta-Ulam Model (FPU) consists of a one-dimensional chain of N particles, which interact through a nearest-neighbor potential. The system was at first conceived as a simple numerical tool to probe the spread of chaos in nonlinear dynamical systems. It can be simply interpreted as the backbone structure of a nonlinear crystal, while at the same time it can map a broad class of other realistic systems such as DNA structures [1] and polymer chains [2]; even the dynamics of growth models evolves according to similar differential equations in one dimension [3].

In the case of harmonic interactions the system is integrable, and it can be explicitly decoupled into independent normal modes; a maximal set of commuting variables for this limit case are the modes’ energies. If a nonlinearity is included in the interactions, the system becomes chaotic. Energy, which initially is not uniformly spread between the normal frequencies, will eventually relax to the expected equipartition. The time-evolution of this relaxation process is intriguing and has been the topic of scientific debate for more than 60 years (see [4] for a review). The results of the very first study E. Fermi, J. Pasta, S. Ulam and M. Tsingou were published in 1955 [5]. The authors considered the case of a small anharmonic interaction; they showed that below a certain threshold energy does not spread uniformly between all the normal modes if only a small subset of frequencies is excited at the initial time. This unexpected result turned out to be in apparent contrast with the classical results from Ergodic Theory: Fermi himself in [6] generalized a Poincaré theorem proving that any arbitrarily small perturbation of an integrable Hamiltonian suffices to ensure equipartition of energy. An intense and fruitful debate on the nature of the dynamical localization led to an interpretation of the phenomenology within the KAM Theorem for discrete lattices [7], while in the continuum limit the quasi-integrability behavior was related to the energy conservation of solitary waves [8]. In general, the relation between conservation laws and and localization phenomena in the system turns out to be a quite involved issue [9]. Sixty year after its original formulation, the “FPU Problem” is still an open and intriguing challenge for the foundation of the Theory of Dynamical Systems.

A question one could ask is whether an analogue of the phenomenology encountered in such a strongly out-of-equilibrium setting can be seen by considering more typical conditions, e.g. by sampling a canonical initial state. In that case it has been shown in [10] that the system exhibits localization phenomena via a nontrivial decay of the energy correlation function.

In either of these settings, the dynamics of the system is history-dependent. A powerful approach for the study of memory effects in complex systems is the Mori-Zwanzig formalism [11], [12]. Via projection operator techniques, it allows to construct a generalized Langevin equation (GLE) for the time evolution of any dynamical variable. This equation of motion depends on time via an integro-differential structure, accounting for the fact that instantaneous realizations of the system depend on the past states.

In the context of glasses, the intermediate scattering function (ISF) is often studied as a relevant correlation function for the analysis of memory problems within this formalism [13]. We therefore study the FPU problem through the...
dynamics of the ISF of for a single tagged degree of freedom (d.o.f.) of the chain. We choose canonical equilibrium conditions such that the reconstruction of the dynamics becomes intrinsically time-independent, but still challenging from an analytical and numerical perspective.

2 The Model

Consider a one-dimensional chain of \( N \) identical particles with mass \( m \) each, interacting through a nearest-neighbor nonlinear potential. The Hamiltonian of the system can be written as:

\[
H = \sum_{j=0}^{N-1} \frac{p_j^2}{2m} + \sum_{j=1}^{N-1} V_\eta(q_j - q_{j-1})
\]

We set boundary conditions of Dirichlet type

\[
q_0 = 0 \quad , \quad q_{N-1} = L
\]

The total length \( L \) is fixed to a value which is comparable to the canonical equilibrium value, i.e. \( L \approx N \langle r \rangle \beta \). We use a quartic nonlinear potential with

\[
V_\eta(r) = \alpha \left[ \left( \frac{r}{\sigma} \right)^2 + A(\eta) \left( \frac{r}{\sigma} \right)^3 + B(\eta) \left( \frac{r}{\sigma} \right)^4 \right]
\]

and coefficients

\[
A(\eta) = -2 - 4\eta \quad \quad B(\eta) = 1 + 3\eta
\]

We have chosen this particular form of the potential, such that the positions of the minima remain fixed while \( \eta = -V(\sigma)/\alpha \) controls the unbalance between their depths (see Appendix A.1).

![Figure 1: Shape of the two body interaction potential for three different values of the parameter \( \eta \)](image.png)

The main observable discussed in this paper is the intermediate scattering function, which we construct in the following way: the spacial density of the \( j \)-th d.o.f. of the system

\[
\rho^j(r) = \delta(r_j - r)
\]
is Fourier-transformed into the density fluctuation
\[ A_K^j = e^{iK r_j} \, . \]

The time propagation of this variable is expanded in time as
\[ e^{iK r_j(t)} = e^{i\mathcal{L}t} e^{iK r_j} = \sum_{n=0}^{+\infty} \frac{(i\mathcal{L}t)^n}{n!} e^{iK r_j} \tag{2} \]

where the Liouvillian \( i\mathcal{L} \) is defined as the operator acting on the phase space points \( \Gamma = (q, p) \) as
\[ i\mathcal{L} = \dot{\Gamma} \frac{\partial}{\partial \Gamma} = \sum_{i=0}^{N-1} \dot{q}_i \frac{\partial}{\partial q_i} + \dot{p}_i \frac{\partial}{\partial p_i} \]

and \( e^{i\mathcal{L}t} \) is the time evolution operator under Hamilton’s dynamics. The magnitude of \( 1/K \) fixes the length-scale at which we inspect the dynamics. In the following we will stick to \( \mathcal{O}(1/K) \sim \mathcal{O}(\sigma) \). The time autocorrelation function of \( A_K^j \) is defined as
\[ C(t) = \int d\mu \left[ e^{i\mathcal{L}t} A_K^j(\Gamma) \right] A_K^{j\ast}(\Gamma) = \left\langle e^{iK(r_j(t)-r_j(0))} \right\rangle_\beta \tag{3} \]

where \( d\mu = d\Gamma \rho_\beta(\Gamma) \) is the measure element on the phase space. The series expansion of the \( C(t) \) can be naturally deduced from the Taylor series of the time evolution operator:
\[ C(t) = \sum_{n=0}^{+\infty} \frac{1}{n!} \left\langle (i\mathcal{L}t)^n e^{iK r_j} \right\rangle_\beta = \sum_{n=0}^{+\infty} \frac{(-1)^n}{(2n)!} \left\langle (i\mathcal{L}t)^n e^{iK r_j} \right\rangle_\beta = \sum_{n=0}^{+\infty} \frac{t^{2n}}{(2n)!} \omega_{2n} \tag{4} \]

which implies
\[ \omega_{2n+1} = 0 \quad \forall n \geq 0 \tag{5} \]

The second identity in eqn. 4 is a consequence of the anti-Hermitianity of the Liouvillian with respect to the scalar product induced by the canonical phase average, which does not evolve in time; in the last identity we introduced the dynamical correlators
\[ \omega_{2n} \equiv \left\langle (i\mathcal{L})^{2n} e^{iK r_j} \right\rangle_\beta = (-1)^n \left\langle (i\mathcal{L})^n e^{iK r_j} \right\rangle_\beta \tag{6} \]

The knowledge of the series of these coefficients would in principle allow to reconstruct the whole dynamics of \( C(t) \). The solution of the \( C(t) \) for an ideal gas (with a purely kinematic Hamiltonian) can be computed exactly via the knowledge of the series of the respective \( \{\omega_n\}_n \) (see A.2.1):
\[ C^{id}(t) = \sum_{n=0}^{+\infty} \frac{t^{2n}}{(2n)!} \omega_{2n} = \frac{1}{\sqrt{\pi}} \sum_{n=0}^{+\infty} (-1)^n \left( \frac{4K^2\alpha}{m\beta} \right)^n \frac{(2n)!}{4^n n!} \frac{t^{2n}}{(2n)!} = e^{-\frac{m\beta t^2}{4K^2}} = e^{-\frac{\tau^2}{2}} \tag{7} \]

where we defined the natural timescale
\[ \tau = \sqrt{\frac{m\beta}{\alpha K^2}} \]

that will ease the comparison of correlation functions with different values of \( \beta \) and \( K \) in the next section.

In case a potential term is introduced into the Hamiltonian, the dynamics is defined as mixing if the time-correlation of any couple of dynamical variables converges to its phase average:
\[ \langle f(t), g \rangle - \langle f \rangle \langle g \rangle \to 0 \quad \text{for} \ t \to +\infty \quad \forall f, g \in \mathcal{L}^2(\text{d}\mu) \tag{8} \]

A mixing dynamical system is in particular ergodic. In the case of our observable, eqn. 8 reads as:
\[ C(t) = \left\langle e^{iK r_j(t)} (e^{iK r_j})^\ast \right\rangle_\beta \to _{t \to +\infty} = \left\langle e^{iK r_j} \right\rangle_\beta (e^{iK r_j})^\ast = \langle \cos(K r_j) \rangle_\beta + \langle \sin(K r_j) \rangle_\beta^2 \equiv C_\beta \tag{9} \]
For the analysis of the decay to equilibrium of a correlation function, it is convenient to subtract the long time limit from $C(t)$ and to define the ISF

$$F(t) = \frac{C(t) - C_{\beta}}{C(0) - C_{\beta}}$$

We get in particular for the kinematic regime $F_{\text{id}}(t) = C_{\text{id}}(t)$. Note that all the correlation functions considered here are bounded: as $A_{K_j} \in L^2(d\mu)$ we have

$$\left| \left\langle A_{K_j}^j(t) A_{K_j}^j \right\rangle_{\beta} \right| = |C(t)| \leq C(0) = \left\langle |A_{K_j}^j|^2 \right\rangle_{\beta} < +\infty$$

$$\left| \left\langle A_{K_j}^j \right\rangle_{\beta} \right| < +\infty$$

The inequality in eqn. (10) is easily proven in [14].

In the next section we present a numerical study of the dynamics of the ISF $F(t)$. We will see that the relaxation dynamics strongly depend on temperature. This effect is a consequence of a dynamical-localization transition in the confining potential. An analytical approach for a perturbative construction the ISF is discussed in Section 4.

3 Numerical Simulations

To study the time evolution of the ISF, we run molecular dynamics simulations for a chain of $N = 32,768$ particles with equal masses $m = 1$. The parameters of the potential are set to $\alpha = 9.5$, $\sigma = 1$, $\eta = 0.01$. The set of initial configurations is generated according to the Boltzmann distribution

$$\rho_{\beta}(r) = \frac{1}{Z(\beta)} e^{-\frac{\beta}{\alpha} \sum_{j=1}^{N-1} V_0(r_j)} = \frac{1}{Z_{1}(\beta)} \prod_{j=1}^{N-1} e^{-\frac{\beta}{\alpha} V_0(r_j)}$$

which we factorized into single particle distributions, each associated to the same partition function

$$Z_{1}(\beta) \equiv \int_{-\infty}^{+\infty} dr e^{-\frac{\beta}{\alpha} V_0(r)}$$

The initial configurations of the particles are then determined by eqn. (33)

$$q_j = \sum_{k=0}^{j} r_k, \quad 1 \leq j \leq N - 1$$

while the initial velocities are drawn from the Maxwell distribution at inverse temperature $\beta/\alpha$. The trajectories of the particles $q_j$, $1 \leq j \leq N - 2$ are computed via the symplectic integration scheme leap-frog [15], while keeping the first and last particle of the system fixed to their initial positions $q_0 = 0$, $q_{N-1} = L$.

The total length of the chain is a constant of motion at the trajectory level. However, phase averages are computed over bundles of initial configurations for which the lengths $L$ are not identical – but due to the large size of the system they are very close to a unique function of the temperature $L = L(\beta)$.

Figure 2 shows the ISF $F(t)$ as a function of the temperature-rescaled time $t/\tau$; each curve corresponds to a different value of the inverse temperature $\beta$. Here and in the following graphs we show the dynamics of the central coordinate $j = \lfloor \frac{N}{2} \rfloor$, the farthest from the boundaries of the system. The dotted line refers to the Gaussian relaxation of the kinematic regime eqn. (7). We can see that for increasing values of $\beta$ all the correlations converge faster (in the rescaled time) to their equilibrium value, while preserving a Gaussian decay. Figure 3 shows the ISF for different wavenumbers. As $K$ is the inverse of the wavelength at which the system is probed, the system tends to equilibrate faster at smaller $K$, i.e. averaging the details of the microscopic dynamics over larger length-scales.

Fig. 4 shows the time series of the ISF for higher values of $\beta$ than in Fig. 2. In this case the equilibration time steadily increases for decreasing temperatures, in contrast to Fig. 2. We can interpret this process as a dynamical
localization transition exhibited in the temperature range where the details of the two-body potential become relevant; the microscopic forces felt by the particles take over the kinematics, inhibiting the relaxation. The effects become stronger when the temperature of the system is decreased.

For increasing values of $\beta$, the distribution of the inter-particle distances becomes more and more localized around the global minimum of the potential in $r = \sigma = 1$ (see Fig. 2). We can quantify this temperature-driven localization by computing the probabilities

$$P_0(\beta) = \int_{-\infty}^{r_c} dr \rho_\beta(r)$$

$$P_1(\beta) = \int_{r_c}^{+\infty} dr \rho_\beta(r)$$

where $r_c$ is the central local maximum in the two body potential, and of course $P_0(\beta) + P_1(\beta) = 1$. We can see in Fig. 5 that the probability ratio $P_0/P_1$ is a monotonically decreasing function of $\beta$. In the same picture are also
displayed the long time limit of the correlation function $C_\beta$ computed with the theoretical phase average of the function eqn. 9 and its value extracted from the numerical simulations $C_{\beta}^{MD}$. We can see that the main drop of the probability ratio is in the range $10 \leq \beta \leq 10^2$, in accordance with the temperature range of the plateau in $C_\beta$. Within this temperature range we also observe a qualitative change of behavior by the curves in Fig. 2 and 4.

Figure 5: Solid line: probability ratio $P_0(\beta)/P_1(\beta)$; dotted line: phase average of the ISF; markers: long-time average of the ISF from the numerical simulations

In this section we presented numerical evidence that the intermediate scattering function is a useful tool for the analysis of the dynamics of the FPU chain. The evolution of the ISF is sensitive to temperature, and a critical inverse temperature $\beta = \beta_c \sim 10$ could be identified as a separator between two behaviors: fast decay in Fig. 2 and diverging decay time in Fig. 4.

If one can reconstruct the sequence of the dynamical correlators (eqn. 6), one would be able to compute the ISF without the need of the explicit integration of the equations of motion of the system. In general, it is a complex task to compute these Taylor coefficients as they involve many-body integrals over the microscopic phases. However, due to the convenient reformulation of the ISF in eqn. 12 we can make progress in this direction. In the next section we present a detailed description of this approach.

4 Construction of the Dynamics

We present here an iterative method for the exact reconstruction of the ISF via the calculation of the correlators, as defined in eqn. 4. This approach is based on a direct evaluation of the action of $(i\mathcal{L})^n$ on the density fluctuations. When dealing with the full microscopic dynamics, we need to choose a proper set of coordinates to control the coupling between the different d.o.f., and to reduce the complexity of the many-body problem. As the potential depends only on the distances between nearest-neighbors (eqn. 1), the displacements

$$r_j = q_j - q_{j-1}$$

appear to be a natural set of configurations. In Appendix A.3 we prove that

$$\pi_j = \sum_{n=j}^{N-1} p_j$$

are the conjugated momenta to these configurations. However, due to the many body sum in eqn. 12 the calculation of the momenta of the $\pi_j$’s is unfortunately nontrivial; it is much simpler for our analytical and numerical purposes
to use the non-canonical set of coordinates \((r, p)\). The Liouville operator is then rewritten as

\[
i\mathcal{L} = \sum_{i=1}^{N-2} \left[ -\frac{\partial V(q_i)}{\partial q_i} \frac{\partial}{\partial p_i} + \frac{p_i}{m} \frac{\partial}{\partial q_i} \right] = \\
\sum_{i=1}^{N-1} \left[ -\frac{\partial V(r_i)}{\partial r_i} \left( \frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_{i-1}} \right) + \frac{1}{m} (p_i - p_{i-1}) \frac{\partial}{\partial r_i} \right]
\]

(13)

The extended change of variables is presented in Appendix A.3.

The action of the \((i\mathcal{L})^n\) on the density fluctuations can in general be written as the following complex polynomial in the coordinates

\[
(i\mathcal{L})^n e^{iK r_j} \equiv \sum_{m_1 \leq \cdots \leq m_{k_{\text{max}}}} \sum_{s_1 \leq \cdots \leq s_{k_{\text{max}}}} \mathcal{I}^{(n)}_{m_1 \cdots m_{k_{\text{max}}}, s_1 \cdots s_{k_{\text{max}}}} (r_{m_1}^{\text{min}} \cdots r_{k_{\text{max}}}^{\text{max}}) (p_{l_1}^{\text{min}} \cdots p_{l_{\text{max}}}^{\text{max}}) \equiv \sum_{m,s} \mathcal{I}^{(n)}_{m,s} r^m p^s
\]

(14)

with complex coefficients \(\mathcal{I}^{(n)}_{m,s} = \mathcal{I}^{(n,\mathcal{R})}_{m,s} + i\mathcal{I}^{(n,\mathcal{I})}_{m,s}\).

It would be computationally difficult to tackle eqn. 14 in case all the degrees of freedom of the system participated in the expansion at any order. Conveniently, the interaction at the lowest orders is restricted to a relatively small subset of coordinates around the tagged \(j\)-th degree of freedom. This is a direct consequence of the nearest-neighbor nature of the interaction. In the following we will formalize this observation. From the expansion of \((i\mathcal{L})^n e^{iK r_j}\) we can identify relevant products of differentials that control the propagation of the interaction from \(r_j\) to any other d.o.f. of the chain; we will refer to these contributions as spreading operators. Via these cross derivatives we can perform a systematic study of the extent of the non-locality as a function of the order \(n\). For example, the composition of derivatives connecting the configuration \(r_j\) of the tagged particle to another generic coordinate \(r_k\) located on the right (R) of \(r_j\) \((k > j)\) is given by

\[
\sigma^R(n, j, k - j) \equiv \theta \left( \left\lfloor \frac{n}{2} \right\rfloor - k + j \right) \left[ \left( -\frac{\partial V}{\partial r_k} \right) \left\{ \frac{\partial}{\partial p_k} - \frac{\partial}{\partial p_{k-1}} \right\} \right]^{\theta(n-2)} \times \\
\times \left\{ \prod_{i=0}^{k-j-2} \left[ \frac{1}{m} (p_{j+i+1} - p_{j+i}) \frac{\partial}{\partial r_{j+i+1}} \right] \left[ \left( -\frac{\partial V}{\partial r_{j+i+1}} \right) \left\{ \frac{\partial}{\partial p_{j+i+1}} - \frac{\partial}{\partial p_{j+i}} \right\} \right] \right\}^{\theta(n-4)} \left[ \frac{1}{m} (p_j - p_{j-1}) \frac{\partial}{\partial r_j} \right]^{\theta(n-2)}
\]

(15)

The prefactor \(\theta \left( \left\lfloor \frac{n}{2} \right\rfloor - k + j \right)\) reduces the operation to the subset of coordinates that participate in the propagation at order \(n\). In Appendix A.3 we show a derivation of a symmetric expression for \(\sigma^L(n, j, k - j)\), connecting \(r_j\) to another coordinate \(r_k\) with \(k < j\), as well as the expressions of the analogous operators for the momenta \(\sigma^L_p(n, j, k - j)\).

Using the spreading operators is straightforward to list the subset of configurations entering the interaction at order \(n\):

\[
K_r(n, j) \equiv \left\{ j - \left\lfloor \frac{n}{2} \right\rfloor, \ldots, j + \left\lfloor \frac{n}{2} \right\rfloor \right\} \in \mathbb{N}^{\left\lfloor \frac{n}{2} \right\rfloor + 1} \equiv \{k_{\text{min}}, \ldots, k_{\text{max}}\}
\]

(16)

The analogous expressions for the momenta are given in eqn. 14.

The boundaries of the sums in eqn. 14 can again be determined by the identification of the relevant differential operators of \((i\mathcal{L})^n\). We can define \(\mathcal{M}_r(n, j, |j - k|)\) and \(\mathcal{S}_p(n, j, |j - l|)\) as the leading power respectively for a configuration \(r_k\) and a momentum \(p_l\) in the sum. In vector notation these definitions read as:

\[
m = \begin{pmatrix}
m_{k_{\text{min}}} \\
m_{k_{\text{max}}}
\end{pmatrix} \leq \begin{pmatrix}
\mathcal{M}_r(n, j, j - k_{\text{min}}) \\
\mathcal{M}_r(n, j, k_{\text{max}} - j)
\end{pmatrix} \equiv \mathbf{M}
\]

and analogously for the momenta

\[
s = \begin{pmatrix}
s_{l_{\text{min}}} \\
s_{l_{\text{max}}}
\end{pmatrix} \leq \begin{pmatrix}
\mathcal{S}_p(n, j, j - l_{\text{min}}) \\
\mathcal{S}_p(n, j, l_{\text{max}} - j)
\end{pmatrix} \equiv \mathbf{S}
\]

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The boundaries of the sums in equation eqn. [13] are then fixed according to

\[(i\mathcal{L})^n e^{iKr_j} = \sum_{m \leq M, n \leq S} \tau^{(n)}_{ms} p^m e^{iKr_j} = \left[ p^{R}_n(r, p) + ip^{\gamma}_n(r, p) \right] e^{iKr_j} \tag{17} \]

where we additionally split the real and imaginary part of the polynomial expansion in the terms \(p^{R}_n(r, p)\) and \(p^{\gamma}_n(r, p)\); by averaging on the phase space we obtain as a the final expression of the dynamical correlators

\[
\omega_{2n} = (-1)^n \left\langle (i\mathcal{L})^n e^{iKr_j} \right\rangle^2 = (-1)^n \left\langle \left[ p^{R}_n(r, p) + ip^{\gamma}_n(r, p) \right]^2 \right\rangle = (-1)^n \left[ \left\langle \left( p^{R}_n(r, p) \right)^2 \right\rangle + \left\langle \left( p^{\gamma}_n(r, p) \right)^2 \right\rangle \right] =
\]

\[
= (-1)^n \sum_{m, m', s, s' \in M \atop s, s' \in S} \left( \mathcal{I}^{(\sigma, \beta)}_{ms} \mathcal{I}^{(\sigma', \beta')}_{ms'} + \mathcal{I}^{(\gamma, \beta)}_{ms} \mathcal{I}^{(\gamma', \beta')}_{ms'} \right) \left\langle r^{m+m'} p^s e^{is} \right\rangle = \mathcal{I}^{(\sigma + \gamma, \beta + \beta')}_{ms} \left\langle r^{m+m'} p^s e^{is} \right\rangle \tag{18} \]

Note that, as a consequence of the assumption of stationarity, knowledge of the \(n\)-th order tensor of coefficients \(\mathcal{I}^{(n)}\) suffices to calculate \(\omega_{2n}\).

The entries of \(\mathcal{I}^{(n)}\) can be determined with a recursive method for increasing orders. This procedure can be identified from the fact that we can extract a relation \(\mathcal{I}^{(n)} \rightarrow \mathcal{I}^{(n+1)}\) directly from the action of the Liouvillian:

\[(i\mathcal{L})^{n+1} e^{iKr_j} = \sum_{m \leq M, n \leq S} \mathcal{I}^{(n+1)}_{ms} r^{m} p^s e^{iKr_j} = (i\mathcal{L})(i\mathcal{L})^n e^{iKr_j} = i\mathcal{L} \sum_{m \leq M, n \leq S} \mathcal{I}^{(n)}_{ms} r^{m} p^s e^{iKr_j} \]

As an example, we can isolate from \(i\mathcal{L}\) the contribution of \(i\mathcal{L}^\gamma\) to \(\mathcal{I}^{(n+1)}_{ms}\) is then given by

\[
i\mathcal{L}^\gamma \left[ r_{m_{\text{min}}} \cdots r_{m_{\gamma}} \cdots r_{m_{\text{max}}} \right] \left( p^{s_{\text{min}}} \cdots p^{s_{\gamma-1}} p^{s_{\gamma}} \cdots p^{s_{\text{max}}} \right) =
\]

\[
= -\frac{\alpha}{\sigma^2} \left[ 2r_{\gamma} + 3A(\eta) \frac{r^2_{\gamma}}{\sigma} + 4B(\eta) \frac{r^3_{\gamma}}{\sigma^2} \right] \left[ r_{m_{\text{min}}} \cdots r_{m_{\gamma}} \cdots r_{m_{\text{max}}} \right] \left( p^{s_{\text{min}}} \cdots p^{s_{\gamma-1}} p^{s_{\gamma}} \cdots p^{s_{\text{max}}} \right) =
\]

\[
= -\frac{\alpha}{\sigma^2} \left[ r_{m_{\text{min}}} \cdots \left( 2r_{m_{\gamma}+1} + 3A(\eta) \frac{r^2_{m_{\gamma}+1}}{\sigma} + 4B(\eta) \frac{r^3_{m_{\gamma}+1}}{\sigma^2} \right) \cdots r_{m_{\text{max}}} \right] \left[ p^{s_{\text{min}}} \cdots \left( p^{s_{\gamma-1}} p^{s_{\gamma-1}} - s_{\gamma-1} p^{s_{\gamma-1}} - s^{s_{\gamma-1}} p^{s_{\gamma-1}} \right) \cdots p^{s_{\text{max}}} \right] \tag{19} \]

The contribution of \(i\mathcal{L}^\gamma\) to \(\mathcal{I}^{(n+1)}_{ms}\) is then given by

\[
\mathcal{I}^{(n+1)}_{ms} \bigg|_{p, \gamma} = \alpha \sum_{k=0,1} (-1)^{k+1} s_{\gamma-k} \left[ \frac{2}{\sigma^2} \mathcal{T}^{(n)}_{ms + \gamma, s - \gamma, -k} + \frac{3}{\sigma^2} A(\eta) \mathcal{T}^{(n)}_{m+2s, s - \gamma, -k} + \frac{4}{\sigma^2} B(\eta) \mathcal{T}^{(n)}_{m+3s, s - \gamma, -k} \right] \tag{20} \]

The other terms of the recursion relation are derived in Appendix A.6. In Appendix A.8 we present a general method for the numerical management of high dimensional tensors.

In Fig. [6] we show the dynamical correlators normalized by the analytically known values of the ideal gas (eqn. [29]). The numerical coefficients are determined by the calculation of high order time derivatives in the trajectories of the density fluctuation, according to

\[
(i\mathcal{L})^n e^{iKr_j(t)} = \frac{d^n}{dt^n} e^{iKr_j(t)} \]

We observe optimal agreement between the recursive approach and the numerical values. The magnitude of \(\omega_2\) is the same in the kinematic and the dynamic regime (and is therefore analytically known); the analytical value of \(\omega_4\) in presence of nonlinearities is computed in the Appendix A.2.2.
Figure 6: $\omega_n/\omega_n^{id}$ from the MD simulations (triangles) and via the recursion relation derived in the work (circles); comparison with the analytical result for $n = 2, 4$ (see A.2.2); the inverse temperature is fixed to $\beta = 0.1$.

Via the procedure presented in this section it is possible to compute the first orders of the dynamics of the ISF exactly; increased computational power would, in principle, permit the reconstruction of higher orders of Taylor coefficients. Instead of pushing in this direction, in the next section we will describe a combined numerical and analytical approach that enables us to study a larger temperature range without needing more computational power. In particular, it will enable us to extract information of the memory effects encapsuled in the evolution of this relevant correlation function.

# 5 The Generalized Langevin Equation

Given a general dynamical variable $A$, it is possible to derive via projection operator techniques the following equation of motion for the correlation $C_A(t) = \langle A(t)A^*(0) \rangle$ [13], [16]:

$$\dot{C}_A(t) = \omega_1(t)C_A(t) + \int_0^t dt'K_A(t,t')C_A(t')$$

(20)

where $K_A$ is the memory kernel of the process and

$$\omega_1^A(t) = \frac{\langle [i\mathcal{L}A(t)]A^*(t) \rangle_\beta}{\langle |A(t)|^2 \rangle_\beta}$$

generalizes the first of the dynamical correlators (eqn. [6]) to the case of initial conditions arbitrarily far from equilibrium. By fixing $A = A_K^j = e^{iKr_j}$ we can identify $C_A = C$, according to the definition given in eqn. [3]. In stationary processes the memory kernel is invariant under time translation [16]:

$$K(t, t') = K(t - t')$$

and therefore in the equilibrium regime eqn. [20] simplifies to

$$\dot{C}(t) = \int_0^t dt'K(t-t')C(t')$$

(21)

The memory kernel contains the information to which extent the dynamics of the system at a certain time depends on the evolution at previous times. In case of a Markovian (memory-less) process $K(t - t') = \delta(t - t')$, meaning
that the solution of eqn. 21 decays exponentially; in our case we can see from the numerical results in section 3 that the dynamics of the system is far from the Markovian limit. It is therefore interesting to study the shape of the kernel and its temperature dependence.

It might seem to be straightforward to extract the (Fourier-)Laplace transform of the kernel from the MD-time series of the correlation function. We could then reconstruct the kernel in the time domain with the inverse transformation; unfortunately, this last procedure is highly unstable and frequently subject to considerable numerical errors. To overcome these limitations, we consider here a different approach. In [16] has been introduced a novel coarse-graining technique which allows a systematic reconstruction of the kernel from its Taylor coefficients

\[ \kappa_n = \frac{d}{dt} K(t) \bigg|_{t=0} \]

with no need to apply any integral transformation. The main result of [16] consists in the derivation of a systematic relation between the coefficients \( \kappa_n \) and a subset of the dynamical correlators out-of-equilibrium; for the case of a stationary process this relation is implicitly given by

\[ \kappa_n = \mathcal{F}_n(\omega_0, \omega_2, \cdots, \omega_{n+2}) \quad (22) \]

being \( \mathcal{F}_n \) a nonlinear combination of its arguments [14]. The reconstruction of \( K \) from its series expansion is simplified, because the odd Taylor coefficients are identically null in equilibrium. This can be proved via dimensional analysis: As a notation, we refer to the physical dimension of a function or constant by enclosing it in square brackets \([\cdot]\). It can be seen from definition in eqn. 6 that \([\omega_{2n}] = T^{-2n}\), where \( T \) denotes a time unit. From eqn. 21 it follows that \([K] = T^{-2}\), therefore the \( n \)-th Taylor coefficient of \( K \) must have dimension \([\kappa_n] = T^{-n-2}\). These coefficients can be expressed as a nonlinear combination of dynamical correlators, according to eqn. 22. It follows that each contribution to \( \kappa_n \), with \( n \) odd must be proportional to an odd number of odd dynamical correlators; these are identically null, according to eqn. 5.

The construction of the memory kernel discussed in the previous section relies on the knowledge of the high-order series coefficients of \( C(t) \). This task can be simplified by introducing an interpolating approximation for the correlation function \( C^i \in C^\infty(\mathbb{R}^+) \), such that its derivatives in \( t = 0 \) provide an estimate of the required Taylor coefficients. To determine a proper functional expression of the ISF we can proceed as follows. We can see from the main plot in Figure 2 that for sufficiently high temperature (for \( \beta \lesssim 2 \)) the initial decay of \( F(t) \) preserves the Gaussian shape of the ideal gas (eqn. 7). It appears therefore convenient in this low-\( \beta \) regime to introduce the following interpolating ansatz:

\[ C^i(t) \equiv (1 - C_\beta)e^{-at^2} + C_\beta \quad (23) \]

The long time limit \( C_\beta \) is fixed by eqn. 9, while the Gaussian parameter \( a = a(\beta) \) can be extracted from the time series of \( C(t) \) in the numerical simulations:

\[ a = \frac{1}{2(C_\beta - 1)} \frac{d^2 C^i(t)}{dt^2} \bigg|_{t=0} \quad (24) \]

Via eqn. 24 we can quantify the deviation from time-temperature superposition in presence of the interaction. (At this level of description we explicitly choose to neglect the oscillatory transients at \( t \approx \tau \) exhibited in the curves in Figures 2 and 3 before the final relaxation; we can interpret those as higher-order dynamical effects.) Let us remark that the shape of the ansatz eqn. 23 is compliant with the requirement that all, and only, the even series coefficients of the ISF are non null. We recall from eqn. 4 that this restriction is a direct consequence of property of anti-Hermitianity of the Liouville operator at equilibrium. This would not be the case if we used a general stretched exponential

\[ f(t) = (1 - A)e^{t^\alpha} + A \quad (25) \]

with \( \alpha \neq 2 \). This class of functions are frequently used as phenomenological curves for the interpolation of a broad class of relaxation processes [17]. The applicability of such an ansatz is however restricted to regimes where the Liouville operator is not anti-Hermitian (as it happens in general out-of-equilibrium processes).
The Taylor coefficients of $C_i$ are given by:

$$
\omega_i^{2n} = \left. \frac{d^{2n} C^i(t)}{dt^{2n}} \right|_{t=0} = (1 - C_\beta) a^n \left( \frac{d}{d(\sqrt{\alpha t})} \right)^{2n} e^{-(\sqrt{\alpha t})^2} \bigg|_{t=0} + \delta_{n,0} C_\beta =
$$

$$
= (1 - C_\beta) a^n (-1)^{2n} H_{2n}(\sqrt{\alpha t}) e^{-(\sqrt{\alpha t})^2} \bigg|_{t=0} + \delta_{n,0} C_\beta = (1 - C_\beta) a^n H_{2n}(0) + \delta_{n,0} C_\beta
$$

(26)

where we introduced the Hermite numbers $H_n \equiv H_n(0)$, being $H_n(x)$ the $n$-th Hermite polynomial. From the recursion relation $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$ and the initial conditions $H_0(0) = 1, H_1(0) = 0$, we can write the closed form:

$$
H_n = \begin{cases} 
(-2)^{n/2}(n-1)!! & \text{n even} \\
0 & \text{n odd}
\end{cases}
$$

We can easily insert the estimates from eqn. 26 into eqn. 22 to compute the Taylor coefficients of the memory kernel for $n \lesssim 40$. Above this order, the calculations become computationally expensive, due to the increased complexity of the combinatorics involved in $F_n$. However for sufficiently large values of $n$ it is possible to identify numerically the leading term of the expansion eqn. 22. The following relation

$$
\kappa_{2n} \simeq \omega_n^{i+2} \quad n \gtrsim 40
$$

(27)

is indeed verified in Fig. 7 by computing for increasing values of $n$ the ratio between the Taylor coefficient $\kappa_n$ and the maximum dynamical correlator $\omega_{n+2}^i$ entering the expansion in eqn. 22.

![Figure 7](image)

Figure 7: Ratio $\kappa_n/\omega_{n+2}^i$ as a function of $n$, for different values of the inverse temperature $\beta$

With this additional approximation we can now compute the short time of the kernel

$$
K_{N_{\text{max}}} (t - \tau) \equiv \sum_{n=0}^{N_{\text{max}}} \kappa_{2n} \frac{(t - \tau)^{2n}}{(2n)!}
$$

(28)

till order $N_{\text{max}} = 180$. The results for different values of $\beta$ are shown in Fig. 8.
Figure 8: Reconstruction of the memory kernel of the GLE (eqn. 21) for different values of $\beta$ and $K = 1$, as a function of the rescaled time $\tau$.

The polynomial in eqn. 28 is intrinsically divergent, as it can be noticed from the dotted lines in the picture. The finite continuation of the functions to erase their divergence is determined according to the arguments discussed in Appendix A.7. We can see in Figure 8 that the strength of the memory, identified by the global minimum of the function, becomes stronger for decreasing temperature. The double normalization in the pictures ease the comparison of the curves at different temperatures, in analogy to the rescalings performed for the ISF.

6 Conclusions

In this work we presented a combined numerical and analytical approach to construct of the dynamics of the intermediate scattering function of the FPU chain, with no restrictions on the strength of the anharmonicity; the method is based on a direct control of the action of the Liouville operator on the density fluctuations. The reduction of the many-body scattering function to its single-particle counterpart allowed us to develop a recursive approach for the construction of the dynamical correlators of the function. Numerical simulations have been coupled to the analytical treatment; they confirm the relevance of the ISF as a tool to study the response and relaxation properties of the system. We hope that the detailed description of the methods presented here can be the starting point for future studies of the FPU problem in the coupled framework between the Theory of Dynamical Systems and Liquid State Physics.

A Appendix

A.1 Two body potential

In this section we derive the expression for the two-body interaction potential in eqn. 1 used in this work. We aim at a parametrization for a quartic potential such that we can isolate a global energy scale, a length scale and a parameter controlling the unbalance between the two wells. We define

$$V(r) = \alpha \left[ \left( \frac{r}{\sigma} \right)^2 + A \left( \frac{r}{\sigma} \right)^3 + B \left( \frac{r}{\sigma} \right)^4 \right]$$
We then require that the distance \( r = \sigma \) corresponds to an equilibrium position, such that \( V(\sigma) = -\epsilon \); the two conditions read as:

\[
\frac{dV(r)}{dr}\bigg|_{r=\sigma} = 0 = \frac{\alpha}{\sigma} [2 + 3A + 4B] \\
V(\sigma) = -\epsilon = \alpha[1 + A + B]
\]

Which is solved by

\[
A = A(\eta) = -2 - 4\eta \\
B = B(\eta) = 1 + 3\eta
\]

With the dimensionless parameter \( \eta = \frac{\sigma}{\alpha} \) taking positive values in case the minimum in \( r = \sigma \) is negative.

### A.2 Analytical expression for \( \omega_n \)

In this appendix we present the analytical expressions of the dynamical correlators \( \omega_n \); while an exact solution is easily determined at any order in the ideal gas regime, a general expression is not available in case a nonlinear interaction is added to the dynamics. For the non-integrable regime, we can still derive the analytical solution of the lowest orders; we present in the following the explicit calculation of \( \omega_n \), which is the first coefficient dependent on the dynamics. By expanding the kinematic part of the Liouvillian (eqn. 13) in the general expression in eqn. 6 we get:

#### A.2.1 Ideal gas regime

\[
\omega_n^{\text{id}} = \left\langle \left[ \left( 1 + \sum_{\gamma=1}^{n-2} (p_{\gamma} - p_{\gamma-1}) \frac{\partial}{\partial r_{\gamma}} \right)^n e^{iKr_j} \right] e^{-iKr_j} \right\rangle = \left( \frac{iK}{m} \right)^n \langle (p_j - p_{j-1})^n \rangle_{\beta} = \left( \frac{iK}{m} \right)^n \sum_{k=0}^n \left( \begin{array}{c} n \\ k \end{array} \right) \langle p_j^k \rangle_{\beta} \langle (-p_{j-1})^{n-k} \rangle_{\beta} =
\]

\[
= \frac{1}{\pi} \left( \frac{\beta}{2m\alpha} \right) \left( \frac{iK}{m} \right)^n \sum_{k=0}^n \left( \begin{array}{c} n \\ k \end{array} \right) \frac{(-1)^n}{k!} \int_{-\infty}^{+\infty} dp_j e^{-\beta \frac{p^2}{m\alpha}} \left[ \int_{-\infty}^{+\infty} dp_{j-1} e^{-\beta \frac{p_{j-1}^2}{m\alpha}} p_j^{n-k} \right] =
\]

\[
= \frac{1}{\pi} \left( \frac{\beta}{2m\alpha} \right) \left( \frac{iK}{m} \right)^n \sum_{k=0}^n \frac{(-1)^n}{k!} \frac{1}{2} \left[ \sum_{k=0}^n \left( \begin{array}{c} n \\ 2k \end{array} \right) \Gamma \left( k + \frac{1}{2} \right) \Gamma \left( \frac{n}{2} - k + \frac{1}{2} \right) \right] =
\]

\[
= \frac{1}{\pi} \frac{(-1)^n}{2} \left( \frac{2K^2\alpha}{m\beta} \right)^{\frac{n}{2}} \frac{1}{2} \sqrt{\pi} 2^{\frac{n}{2}} \Gamma \left( \frac{n+1}{2} \right) = \frac{1}{\sqrt{\pi}} \frac{(-1)^{\frac{n}{2}}}{2} \left( \frac{4K^2\alpha}{m\beta} \right)^{\frac{n}{2}} \frac{1}{2} \sqrt{\pi} 2^{\frac{n}{2}} \Gamma \left( \frac{n+1}{2} \right)
\]

where we used

\[
\langle p_j^m \rangle_{\beta} = \left( \frac{2m\alpha}{\beta} \right)^{\frac{m}{2}} \frac{1}{\sqrt{\pi}} \frac{(-1)^m}{2} \Gamma \left( \frac{m+1}{2} \right)
\]

and

\[
\sum_{k=0}^{\frac{n}{2}} \left( \begin{array}{c} n \\ 2k \end{array} \right) \Gamma \left( k + \frac{1}{2} \right) \Gamma \left( \frac{n}{2} - k + \frac{1}{2} \right) = \frac{\pi n!}{4^{\frac{n}{2}} \Gamma \left( \frac{n}{2} \right)!} \cdot \frac{\sqrt{\pi} (2k)!}{4k!} \cdot \frac{\sqrt{\pi} (n-2k)!}{4^{\frac{n}{2} - k} \left( \frac{n}{2} - k \right)!} = \frac{\pi n!}{4^{\frac{n}{2}} \left( \frac{n}{2} \right)!} \cdot \frac{\sqrt{\pi} (2k)!}{4k!} \cdot \frac{\sqrt{\pi} (n-2k)!}{4^{\frac{n}{2} - k} \left( \frac{n}{2} - k \right)!} = \pi n! \sqrt{\pi} \frac{2^{\frac{n}{2}}}{4^{\frac{n}{2} \left( \frac{n}{2} \right)!} \cdot \frac{\sqrt{\pi} n!}{4^{\frac{n}{2} \left( \frac{n}{2} \right)!}} = \sqrt{\pi} 2^{\frac{n}{2}} \Gamma \left( \frac{n+1}{2} \right)
\]
A.2.2 Anharmonic regime

Let’s decompose the Liouville operator into kinematic and potential part

\[ i\mathcal{L} = i\mathcal{L}_r + i\mathcal{L}_p \]

where the pedices stand for the observables which are differentiate, and the apex on the second term reflect the fact that the anharmonicities enter only via this contribution. The fourth dynamical correlator is then given by:

\[
\omega_4 = (-1)^2 \left\langle \left| (i\mathcal{L}_r^a) e^{iK_\gamma r} \right|^2 \right\rangle_{\beta} = \left\langle \left| \left( i\mathcal{L}_r^a + i\mathcal{L}_p^a \right) e^{iK_\gamma r} \right|^2 \right\rangle_{\beta} = \left\langle \left( \left( i\mathcal{L}_r^a \right)^2 + (i\mathcal{L}_p^a)^2 + i\mathcal{L}_r^a i\mathcal{L}_p^a + i\mathcal{L}_p^a i\mathcal{L}_r^a \right) e^{iK_\gamma r} \right|^2 \right\rangle_{\beta} = \\
\left\langle \sum_{\gamma, \gamma'=1}^{N-2} \left[ \frac{1}{m^2} (p_\gamma - p_{\gamma-1}) (p_{\gamma'} - p_{\gamma'-1}) \frac{\partial^2}{\partial r_\gamma r_{\gamma'}} + \frac{\alpha}{m} (-2r_\gamma - 3A(\eta)r_\gamma^2 - 4B(\eta)r_\gamma^3) \left( \frac{\partial}{\partial p_\gamma} - \frac{\partial}{\partial p_{\gamma-1}} \right) (p_{\gamma'} - p_{\gamma'-1}) \frac{\partial}{\partial r_{\gamma'}} \right] e^{iK_\gamma r} \right|^2 \right\rangle_{\beta} = \\
\left\langle \left( \frac{iK}{m} \right)^2 (p_j - p_{j-1})^2 + \frac{i\kappa}{m} \sum_{\gamma=1}^{N-2} \left( -2r_\gamma - 3A(\eta)r_\gamma^2 - 4B(\eta)r_\gamma^3 \right) \left( \delta_\gamma, \gamma' - \delta_\gamma, \gamma' - \delta_{\gamma-1, \gamma'} + \delta_{\gamma-1, \gamma'} \right) \delta_{\gamma', j} \right\rangle_{\beta} = \\
\left\langle \left( \frac{iK}{m} \right)^2 (p_j - p_{j-1})^2 + \frac{i\kappa}{m} \sum_{\gamma=1}^{N-2} \left( -2r_\gamma - 3A(\eta)r_\gamma^2 - 4B(\eta)r_\gamma^3 \right) \left( 2\delta_\gamma, j - \delta_{\gamma, j-1} - \delta_{\gamma, j+1} \right) \right\rangle_{\beta} = \\
\left\langle \left( \frac{iK}{m} \right)^2 (p_j - p_{j-1})^2 + \frac{i\kappa}{m} \left[ 2 \left( -2r_j - 3A(\eta)r_j^2 - 4B(\eta)r_j^3 \right) - \left( -2r_{j-1} - 3A(\eta)r_{j-1}^2 - 4B(\eta)r_{j-1}^3 \right) + \left( -2r_{j-1} - 3A(\eta)r_{j-1}^2 - 4B(\eta)r_{j-1}^3 \right) \right] \right\rangle_{\beta} = \\
\left\langle \left( \frac{iK}{m} \right)^4 (p_j - p_{j-1})^4 \right\rangle_{\beta} + \left\langle \frac{\kappa}{m} \right\rangle_{\beta} \left\langle 6 \left( -2r - 3A(\eta)r^2 - 4B(\eta)r^3 \right) \right\rangle_{\beta} - 6 \left\langle -2r - 3A(\eta)r^2 - 4B(\eta)r^3 \right\rangle_{\beta}^2 = \\
\left\langle \frac{K}{m} \right\rangle_{\beta}^4 \left\langle (p_j - p_{j-1})^4 \right\rangle_{\beta} + 6 \left\langle \frac{K}{m} \right\rangle_{\beta}^2 \sigma^2(F_\eta, F_\eta) = \left\langle \frac{K}{m} \right\rangle_{\beta}^4 \left[ 2 \left\langle p^4 \right\rangle_{\beta} + 6 \left\langle p^2 \right\rangle_{\beta}^2 \right] + 6 \left\langle \frac{K}{m} \right\rangle_{\beta}^2 \left\langle F_\eta^2 \right\rangle_{\beta}
\]

where we defined the force acting on a single d.o.f. with

\[ F_\eta(r) = -\frac{dV_\eta(r)}{dr} \]

and the equilibrium variance \( \sigma^2(A, B) = \langle AB \rangle - \langle A \rangle \langle B \rangle \). In the last line we noticed that \( \sigma^2(F_\eta, F_\eta) = \langle F_\eta^2 \rangle_{\beta} \) being \( \langle F_\eta \rangle_{\beta} = 0 \).

A.3 A canonical change of coordinates

Due to the nearest neighbors nature of the interaction potential, the configurations of the systems could be naturally expressed in terms of the distances \( r_j = q_j - q_{j-1} \) between adjacent particles. In this appendix we aim to construct a set of momenta such that the set of coordinates \( \{r_j, \pi_j\}_{i,j=1,...,N-1} \) is canonical; a change of coordinates of this kind, not mixing configurations and momenta, is called point transformation. Recall that a necessary and sufficient condition for a transformation to be canonical is that it preserves the Poisson brackets w.r.t. the original coordinates. We will look for a linear transformation in the momenta:

\[ \pi_j = \sum_{k=1}^{N-1} \alpha_{j,k} p_k \quad j \in \{1, ..., N-1\} \] (30)
We can then impose $\forall \ i, j \in \{1, \cdots, N - 1\}$:
\[
\{r_i, \pi_j\} = \delta_{ij} \quad \iff \quad \sum_{k=1}^{N-1} \frac{\partial r_i}{\partial q_k} \frac{\partial \pi_j}{\partial p_k} = \delta_{ij}
\]
\[
\frac{\partial \pi_j}{\partial p_i} - \frac{\partial \pi_j}{\partial p_{i-1}} = \delta_{ij}
\]
\[
(31)
\]
By inserting in eqn. 31 the ansatz in eqn. 30 we get the following recursion relation
\[
\alpha_{j,i} = \alpha_{j,i-1} + \delta_{ij}
\]
\[
(32)
\]
for $1 \leq j \leq N - 1$ and $2 \leq i \leq N - 1$.
In case of point transformations these fundamental Poisson bracket relations are easily satisfied:
\[
\{r_i, r_j\} = \sum_{k=1}^{N-1} \frac{\partial r_i}{\partial q_k} \frac{\partial r_j}{\partial p_k} = 0
\]
\[
\{\pi_i, \pi_j\} = \sum_{k=1}^{N-1} \frac{\partial \pi_i}{\partial q_k} \frac{\partial \pi_j}{\partial p_k} = 0
\]
In order to determine a matrix $\alpha$ fulfilling eqn. 32 we need to specify arbitrary initial conditions on $\alpha_{j,1}$, $\forall \ j \in \{1, \cdots, N - 1\}$. By choosing $\alpha_{j,1} = \delta_{j,1}$, we obtain a symmetric solution for eqn. 32 in fact, the relation is solved by the upper triangular matrix $(N - 1) \times (N - 1)$ with unit entries:
\[
P = \begin{pmatrix}
1 & 1 & \cdots & 1 & 1 \\
0 & 1 & \cdots & 1 & 1 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & \cdots & 1 & 1 \\
0 & 0 & \cdots & 0 & 1 \\
\end{pmatrix}
\]
such that
\[
\pi = P \cdot p
\]
\[
\pi_j = \sum_{k=j}^{N-1} p_k \quad \forall j \in \{1, \cdots, N - 1\}
\]
The inverse of the momenta transformation matrix is given by:
\[
P^{-1} = \begin{pmatrix}
1 & -1 & 0 & \cdots & 0 \\
0 & 1 & -1 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & \cdots & 1 & -1 \\
0 & 0 & \cdots & 0 & 1 \\
\end{pmatrix}
\]
and therefore
\[
p_j = \pi_j - \pi_{j+1} \quad \forall j \in \{1, \cdots, N - 1\}
\]
In a similar fashion, we can define the $(N - 1) \times (N - 1)$ transformation matrix for the coordinates
\[
Q = \begin{pmatrix}
1 & 0 & 0 & \cdots & 0 \\
-1 & 1 & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & -1 & 1 & 0 \\
0 & 0 & \cdots & -1 & 1 \\
\end{pmatrix}
\]
such that
\[ r = Q \cdot q \]

with inverse
\[
Q^{-1} = \begin{pmatrix}
1 & 0 & \cdots & 0 & 0 \\
1 & 1 & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
1 & 1 & \cdots & 1 & 0 \\
1 & 1 & \cdots & 1 & 1
\end{pmatrix}
\]

meaning
\[ q_j = \sum_{k=1}^{j} r_k = \sum_{k=1}^{j} (q_k - q_{k-1}) \quad \forall j \in \{1, \cdots, N-1\} \quad (33) \]

Note that the \( r_j \)'s and \( \pi_j \)'s are defined for \( j \in \{1, \cdots, N-1\} \); in order to set the proper number of \( N-2 \) d.o.f. we only need one additional condition on the momenta and one on the configurations; these are:
\[
\begin{aligned}
\sum_{j=1}^{N-1} r_j &= L \\
\pi_{N-1} &= p_{N-1} = 0
\end{aligned}
\]

The Hamiltonian in the new coordinates is rewritten as
\[ H(r, \pi) = \sum_{j=1}^{N-1} \left[ \frac{1}{2m} (\pi_j - \pi_{j-1})^2 + V_q(r_j) \right] \]

In the following we prove that the new set of coordinates preserves the Hamilton’s equations. In order to write them on an equal footing \( \forall \ 1 \leq j \leq N-2 \), we can define an additional fictitious momentum \( \pi_0 \equiv \pi_1 \). This label does not refer to a real d.o.f., therefore it is not supposed to be related to any coordinate \( r_0 \). Then \( \forall \ j \in \{1, \cdots, N-2\} \) the following relation is well defined:
\[
\frac{\partial H}{\partial \pi_j}(r, \pi) = \frac{1}{m} [2\pi_j - \pi_{j-1} - \pi_{j+1}]
\]

We can now prove:

**Lemma 1.**
\[
\dot{q}_j = \frac{\partial H}{\partial p_j} \iff \dot{r}_j = \frac{\partial H}{\partial \pi_j} \quad \forall j \in \{1, \cdots, N-2\}
\]

**Proof:**

\[ \Rightarrow \dot{r}_j = \dot{q}_j - \dot{q}_{j-1} = \frac{\partial H}{\partial p_j} - \frac{\partial H}{\partial p_{j-1}} = \frac{1}{m} (p_j - p_{j-1}) = \frac{1}{m} [(\pi_j - \pi_{j+1}) - (\pi_{j-1} - \pi_j)] = \frac{\partial H(\pi)}{\partial \pi_j} \]

\[ \Leftarrow \dot{q}_j = \sum_{k=1}^{j} \dot{r}_k = \sum_{k=1}^{j} \frac{\partial H}{\partial \pi_k} = \frac{1}{m} \sum_{k=1}^{j} [(\pi_k - \pi_{k+1}) - (\pi_{k-1} - \pi_k)] = \frac{1}{m} \sum_{k=1}^{j} (p_k - p_{k-1}) = \frac{p_j}{m} = \frac{\partial H(\pi)}{\partial p_j} \]

**Lemma 2.**
\[
\dot{p}_j = -\frac{\partial H}{\partial q_j} \iff \dot{\pi}_j = -\frac{\partial H}{\partial r_j} \quad \forall j \in \{1, \cdots, N-2\}
\]
Proof:

\[ \hat{\pi}_j = \sum_{k=j}^{N-2} \dot{\pi}_k = - \sum_{k=j}^{N-2} \frac{\partial H}{\partial q_k} = - \sum_{k=j}^{N-2} \frac{\partial}{\partial q_k} \left\{ \sum_{l=1}^{N-2} V_q(q_l - q_{l-1}) \right\} = - \sum_{k=j}^{N-2} \left( \frac{\partial V_q(q_k - q_{k-1})}{\partial q_k} - \frac{\partial V_q(q_{k+1} - q_k)}{\partial q_k} \right) = \]

\[ = - \frac{\partial r_j}{\partial q_j} \frac{\partial V_q(r_j)}{\partial r_j} + \frac{\partial r_{N-1}}{\partial q_{N-1}} \frac{\partial V_q(r_{N-1})}{\partial r_{N-1}} = - \frac{\partial V_q(r_j)}{\partial r_j} - \frac{\partial V_q(r_{N-1})}{\partial r_{N-1}} = - \frac{\partial V_q(r_j)}{\partial r_j} + \dot{r}_{N-1} = \]

\[ = - \frac{\partial V_q(r)}{\partial r_j} = - \frac{\partial H}{\partial r_j} \]

\[ \hat{p}_j = \hat{\pi}_j - \hat{\pi}_{j+1} = - \frac{\partial H}{\partial r_j} + \frac{\partial H}{\partial r_{j+1}} = - \frac{\partial V_q(r_j)}{\partial r_j} + \frac{\partial V_q(r_{j+1})}{\partial r_{j+1}} = - \frac{\partial}{\partial q_j} \left( V_q(q_j - q_{j-1}) + V_q(q_{j+1} - q_j) \right) = \]

\[ = - \frac{\partial V_q(q)}{\partial q_j} = - \frac{\partial H}{\partial q_j} \]

A.4 Liouvillean in non canonical coordinates

We derive here a symmetric expression for the Liouvillean in the set of non canonical coordinates \((r,p)\) used in the work.

\[ i\mathcal{L} = \sum_{j=1}^{N-2} \left[ - \frac{\partial V(q)}{\partial q_j} \frac{\partial}{\partial p_j} + \frac{p_j}{m_p} \frac{\partial}{\partial q_j} \right] = \sum_{j=1}^{N-2} \left[ - \frac{\partial r_k}{\partial q_j} \frac{\partial V(q)}{\partial r_k} + \frac{p_j}{m_p} \frac{\partial}{\partial q_j} \right] \]

\[ = \sum_{j,k=1}^{N-2} \left[ \frac{(\delta_{j-k} - \delta_{j,k-1})}{\partial q_j} \frac{\partial V(q)}{\partial r_k} \right] \frac{\partial}{\partial p_j} + \frac{p_j}{m_p} \frac{\partial}{\partial q_j} \frac{\partial}{\partial r_k} \]

\[ = \sum_{j,k=1}^{N-2} \left[ - \left\{ \frac{\partial V(q)}{\partial r_j} - \frac{\partial V(q)}{\partial r_{j+1}} \right\} \frac{\partial}{\partial p_j} + \frac{p_j}{m_p} \left( \frac{\partial}{\partial r_j} - \frac{\partial}{\partial r_{j+1}} \right) \right] \]

\[ = - \left\{ \frac{\partial V(q)}{\partial r_1} - \frac{\partial V(q)}{\partial r_2} \right\} \frac{\partial}{\partial p_1} + \frac{p_1}{m_p} \left( \frac{\partial}{\partial r_1} - \frac{\partial}{\partial r_2} \right) - \left\{ \frac{\partial V(q)}{\partial r_2} - \frac{\partial V(q)}{\partial r_3} \right\} \frac{\partial}{\partial p_2} + \frac{p_2}{m_p} \left( \frac{\partial}{\partial r_2} - \frac{\partial}{\partial r_3} \right) \cdots + \]

\[ - \left\{ \frac{\partial V(q)}{\partial r_{N-2}} - \frac{\partial V(q)}{\partial r_{N-1}} \right\} \frac{\partial}{\partial p_{N-2}} + \frac{p_{N-2}}{m_p} \left( \frac{\partial}{\partial r_{N-2}} - \frac{\partial}{\partial r_{N-1}} \right) \]

\[ = - \frac{\partial V(q)}{\partial r_1} \left( \frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_0} \right) + \frac{1}{m_p} (p_1 - p_0) \frac{\partial}{\partial r_1} + \cdots - \frac{\partial V(q)}{\partial r_{N-1}} \left( \frac{\partial}{\partial p_{N-1}} - \frac{\partial}{\partial p_{N-2}} \right) + \frac{1}{m_p} (p_{N-1} - p_{N-2}) \frac{\partial}{\partial r_{N-1}} = \]

\[ = \sum_{j=1}^{N-1} \left[ - \frac{\partial V(r_j)}{\partial r_j} \left( \frac{\partial}{\partial p_j} - \frac{\partial}{\partial p_{j-1}} \right) + \frac{1}{m_p} (p_j - p_{j-1}) \frac{\partial}{\partial r_j} \right] \]
A.5 Polynomial expansion of the dynamical correlators

We present here the expression of the spreading operators that, along with eqn. 19 control the propagation of the non-locality of the dynamics of the ISF.

\[
\sigma^T(n, j, k) = \theta \left( \left\lfloor \frac{n}{2} \right\rfloor - k + j \right) \left( \frac{\partial V}{\partial r_k} \right) \left( \frac{\partial}{\partial p_k} - \frac{\partial}{\partial p_{k-1}} \right)^\theta(n-2) \times \left\{ \prod_{i=0}^{j-k-2} \left[ \frac{1}{m}(p_{j-i-1} - p_{j-i-2}) \frac{\partial}{\partial r_{j-i-1}} \right] \left[ \left( - \frac{\partial V}{\partial r_{j-i-1}} \right) \left( \frac{\partial}{\partial p_{j-i-1}} - \frac{\partial}{\partial p_{j-i-2}} \right) \right] \right\}^{\theta(n-4)} \left[ \frac{1}{m}(p_j - p_{j-1}) \frac{\partial}{\partial r_j} \right]^{\theta(n-2)}
\]

\[
\sigma^n_p(n, j, l - j) = \theta \left( \left\lfloor \frac{n-1}{2} \right\rfloor - j + l \right) \left\{ \prod_{i=0}^{j-l-2} \left[ \frac{1}{m}(p_{j+i-1} - p_{j+i-2}) \frac{\partial}{\partial r_{j+i-1}} \right] \left[ \left( - \frac{\partial V}{\partial r_{j+i-1}} \right) \left( \frac{\partial}{\partial p_{j+i-1}} - \frac{\partial}{\partial p_{j+i-2}} \right) \right] \right\}^{\theta(n-3)} \times \left[ \frac{1}{m}(p_j - p_{j-1}) \frac{\partial}{\partial r_j} \right]^{\theta(n-1)}
\]

From eqn. 35 and eqn. 36 we can construct the list of the index of the momenta entering the dynamics at order \( n \):

\[
L_p(n, j) \equiv \left\{ j - \left\lfloor \frac{n+1}{2} \right\rfloor, \ldots, j + \left\lfloor \frac{n-1}{2} \right\rfloor \right\} \in \mathbb{N}(\left\lfloor \frac{n}{2} \right\rfloor, \left\lfloor \frac{n}{2} \right\rfloor + 1) \equiv \{ l_{\text{min}}, \ldots, l_{\text{max}} \}
\]

Via additional manipulations of the spreading operators we can fix the leading power of each of the degrees of freedom at order \( n \) in the polynomial expansion; this ensures a more efficient computational management of the problem. The calculation is easily performed if we are interested in the leading power of \( r_k \) for \( |k-j| \leq 1 \), because we don’t need to explicitly propagate the dynamics via the spreading operators; the factor of \((i\mathcal{L})^n\) providing this maximal power is simply

\[
\left[ \left( - \frac{\partial V}{\partial r_k} \right) \left( \frac{\partial}{\partial p_k} - \frac{\partial}{\partial p_{k-1}} \right) (p_j - p_{j-1}) \frac{\partial}{\partial r_j} \right]^n
\]

such that the maximum power in \( r_k \) is \( 2 \left( \left\lfloor \frac{n}{2} \right\rfloor - 1 \right) + 3 = 2 \left\lfloor \frac{n}{2} \right\rfloor + 1 \).

Analogously, it is straightforward to note that the contribution of \((i\mathcal{L})^n\) associated to leading power of \( p_l \) for \( l \in \{ j, j-1 \} \) is given

\[
\left[ (p_j - p_{j-1}) \frac{\partial}{\partial r_j} \right]^n
\]

In the general case we proceed as before by defining suitable chains of differential operators in \((i\mathcal{L})^n e^{i\mathcal{K}r_j}\). A subset of \(\mathcal{N}_{r/p}^{(R/L)} < n\) differentials must be devoted to the spreading of the interaction till the freedom under interest is reached. By direct counting we get:

\[
\mathcal{N}^R_R(n, j, k - j) = \theta \left( \left\lfloor \frac{n}{2} \right\rfloor - k + j \right) [2\theta(n-2) + 2(k-j-1)\theta(n-4)]
\]

\[
\mathcal{N}^T_R(n, j, j - k) = \theta \left( \left\lfloor \frac{n}{2} \right\rfloor - j + k \right) [2\theta(n-2) + 2(j-k-1)\theta(n-4)]
\]

\[
\mathcal{N}^R_P(n, j, l - j) = \theta \left( \left\lfloor \frac{n-1}{2} \right\rfloor - l + j \right) \theta(n-3) [1 + 2(l-j)]
\]

\[
\mathcal{N}^T_P(n, j, l - j) = \theta \left( \left\lfloor \frac{n+1}{2} \right\rfloor - j + l \right) [\theta(n-1) + 2(j-l-1)\theta(n-3)]
\]
with
\[
\begin{align*}
\mathcal{N}_p^{(R/L)}(n, j, |l-j|) &= \left[ \frac{n - \mathcal{N}_p^{(R/L)}(n, j, |l-j|)}{2} \right] \left( \frac{n - \mathcal{N}_p^{(R/L)}(n, j, |l-j|)}{4} \right) \in \{0, 1\}
\end{align*}
\]

Let us notice that eqn. [40] and eqn. [41] are symmetric w.r.t. the index $j$, in contrast to the expression of the spreading operators themselves. We are now almost able to write the explicit expression of the functions $\mathcal{M}_r(n, j, |k-j|)$ and $\mathcal{S}_p(n, j, |k-j|)$, returning respectively the maximum power of $r_k$ and $p_l$ at order $n$.

This can be done by direct counting from eqn. [40] and eqn. [41]. We have to distinguish three different cases:

1. \[
\left| \frac{n - \mathcal{N}_r^{(R/L)}(n, j, |k-j|)}{2} \right| = 0 \implies \mathcal{M}_r(n, j, |k-j|) = 3\theta(n-2)
\]
2. \[
\left| \frac{n - \mathcal{N}_r^{(R/L)}(n, j, |k-j|)}{2} \right| = 1 \implies \mathcal{M}_r(n, j, |k-j|) = 2 + 3\theta(n-2)
\]
3. \[
\left| \frac{n - \mathcal{N}_r^{(R/L)}(n, j, |k-j|)}{2} \right| \geq 2 \implies \mathcal{M}_r(n, j, |k-j|) = 3\theta(n-2) + 2 \left( \left| \frac{n - \mathcal{N}_r^{(R/L)}(n, j, |k-j|)}{2} \right| - 1 \right) + 3
\]

and therefore

\[
\mathcal{M}_r(n, j, |k-j|) = \begin{cases} 2 \left| \frac{n}{2} \right| + 1, & 0 \leq |j-k| \leq 1 \\ \theta \left( \left| \frac{n}{2} \right| - |k-j| \right) \left( 3\theta \left( \left| \frac{n - \mathcal{N}_r^{(R/L)}(n, j, |k-j|)}{2} \right| \right) \theta(n-2) + 2\theta \left( \left| \frac{n - \mathcal{N}_r^{(R/L)}(n, j, |k-j|)}{2} \right| - 1 \right) + 2 \left( \left| \frac{n - \mathcal{N}_r^{(R/L)}(n, j, |k-j|)}{2} \right| - 1 \right) \\ 0 \leq |j-k| \leq 1 \\ 2 \left( \left| \frac{n}{2} \right| - |k-j| \right) \left( 3\theta \left( \left| \frac{n - \mathcal{N}_r^{(R/L)}(n, j, |k-j|)}{2} \right| \right) \theta(n-2) + 2\theta \left( \left| \frac{n - \mathcal{N}_r^{(R/L)}(n, j, |k-j|)}{2} \right| - 1 \right) + 2 \left( \left| \frac{n - \mathcal{N}_r^{(R/L)}(n, j, |k-j|)}{2} \right| - 1 \right) \\ \text{otherwise}
\end{cases}
\]

Analogously we can write for the momenta:

1. \[
\left| \frac{n - \mathcal{N}_p^{(R/L)}(n, j, |l-j|)}{4} \right| = 0 \implies \mathcal{S}_p(n, j, |l-j|) = \theta \left( \left| \frac{n+1}{2} \right| \right) + \theta \left( \mathcal{N}_p^{(R/L)}(n, j, |l-j|) - 1 \right)
\]
2. \[
\left| \frac{n - \mathcal{N}_p^{(R/L)}(n, j, |l-j|)}{4} \right| = 1 \implies \mathcal{S}_p(n, j, |l-j|) = \theta \left( \left| \frac{n+1}{2} \right| \right) + 2\theta \left( \mathcal{N}_p^{(R/L)}(n, j, |l-j|) - 1 \right)
\]
3. \[
\left| \frac{n - \mathcal{N}_p^{(R/L)}(n, j, |l-j|)}{4} \right| \geq 2 \implies \mathcal{S}_p(n, j, |l-j|) = \theta \left( \left| \frac{n+1}{2} \right| \right) + 2 \left( \left| \frac{n - \mathcal{N}_p^{(R/L)}(n, j, |l-j|)}{4} \right| - 1 \right) + 3\theta \left( \mathcal{N}_p^{(R/L)}(n, j, |l-j|) - 1 \right) + 4\theta \left( \mathcal{N}_p^{(R/L)}(n, j, |l-j|) - 1 \right)
\]

The different cases above can be expressed together to get:
We can then infer the following recursion relation:

\[ S_p(n, j, |l - j|) = \begin{cases} 
  n, & l \in \{j, j - 1\} \\
  \theta \left(\left\lfloor \frac{n+1}{2} \right\rfloor - |j - l|\right) & + 2\theta \left(\left\lfloor \frac{n_N^R(L)}{2} \right\rfloor - |n - \frac{n_N^R(L)}{2}| - 1\right) + \theta \left(\left\lfloor \frac{n_N^R(L)}{2} \right\rfloor - |n - \frac{n_N^R(L)}{2}| - 2\right) \times \\
  & + 2\left[2 - \frac{n_N^R(L)}{2} \right] + 3\theta \left(-\frac{n_N^R(L)}{2} \right) + \theta \left(-\frac{n_N^R(L)}{2} \right) - 1 \right) \\
  \end{cases} \]

where the upper/lower sign refer respectively to the right/left (R/L) directions of the spreading.

### A.6 Recursive construction of the dynamical tensor

We present here the derivation of the recursion relations for the construction of the tensor \( \mathcal{I}^{(n)} \) in eqn. 14. The action of \( i\mathcal{L}_p \) on the iterative scheme has been derived in eqn. 19. We can proceed in the same fashion for the calculation of the other contributes. Let’s first consider the operator

\[ i\mathcal{L}_p \equiv \frac{1}{m} (p_{\gamma} - p_{\gamma-1}) \frac{\partial}{\partial r_{\gamma}} \]

on a generic monomial of the expansion at order \( n \), given \( k_{\min} \leq \gamma \leq k_{\max} \); we have:

\[ \left\{ i\mathcal{L}_p \left[ r_{k_{\min}} \ldots r_{\gamma} \ldots r_{k_{\max}} \right] \left[ p_{l_{\min}} \ldots p_{l_{\gamma}} \ldots p_{l_{\max}} \right] \right\} e^{iK_{r,j}} = \frac{m_N}{m} \left\{ r_{k_{\min}} \ldots r_{\gamma-1} \ldots r_{k_{\max}} \right\} \left[ p_{l_{\min}} \ldots p_{l_{\gamma-1}} \ldots p_{l_{\max}} \right] \}

We can then infer the following recursion relation:

\[ \mathcal{I}^{(n+1)}_{m,s} \mid_{r_{j}, \gamma} = \frac{m}{m_N} \sum_{k=0}^{k_{\max}} (-1)^k \mathcal{I}^{(n)}_{m,s+\hat{e}_{r_{j}-k}} \]

We finally have to consider separately the action on \( i\mathcal{L}_p \) on \( e^{iK_{r,j}} \):

\[ \left\{ i\mathcal{L}_p \left[ r_{k_{\min}} \ldots r_{\gamma} \ldots r_{k_{\max}} \right] \left[ p_{l_{\min}} \ldots p_{l_{\gamma}} \ldots p_{l_{\max}} \right] \right\} i\mathcal{L}_p e^{iK_{r,j}} = \frac{iK}{m} \left\{ r_{k_{\min}} \ldots r_{\gamma} \ldots r_{k_{\max}} \right\} \left[ p_{l_{\min}} \ldots p_{l_{\gamma}} \ldots p_{l_{\max}} \right] \]

and therefore

\[ \mathcal{I}^{(n+1)}_{m,s} \mid_{r_{j}, K} = \frac{iK}{m} \sum_{k=0}^{k_{\max}} (-1)^k \mathcal{I}^{(n)}_{m,s+\hat{e}_{j}-k} \]

The final expression for the dynamical tensor at order \( n + 1 \) is obtained by summing the contributions of eqn. 19, eqn. 42 and eqn. 43 over the subset \( \boldsymbol{\Gamma} \) of the coordinates entering the interaction at order \( n \):

\[ \mathcal{I}^{(n+1)}_{m,s} = \sum_{\gamma \in \boldsymbol{\Gamma}} \left( \mathcal{I}^{(n+1)}_{m,s} \mid_{r_{j}, \gamma} + \mathcal{I}^{(n+1)}_{m,s} \mid_{r_{j}, \gamma} + \mathcal{I}^{(n+1)}_{m,s} \mid_{r_{j}, \gamma} \right) \]

with the initial condition

\[ \mathcal{I}^{(0)}_{m,s} = \begin{cases} 
  1, & \text{for } m = e_j \\
  0, & \text{elsewhere} 
\end{cases} \]

Let us call \( n_{\max} \) the maximum order of \( \mathcal{I}^{(n)} \) we aim to compute. The set \( \boldsymbol{\Gamma} \) can be fixed once for all for any \( n \in \{0, \ldots, n_{\max}\} \):

\[ \boldsymbol{\Gamma} \leq \{ \min\{K_r(n_{\max}, j), L_p(n_{\max}, j)\}, \ldots, \max\{K_r(n_{\max}, j), L_p(n_{\max}, j)\} \} = \left\{ j - \left\lfloor \frac{n_{\max} + 1}{2} \right\rfloor, \ldots, j + \left\lfloor \frac{n_{\max}}{2} \right\rfloor \right\} \]
A.7 Long-time decay of the memory kernel

In this appendix we derive an analytical estimate of the long-time tail of the memory kernel. Note beforehand that the increasing magnitude of the kernel coefficients can give rise to numerical limitations above a certain order in the expansion. It is therefore a matter of convenience to rescale in the first place the terms by the factorial weight of the series expansion. This allows the following simplifications:

\[
\frac{\kappa_{2n-2}^{ij}}{(2n-2)!} \begin{cases} 
\sum_{n \geq 1} \frac{\omega_n^{ij}}{(2n)!} = (1 - C_\beta) a^n (-2)^n n \Gamma (n + \frac{3}{2}) = (1 - C_\beta) a^n (-2)^n 2^n \sqrt{\pi} = (1 - C_\beta) a^n (2n)! \sqrt{\pi} (2n-2)! = (1 - C_\beta) a^n 2^n \sqrt{\pi} (2n-2)! 4^n n! 
\end{cases} = \...
\]

The same rescaling applies to the high-order coefficients in the ideal gas regime to reduce their total magnitude:

\[
\frac{\kappa_{2n-2}^{ij}}{(2n-2)!} = \frac{\omega_{2n}^{ij}}{(2n-2)!} = \frac{1}{\sqrt{\pi}} (-1)^n \left( \frac{4K^2 \alpha}{m \beta} \right)^n n \Gamma (n + \frac{3}{2}) = \frac{1}{\sqrt{\pi}} (-1)^n \left( \frac{4K^2 \alpha}{m \beta} \right)^n \frac{n! 2^n \sqrt{\pi}}{4^n n! (2n-2)!} = \...
\]

according to the fact that in the kinematic regime it holds \( C_\beta = 0, a = \frac{K^2 \alpha}{m \beta} \).

An analytical expression for the memory kernel at long-times can be determined by extending the estimate in eqn. [7] to the whole series of the Taylor coefficients. This approximation is known to fail at low orders, according to the discussion about Fig. [7] however this does not affect the reconstruction of \( K(t) \) for \( t \gg 1 \), when the first contributions become negligible. We then get:

\[
K(t) \approx t \sum_{n=0}^{\infty} \frac{t^{2n}}{(2n)!} \omega_{2n+2}^{ij} = \sum_{n=0}^{\infty} \frac{t^{2n}}{(2n)!} \left[ (1 - C_\beta) a^{n+1} H_{2n+2} + \delta_{n+1,0} C_\beta \right] =
\]

\[
= \sum_{n=0}^{\infty} \frac{t^{2n}}{(2n)!} \left[ (1 - C_\beta) a^{n+1} (2n + 1)! \Gamma (n + \frac{3}{2}) = (1 - C_\beta) \sum_{n=0}^{\infty} \frac{t^{2n}}{(2n)!} a^{n+1} (2n + 1)! \right]
\]

\[
= (1 - C_\beta) a \sum_{n=0}^{\infty} \frac{t^{2n}}{(2n)!} \left( \frac{4n + 1}{4(n + 1)} \right) = (1 - C_\beta) a (at^2)^n \frac{2n + 1}{(n + 1)!} = 2(1 - C_\beta) a e^{-at^2} (2at^2 - 1)
\]

which means

\[
\frac{K(t)}{K(0)} \approx e^{-at^2} (1 - 2at^2)
\]

According to eqn. [46] we can fix the following ansatz for the long time behavior of the function:

\[
K_{LT}(t) \equiv A t^2 e^{-Bt^2}
\]

We can notice that the divergences of all the curves in Figure [8] occur after the instant when the second derivative vanishes for the third time by increasing times. Let us define this critical time \( t^* \) and take this as a starting point for the estimate of the tail. By imposing continuity of the function and its derivative in this point the parameters of the ansatz are given by

\[
A = \frac{K^*}{t^2 \exp(\frac{K^* t^*}{2K^*})}
\]

\[
B = \frac{2K^* - K^* t^*}{2K^* t^*}
\]
\[ K^* \equiv K_{N_{max}}(t^*) \]
\[ K*^* \equiv \sum_{n=0}^{N_{max}} \frac{K_{2n}}{(2n)!} t^{*2n-1} \]

### A.8 Management of high-dimensional tensors

The components of \( \mathcal{T}_{\text{ms}}^{(n)} \) can be stored in a one-dimensional pointer in row-major order; via this sorting the list of the sequence of the indexes increases progressively in a natural fashion. For example the indexes of a \( 3 \times 3 \times 3 \) tensor would be sorted as
\[ \{000, 001, 002, 010, 011, 012, 021, \cdots, 222\} \]
and by mapping the sequence of the indexes into integer numbers according to
\[ (i, j, k) \rightarrow i \cdot 10^2 + j \cdot 10 + k \]
we get a monotonically increasing sequence.

We can generalize this approach for a generic number of \( n_{\text{ind}} \in \mathbb{N} \) indexes, with dimensions \( \mathbf{D} = \{D_0, \cdots, D_{n_{\text{ind}}-1}\} \). Let us label a general multi-index of the tensor with the vector
\[ \mathbf{v} = \{v_0, \cdots, v_{n_{\text{ind}}-1}\} \]
with \( v_j \leq D_j - 1 \ \forall \ j = 0, \cdots, n_{\text{ind}}-1 \). It is possible to map this into the index of a one dimensional array via the function
\[
\text{map}(\mathbf{v}, \mathbf{D}, n_{\text{ind}}) = v_0 \prod_{\beta_0=1}^{n_{\text{ind}}-1} D_{\beta_0} + v_1 \prod_{\beta_1=2}^{n_{\text{ind}}-1} D_{\beta_1} + \cdots v_{n_{\text{ind}}-1} = \sum_{\alpha=0}^{n_{\text{ind}}-1} v_\alpha \prod_{\beta_\alpha=\alpha+1}^{n_{\text{ind}}-1} D_{\beta_\alpha} \tag{48}
\]

It is straightforward to determine the map of last index of the tensor \( \mathbf{v}_{\text{last}} \equiv \{D_0 - 1, D_1 - 1, \cdots, D_{n_{\text{ind}}-1} - 1\} \):
\[
\text{map}(\mathbf{v}_{\text{last}}, \mathbf{D}, n_{\text{ind}}) = \sum_{\alpha=0}^{n_{\text{ind}}-1} (D_\alpha - 1) \prod_{\beta_\alpha=\alpha+1}^{n_{\text{ind}}-1} D_{\beta_\alpha} = [(D_0 - 1)D_1D_2 \cdots D_{n_{\text{ind}}-1}] + \\
+ [(D_1 - 1)D_2 \cdots D_{n_{\text{ind}}-1}] + \cdots + D_{n_{\text{ind}}-1} - 1 = \prod_{\gamma=0}^{n_{\text{ind}}-1} D_\gamma - 1
\]

Last identity follows being the sum telescopic.

In the implementation of the recursion relations in Section 4, we are interested in integer increments (let us say by \( l \in \mathbb{N} \)) of a generic \( i \)-th 'column' of the coefficients tensor: \( \mathcal{T}_{\text{ms}}^{(n)} \rightarrow \mathcal{I}_{\text{ms}+l\delta_i}^{(n)} \). By imposing \( v_i \equiv l \in \{0, \cdots, D_i - 1\} \) we can easily extract the following shifting rule:
\[
\text{map}(\{v_0, \cdots, v_{i-1}, l, v_{i+1}, \cdots, v_{n_{\text{ind}}-1}\}, \mathbf{D}, n_{\text{ind}}) = \sum_{\alpha=0}^{n_{\text{ind}}-1} v_\alpha \prod_{\beta_\alpha=\alpha+1}^{n_{\text{ind}}-1} D_{\beta_\alpha} + l \prod_{\beta_i=i+1}^{n_{\text{ind}}-1} D_{\beta_i} \tag{49}
\]

It is moreover possible to determine the inverse map that, given an entry of a one-dimensional mapping and the list of the related dimensions, returns the multi-index associated to that component. For this we can proceed recursively, from the extraction of the last index \( v_{n_{\text{ind}}-1} \) backwards. From eqn. 48 we get:
\[
\begin{align*}
    n_{\text{map}} & \equiv \text{map}(\mathbf{v}, \mathbf{D}, n_{\text{ind}}) = \left( \sum_{\alpha=0}^{n_{\text{ind}}-2} v_\alpha \prod_{\beta_\alpha=\alpha+1}^{n_{\text{ind}}-1} D_{\beta_\alpha} \right) + v_{n_{\text{ind}}-1} = \left( \sum_{\alpha=0}^{n_{\text{ind}}-2} v_\alpha \prod_{\beta_\alpha=\alpha+1}^{n_{\text{ind}}-2} D_{\beta_\alpha} \right) D_{n_{\text{ind}}-1} + v_{n_{\text{ind}}-1} \tag{49} \\
    v_{n_{\text{ind}}-1} & \equiv n_{\text{map}} \mod D_{n_{\text{ind}}-1} \tag{50}
\end{align*}
\]
Eqn. 50 follows from eqn. 49 being \( v_{n_{\text{ind}}}^{n_{\text{ind}}-1} < D_{n_{\text{ind}}}^{n_{\text{ind}}-1} \). We can proceed with the extraction of the second last component of \( v_{n_{\text{ind}}}^{n_{\text{ind}}-2} \) via the knowledge of \( v_{n_{\text{ind}}}^{n_{\text{ind}}-1} \):

\[
A_{n_{\text{ind}}-1} \equiv \frac{n_{\text{map}} - v_{n_{\text{ind}}-1}}{D_{n_{\text{ind}}-1}} = \left( \sum_{\alpha=0}^{n_{\text{ind}}-3} v_{\alpha} \prod_{\beta_{\alpha}=\alpha+1}^{n_{\text{ind}}-3} D_{\beta_{\alpha}} \right) D_{n_{\text{ind}}-2} + v_{n_{\text{ind}}-2}
\]

\[
v_{n_{\text{ind}}-2} = A_{n_{\text{ind}}-1} \mod D_{n_{\text{ind}}-2}
\]

A recursion relation can then be established \( \forall \ i \in \{0, \ldots, n_{\text{ind}}-1\} \):

\[
v_{n_{\text{ind}}-i-1} = A_{n_{\text{ind}}-i} \mod D_{n_{\text{ind}}-i-1}
\]

\[
A_{n_{\text{ind}}-i-1} = \frac{A_{n_{\text{ind}}-i} - v_{n_{\text{ind}}-i-1}}{D_{n_{\text{ind}}-i-1}}
\]

with initial condition \( A_{n_{\text{ind}}} = n_{\text{map}} \).

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