Fractional equation description of an open anomalous heat conduction set-up

Aritra Kundu$^1$, Cédric Bernardin$^2$, Keji Saito$^3$, Anupam Kundu$^1$ and Abhishek Dhar$^1$

$^1$ International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bengaluru 560089, India
$^2$ Université Côte d’Azur, CNRS, LJAD Nice Cedex 02, France
$^3$ Department of Physics, Keio University, Yokohama 223-8522, Japan

E-mail: aritrak@icts.res.in, cedric.bernardin@unice.fr, saitoh@rk.phys.keio.ac.jp, anupam.kundu@icts.res.in and abhishek.dhar@icts.res.in

Received 19 September 2018
Accepted for publication 29 November 2018
Published 4 January 2019

Abstract. We provide a stochastic fractional diffusion equation description of energy transport through a finite one-dimensional chain of harmonic oscillators with stochastic momentum exchange and connected to Langevin type heat baths at the boundaries. By establishing an unambiguous finite domain representation of the associated fractional operator, we show that this equation can correctly reproduce equilibrium properties like the Green–Kubo formula as well as non-equilibrium properties like the steady state temperature and current. In addition, this equation provides the exact time evolution of the temperature profile. Taking insights from the diffusive system and from numerical simulations, we pose a conjecture that these long-range correlations in the steady state are given by the inverse of the fractional operator. We also point out some interesting properties of the spectrum of the fractional operator. All our analytical results are supplemented with extensive numerical simulations of the microscopic system.

Keywords: current fluctuations, heat conduction, stationary states, transport properties
1. Introduction

Energy transport across an extended system is a fundamental non-equilibrium phenomenon which is often described by the phenomenological Fourier law. This law leads to the heat equation for the evolution of the temperature field \( T(y, t) \), which in one dimension is given by

\[
\partial_t T(y, t) = \frac{\kappa}{c} \partial_y^2 T(y, t),
\]

where \( c \) is the specific heat capacity and \( \kappa \) the heat conductivity (assumed, for simplicity to be temperature independent). This equation plays a central role in understanding
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heat transport through macroscopic materials in several contexts. However, various studies have established that for a large class of one and two dimensional systems with momentum conservation, energy transport is not diffusive but super-diffusive—this is referred to as anomalous transport [1–3]. There are several signatures of anomalous transport which include the super-diffusive spreading of localized heat pulses and the form of spatio-temporal correlations in equilibrium set-up as well as diverging thermal conductivity in non-equilibrium (boundary driven) set-up. Unlike diffusive transport, currently there is no general framework to understand these features of anomalous transport completely except for a recent development based on non-linear fluctuating hydrodynamics theory [4–7]. This theory, based on some phenomenological assumptions, provides a framework to understand the super-diffusive energy transport in a wide class of one-dimensional anharmonic classical Hamiltonian systems such as the Fermi–Pasta–Ulam–Tsingou (FPUT) system and hard-particle gases [4–9].

One picture that has emerged from many studies is that, for systems with anomalous transport, the standard heat diffusion equation has to be replaced by some fractional diffusion equation [1, 10–15]. A particular model of anomalous transport where some rigorous results have been obtained is that of the harmonic chain whose Hamiltonian dynamics is supplemented by a stochastic part that keeps the conservation laws (volume, energy, momentum) intact—we will refer this model as the harmonic chain momentum exchange (HCME) model. For the infinite HCME system, it was shown exactly that at equilibrium the energy current autocorrelation has a $\sim t^{-1/2}$ decay [16]. It was also shown that, in contrast to equation (1), in infinite volume, the evolution of a localized energy perturbation $e(y, t)$, is described by a non-local fractional diffusion equation $\partial_t e(y, t) = -\tilde{\kappa}(-\Delta)^{3/4}e(y, t)$, where $\tilde{\kappa}$ is some constant which depends on microscopic parameters [14]. The fractional Laplacian operator $(-\Delta)^{3/4}$ in the infinite space is defined by its Fourier spectrum: $|q|^{3/2}$ which for the normal Laplacian operator $-\Delta \equiv -\partial_y^2$ is $q^2$.

While most of the studies in HCME model consider evolution in infinite systems, it is also of interest to study transport across a finite system connected to two reservoirs of different temperatures at its two ends. For diffusive systems in this set-up, the heat equation continues to describe both non-equilibrium steady state (NESS) and time-dependent properties. However, for anomalous transport, it is a priori not clear how to write a corresponding evolution equation in a finite domain. Since we expect this evolution to be governed by a fractional Laplacian which is a non-local operator, it is difficult to guess its representation in a finite system from its representation in the infinite system. Note that in the finite system one has to include the effects of the boundary conditions which are important as the operator itself is non-local. Hence, extending its definition to a finite domain is a non-trivial problem. Several studies have addressed this problem of obtaining and studying fractional diffusion description in finite domain [17–19].

In this paper, we study heat transfer across the HCME model connected to two reservoirs at its two ends. It has been observed and proved that in this model, heat current scaling with system size is anomalous and the steady state temperature profile is inherently non-linear [1, 11, 20]. In the present work we provide a fractional equation description of the anomalous heat transfer both in the stationary as well as in the non-stationary state. Using this fractional description we derive new results related to
the evolution of temperature profile, equilibrium current fluctuations and to two-point
correlations in NESS. Below we summarise the main results of our work along with the
plan of the paper:

• In section 2 we first review previous studies on the HCME model. These studies
show that the macroscopic time evolution of two-point correlations is described
by a set of coupled local linear PDEs [11, 12]. Starting from these PDEs, it can be
shown that they naturally give rise to an evolution equation for the temperature
profile $T(y, \tau)$

$$\partial_\tau T(y, \tau) = -\bar{\kappa} \mathcal{L} T(y, \tau),$$

governed by a fractional Laplacian $\mathcal{L}$ defined in a finite domain, where $\tau$ is a
scaled time (see later). The operator $\mathcal{L}$ is defined in the domain $0 \leq y \leq 1$
through its action

$$\mathcal{L} | \phi_n \rangle = \lambda_n^{3/4} | \phi_n \rangle,$$

on the complete Neumann basis $\langle y | \phi_n \rangle = \phi_n(y) = \sqrt{2} \cos(n\pi y)$ for $n \geq 1$ and
$\langle y | \phi_0 \rangle = \phi_0(y) = 1$ with $\lambda_n = (n\pi)^2$. Using this representation, we show that one
can recover the exact results [11] for the steady state temperature and current
profiles in the HCME.

• Next in section 3 we discuss in detail the time evolution of the temperature
profile to the long-time NESS profile which was discussed briefly in [12]. In order
to solve the fractional diffusion equation with Dirichlet boundary conditions for
an arbitrary time we are required to find the eigenvalues and eigenvectors of
the fractional operator $\mathcal{L}$ with Dirichlet boundary conditions. We describe an
efficient procedure to compute this Dirichlet eigensystem. We also provide a
detailed discussion of some properties of the eigensystem that distinguish them
from the eigensystem of the normal Laplacian operator with the same boundary
conditions.

• Inspired by the fluctuating equations for energy evolution in diffusive systems
[21, 22], in section 4 we extend the definition of the fractional equation to include
fluctuations and noise in equilibrium such that fluctuation-dissipation relation
holds locally.

• Using the fluctuating fractional equation description, in section 4.2, we first verify
the validity of the equilibrium Green–Kubo relation in finite systems where we
encounter some interesting mathematical identities that we establish numerically.
This motivates and enables us to study the long-range correlations in NESS in
section 4.4, where we propose a conjecture on the relation between these correla-
tions and the Green’s function of the operator $\mathcal{L}$.

• Finally, in section 5 we conclude our paper.
2. Definition of model and survey of earlier results

We consider the so-called harmonic chain momentum exchange model (HCME), which considers an added stochastic component in the usual Hamiltonian dynamics of a harmonic chain. The stochastic part is such that it preserves volume, momentum and energy conservation but the other conserved variables of the harmonic chain are no longer conserved. Thus the stochastic model restores ergodicity while preserving the important conservation laws. Here we are interested in the open system where the system is driven by two Langevin-type heat baths. Specifically we consider a system consisting of \( N \) particles and attached to two heat baths. The Hamiltonian plus heat bath part of the dynamics is described by the following equations

\[
\begin{align*}
\dot{q}_i &= p_i, \quad \dot{p}_i = \omega^2 (q_{i+1} - 2q_i + q_{i-1}), \quad 1 < i < N, \\
\dot{p}_1 &= \omega^2 (q_2 - 2q_1) - \lambda p_1 + \sqrt{2Nt} \eta_L, \\
\dot{p}_N &= \omega^2 (q_{N-1} - 2q_N) - \lambda p_N + \sqrt{2Nt} \eta_R, \\
\end{align*}
\]

where \( \{q_i, p_i\}, \ i = 1, 2, \ldots, N, \) are the positions and momenta of the particles, \( T_L, T_R \) are the temperatures of the left and the right Langevin baths and \( \eta_L, \eta_R \) are Gaussian white noise terms. Additionally there is a stochastic noise, such that the momenta of nearest neighbour particles are exchanged (i.e. \( p_{i+1} \leftrightarrow p_i \)) at a rate \( \gamma \). For this model the two point correlation functions satisfy a closed set of equations.

Following [12] let us denote the possible correlation matrices by \( U_{ij} = \langle q_i q_j \rangle \), \( V_{ij} = \langle p_i p_j \rangle \), and \( Z_{ij} = \langle q_i p_j \rangle \). One can show that the time evolution of these correlation functions is given by linear equations involving only these sets of correlations and source terms arising from the boundary driving [12]. Let us also define the correlation \( z_{i,j}^+ = (Z_{i,j} - Z_{i-1,j} + Z_j,i - Z_{j-1,i})/2 \). The most interesting physical observables involve the correlations \( T_i = V_{ii} \), which can be taken as the definition of local temperature and the energy current \( J = \omega^2 z_{i+1}^+ + (\gamma/2) (V_{i+1,i+1} - V_{i,i}) \). In the \( N \to \infty \) limit, one observes that the fields \( T_i \) and \( z_{ij}^+ \) have the scaling forms \( T_i(t) = T(i/N, t/N^3/2) \) and \( z_{ij}^+ = 1/\sqrt{N}\ C ((i - j)/N^{1/2}, (i + j)/2N, t/N^3/2) \). In terms of the following scaling variables \( u = |i - j|/N^{1/2}, y = (i + j)/(2N), \tau = t/N^3/2 \), it has been shown in [12] that the fields \( T(y, \tau) \) and \( C(u, y, \tau) \) satisfy the following coupled set of PDEs:

\[
\begin{align*}
\gamma^2 \partial_u^4 C(u, y, \tau) &= \omega^2 \partial_y^2 C(u, y, \tau), \\
\partial_y T(y, \tau) &= -2\gamma \partial_u C(u, y, \tau)|_{u \to 0}, \\
\partial_\tau T(y, \tau) &= \omega^2 \partial_y C(u, y, \tau)|_{u \to 0},
\end{align*}
\]

with boundary conditions \( C(u, 0, \tau) = C(u, 1, \tau) = 0, C(\infty, y, \tau) = 0, \partial_u^4 C(0, y, \tau) = 0 \) and \( T(0, \tau) = T_L \) and \( T(1, \tau) = T_R \) where, the domain of variables are \( u \in [0, \infty) \) and \( y \in [0, 1] \) (note that in [12] \( y \in (-1, 1) \)). To study the time-evolution of the fields \( C(u, y, \tau) \) and \( T(y, \tau) \), one has to subtract the steady state solutions \( J_{ss}(u, y) \) and \( T_{ss}(y) \) of the above equations (whose explicit forms are given in [11]). The boundary conditions suggest that one expands the difference fields using the complete Dirichlet basis \( \langle y|\alpha_n \rangle = \alpha_n(y) = \sqrt{2}\sin(n\pi y) \) for \( n \geq 1 \).
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\[ C(u, y, \tau) - C_{ss}(u, y) = \sum_{n=1}^{\infty} \hat{c}_n(u, \tau)\alpha_n(y), \]  
\[ T(y, \tau) - T_{ss}(y) = f(y, \tau) = \sum_{n=1}^{\infty} \hat{f}_n(\tau)\alpha_n(y). \]

Following [12] one then gets (see appendix B) the following matrix equation for the evolution of the components \( f_n \):

\[ \dot{\hat{f}}_n = -\kappa \sum_{k=1}^{\infty} \mathbb{L}_{nk}\hat{f}_k, \quad n = 1, 2, \ldots, \infty, \]  
\[ \text{where, } \mathbb{L}_{nk} = [\mathcal{T} \Lambda^{3/4} \mathcal{T}]_{nk}, \]

with \( \mathcal{T}_{nl} = \langle \alpha_n | \phi_l \rangle = \int_0^\infty dy \alpha_n(y)\phi_l(y) \), where \( \phi_m(y) = \sqrt{2} \cos(m\pi y) \) for \( m > 0 \), \( \phi_0(y) = 1 \) and \( \Lambda_{ml} = \lambda_m \delta_{ml} \) is a diagonal matrix with \( \lambda_n = (n\pi)^2 \). The constant \( \kappa = \omega^{3/2}/(2\sqrt{2}) \).

Therefore, the function \( f(x, \tau) \) with homogeneous boundaries \( f(0, \tau) = f(1, \tau) = 0 \) satisfies

\[ \partial_\tau f(y, \tau) = -\kappa \mathbb{L} f(y, \tau). \]

From equation (7), one notices that \( \mathbb{L}_{nk} \) can be written as

\[ \mathbb{L}_{nk} = \langle \alpha_n | \mathbb{L} | \alpha_k \rangle = \langle \alpha_n | \left[ \sum_{m=0}^{\infty} \lambda_m^{3/4} | \phi_m \rangle \langle \phi_m | \right] | \alpha_k \rangle, \quad \forall \ n, k = 1, 2, \ldots, \infty, \]

which allows us to identify the action of the operator \( \mathbb{L} \) acting on the set of basis functions \( \phi_m \) (which satisfy Neumann boundary conditions):

\[ \mathbb{L} | \phi_m \rangle = \lambda_m^{3/4} | \phi_m \rangle. \]

It is important to notice that the above representation of the operator \( \mathbb{L} \) is not the ‘spectral fractional Laplacian with Dirichlet boundary conditions’ which would consist of replacing \( \phi_n \) by \( \alpha_n \) in (9). The definition in equation (9) has been mentioned in [1] and a more mathematically rigorous derivation has been obtained [19]. The above results imply that the temperature field \( T(y, \tau) \) evolves according to the fractional equation

\[ \partial_\tau T(y, \tau) = -\kappa \mathbb{L} T(y, \tau) = -\mathbb{L}_\kappa T(y, \tau), \]

where we have defined \( \mathbb{L}_\kappa = \kappa \mathbb{L} \) and the steady state is required to satisfy the condition \( \mathbb{L}_\kappa T_{ss}(y) = 0 \). To describe the evolution of the temperature profile, one is specifically interested in finding the eigenvectors of the operator \( \mathbb{L} \) which satisfy Dirichlet boundary conditions. This can be obtained by diagonalizing the infinite-dimensional matrix in equation (7). Let the eigenvector components of this matrix be denoted by \( \psi_n^{(m)} \), corresponding to eigenvalue \( \mu_n \), so that \( \sum_k \mathbb{L}_{mk}\psi_n^{(k)} = \mu_n \psi_n^{(m)} \) or equivalently,

\[ \mathbb{L} | \psi_n \rangle = \mu_n | \psi_n \rangle. \]

Then the eigenvector in the position basis is given by \( \psi_n(y) = \sum_m \psi_n^{(m)} \alpha_m(y) \). In section 3 we provide an alternate and more efficient method of computing eigenvalues.
and eigenvectors. This method involves finding roots of a transcendental equation and avoids diagonalization of infinite dimensional matrices. We also discuss various properties of the spectrum there. We now describe several results that follow for the steady state and the time evolution towards it.

### 2.1. Steady state results

Let us write the steady state temperature in the form

$$T_{ss}(y) = \bar{T} + \delta T \Theta(y),$$

where $\bar{T} = (T_L + T_R)/2$, $\delta T = T_L - T_R$ and the function $\theta(y)$ satisfies the boundary conditions, $\Theta(0) = 1/2$, $\Theta(1) = -1/2$. Then expanding $\Theta(y) = \sum_n \hat{\Theta}_n \phi_n(y)$, the stationarity condition $\bar{\kappa} \Theta = 0$ along with equation (9) gives

$$\sum_n \lambda_n^{3/4} \hat{\Theta}_n \phi_n = 0.$$  \hfill (13)

Now we note the identities (see appendix C), which have to be understood in a distributional sense:

$$\sum_{n \text{ odd}} \phi_n(y) = 0, \quad \sum_{n \text{ even}} \phi_n(y) = -1/\sqrt{2}. \hfill (14)$$

Using these and the boundary conditions $\Theta(0) = -\Theta(1) = 1/2$ we finally get

$$\Theta(y) = \sum_{n \text{ odd}} \frac{c}{\lambda_n^{3/4}} \phi_n(y),$$

with $c = \frac{\pi^{3/2}}{[\sqrt{8} - 1] \zeta(3/2)}$, \hfill (15)

where $\zeta(s)$ is the Riemann-Zeta function. The temperature profile matches with the one presented in [1, 11, 20]:

$$T_{ss}(y) = \bar{T} + \delta T \frac{\pi^{3/2}}{[\sqrt{8} - 1] \zeta(3/2)} \sum_{n \text{ odd}} \phi_n(y) \lambda_n^{3/4}.$$ \hfill (16)

A comparison of the above equation with the microscopic simulation of the system equation (2) in figure 1 shows a very good agreement. The systematic differences are due to finite size effects, as was already noted in [11]. We next consider the steady state current. First, we observe that the fractional Laplacian $\bar{\kappa}$ can be expressed in the form of a divergence, namely in the form $\bar{\kappa} = \bar{\kappa} \partial_y \hat{A}$ where the operator $\hat{A}$ is defined through the following action on Neumann basis vectors

$$\hat{A} | \phi_n \rangle = \lambda_n^{1/4} | \alpha_n \rangle.$$ \hfill (17)

We then see that (10) is in the form of a continuity equation $\partial_y T(y, \tau) = -\partial_y j(y, \tau)$ with the non-local energy current defined as $j(y, \tau) = \bar{\kappa} \hat{A} T(y, \tau)$. Using this definition of the current and the steady state temperature profile in (16) we immediately get the steady state current as
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\[ \frac{\delta T}{\delta T} = \bar{\kappa} A T_{ss}(y) = \frac{\bar{\kappa} c}{2\sqrt{2}}, \]  \hspace{1cm} (18)

where we used the identity \( \sum_{n \in \text{odd}} \alpha_n(y)/\lambda_n = 1/(2\sqrt{2}) \) (appendix C). Note that this gives us the scaled current while the actual current is given by \( J = j/\sqrt{N} \), in agreement with results obtained in [11].

3. Time evolution of temperature profile

The fractional Laplacian equation (10) allow us to study the time evolution of the temperature profile, starting from given initial and boundary conditions, and the eventual approach to the steady state at large times. Here we address the problem of describing the system’s time evolution. As before, the temperature profile at any time \( \tau \) in the form \( T(y, \tau) = T_{ss}(y) + f(y, \tau) \), where again \( f(y, \tau) \) satisfies equation (10) but with vanishing Dirichlet boundary conditions, \( f(0, \tau) = f(1, \tau) = 0 \). Let \( \{\psi_n\} \) be the eigenvectors with corresponding eigenvalues \( \mu_1 < \mu_2 < \mu_3 \ldots \) of \( L \), satisfying the equation

\[ \langle L \psi_n \rangle = \mu_n \langle \psi_n \rangle, \]  \hspace{1cm} (19)

and boundary conditions \( \psi_n(0) = \psi_n(1) = 0 \). It can be shown that the operator \( L \) has a non-degenerate and positive spectrum (see below). We can then immediately write the solution for \( f(y, \tau) \) as

\[ f(y, \tau) = \sum_{n=1}^{\infty} \hat{f}_n(0)e^{-\bar{\kappa} \mu_n \tau} \psi_n(y), \]

where \( \hat{f}_n(0) = \int_0^1 dy f(y, 0) \psi_n(y) \),  \hspace{1cm} (20)

Figure 1. Temperature profile from equation (16) (solid black line) compared with direct numerical simulations of microscopic system for system sizes \( N = 128, 256, 512 \). In the inset the difference between equation (16) and numerical simulations is plotted for various system size.
are ‘fractional-Fourier coefficients’ for the initial field \( f(y, 0) \). In the first section we outlined the procedure followed in [12] to find the Dirichlet eigenfunctions expanding the eigenfunctions \( \psi_n \) in the orthogonal basis of \( \{ \alpha_l \}_{l \geq 1} \) as \( \psi_n(y) = \sum_{l \geq 1} \xi_n \alpha_l(y) \). We show here that much simplification and better accuracy is achieved if one expands \( \psi_n \) directly in the Neumann basis \( \{ \phi_m \}_{m \geq 0} \).

\[
\psi(y) = \sum_m \hat{\chi}_m \phi_m(y). \tag{21}
\]

From equation (19), and using the definition of \( L \) in equation (9), we have

\[
\sum_{m \geq 0} (\mu - \lambda_m^{3/4}) \hat{\chi}_m \phi_m(y) = 0. \tag{22}
\]

There are two sets of solution for this equation. The first set is given by

\[
\hat{\chi}_0 = -\frac{b}{\sqrt{2} \mu}, \quad \hat{\chi}_{2k} = \frac{b}{\lambda_{2k}^{3/4} - \mu}, \quad k \geq 1, \quad \hat{\chi}_{2k+1} = 0, \quad k \geq 0, \tag{23}
\]

where we have made use of the identity \( \sum_{m=1}^{\infty} \phi_{2m}(x) = -1/\sqrt{2} \). The second solution set is given by

\[
\hat{\chi}_{2k+1} = \frac{b}{\lambda_{2k+1}^{3/4} - \mu}, \quad k \geq 0, \quad \hat{\chi}_{2k} = 0, \quad k \geq 0, \tag{24}
\]

where we have used the identity \( \sum_{m=0}^{\infty} \phi_{2m+1}(y) = 0 \) (appendix C). So far, \( b \) and \( \mu \) are un-determined. We now use the Dirichlet boundary condition \( \psi(0) = \hat{\chi}_0 + \sqrt{2} \sum_{k \geq 1} \hat{\chi}_{2k} + \sum_{k \geq 0} \hat{\chi}_{2k+1} = 0 \). From our first solution set equation (23) we then get the following equation satisfied by \( \mu \)

\[
\sum_{k \geq 1} \frac{1}{\lambda_{2k}^{3/4} - \mu} = \frac{1}{2 \mu}. \tag{25}
\]

Similarly, from the second solution set equation (24), we get

\[
\sum_{k \geq 0} \frac{1}{\lambda_{2k+1}^{3/4} - \mu} = 0. \tag{26}
\]

The solution of either of the above two equations gives us the required eigenvalue, while equations (23) and (24) provide us with the corresponding eigenfunction, with the constant \( b \) fixed by normalization. We label the first set of solutions by \( \mu_{2n+1}, \psi_{2n+1}, n \geq 0 \) and the second set by \( \mu_{2n}, \psi_{2n+2}, n \geq 0 \). From the structure of the eigenvalue equations it is clear that the roots are ordered set of numbers such that \( \lambda_{2n}^{3/4} < \mu_{2n+1} < \lambda_{2n+2}^{3/4} \) and \( \lambda_{2n-1}^{3/4} < \mu_{2n} < \lambda_{2n+1}^{3/4} \). Finally, using the notation, \( \langle f | g \rangle = \int_0^1 dx' f(x') g(x') \), such that \( \langle x | \psi_n \rangle = \int_0^1 dx \delta(x - x') \psi_n(x') = \psi_n(x) \), the eigenvectors can now be written explicitly as

\[
| \psi_{2n+1} \rangle = D_{2n+1} \left(-\frac{1}{\sqrt{2} \mu_{2n+1}} | \phi_0 \rangle + \sum_{m \geq 1} \frac{1}{\lambda_{2m}^{3/4} - \mu_{2n+1}} | \phi_{2m} \rangle \right), \tag{27}
\]

https://doi.org/10.1088/1742-5468/aaf630


\[ | \psi_{2n+2} \rangle = D_{2n+2} \left( \sum_{m \geq 0} \frac{1}{\lambda_{2m+1}^{3/4} - \mu_{2n+2}} | \phi_{2m+1} \rangle \right), \]

where \( D_n \), found from the normalizing condition \( \langle \psi_n | \psi_n \rangle = 1 \), is explicitly given as,

\[
D_{2n+1} = \left[ \frac{1}{2\mu_{2n+1}^2} + \sum_{m \geq 1} \frac{1}{(\lambda_{2m}^{3/4} - \mu_{2n+1})^2} \right]^{-1/2},
\]

\[
D_{2n+2} = \left[ \sum_{m \geq 0} \frac{1}{(\lambda_{2m+1}^{3/4} - \mu_{2n+2})^2} \right]^{-1/2}.
\]

Thus, as promised, we have managed to obtain a much efficient method for computing the Dirichlet spectrum of the fractional operator \( L \). The roots of the eigenvalue equations (25) and (26) are solved numerically using Newton–Raphson method scanning in between these intervals. This procedure gives a fast and efficient way to compute the eigenvector while avoiding diagonalizing infinite dimensional matrices. For large \( k \), we have, \( \mu_k \approx \lambda_k^{3/4} \).

This procedure can be generalized to a fractional operator defined through the equation

\[ L^{(\beta)} | \phi_n \rangle = \lambda_n^{\beta} | \phi_n \rangle, \]

for arbitrary \( \beta \). For diffusive case (\( \beta = 1 \)) one can obtain exact results and recover the expected result \( \mu_k^{(\beta=1)} = \pi^2 k^2 \) and \( \psi_k(y) = \alpha_k(y) \).

### 3.1. Properties of Dirichlet eigensystem of the fractional operator in bounded domain

The numerical values of the computed eigenvalues are plotted in figure 2 in log–log scale, where we find that for large \( n \) \( \mu_n \approx (n\pi)^{3/2} \), while for smaller values \( n \), there is a systematic deviation from the scaling due to the fact we are now working in a bounded domain. The first three eigenvalues \( (\mu_n) \) are approximately \( \mu_1 \approx 2.75, \mu_2 \approx 12.02, \mu_3 \approx 24.22 \). The first eigenvalue we have \( |\mu_1 - \pi^{3/2}|/\pi^{3/2} \approx 0.5046 \) (see inset in figure 2). This eigenvalue spectrum is expected to be identical to that in [12], up to a constant factor (see discussion in the previous section). The first few numerically computed eigenvectors are shown in figure 3. The eigenvectors are similar to sin functions but have divergent derivatives near the left and right boundaries. In order to compare it with corresponding sin functions, we plot in figure 4 the overlap of integral between \( \psi_n(y) \) and \( \sqrt{2} \sin(n\pi y) \) defined as \( I_n = 1 - \int_0^1 \psi_n(y) \sqrt{2} \sin(n\pi y) \, dy \). This increases and saturates to a particular value, suggesting that the wave functions are quite different from sin functions even for large \( n \). Also the eigenfunctions show a non-analytic behavior at the boundaries, for example near the left boundary one finds \( \lim_{y \to 0^+} \psi_n(y) \sim \sqrt{y} \) (see figure 4(b)), in contrast to sin-functions for which \( \lim_{y \to 0^+} \sin(n\pi y) \sim y \).

The eigenspectrum of fractional operator in bounded domain has been discussed earlier in the literature, using somewhat phenomenological approaches [18, 23–25]. It is not clear if those approaches can be related to that presented in this paper.

https://doi.org/10.1088/1742-5468/aaf630
3.2. Comparison of time evolution formula with numerical simulations of the HCME model

We now compare the prediction from equation (20), with \( \tilde{\kappa} = 1/(2\sqrt{2}) \), with results from direct microscopic simulations, described by equation (2) with the additional
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stochastic exchange dynamics. Initially the system of size $N$ is prepared in a step initial condition, given by

$$T_i = T_L, \ 1 \leq i < N/2,  
\quad = T_R, \ N/2 \leq i \leq N + 1. \quad (31)$$

At large times it reaches a steady state described by equation (16). At various intermediate times, we plot the function $\Theta(y, \tau) = T(y, \tau) - Tss(y) + f(y, \tau) - T$, such that $\Theta(0, \tau) = 1/2 = -\Theta(1, \tau)$. In figure 5 we show the temperature profile at intermediate times from microscopic simulation with scaled space ($y = i/N$) and times ($\tau = t/N^{3/2}$) for various system sizes. We note that with increasing system size, the data converges to the prediction from equation (20). The difference between the numerical profiles and the predicted theoretical profile is shown in the inset. As we increase the system size, this difference systematically decreases. We also demonstrate that using standard Dirichlet $\sin$-functions, instead of the $\psi$-functions, leads to significant differences, especially near the boundaries.

4. Adding noise satisfying fluctuation dissipation to describe equilibrium fluctuations in finite system

In [21], the harmonic chain with random momentum flips (HCMF model) was studied. In the HCMF, the stochastic dynamics flips the momentum of the particle and is embedded in the Hamiltonian dynamics such that the macroscopic dynamics is diffusive. It was shown that the equilibrium energy fluctuations $\epsilon(x, t) = E(x, t) - \langle E(x, t) \rangle$, where $E(x, t)$ is the local energy of the system at time $t$, satisfies the noisy diffusion equation

$$\partial_\tau \epsilon(x, t) = \partial_x^2 \epsilon(x, t) + \partial_x (DT(x, t) \eta(x, t)),$$

with $\eta$ a space-time mean zero white noise. The aim of this section is to establish a fractional fluctuating equation for the
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The HCME model, which has anomalous diffusion properties. Using this equation, we establish a Green–Kubo formula relating the equilibrium current fluctuations to the non-equilibrium current. Next, we discuss the long-range correlations and conjecture a form for the long-range correlations of energy and test it using simulations.

The generalized equation, which we hypothesize in equilibrium at temperature $T$ is

$$\partial_t | e_t \rangle = -\mathbb{L}_\kappa | e_t \rangle + \sqrt{2 \kappa} \nabla (B T | \eta_t \rangle),$$  

(32)

where $\eta(x, t)$ is a white Gaussian noise with $\langle \eta(x) \rangle = 0, \langle \eta(x, t) \eta(y, t') \rangle = \delta(x - y) \delta(t - t')$ and $\mathbb{L}_\kappa$ is the fractional Laplacian as defined in equation (11). The explicit form for the operator $B B^1$ is established through the requirement that energy fluctuations must respect the fluctuation dissipation (FD) in equilibrium. We define the Green function satisfying

$$\partial_t G_t = -\mathbb{L}_\kappa G_t, \quad \langle x | G_0 | x' \rangle = G_0^{xx'} = \delta(x - x'),$$  

(33)

with Dirichlet boundary conditions in $x \in [0, 1]$. This can then be easily expressed in terms of the basis states $\{ \psi_n \}_{n \geq 1}$ as $G_t^{xx'} = \sum_{n=1}^{\infty} \psi_n(x) \psi_n(x') e^{-\kappa \lambda_n^3 t}$. The long-time solution to equation (32) is then given by

$$e(x, t) = \sqrt{2 \kappa} \int_{-\infty}^{t} ds \langle x | G_{t-s} | \nabla (B T \eta_s) \rangle,$$

$$= -\sqrt{2 \kappa} \int_{-\infty}^{t} ds \langle x | \nabla G_{t-s} | (B T \eta_s) \rangle.$$

(34)

The equal time correlation function in equilibrium defined as $C_{eq}(x, y) = \langle e(x, t) e(y, t) \rangle$ then is given as

Figure 5. The time evolution of temperature starting from an initial step profile. The function $\Theta(y, \tau) = T(y, \tau) - T = T_m(y) + f(y, \tau) - T$ is plotted and compared with numerical simulations. In the left figure, dashed lines indicate simulation results for the time-evolution, for system sizes $N = 128$ (red), $N = 256$ (blue), $N = 512$ (magenta). The solid lines at different scaled times ($\tau$) are generated from equation (20) by summing over 600 basis states. (right) The same, but now with the theoretical curves computed using the sin-functions instead of the $\psi$-functions, and eigenvalues $\lambda_n^{3/4}$ instead of $\mu_n$. We notice that they do not match well with simulations, specially the deviations are prominent near the two boundary.

https://doi.org/10.1088/1742-5468/aaf630
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\[
C_{eq}(x, y) = 2\kappa \int_{-\infty}^{t} ds \int_{-\infty}^{t} ds' \langle \left. x \mid \nabla G_{t-s} \right| BT\eta \rangle \langle \eta_s \nabla G_{t-s'} \mid y \rangle,
\]

\[
= 2\kappa T^2 \int_{-\infty}^{t} ds \langle \left. x \mid \nabla G_{t-s} BB^\dagger \nabla G_{t-s} \right| y \rangle,
\]

\[
= -2\kappa T^2 \int_{-\infty}^{t} ds \langle \left. x \mid G_{t-s} \nabla BB^\dagger \nabla G_{t-s} \right| y \rangle,
\]

(35)

where the statistical average is used and we integrate out the space time white noise to give \( \langle \left. x' \right| BT\eta \rangle \langle \eta \nabla B \mid y' \rangle = \langle B\eta(s)B\eta(s') \rangle = \delta(s-s')BB^\dagger(x', y') \) followed by an integration by parts. Here, the big angular brackets, \( \langle \ldots \rangle \) denote average over space-time white noise profiles whereas \( \langle .. \rangle \) and \( \langle .. \rangle \) denote the bra-ket notation, e.g. \( \langle x|e \rangle = e(x, t) \). If we identify \(-\kappa \nabla BB^\dagger \nabla = L_{\kappa}\), and using equation (33) we recover FD relation in equilibrium

\[
C_{eq}(x, y) = T^2 \int_{-\infty}^{t} ds \langle \left. x \mid G_{t-s} \nabla \nabla G_{t-s} \right| y \rangle + \langle y \mid G_{t-s} \nabla \nabla G_{t-s} \mid x \rangle,
\]

\[
= T^2 \int_{-\infty}^{t} ds \partial_s \langle \left. x \mid G_{t-s} \nabla \nabla G_{t-s} \right| y \rangle = T^2 \delta(x-y),
\]

(36)

where we used the fact that changing \( x \leftrightarrow y \) would not change the correlation function due to time reversal symmetry of the microscopic dynamics. The operator \( BB^\dagger \) can consistently be defined on a function \( g(x) \), expanded in \( \{\alpha_n\}_{n \geq 1} \) basis, as \( g(x) = \sum_n \hat{g}_n \alpha_n(x) \). Again, using the definition of \( L_{\kappa} = -\kappa \nabla BB^\dagger \nabla \) in equation (9), we define the symmetric operator \( BB^\dagger \) as,

\[
\int_0^1 dx' BB^\dagger(x, x')g(x') = \sum_{n=1}^{\infty} \frac{1}{(\lambda_n)^{1/4}} \hat{g}_n \alpha_n(x).
\]

(37)

Note that we do not assume anything about the form of the operator \( B \), which would be important if we were to study non-equilibrium phenomena where temperature is not constant in space.

The connection between the \( \nabla \) operator with the \( BB^\dagger \) allows one to identify the current (through continuity equation) as

\[
j(x, t) = -\kappa \int_0^1 dx' BB^\dagger(x, x')\partial_x e(x', t).
\]

Note that the above equation is a linear response relation, but in contrast to the diffusive case, this relation is non-local. Such non-local linear response relations have recently been reported in [20], where an alternate series representation of the kernel \( BB^\dagger(x, x') \) has been provided for HCME model with general boundary conditions. In appendix D, we show that the spectral representation in equation (37) is completely consistent with the series representation in [20] for fixed boundary condition.
4.1. Spatio-temporal equilibrium energy correlations

We compute the two time spatio-temporal energy correlations in equilibrium defined as
\[ C_{eq}(x, t, y, t') = \langle e(x, t)e(y, t') \rangle \] and show that at large times it is given in terms of the Green functions. The two time correlations can be analogously written down as,
\[ C_{eq}(x, t, y, t') = 2\bar{\kappa} \int_{-\infty}^{t} ds \int_{-\infty}^{t'} ds' \langle x | \nabla G_{t-s} | BT\eta_s \rangle \langle \eta_{s'}TB^\dagger | \nabla G_{t'-s'} | y \rangle. \]

Taking \( t > t' \), and performing the \( s' \) integral we have,
\[ C_{eq}(x, t, y, t') = -2\bar{\kappa}T^{2} \int_{-\infty}^{t} ds \langle x | G_{t-s} \nabla BB^\dagger \nabla G_{v-s} | y \rangle \theta(t - t'), \]
where \( \theta(t) \) is the Heaviside theta function. Proceeding as before and identifying \(-\bar{\kappa} \nabla BB^\dagger \nabla = L_{\bar{\kappa}}\) and interchanging \( x, y \)
\[ C_{eq}(x, t, y, t') = T^{2} \int_{-\infty}^{t'} ds \langle x | G_{t-s}L_{\bar{\kappa}}G_{v-s} | y \rangle + \langle y | G_{t-s}L_{\bar{\kappa}}G_{v-s} | x \rangle, \]
\[ = T^{2} \int_{-\infty}^{t'} ds \partial_s \langle x | G_{t-s}G_{v-s} | y \rangle = T^{2}G_{t-v}^{\tau y}(t - t'). \]

Along with a similar term for \( t < t' \), we can write the two time correlations as,
\[ C_{eq}(x, t, y, t') = \langle x | T^{2}G_{t-v}^\tau \theta(t - t') + T^{2}G_{t-v}^\tau \theta(t' - t) | y \rangle. \]

4.2. Current fluctuations in equilibrium

Here we define the fluctuating current in the system and then establish Green–Kubo relation for the system connecting the equilibrium current fluctuations and non-equilibrium current in the system. We expect that since the total energy in the isolated system is conserved, the energy flow across the system must be in continuity form \( \partial_t \epsilon(x, t) + \partial_x j(x, t) = 0 \). Along with the definition of current in equation (17), the fluctuating current operator is defined as,
\[ | j_t \rangle = \bar{\kappa}A | e_t \rangle - \sqrt{2\bar{\kappa}} | BT\eta_t \rangle. \]

From the previous section, it follows that the definition of current operator as \( A = -BB^\dagger \nabla \). We also note that since the current operator is odd in derivatives, the adjoint current operator has the property, \( A^\dagger = -A \). Now we expect that [26] the second moment of equilibrium total current fluctuations is related to the current in NESS through the Green–Kubo formula. A precise statement is:
\[ \lim_{\tau \to \infty} \frac{q(\tau)^2}{2\tau T^2} = \lim_{\tau \to 0} \frac{\langle j \rangle}{\delta(T)}, \]

where \( q(\tau) = \int_0^\tau dt \int_0^1 dx j(x, t) \). In order to verify this relation, we first express \( \langle q^2 \rangle \), in terms of the integrals of the unequal time current correlations:
\begin{equation}
\frac{\langle q^2 \rangle_{\tau=0}}{\tau} = \frac{1}{\tau} \int_{0}^{\tau} dt \int_{0}^{r} dt' \int_{0}^{1} dx \int_{0}^{1} dy \langle j(x, t) j(y, t') \rangle. \tag{43}
\end{equation}

Using equation (41) the current correlations can be split into four parts:
\begin{align*}
\langle j(x, t) j(y, t') \rangle &= \bar{\kappa}^2 \left( \langle x | \mathbb{A} | e_t \rangle \langle e_{t'} | \mathbb{A}^\dagger | y \rangle \right) + 2\bar{\kappa} T^2 \langle x | \mathbb{B} \mathbb{B}^\dagger | y \rangle \delta(t-t') \\
&\quad - \sqrt{2}\bar{\kappa}^{3/2} \left( \langle x | \mathbb{A} | e_t \rangle \langle \eta \mathbb{TB}^\dagger | y \rangle \right) + \sqrt{2}\bar{\kappa}^{3/2} \left( \langle x | \eta \mathbb{TB}^\dagger | y \rangle \right). \tag{44}
\end{align*}

Part III in the above equation can be simplified to
\begin{align*}
\sqrt{2}\bar{\kappa}^{3/2} \left\langle x | \mathbb{A} | e_t \rangle \langle \eta \mathbb{TB}^\dagger | y \rangle \right\rangle &= 2\bar{\kappa} T^2 \int_{-\infty}^{t} ds \langle x | \mathbb{G}_{t-s} | \nabla (\eta \mathbb{TB}) \rangle \langle \eta \mathbb{TB}^\dagger | y \rangle, \\
&= -T^2 2\bar{\kappa}^2 \langle x | (\mathbb{A} \nabla \mathbb{G}) \mathbb{B} \mathbb{B}^\dagger | y \rangle \theta(t-t'), \\
&= T^2 2\bar{\kappa}^2 \langle x | \mathbb{A} \mathbb{G} \mathbb{A}^\dagger | y \rangle \theta(t-t'). \tag{45}
\end{align*}

Similarly part IV is given by
\begin{align*}
\sqrt{2}\bar{\kappa}^{3/2} \left\langle x | \mathbb{B} \mathbb{G} \mathbb{B}^\dagger | y \rangle \right\rangle &= 2\bar{\kappa} T^2 \int_{-\infty}^{t} ds \langle x | \mathbb{B} \eta \mathbb{G}_{t-s} \rangle \langle \mathbb{G}_{t-s} \mathbb{A}^\dagger | y \rangle, \\
&= -T^2 2\bar{\kappa}^2 \langle x | \mathbb{B} \mathbb{B}^\dagger \nabla \mathbb{G} \mathbb{A}^\dagger | y \rangle \theta(t-t'), \\
&= T^2 2\bar{\kappa}^2 \langle x | \mathbb{A} \mathbb{G} \mathbb{A}^\dagger | y \rangle \theta(t-t'),
\end{align*}

while part I, on using (40), gives
\begin{equation}
\bar{\kappa}^2 \langle x | \mathbb{A} | e_t \rangle \langle e_{t'} | \mathbb{A}^\dagger | y \rangle = T^2 \bar{\kappa}^2 \left[ \langle x | \mathbb{A} \mathbb{G} \mathbb{A}^\dagger \theta(t-t') + \mathbb{A} \mathbb{G} \mathbb{A}^\dagger \theta(t'-t) | y \rangle \right]. \tag{46}
\end{equation}

We see that III + IV = 2I. The first term explicitly gives,
\begin{align*}
I &= \bar{\kappa}^2 \int_{0}^{1} dx' \int_{0}^{1} dy' \delta(x, x') \langle e_t(x') e_{t'}(y') \rangle \mathbb{A}^\dagger (y', y), \\
&= \bar{\kappa}^2 T^2 \int_{0}^{1} dx' \int_{0}^{1} dy' \delta(x, x') \mathbb{A}(y, y') \mathbb{G}_{t-t'}(x', y'), \\
&= \bar{\kappa}^2 T^2 \sum_{n,l,l'} \hat{\chi}_{nl} \hat{\chi}_{nl'} (\lambda_l \lambda_{l'})^{1/4} e^{-\bar{\kappa} \mu_n |l-t'|} \alpha_l(x) \alpha_{l'}(y). \tag{47}
\end{align*}

Therefore, the contribution of the parts I − III − IV = −I in (43) gives, after doing the space and time integrals:
\begin{equation}
\int_{0}^{r} dt' \int_{0}^{r} dt \int_{0}^{1} dx \int_{0}^{1} dy (-1) = -16\bar{\kappa}^2 T^2 \sum_{n} \sum_{l' \text{ odd}} \frac{1}{\bar{\kappa} \mu_n} \left[ \tau + \frac{(e^{-\mu_n \tau} - 1)}{\mu_n} \right] \hat{\chi}_{nl} \hat{\chi}_{nl'} (\lambda_l \lambda_{l'})^{1/4}. \tag{48}
\end{equation}

On using (37), the contribution of part II in (43) gives
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\[ \int_0^\tau dt' \int_0^\tau dt \int_0^1 dx \int_0^1 dy (\Pi) = 2\bar{\kappa}T^2 \int_0^\tau dt' \int_0^\tau dt \int_0^1 dx \int_0^1 dy B B^\dagger (x, y) \delta (t - t'), \]

\[ = 2\bar{\kappa}T^2 \tau \int_0^1 dx \int_0^1 dy \sum_n \frac{\alpha_n (x) \alpha_n (y)}{\lambda_n^{1/4}}, \]

\[ = 16\bar{\kappa}T^2 \tau \sum_{n \text{ odd}} \frac{1}{\lambda_n^{5/4}}. \] (49)

Combining the above results we finally have

\[ \lim_{\tau \to \infty} \frac{\langle q^2 \rangle_{\delta T = 0}}{2\tau T^2} = \bar{\kappa} \left( 8 \sum_{n \text{ odd}} \frac{1}{\lambda_n^{5/4}} - \sum_n \sum_{l' \text{ odd}} \frac{8}{\mu_n (\lambda_l \lambda_{l'})^{1/4}} \right). \] (50)

The first summation yields 0.5050... and the second yields \( \approx 0.0931 \), hence we get

\[ \lim_{\tau \to \infty} \frac{\langle q^2 \rangle_{\delta T = 0}}{2T^2} \approx 0.4119\bar{\kappa}, \] (51)

which, up to numerical accuracy is consistent with the numerical value of steady state current (\( j/\delta T = 0.4124\bar{\kappa} \)) we found in (18), thus validating the Green–Kubo formula in (42).

Note that in order to get the expected scaling in system size \( N \), we need to put in the appropriate length scaling of the eigenvalues and eigenfunctions, for example \( \lambda_n \to \lambda_n/N^2 \) and \( \mu_n \to \mu_n/N^{3/2} \). We also need to consider the integrated

\[ \text{Figure 6. For the microscopic HCME model, we compute the two quantities, } J/\delta T \text{ computed from non-equilibrium simulations connected to heat baths and } \langle Q^2 \rangle/(2\tau T^2) \text{ computed from equilibrium simulations, are plotted as a function of } N. \text{ The black dashed curve is for the theoretical current with appropriate scaling as given in equation (18). We find that for small } N, \text{ these two do not match, and the difference between the two decays as } 1/N \text{ (inset), which is due to the contribution of current from the stochastic part. This signifies that at large } N, \text{ Green–Kubo holds while for small } N, \text{ it fails.} \]
current $Q(\tau) = \int_0^\tau dt \int_0^N dx \dot{j}(x, t)$ and then one gets $\lim_{\tau \to \infty} (Q^2)_{\delta T=0} = \frac{1}{2T^2} \approx 0.4119$ and $\frac{\dot{j}}{\delta T} = \frac{1}{\sqrt{N} \delta T} \approx 0.4124$.

The above verification of the Green–Kubo identity was obtained using the fluctuating fractional diffusion equation, which is valid in the limit of large system size. A natural question is as to whether the identity is true even for a small chain with the microscopic dynamics (HCME), as would be expected from the fluctuation theorem. In figure 6, we present a numerical comparison of the equilibrium current fluctuations, with the non-equilibrium current, both computed from the microscopic model for finite systems. We see clear evidence that for small $N$, the Green–Kubo relation is violated in the HCME model. We also find that the difference between the fluctuation and response parts decreases with system size as $\sim 1/N$. Somewhat surprisingly, the numerically obtained fluctuations (from HCME simulations) are very close to the response computed from the fractional diffusion equation description. A possible reason for the failure of fluctuation theorem for small systems could be that in this model, the Hamiltonian part of current ($J_{\text{ham}} = \frac{1}{2} (p_{i+1} + p_i)(q_i - q_{i+1})$) and the stochastic part of the current ($J_{\text{stochastic}} = \frac{\Gamma}{2} (p_i^2 - p_{i+1}^2)$, where $\Gamma$ is a Poisson process.) have different time reversal symmetries. In fact, at large system size this leads to the current decay of the Hamiltonian part as $1/\sqrt{N}$, while the decay of stochastic part goes as $\sim 1/N$.

### 4.3. General fractional power

In this section, we discuss a possible generalization of the results of the previous section for the Green–Kubo identity to the case of arbitrary fractional power $\beta$ of the Laplacian. There is currently no microscopic model in which heat transfer can be described by a fractional equation with arbitrary $\beta$—nevertheless it is an interesting exercise as it leads to some general mathematical identities involving Riemann-zeta functions. Using the definition of fractional Laplacian in equation (30), namely through the operation $L(\beta) \phi_n(x) = \lambda_n^\beta \phi_n(x)$, we can proceed in a similar way as for the $\beta = 3/4$ case and compute steady state properties in NESS as well as equilibrium current fluctuations.

Corresponding to equation (18) we then get
\begin{equation}
\frac{\dot{j}}{\delta T} = \frac{1}{8 (2^{2\beta} - 1)(2\pi)^{2\beta} \zeta(2\beta)},
\end{equation}
and corresponding to equation (50) we get
\begin{equation}
\lim_{\tau \to \infty} \frac{(q^2)_{\delta T=0}}{2T^2} = 8 \left(1 - 2^{2\beta-4}\right) \pi^{2\beta-4} \zeta(4 - 2\beta) - \sum_{n \text{ even}} \sum_{l' \text{ odd}} \frac{8}{\mu_n^{2\beta}} \hat{\chi}_{nl}^{(\beta)} \hat{\chi}_{nl'}^{(\beta)} (l \lambda_{l'}^{(\beta)})^{1-\beta},
\end{equation}
where due to structure of $\hat{\chi}_{nl}^{(\beta)}$, only the terms with even $n$ survives for odd $l$. This is computed as before but now with power $\beta$ and is explicitly given as
\begin{equation}
\hat{\chi}_{2k+1,2m+1}^{(\beta)} = \frac{D_{2k+2}^{(\beta)}}{\lambda_{2m+1}^{\beta} - \mu_{2k+2}^{(\beta)}}, \quad k, m \geq 0,
\end{equation}

https://doi.org/10.1088/1742-5468/aaf630
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where

\[ D_{2k+2}^{(\beta)} = \left[ \sum_{m \geq 0} \frac{1}{(\lambda_{2m+1}^{\beta} - \mu_{2k+2}^{(\beta)})^2} \right]^{-1/2} \]  \tag{55} 

and \( \{\mu_{2n}^{(\beta)}\}_{n \geq 1} \) are the ordered roots of the equation

\[ \sum_{k \geq 0} \frac{1}{\lambda_{2k+1}^{\beta} - \mu^{(\beta)}} = 0. \]  \tag{56} 

All the coefficients in the above expressions are explicit and we have evaluated numerically the right hand sides of equations (52) and (53) for values of \( \beta \in (0.5, 1.5) \). In figure 7, we plot these quantities and find that they are very close to each other, hence verifying the Green–Kubo formula equation (42) for general \( \beta \). The differences arise from numerical error due to truncation of series and also use of a finite number of basis functions. For \( \beta = 1 \), this leads to diffusive results for which the double summation can be computed explicitly. Conversely, on the basis of the validity of the Green–Kubo formula we are then led to conjecture a mathematical identity between the right hand sides of equations (52) and (53). For \( \beta < 1/2 \), one has a non-convergent series summation in equation (53), which leads to a breakdown of the identity in this form. This corresponds to defining zeta function for power less than 1, and possibly analytic continuation could extend the definition to other values of \( \beta \). We believe that the relation holds true at least in the open interval \( \beta \in (1/2, 3/2) \). However, proving it remains an open problem.

Figure 7. The numerically evaluated expressions in equations (52) and (53) are plotted as a function of general fractional power \( \beta \). The two quantities match numerically to a very good precision. The relative error between the two is plotted in the inset.

https://doi.org/10.1088/1742-5468/aaf630
4.4. Long range correlations in NESS

For a non-equilibrium current carrying steady state, it is expected that fluctuations across the system will develop non-zero long-range correlations. These long-range correlations is a distinguishing feature of non-equilibrium systems with conservative dynamics [27]. In some diffusive lattice gas as well as some Hamiltonian systems, these long-range correlations have been studied [21, 28–31]. The energy correlation in the velocity flip model (HCMF) in NESS is defined as $C_{NESS}(x, y) = \langle e(x, t) e(y, t) \rangle$, where the average is taken in NESS (as $t \to \infty$). It was shown that $C_{NESS}(x, y) = \delta T^2 \Delta^{-1}(x, y)$, where $\Delta$ is the Laplacian operator with Dirichlet boundary conditions. From the definition of fluctuating fractional equation to non-equilibrium case, it is tempting to extend the definition of fluctuating fractional equation to non-equilibrium case, where the temperature is space-dependent:

$$\partial_t | e_t \rangle = -L \delta \langle e_t \rangle + \sqrt{2\kappa} \nabla (BT_{NESS}) | \eta_t \rangle. \quad (57)$$

We note that there is an ambiguity regarding the relative position of the operator $B$ and $T_{NESS}$, and also with the definition for operator $B$ and $B^\dagger$ separately. If we anyway proceed with a naive replacement of $T$ by $T_{NESS}(x)$ in equation (32), to get (57), we can perform the computation of $C_{NESS}(x, y)$ and find that this does not agree with the results from direct simulations. However, in analogy to the HCMF model, we conjecture that the NESS energy correlations $C_{NESS}(x, y)$ are given (upto a constant factor $\nu$) by the inverse of the fractional Laplacian (in Dirichlet basis):

$$\delta T^2 C(x, y) = \frac{\delta T^2}{\nu} \xi^{-1} = \frac{\delta T^2}{\nu} \sum_{n \geq 1} \psi_n(x) \psi_n(y) \mu_n, \quad (58)$$

where we have defined $\delta T^2 C(x, y) = C_{NESS}(x, y) - T_{NESS}(x)^2 \delta(x - y)$, with the local same-site correlation $T_{NESS}(x)^2 \delta(x - y)$ subtracted from correlations.

**Numerical verification of equation (58):** We simulate the microscopic system in non-equilibrium with two Langevin heat baths kept at different temperature. After the system is in the steady state, we compute $C(x, y) = N \langle e(i/N)e(j/N) \rangle$, where $e(i/N) = E(i/N) - \langle E(i/N) \rangle$. In figure 8 we compare our conjectured form from equation (58) with the results from microscopic simulations. We see that with the constant $\nu \approx 3.77$, the two numerical curves (for $y = 1/4$ and $y = 1/2$) match well with the inverse of fractional Laplacian. The constant $\nu$ is related to the total energy fluctuations in the system at NESS as

$$\int_0^1 dx \int_0^1 dy \frac{\delta T^2}{\nu} \Sigma^{-1}(x, y) + \int_0^1 dx T_{NESS}^2(x) = \int_0^1 dx \int_0^1 dy C_{NESS}(x, y) = \langle \Delta E^2_{tot} \rangle_{NESS}.$$

By evaluating the integrals on the LHS and finding the RHS from numerical simulations in the NESS, we can use the above equation to independently evaluate $\nu$. We find that the fluctuations $\langle \Delta E^2_{tot} \rangle_{NESS}$ obtained from simulations in NESS, converges very slowly and with the final accessed simulation time ($2 \times 10^9$ time with $10^6$ samples) we estimate $3.51 \leq \nu \leq 4.2$. The value $\nu \approx 3.77$, obtained by fitting the long range correlations data from simulation, is well within the limits of the above estimate. We have tested (see appendix F) that the constant $\nu$ does not change substantially with $\delta T$.
and \( \bar{T} \), within the numerical accuracy and finite size effects. We note in appendix F, that if we did the same computation with \( \sin(n\pi x) \) basis, then the results would differ significantly. We close this section by making a comment that proving our conjecture on the equality between the long-range correlations and the inverse fractional operator is an open question.

5. Conclusions

We have shown that in a particular analytically tractable model of heat conduction in one dimension, the macroscopic evolution of energy in an open system is governed by the fractional diffusion equation. This gives us a definition of the fractional operator in a finite domain and also gives a meaning to the fractional operator in terms of linear PDE’s (similar to the harmonic extension of a fractional operator). We describe an efficient procedure to numerically construct the eigenspectrum of this operator. In terms of this operator, we compute the steady state and time evolution of temperature field, which we compare with microscopic simulations of the system. We defined the fluctuating fractional equation and used it to verify the Green–Kubo relation in the system. We also generalize the Green–Kubo for general fractional power which leads to some general mathematical identity involving zeta functions. This identity is verified numerically. We also conjecture that the long-range correlations are given by the inverse of a fractional operator. Proving this conjecture in equation (58), as well as finding the correct equation to replace equation (57) are open problems. The other interesting question would be to consider the use of the fractional operator in studying the dynamics of other Hamiltonian systems such as the FPUT model and also the HCME model with other boundary conditions. Another very interesting aspect is to study the usefulness of the eigensystem of the fractional operators in studying other

Figure 8. Non-equilibrium energy correlation function \( \mathcal{C}(x, y) \) in steady state of Harmonic chain momentum exchange model for \( y = 1/4 \) (left figure) and \( y = 1/2 \) (right figure). The system size considered here are for \( N = 128, 256 \) with \( T_L = 2, T_R = 1 \). The inverse of the fractional Laplacian (summed up to 600 basis states) and with an arbitrary constant factor (\( \nu = 3.77 \)), is plotted (black solid) along with the simulation results.

https://doi.org/10.1088/1742-5468/aaf630
applications where the underlying dynamics can be modelled as Levy flights or Levy walks.

Acknowledgments

The authors are very grateful to G Basile, T Komorowski and S Olla to send them their unpublished notes [19] on which a part of this work is based. Aritra Kundu would like to thank the hospitality of Nice Sophia-Antipolis University Laboratoire Dieudonné and Institut Henri Poincaré—Centre Emile Borel during the trimester ‘Stochastic Dynamics Out of Equilibrium’ where part of the work was done. This work benefited from the support of the project EDNHS ANR-14-CE25-0011 of the French National Research Agency (ANR), and also in part by the International Centre for Theoretical Sciences (ICTS) during a visit for participating in the program Non-equilibrium statistical physics (Code: ICTS/Prog-NESP/2015/10). Cédric Bernardin thanks the French National Research Agency (ANR) for its support through the grant ANR-15-CE40-0020-01 (LSD) and the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovative programme (grant agreement No 715734). Anupam Kundu (AK) would like to acknowledge the support from DST grant under project No. ECR/2017/000634. AK, AD and CB would like to acknowledge the support from the project 5604-2 of the Indo-French Centre for the Promotion of Advanced Research (IFCPAR). KS was supported by JSPS Grants-in-Aid for Scientific Research (JP16H02211 and JP17K05587).

Appendix A. Connection coefficients between sine and cosine

We can expand sin in the complete basis of cos as, $\alpha_n(y) = \sum_l T_{nl} \phi_l(y)$, with explicit coefficients $T_{nl} = \int_0^1 dy \alpha_n(y) \phi_l(y)$. The coefficients are given as,

$$T_{nl} = \begin{cases} 0 & \text{if } l = 0, n \text{ is even}, \\ \frac{2\sqrt{2}}{\pi n} & \text{if } l = 0, n \text{ is odd}, \\ \frac{2}{\pi} \left( \frac{\delta(n+l)_{\text{odd}}}{n+l} + \frac{\delta(n-l)_{\text{odd}}}{n-l} \right) & \text{if } l > 0. \end{cases} \tag{A.1}$$

Appendix B. Derivation of matrix equations of fractional operator

Here we enumerate the steps involved in going from the set of PDE’s to the matrix representation of $L$ as stated in the main text. The correlation and temperature fields are expanded as, $C(u, y, \tau) - C_{ss}(u, y) = \sum_{n=1}^{\infty} \hat{C}_n(u, \tau) \alpha_n(y)$ and $T(y, \tau) - T_{ss}(y) = f(y, \tau) = \sum_{n=1}^{\infty} \hat{T}_n(\tau) \alpha_n(y)$. Following [12], the first of the equations in (3) implies $\partial_{\delta_n} \hat{C}_n(u) = -4\delta_n \hat{T}_n(u)$, where $\delta_n = \sqrt{n\pi \omega/(2\gamma)}$. Solving these equations with the appropriate boundary conditions one eventually gets,

$$\hat{C}_n(u, \tau) = \hat{A}_n(\tau) e^{-\delta_n u} \left[ \sin(\delta_n u) - \cos(\delta_n u) \right], \tag{B.1}$$

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using the PDE’s one gets

\[ \dot{A}_n(\tau) = -\frac{1}{4\gamma_n} \sum_{k=1}^{\infty} T^\dagger_{kn} \sqrt{\lambda_k} f_k \]

\[ \dot{f}_m = \omega^2 \sum_{n=1}^{\infty} T_{mn} \sqrt{\lambda_n} A_n(\tau) \]

\[ = -\frac{\omega^2}{4\gamma} \sum_{n,k=1}^{\infty} T_{mn} \sqrt{\lambda_n} \frac{1}{\delta_n} T^\dagger_{kn} \sqrt{\lambda_k} f_k \]

\[ = -\frac{\omega^2}{4\gamma} \sum_{n,k=1}^{\infty} T_{mn} \frac{\lambda_n}{\delta_n} T^\dagger_{nk} f_k \]

\[ = -\kappa \left[ T \Lambda^{3/4} T^\dagger \right]_{mk} f_k \] \hspace{1cm} (B.2)

where we used the property of transformation element, \( T^\dagger_{kn} \sqrt{\lambda_k} = T_{kn} \sqrt{\lambda_n} \) with \( T_{nl} = \langle \alpha_n | \phi_l \rangle = \int_0^1 dy \alpha_n(y) \phi_l(y) \) and the constant \( \kappa \).

Appendix C. Formal identities of cos and sin series

Consider the two Fourier cosine series on \([0, 1]\),

\[ q = \frac{1}{2} + \sum_{m \text{ odd}} -\frac{2\sqrt{2}}{\pi^2 m^2} \sqrt{2} \cos(m\pi y), \]

\[ q^2 - q = -\frac{1}{6} + \sum_{m \text{ even}, m > 1} \frac{2\sqrt{2}}{\pi^2 m^2} \sqrt{2} \cos(m\pi y), \]

\[ q^2 - q = \sum_{m \text{ odd}} -\frac{4\sqrt{2}}{(n\pi)^3} \sqrt{2} \sin(n\pi y). \] \hspace{1cm} (C.1)

Formally differentiating these two equations with respect to \( q \) on both sides we get two formal identities (which needs to be interpreted as distributional sense):

\[ \sum_{m \text{ odd}} \cos(m\pi q) = 0 \] \hspace{1cm} (C.2)

\[ \sum_{m \text{ even}, m > 1} \sqrt{2} \cos(m\pi q) = -\frac{1}{\sqrt{2}}, \] \hspace{1cm} (C.3)

\[ \sum_{m \text{ odd}} \frac{\sqrt{2}}{\sqrt{\lambda_n}} \frac{\sin(m\pi q)}{\sqrt{\lambda_n}} = \frac{1}{2\sqrt{2}}. \] \hspace{1cm} (C.4)

Appendix D. Alternate series representation of \( BB^\dagger \) and connection with equation (37)

As mentioned in the main text the kernel operator \( BB^\dagger \) has appeared earlier in the context of heat conduction through HCME model [20]. Using non-linear hydrodynamics

https://doi.org/10.1088/1742-5468/aaf630
theory in [20], the non-local linear response relation has been established for general boundary conditions characterized by a reflection coefficient \( R = \left( \frac{\omega}{\lambda} \right)^2 \) which vary from 0 to 1. For given \( R \), the expression for the kernel is given as [20]

\[
BB^I(x, x') = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \left[ \frac{R^{2n}}{\sqrt{|2n + x - x'|}} - \frac{R^{2n+1}}{\sqrt{|2n + x + x'|}} \right]. \tag{D.1}
\]

The value \( R = 0 \) corresponds to the resonance condition \( \omega = \lambda \) for free boundary condition i.e. \( q_0 = q_1 \) and \( q_N = q_{N+1} \). On the other hand, \( R = 1 \) corresponds to fixed boundary condition. For \( R = 1 \), one can explicitly check with the above representation that

\[
\int_0^1 dx' \ BB^I(x, x') \alpha_m(x') = \frac{1}{\lambda_n^{1/4}} \alpha_m(x), \tag{D.2}
\]

which is same as equation (37). The proof is as follows. The LHS of equation (D.2) can be written as,

\[
\text{LHS} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dy \left[ \frac{1}{\sqrt{|x - y|}} + \sum_{n=1}^{\infty} \frac{1}{\sqrt{2n + x - y}} + \frac{1}{\sqrt{2n - x + y}} - \frac{1}{\sqrt{2n - 2 + y}} - \frac{1}{\sqrt{2n - y}} \right] \sin(m\pi y). \tag{D.3}
\]

Using change of variables and separating the part in absolute value we have,

\[
\text{LHS} = \frac{1}{\sqrt{\pi}} \left[ \int_0^x dz \frac{\sin(m\pi(x - z))}{\sqrt{z}} + \int_0^{1-x} dz \frac{\sin(m\pi(x + z))}{\sqrt{z}} + \sum_{n=1}^{\infty} \left( \int_{2n-1}^{2n+1-x} dz \frac{\sin(m\pi(2n + x - z))}{\sqrt{z}} + \int_{2n-x}^{2n+1} dz \frac{\sin(m\pi(z - 2n + x))}{\sqrt{z}} - \int_{2n-2-x}^{2n+1} dz \frac{\sin(m\pi(z - 2n + 2 - x))}{\sqrt{z}} - \int_{2n-1-x}^{2n-x} dz \frac{\sin(m\pi(2n - x - z))}{\sqrt{z}} \right) \right].
\]

Upon using trigonometric identities this can be reduced to,

\[
\text{LHS} = \frac{1}{\sqrt{\pi}} \left[ \left( \int_0^x dz + \sum_{n=1}^{\infty} \left( \int_{2n-2-x}^{2n+1} dz + \int_{2n-1-x}^{2n-x} dz \right) \right) \frac{\sin(m\pi(x - z))}{\sqrt{z}} + \left( \int_0^{1-x} dz + \sum_{n=1}^{\infty} \left( \int_{2n-1-x}^{2n-x} dz + \int_{2n-2-x}^{2n+1-x} dz \right) \right) \frac{\sin(m\pi(x + z))}{\sqrt{z}} \right] \tag{D.4}
\]

which, upon simplifying further provides the RHS of equation (D.2),

\[
\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz \left[ \frac{\sin(m\pi(x - z))}{\sqrt{z}} + \frac{\sin(m\pi(x + z))}{\sqrt{z}} \right] = \frac{1}{\sqrt{m\pi}} \sqrt{2} \sin(m\pi x). \tag{D.5}
\]
Appendix E. Explicit expressions of some equations mentioned in main text

The total fractional equation (32) can be written explicitly as,
\[ \partial_t e(x, t) = \nabla_x \int dx' [A(x', t)e(x', t) - B(x', t)T\eta(x', t)]. \]  
(E.1)

The equation for the two time equilibrium spatio-temporal correlation (equation (40)) can be written as,
\[ C_{eq}(x, t, y, t') = 2\bar{\kappa} \int_{-\infty}^{t} ds \int_{-\infty}^{t'} ds' \int dx' \int dy' \nabla_x G^{x'y'}_{\tau-t-s} \langle (BT\eta)(x', s)(BT\eta)(y', s') \rangle \nabla_y G^{y'y'}_{\tau-t-s}. \]  
(E.2)

The spatio-temporal current correlations in equation (44) can be explicitly written as,
\[ \langle j(x, t) j(y, t') \rangle = \int dx' \int dy' \bar{\kappa}^2 A(x, x') A(y, y') \langle e(x', t) e(y', t') \rangle \]  
(E.3)

\[ + 2\kappa T^2 B(x, x') B(y, y') \langle \eta(x', t) \eta(y', t') \rangle \]  
(E.4)

\[ - \sqrt{2}\kappa^{2/3} T A(x, x') B(y, y') \langle e(x', t) \eta(y', t') \rangle \]  
(E.5)

\[ - \sqrt{2}\kappa^{2/3} T B(x, x') A(y, y') \langle \eta(x', t) e(y', t') \rangle. \]  
(E.6)

Since it might be a bit confusing using the symbolic vector notation for the operations in the main text, here we show explicitly the expressions for individual terms and show the 2nd and 3rd terms give a similar term to 1st. Equation (E.3) gives,
\[ \bar{\kappa}^2 \int dx' \int dy' A(x, x') A(y, y') G^{x'y'}_{\tau-t-s} = \bar{\kappa}^2 \int dx' \int dy' BB^\dagger(x, x') \partial_{x'} BB^\dagger(y, y') \partial_{y'} G^{x'y'}_{\tau-t-s} \] 
\[ = \bar{\kappa}^2 \int dx' \int dy' A(x, x') G^{x'y'}_{\tau-t-s} A^\dagger(y, y) \]  
(E.7)

where we used the adjoint representation for $A^\dagger(y, y') = A(y', y)$. Equation (E.5) gives,
\[ III = \int dx' \int dy' \sqrt{2}\kappa^{2/3} T A(x, x') B(y, y') \langle e(x', t) \eta(y', t') \rangle \] 
\[ = -2\kappa T^2 \int dx' \int dy' \int dx'' \int dy'' \int_{-\infty}^{t} ds BB^\dagger(x, x') \partial_{x'} B(y, y') G^{x'y''}_{\tau-t-s} \partial_{y''} B(x'', y'') \langle \eta(y'', s) \eta(y', t') \rangle \] 
\[ = 2\kappa T^2 \int dx' \int dy' \int dx'' BB^\dagger(x, x') \partial_{x'} B(y, y') \partial_{y'} G^{x'y''}_{\tau-t-s} B(x'', y') \theta(t - t') \] 
\[ = 2\kappa T^2 \int dx' \int dy' \int dx'' A(x, x') G^{x'y''}_{\tau-t-s} A^\dagger(x'', y) \theta(t - t'). \]  
(E.8)
Equation (E.6) gives,
\begin{align*}
IV &= \iiint dx' \int dy' \sqrt{2\kappa^3/2}TB(x, x')A(y, y')\langle \eta(x', t)e(y', t') \rangle \\
&= -2\kappa T^2 \iiint dx' \int dy' \int dx'' \int dy'' \int_{-\infty}^t dsB(x, x')A(y, y')G_{\mu \nu -s} \partial_{\nu'} B(x'', y'')\langle \eta(x', t)\eta(y'', s) \rangle \\
&= 2\kappa T^2 \iiint dx' \int dy' \int dx'' B(x, x')A(y, y')\partial_{\nu'}(G_{\nu' -t}^{y''})B(x'', x')\theta(t' - t) \\
&= 2\kappa T^2 \iiint dx' \int dy' \int dx'' A(y, y')G_{\nu' -t}^{y''}A^+(x'', x)\theta(t' - t). 
\end{align*}
(E.9)

The second term is explicit in the main-text.

Appendix F. Some tests on long-range correlations

In figure F1 we do microscopic simulations for different temperature differences, and absolute temperatures to show, to good accuracy, the constant $\nu$ does not depend on these factors. In figure F2 we test the use of $\alpha(\sin)$ basis instead of the $\psi$ basis for theoretical prediction for the nature of long-range correlations, and show it performs badly.
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\[ \frac{1}{\Gamma(n)} \sum_{n=1}^{\infty} a_n(x^\alpha y^\beta) \lambda_n^{3/4} \]

\[ \frac{1}{\Gamma(n)} \sum_{n=1}^{\infty} a_n(x^\alpha y^\beta) \lambda_n^{3/4} \]

Figure F2. Here we show that instead of using \( \psi_n \) and \( \mu_n \) if we use \( \sin \) and \( \lambda_n^{3/4} \) for construction of inverse of the fractional operator, there are significant differences between the simulations with the formula \( C(x, y) = \sum_{n=1}^{\infty} \frac{a_n(x)}{\lambda_n^{3/4}} \).

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