Stationary time correlations for fermions after a quench in the presence of an impurity

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Abstract – We consider the quench dynamics of non-interacting fermions in one dimension in the presence of a finite-size impurity at the origin. This impurity is characterized by general momentum-dependent reflection and transmission coefficients which are changed from $r_0(k), t_0(k)$ to $r(k), t(k)$ at time $t = 0$. The initial state is at equilibrium with $t_0(k) = 0$ such that the system is cut in two independent halves with $r_R^0(k), r_L^0(k)$, respectively, to the right and to the left of the impurity. We obtain the exact large time limit of the multi-time correlations. These correlations become time translationally invariant, and are non-zero in two different regimes: i) for $x = O(1)$ where the system reaches a non-equilibrium steady state (NESS), ii) for $x \sim t$, i.e., the ray regime. For a repulsive impurity these correlations are independent of $r_R^0(k), r_L^0(k)$, while in the presence of bound states they oscillate and memory effects persist. We show that these nontrivial relaxational properties can be retrieved in a simple manner from the large time behaviour of the single particle wave functions.

Introduction. – There is a fast growing interest in non-interacting fermions in the presence of external potentials as solvable models capturing nontrivial quantum correlations. For fermions at equilibrium, either in a trap [1–5] or in the presence of an impurity [6–8], spatial correlations have been computed using various analytical methods, including determinantal processes and connections to random matrices [3–5,9,10], as well as inhomogeneous bosonisation [11]. Extensions of these methods allow to also obtain the temporal correlations at equilibrium [11,12].

Non-interacting fermions also provide interesting tractable models to study non-equilibrium quantum dynamics. A seminal example is the Landauer-Büttiker theory for transport between two reservoirs [13–15] where the system is assumed to be in a stationary state from the start. A more general setting to study out of equilibrium dynamics and convergence to a stationary state are quantum quenches. Non-interacting fermions have been much studied in this context for translationally invariant systems. The resulting equilibrium state reached at large time can be predicted using the generalised Gibbs ensemble (GGE), which more generally describes integrable interacting systems, see, e.g., [16]. In these cases, the dynamics can also be computed using the generalised hydrodynamics (GHD) [17,18] which predicts correlations in the so-called ray regime $x \sim t$. For non-interacting fermions, the GHD amounts to consider a semi-classical version of the Wigner function. To address the transport properties using quantum quenches a standard protocol is to consider an initial state inhomogeneous in space in one dimension [19–31]. At late time the system reaches a non-equilibrium stationary state (NESS) characterized by stationary currents, density profiles and counting statistics [32].

An important question is how the transport in the NESS as well as in the ray regime is affected by the presence of inhomogeneities in space. The simplest case is a local impurity which has been studied, e.g., in [33–35], or using conformal field theory [36–38]. Recently, for non-interacting fermions in one dimension, several analytical results have been obtained both for discrete [39–44] and continuum [45,46] models. In these models, the system is initially prepared either with a domain wall or partitioned into two separate halves. It then evolves in the presence of an impurity, modeled either by a so-called “conformal
metric (V) We work in units where ℏ ing non-interacting fermions in one dimension prepared in the NESS does not predict the correlations in the NESS (\( \xi \)) probabilities [39,45]. It was shown to predict the correct i.e. proved by taking into account reflection and transmission coefficients. The fermions are confined in a hard box of size \( \ell \) with \( \ell > a \) (i.e., the wave function vanishes outside \([-\ell/2, \ell/2]\)).

The system is prepared at \( t = 0 \) at Gibbs equilibrium and is described by the single particle Hamiltonian \( \hat{H}_0 \)

\[
\hat{H}_0 = -\frac{1}{2} \partial_x^2 + V_0(x),
\]

where \( V_0(x) \) is another potential localized in the region \([-\frac{\ell}{2}, \frac{\ell}{2}]\) and characterized by a scattering matrix

\[
S_0 = \begin{pmatrix}
0 & r_0^R(k) \\
r_0^L(k) & 0
\end{pmatrix}, \quad |r_0^L(k)|^2 = |r_0^R(k)|^2 = 1.
\]

The potential \( V_0(x) \) is sufficiently divergent at \( x = 0 \) so that the system is cut in two halves with \( t_0^R(k) = t_0^L(k) = 0 \). The initial N-body density matrix \( \hat{D} = \hat{D}_L \otimes \hat{D}_R \) is the tensor product of left and right density matrices \( \hat{D}_{L/R} \) each describing equilibrium at temperature \( T_{L/R} \) with chemical potentials \( \mu_{L/R} \). In the zero temperature case, this amounts to consider the ground state with a fixed number of fermions \( N_{L/R} \) on each side.

The normalized eigenfunctions \( \phi^{R/L}_k(x) \) of the initial Hamiltonian \( \hat{H}_0 \) vanish for \( x \in \mathbb{R}^{-/+} \) and can be written outside the interval \([-\frac{\ell}{2}, \frac{\ell}{2}]\)

\[
\phi^{R}_k(x) = c^0_k \cos(k(|x| - \delta^R_k))\theta \left( x - \frac{a}{2} \right), \quad k \in \Lambda^R,
\]

\[
\phi^{L}_k(x) = c^0_k \cos(k(|x| - \delta^L_k))\theta \left( \frac{a}{2} - x \right), \quad k \in \Lambda^L,
\]

with \( c^0_k \sim \sqrt{\frac{2}{\ell}} \) at large \( \ell \) and where \( \theta(x) = 0 \) if \( x \leq 0 \) and \( \theta(x) = 1 \) if \( x > 0 \). The phase shifts \( \delta^{R/L}_k \) are related to the reflection coefficients as

\[
t_0^{R/L}(k) = e^{-2ik\delta^{R/L}_k},
\]

while the lattices \( \Lambda^R \) and \( \Lambda^L \) are defined as follows:

\[
\Lambda^{R/L} = \left\{ k \in \mathbb{R}^+ | \phi^{R/L}_k \left( \pm \frac{\ell}{2} \right) = 0 \right\}.
\]

**Observables.** — We are interested in the space–time \( m \) point density correlation functions, defined for \( 0 \leq t_1 \leq \cdots \leq t_m \) and all distinct space time points \((x_i, t_i)\) as

\[
C_m(x_1, t_1; \cdots ; x_m, t_m) = Tr(\hat{D}\hat{\rho}(x_m, t_m)\cdots \hat{\rho}(x_1, t_1)),
\]

where \( |r(k)| = |t(k)| \).
where \( \hat{\rho}(x, t) \) is the density operator in the Heisenberg representation. For non-interacting fermions they can be expressed as an \( m \times m \) determinant involving the so-called space-time extended kernel (see \([48, 49]\))

\[
C_m(x_1, t_1; \cdots; x_m, t_m) = \det_{1 \leq i, j \leq m} K(x_i, t_i; x_j, t_j). \quad (10)
\]

In particular, the total fermion density reads \( \rho(x, t) = K(x, t; x, t) \). The current correlations can also be obtained from the kernel (see the SM). The space-time extended kernel can be written as the sum

\[
K(x, t; x', t') = K_R(x, t; x', t') + K_L(x, t; x', t'), \quad (11)
\]

where

\[
K_{R/L}(x; t; x', t') = \sum_{k \in \Lambda_{R/L}^0} \left( f_{R/L}(k) - \theta(t' - t) \right) \psi_{k}^{R/L}(x, t) \psi_{k}^{R/L}(x', t'). \quad (12)
\]

Here \( f_{R/L}(k) = 1/(1 + e^{\beta \mu_{R/L} - \frac{\epsilon_k}{2}}) \) are the right and left Fermi factors, and \( \psi_{k}^{R/L}(x, t) \) is the solution of the Schrödinger equation \( i \partial_t \psi_{k}^{R/L}(x, t) = \hat{H} \psi_{k}^{R/L}(x, t) \) with the initial condition \( \psi_{k}^{R/L}(x, 0) = \phi_{k}^{R/L}(x) \), where \( \phi_{k}^{R/L}(x) \) are given in eq. (5).

**Large time limit: the NESS.** We now want to take a double limit: first the thermodynamic limit \( \ell \to +\infty \) with fixed left and right mean densities (i.e., fixed chemical potentials \( \mu_{L,R} \)) and then the large time limit\(^2\). We first consider the system over distances \( x = O(1) \) (i.e., “close to the impurity”). In this regime, the system reaches a NESS where one-point quantities (such as the density) becomes stationary, and multi-time correlations become time-translational invariant. We can compute exactly the large \( \ell \) and large time limit of the kernel starting from the exact formula in eq. (12). Since it is a bit cumbersome (similar to the calculations in \([39, 45]\)) we instead present here a shortcut by studying directly the asymptotic form of the single-particle time evolved initial eigenfunctions, \( \psi_{k}^{R/L}(x, t) \), in the large \( \ell \) and large \( t \) limit. The exact formula for \( \psi_{k}^{R/L}(x, t) \) is an infinite superposition which involves the overlap of \( \phi_{k}^{R/L}(x) \) with all the eigenstates of \( \hat{H} \). The asymptotic form of this superposition is obtained using a contour-integral representation which leads to (see the SM)

\[
\psi_{k}^{R/L}(x, t) = \frac{1}{\sqrt{\ell}} (e^{-\frac{\epsilon_k}{2} t} \chi_{R/L}^{R}(x) + \delta \chi_{k, \ell}^{R/L}(x, t)). \quad (13)
\]

\(^1\)One has \( K(x, t; x', t') = \text{Tr} \hat{D} T \delta_{\epsilon_{k}, \epsilon_{k'}} T \theta(t' \geq t) - \epsilon_{k}, \epsilon_{k'} \theta(t' > t) \).

\(^2\)Note that here we considered a finite box in the large \( \ell \) limit. One can instead consider directly the system on the infinite axis and use the Lippman-Schwinger approach, see, e.g., \([50]\). Although these are equivalent, the present method allows a control of finite-size effects.

where \( \delta \chi_{k, \ell}^{R/L}(x, t) \) decays to zero in the limit of large \( \ell \) followed by large \( t \). In eq. (13), the leading contributions \( \chi_{k}^{R/L}(x) \) are given by

\[
\chi_k^R(x) = \begin{cases}
(e^{-ikx} + r(k)e^{ikx})e^{ik\delta_x^R} & \text{if } x > \frac{a}{2} , \\
t(k)e^{-ikx}e^{ik\delta_x^R} & \text{if } x < -\frac{a}{2}.
\end{cases} \quad (14)
\]

\[
\chi_k^L(x) = \begin{cases}
t(k)e^{ikx}e^{ik\delta_x^L} & \text{if } x > \frac{a}{2} , \\
(e^{ikx} + r(k)e^{-ikx})e^{ik\delta_x^L} & \text{if } x < -\frac{a}{2}.
\end{cases} \quad (15)
\]

where we recall that \( r(k) \) and \( t(k) \) are the reflection and transmission coefficients (2). In this result (13) the time dependence \( e^{-i\frac{\epsilon_k}{2} t} \) is simply the one of a free particle of energy \( \frac{\epsilon_k}{2} \), while the factor \( \frac{1}{\sqrt{\ell}} \) ensures the normalization of \( \psi_{k}^{R/L}(x, t) \). The form of \( \chi_{k}^{R/L}(x) \) in (14) and (15) can be qualitatively understood as follows. Away from the impurity, at time \( t = 0 \), from (5) a particle can have momentum \( k \) or \( -k \) (everywhere \( k > 0 \)). Consider a space point \( x \) with \( x = O(1) > 0 \) and large \( t \) and first ask how a particle starting from the left of the impurity can reach \( x \). As shown in fig. 1(a), there is a single possible initial position such that a particle with initial momentum \( k \) reaches \( x \). Since it crosses the barrier, it collects a factor \( t(k) \). This accounts for the first line in (15). It contains a single term, with phase factor \( e^{ik\delta_x^L} \), since particles with initial momentum \( -k \) escape to \(-\infty \) (the phase factor information they carry \( e^{-ik\delta_x^L} \) is lost). For particle

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starting from the right of the impurity, one similarly interprets the two terms in the first line in (14). Indeed, one sees from fig. 1(b) that there are two possible initial positions such that a particle with initial momentum $-k$ reaches $(x, t)$ either i) directly (leading to the factor $e^{ikx}$) or ii) after one reflection (which changes $-k$ to $k$ leading to the factor $r(k)e^{ikx}$). Of course this semi-classical argument is deceptively simple, since in reality momentum is not a quantum number here and the true wave function is a complicated superposition. However we show here that it becomes exact at large time. Thus, although the final result is intuitively simple, the convergence to the large time limit is nontrivial. It can be extracted from the exact expression for the subleading part $\delta \chi_{R/L}^R(x, t)$ that we provide in (13) — see [45] and the SM. Although we did not perform an exhaustive analysis it is easy to see that the decay is generically algebraic in time (with possible oscillations).

The next step is to compute the space-time kernel from eqs. (11) and (12). It turns out, as we have explicitly checked by an exact independent computation, that in the limit $\ell \to \infty$ and $t \to \infty$, one can simply inject the dominant part of (13) in the formula for the kernel (11) and (12) and replacing the discrete sums in this formula by integrals (in the limit $\ell \to \infty$). This yields the asymptotic limit

$$ K_\infty(x, x', t-\tau) = K_{\infty}(x, x', \tau) $$

as $t \to \infty$

$$ K_{\infty}(x, x', \tau) = \int_{\ell, R, \tau} \frac{dk}{2\pi} \chi^R_k(x)^* \chi^L_k(x') + \int_{R, \tau} \frac{dk}{2\pi} \chi^R_k(x)^* \chi^R_k(x'). $$

(16)

Here and below we use the shorthand notation

$$ \int_{\ell, \tau} \frac{dk}{2\pi} = \int_{0}^{\infty} \frac{dk}{2\pi} (f_{R/L}(k) - \theta(-\tau)), $$

$$ \int_{R, \tau} \frac{dk}{2\pi} = \int_{0}^{\infty} \frac{dk}{2\pi} f_{R}(k) - f_{L}(k) $$

(17)

and we use the convention $\theta(0) = 0$. Injecting the explicit form of the function $\chi_{k/L}^R(x)$ from (14) and (15) in (16) we find

$$ K_\infty \left(x > \frac{a}{2}, x' > \frac{a}{2}, \tau \right) = \int_{\ell, R, \tau} \frac{dk}{2\pi} e^{ik(x-x')/\ell} t(k)^2 + \int_{R, \tau} \frac{dk}{2\pi} e^{ik(x-x')/\ell} \left( \cos(k(x-x')) + \Re[r(k)e^{ikx}] \right) $$

$$ + \int_{L, \tau} \frac{dk}{2\pi} e^{ik(x-x')/\ell} \left( \cos(k(x-x')) + \Re[r(k)e^{ikx}] \right) $$

$$ K_\infty \left(x > \frac{a}{2}, x' < -\frac{a}{2}, \tau \right) = \int_{\ell, R, \tau} \frac{dk}{2\pi} e^{ik(x-x')/\ell} t(k)^2 + \int_{R, \tau} \frac{dk}{2\pi} e^{ik(x-x')/\ell} \left( \cos(k(x-x')) + \Re[r(k)e^{ikx}] \right) $$

$$ + \int_{L, \tau} \frac{dk}{2\pi} e^{ik(x-x')/\ell} \left( \cos(k(x-x')) + \Re[r(k)e^{ikx}] \right) $$

(18)

together with the other regions obtained using the symmetry $K_\infty(x, x', \tau)|_{L,R} = K_\infty(-x, -x', \tau)|_{R,L}$. Note that the initial phase shifts $e^{ikx}$ cancel in the kernel. As expected $K_\infty(x, x', \tau)$ vanishes at large $|\tau|$, with algebraic decay see the SM. In particular, from (19), one obtains the density $\rho_\infty(x) = K_\infty(x, x, 0)$ in the NESS, which reads, for $|x| > a/2$,

$$ \rho_\infty(x) = \int_{L,R} \frac{dk}{2\pi} |t(k)|^2 + \int_{0}^{\infty} \frac{dk}{\pi} f_R(k) \left(1 + \Re[r(k)e^{ikx}]\right). $$

(20)

Similarly, from (19) one also obtains the current in the NESS $J_\infty = \frac{1}{2i}(\partial_{x'} - \partial_k)K_\infty(x, x', 0)|_{x'=x}$, which yields

$$ J_\infty = \int_{L,R} \frac{dk}{2\pi} 2i |t(k)|^2. $$

(21)

For $f_{L}(k) = f_{R}(k)$ the first and fourth line in (19) vanish and one can check that one recovers the thermal equilibrium (in the absence of bound states).

**Large time limit: the ray regime.** — We also computed the asymptotic kernel at large time when distances are scaled with time $x = O(\ell)$, i.e., setting $x = \xi + y$ with $\xi, y = O(1)$. Again we first obtain the asymptotic form of the wave function (SM)

$$ \psi_{k}^{R/L}(x = \xi + y, t) \sim \frac{1}{\sqrt{\ell}} e^{-\frac{1}{\ell} \xi^2} \chi^{R/L}_{\xi,k}(x = \xi + y), $$

(22)

where we have defined

$$ \chi^{R/L}_{\xi,k}(x) = \{ \begin{array}{ll}
\theta(k - \xi) t(k) e^{-ikx} e^{ik\delta^R_k} & \text{if } \xi < 0, \\
\theta(k - \xi) t(k) e^{-ikx} e^{-ik\delta^L_k} & \text{if } \xi > 0, \\
\chi^{R/L}_{\xi,k}(x) = \{ \begin{array}{ll}
\theta(k - \xi) t(k) e^{ikx} e^{ik\delta^R_k} & \text{if } \xi < 0, \\
\theta(k - \xi) t(k) e^{-ikx} e^{-ik\delta^L_k} & \text{if } \xi > 0, \\
\end{array}
\end{array} $$

(23)

(24)

Since $x = \xi + y$ (22) exhibits fast oscillations in time $\propto e^{-\frac{1}{\ell^2} \xi^2 \pm \xi \delta^R_k}$. The forms (23) and (24) can be understood by an extension to the ray regime of the argument given in the NESS, see fig. 1(c) and (d). It can also be summarized by considering the “light cone” with slopes $\pm k$ originating from the impurity, see fig. 2. Outside of it, i.e., for $|\xi| > k$, $\psi_{R/L}(x, t)$ recovers the initial condition up to a time propagation phase $e^{-\frac{1}{\ell^2} \xi^2}$, i.e.,

$$ \frac{1}{\sqrt{\ell}} \chi^{R/L}_{\xi,k}(x) = \tilde{\phi}_{k}^{R/L}(x), \text{ for } |\xi| > k. $$

(25)

Inside the cone, i.e., for $|\xi| < k$, $\psi_{R/L}(x, t)$ is given by the extrapolation to the ray regime (with $x = \xi + y$) of the form obtained above in the NESS (for $x = O(1)$), in eqs. (23) and (24), i.e.,

$$ \chi^{R/L}_{\xi,k}(x) = \chi^{R/L}_{k}(x), \text{ for } |\xi| < k. $$

(26)
Hydrodynamics argument based on the Wigner function [18,39,45], this is not the case for $K^-$ (see footnote 4). Instead, in the present framework, the correlations between $(x,t)$ and $(x',t)$ arise naturally from trajectories which start from the same point (e.g., from the right with moment $-k$) and are either reflected or transmitted. In the kernel, the differences between these two trajectories result from the product of the first and the third line in (23) when computing $\chi^R_{\xi k}(x,t)\chi^R_{\xi k}(x,t)$ (see (16)).

At large time the mean density along rays thus converges $\rho(\xi,t) \to \bar{\rho}(\xi)$ given by

$$\bar{\rho}(\xi > 0) = \rho_R + \int_{L \to R} \frac{dk}{2\pi}[|k|^2\theta(k - |\xi|)],$$

and the same for $\xi < 0$ exchanging $R$ and $L$. Here $\rho_R/L = \int_{0}^{\infty} \frac{dk}{2\pi}[|k|^2\theta(k)]^2$. Similarly the current along rays converges to $J(\xi,t) \to \bar{J}(\xi)$ with

$$\bar{J}(\xi) = \int_{L \to R} \frac{dk}{2\pi}[|k|^2\theta(k - |\xi|)].$$

**Bound states.** Let us now discuss the NESS regime when $V(x)$ admits a sequence of bound states $\phi_n(x)$, $\kappa \in \Lambda$ of energies $-\frac{1}{2} b^2$. In that case the asymptotic large time kernel $K = K_+ + K_b$ is the sum of two pieces: i) one due to scattering states, $K_+$, identical to the one obtained above ii) one due to bound states, $K_b = K_b^R + K_b^L$, where

$$K_b^{R/L}(x,t;x',t') = \sum_{\kappa',\kappa'' \in \Lambda_b} \phi_{\kappa'}(x)\phi_{\kappa''}(x')e^{-i(\xi_x^2 - \xi_y^2) \epsilon}C_{\kappa'\kappa''}^{R/L},$$

with

$$C_{\kappa'\kappa''}^{R/L} = \langle \phi_{\kappa'}|1 + e^{iL/K}(H^{R/L} - \mu n_{L/R})^{-1}|\phi_{\kappa''}\rangle,$$

see the SM. When they are at least two bound states the total NESS kernel exhibits permanent oscillations in time. These oscillations also occur in the density and current, see the SM. Note that these oscillations contain information about the overlap of the initial wave functions with the post-quench bound states (and about the fact that $V_0$ has or not bound states), while in the absence of bound states of $V(x)$, only the scattering coefficients remains relevant at large time. In particular one finds that the post-quench bound states are always partially empty in the NESS. Finally, bound states do not contribute to the kernel in the ray regime since their wave functions decrease exponentially at large $|x|$. For related results in the presence of bound states see [39,41,51].

We now study the connected correlation function of the density at two distinct space-time points in the NESS. It

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3Alternatively one could define the large $t$ limit of $K(\xi t + y, t; \xi(t - r) + y', t - r)$ which amounts to a simple shift $y' \to y' + \xi \tau$ in our formula.

4Indeed an exact calculation of the Wigner function $W(x,p)$, see the SM, unveils the existence of a $\delta(p)$ peak, which is shown to be a quantum signature of the finite limit of the correlations along opposite rays.
is obtained from the kernel in the NESS using (9), (10) as
\[
\lim_{t \to +\infty} \langle \rho(x', t + \tau) \rho(x, t) \rangle^c = -K_\infty(x, x'; -\tau)K_\infty(x', x, \tau). \tag{33}
\]
In the large \( \tau \) limit the behavior of this correlation depends on the ratios \( \zeta = \frac{x}{L} \) and \( \zeta' = \frac{x'}{L} \). As shown in fig. 3 there are several sectors in the \( (\zeta, \zeta') \) plane, where the decay of the correlation at large time is of the form \( \sim \tau^{-\alpha}C(\zeta, \zeta') \) where \( \alpha \) depends on the sector, up to oscillating and diffusive factors respectively of the form \( e^{\pm i k L / (x+x')} \) and \( e^{-i \tau / (x+x')} \) (see the SM for details). As compared to the equilibrium case in the absence of a defect for which \( \alpha = 3/2 \) for all \( (\zeta, \zeta') \) [12], the stationary temporal correlations in the NESS in the presence of an impurity exhibits a richer behavior, in particular regions with a slower decay. In addition, we have shown that the response function reaches a stationary limit \( \lim_{t \to +\infty} \frac{\langle \hat{\rho}(x, t) \rangle}{\rho(x, t)} \bigg|_{\tau=0} \) which we have expressed in terms of the kernel \( K_\infty(x, x'; \tau) \) (see the SM).

In conclusion, we have obtained in eqs. (13) and (22) the limiting forms of the time-evolved single particle wave functions at large time after a quantum quench in the presence of an arbitrary impurity. Here we have presented the case of a symmetric impurity \( V(x) = V(-x) \), the extension to the general case being presented in the SM. These limiting wave functions allow to obtain elegant expressions for the space-time correlation kernel of non-interacting fermions in terms of the scattering coefficients, both in the NESS and in the ray regime. They incorporate the quantum interference effects and allow to overcome the shortcomings of the semi-classical approach. These correlation kernels allow in principle calculation of the full counting statistics and entanglement entropy for arbitrary intervals (see recent developments in [41,43,46,52]). It would be interesting to realize such partitioning protocol in cold Fermi gas transport experiments [53]. In bosonic cold atoms the relaxation after a quantum quench has been observed [54,55], including in the non-interacting limit [56,57]. Our results can also be applied to bosons in the presence of an impurity: i) for non-interacting bosons using our asymptotic wave function replacing the Fermi by the Bose factors; ii) to the Tonks-Girardeau gas since density correlations are related in both systems [30]. Finally, it is possible to extend our 1d calculation to other geometries, such as tubes or 2d sheets.

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