Probabilités et mécanique statistique hors équilibre

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Chapter 1

Introduction

Après l'obtention de mon doctorat en juin 1999, j'ai consacré mes travaux de recherche à l'étude de problèmes mathématiques issus de la physique statistique hors équilibre. Les problèmes traités concernent les propriétés ergodiques d'équations aux dérivées partielles stochastiques, l'étude de la mesure invariante de dynamiques stochastiques hypoelliptiques non-réversibles et de leur grandes déviations, la simulation numérique de systèmes étendus de particules Hamiltoniennes, l'étude de processus de renouvellement Markoviens les modélisant.

1.1 Ergodicité des équations de Navier-Stokes stochastiques.

On se trouve encore relativement loin d'une compréhension théorique détaillée de l'état stationnaire d'un fluide turbulent. Un premier pas dans la description mathématique des ces états est de considérer les équations de Navier-Stokes avec un forçage stochastique et de démontrer que le système est décrit par une mesure invariante unique. Le but ultime serait la compréhension des propriétés des fonctions de corrélations d'une telle mesure. Dans les articles [16, 17, 18], en collaboration avec Jean Bricmont et Antti Kupiainen, nous avons considéré les équations de Navier-Stokes sur un tore bidimensionnel avec une force aléatoire, de type bruit blanc dans le temps (ou à temps discret) et agissant uniquement sur de grandes échelles spatiales et pour un nombre de Reynolds (Re) arbitraire. Nous avons démontré des estimations probabilistes pour le comportement asymptotique en temps des solutions. Ces estimations impliquent des bornes pour l'échelle dissipative et le spectre d'énergie des modes de Fourier lorsque $Re \to +\infty$ [16]. Ensuite, nous avons démontré l'unicité de la mesure invariante [17, 18].

Plus précisément, on considère l'équation de Navier-Stokes stochastique pour le champ de vitesses $u(t,x) \in \mathbb{R}^2$ défini sur le tore $\mathbf{T} = (\mathbb{R}/2\pi\mathbf{Z})^2$:

$$du + ((u \cdot \nabla)u - \nu\nabla^2 u + \nabla p)dt = df, \tag{1}$$

où $f(t,x)$ est un processus de Wiener de covariance

$$\mathbb{E} f_\alpha(t,x) f_\beta(t',y) = \min\{t,t'\} C_{\alpha\beta}(x-y) \tag{2}$$

et $C_{\alpha\beta}$ est une fonction régulière satisfaisant $\sum_\alpha \partial_\alpha C_{\alpha\beta} = 0$. L'équation (1) est complétée par la condition d'incompressibilité $\nabla \cdot u = 0 = \nabla \cdot f$, et nous supposons que les moyennes sur le tore s'annulent. $\int_{\mathbf{T}} u(0,x) = 0 = \int_{\mathbf{T}} f(t,x)$, ce qui implique que $\int_{\mathbf{T}} u(t,x) = 0$ pour tout t.

Il est commode d'introduire des variables sans dimension, de telle sorte que ν devient égal à 1. On introduit donc, $u(t,x) = \nu u'(\nu t, x)$. Alors u' satisfait (1) et (2) où ν est remplacé par 1 et C par

$$C' = \nu^{-3} C.$$

Le paramètre sans dimension de contrôle du système est le taux d'injection d'énergie $\frac{1}{2}\mathrm{tr}\, C'(0)$, que l'on peut écrire comme $(\mathrm{Re})^3$ où Re est le nombre de Reynolds :

$$\mathrm{Re} = \epsilon^{\frac{1}{3}} \nu^{-1},$$

et $\epsilon = \frac{1}{2}\mathrm{tr}\, C(0)$ est le taux d'injection d'énergie dans les unités originales. Ci-dessous, nous travaillons avec ces variables et abandonnons les primes. En deux dimensions, on se débarasse de la condition d'incompressibilité en exprimant le champ de vitesses en termes de la vorticité $\omega = \partial_1 u_2 - \partial_2 u_1$. Tout d'abord, (1) implique l'équation de transport

$$d\omega + ((u \cdot \nabla)\omega - \nabla^2 \omega)dt = db, \tag{3}$$

où $b = \partial_1 f_2 - \partial_2 f_1$ est de covariance

$$\mathbb{E} b(t,x) b(t',y) = \min\{t,t'\}(2\pi)^{-1}\gamma(x-y)$$

avec $\gamma = -2\pi\nu^{-3}\Delta \mathrm{tr} C$.

Ensuite, en utilisant la transformée de Fourier $\omega_k(t) = \frac{1}{2\pi}\int_{\mathbf{T}} e^{ik\cdot x}\omega(t,x)dx$, $k \in \mathbf{Z}^2$; on peut exprimer u comme $u_k = i\frac{(-k_2,k_1)}{k^2}\omega_k$, et écrire l'équation pour la vorticité

$$d\omega(t) = F(\omega(t))dt + db(t), \tag{4}$$

où la dérive est donnée par

$$F(\omega)_k = -k^2\omega_k + \frac{1}{2\pi}\sum_{l \in \mathbf{Z}^2 \setminus \{0,k\}} \frac{k_1 l_2 - l_1 k_2}{|l|^2}\omega_{k-l}\omega_l \tag{5}$$

et les $\{b_k\}$ sont des mouvements Brownien tels que $\bar{b}_k = b_{-k}$ et

$$\mathbb{E} b_k(t) b_l(t') = \min\{t,t'\}\delta_{k,-l}\,\gamma_k.$$

Le paramètre de contrôle sans dimension pour l'équation de vorticité est à présent :

$$R = \sum_{k \in \mathbf{Z}^2} \gamma_k = 2\pi\gamma(0) \tag{6}$$

qui est proportionnel au cube du nombre de Reynolds. Pour étudier les situations turbulentes, on voudrait considérer le cas où on excite seulement un nombre fini de modes:

$$\gamma_k \neq 0\ ,\ k^2 \leq N,$$

où N est d'ordre 1. Nous supposons que

$$N = \kappa R, \tag{7}$$

où κ est une constante sans dimension. Moyennant cette hypothèse, nous sommes parvenus à démontrer l'unicité de la mesure invariante et les propriétés de mélange des équations de Navier-Stokes stochastiques [17, 18]. Nous avons aussi obtenu des bornes intéressantes sur l'échelle de dissipation et le spectre d'énergie [16]. L'échelle dissipative est bornée inférieurement par $R^{-\frac{1}{2}\alpha}$ et le spectre d'énergie $e(k)$ est tel que :

$$e(k) \equiv k^{-1} \int_{S^1} d\widehat{\mathbf{k}} \left\langle |\omega_{\widehat{\mathbf{k}}k}|^2 \right\rangle \leq C R^{\widetilde{\alpha}} k^{-(2r+1)}$$

où $k = |\mathbf{k}|$, et r peut être choisi arbitrairement proche de 1. $\widetilde{\alpha}$,α sont eux strictement plus grand que (mais arbitrairement proches de) $1 + r$.

1.2 Dynamique Hamiltonienne sur réseau couplée à des thermostats stochastiques.

Pour décrire la conduction de la chaleur dans les solides cristallins, on modélise souvent le solide par un réseau d'atomes dont les extrémités sont couplées à des bains de chaleur maintenus à des températures différentes. En une dimension, le système peut être décrit comme ceci : à chaque site i du réseau $\{1, \ldots, N\}$, on attache une particule de vitesse p_i et position q_i. La dynamique est Hamiltonienne à l'intérieur de la chaîne et stochastique aux extrémités à cause du couplage aux bains de chaleur. L'Hamiltonien est de la forme

$$H(\underline{p}, \underline{q}) = \sum_{i=1}^{N} \Big(\tfrac{1}{2} p_i^2 + V(q_i) \Big) + \sum_{i=2}^{N} U(q_i - q_{i-1}) + U(q_1) + U(q_N). \tag{8}$$

Les équations du mouvement sont données par

$$\begin{aligned} dq_i &= p_i dt, \quad i = 1, \ldots, N, \\ dp_i &= -\frac{\partial H}{\partial q_i}(\underline{p}, \underline{q}) dt, \quad i = 2, \ldots, N-1, \end{aligned} \tag{9}$$

et

$$\begin{aligned} dp_1 &= -\frac{\partial H}{\partial q_1}(\underline{p}, \underline{q}) dt - \gamma p_1 dt + \sqrt{2\gamma k T_L}\, dw_l\,, \\ dp_N &= -\frac{\partial H}{\partial q_N}(\underline{p}, \underline{q}) dt - \gamma p_N dt + \sqrt{2\gamma k T_R}\, dw_r\,. \end{aligned} \tag{10}$$

T_L et T_R sont les températures du bain de gauche et du bain de droite. Tandis que w_l and w_r sont des processus de Wiener indépendants.

Il est facile de vérifier que lorsque $T_L = T_R = T = \beta^{-1}$, la mesure invariante du système est donnée par sa densité:

$$\rho(\underline{p}, \underline{q}) = Z^{-1} e^{-\beta H(\underline{p}, \underline{q})}. \tag{11}$$

Lorsque les températures sont différentes, l'existence, l'unicité et la convergence exponentielle ont été établies sous des hypothèses relativement générales sur les potentiels U et V [31, 29, 87]. Dans le cas d'interactions harmoniques, la covariance de l'état stationnaire a été calculée exactement en [77, 90].

Afin de décrire la conduction de la chaleur dans un solide cristallin, on définit une fonction d'énergie locale,

$$h_i(\underline{p},\underline{q}) = \frac{p_i^2}{2} + V(q_i) + \tfrac{1}{2}(U(q_{i+1}-q_i) + U(q_i - q_{i-1})) \tag{12}$$

pour $i \neq 1, N$ tandis que

$$h_1(\underline{p},\underline{q}) = \frac{p_1^2}{2} + V(q_1) + U(q_1) + \tfrac{1}{2}U(q_2 - q_1), \tag{13}$$

et h_N est défini de manière similaire. Le courant de chaleur est défini par l'évolution temporelle de l'énergie locale:

$$\frac{dh_i}{dt} = j_i^+ - j_i^- \tag{14}$$

pour $i \neq 1, N$ et où

$$j_i^+ = \tfrac{1}{2}F(q_i - q_{i+1})(p_i + p_{i+1}), \tag{15}$$

$$j_i^- = \tfrac{1}{2}F(q_{i-1} - q_i)(p_i + p_{i-1}). \tag{16}$$

$F = -U'$ et j_i est défini comme étant le courant microscopique d'énergie entre l'atome i et $i+1$, c'est à dire le taux de transfert d'énergie par unité de temps entre ces atomes. On observe que $j_{i-1}^+ = j_i^-$ et dans la suite nous utiliserons la notation $j_i \equiv j_i^+$.
On utilise aussi la notation $\langle . \rangle$ pour indiquer la moyenne par rapport à l'état stationnaire. On définit la température locale dans la chaîne comme étant:

$$\left\langle p_i^2 \right\rangle \equiv T_i. \tag{17}$$

Le courant moyen est

$$j \equiv \langle j_i \rangle = \frac{\omega^2}{2} \langle F(q_i - q_{i+1})(p_i + p_{i+1}) \rangle \tag{18}$$

qui doit être constant le long de la chaîne par conservation de l'énergie, en vertu de,

$$\left\langle \frac{dh_i}{dt} \right\rangle = \left\langle j_i^+ \right\rangle - \left\langle j_i^- \right\rangle = 0\,,\ i \neq 1, N \tag{19}$$

et $j_{i-1}^+ = j_i^-$.
La loi de Fourier énonce que

$$j = \kappa(T_i)(T_{i+1} - T_i) \tag{20}$$

où κ est la conductivité du cristal. Le problème fondamental est de comprendre comment la partie anharmonique rend cette constante finie dans la limite d'un nombre d'oscillateur tendant vers l'infini. Ensuite, on voudrait être capable de calculer sa valeur comme fonction des interactions microscopiques et de la température locale.

Analyse perturbative.

En collaboration avec Alain Schenkel [59], nous avons développé une théorie de perturbations pour les Hamiltoniens de la forme (8) avec $U(x) = \omega^2 \frac{x^2}{2}$ et $V(x) = \mu^2\omega^2 \frac{x^2}{2} + \lambda \frac{x^4}{4}$ en prenant comme paramètre perturbatif λ. Nous avons calculé la correction au premier ordre des fonctions de corrélation de l'état stationnaire hors équilibre. Nous avons effectué le calcul en démontrant en premier lieu une formule utile pour analyser la matrice de covariance de l'état stationnaire. Nous avons développé une méthode pour résoudre des équations dont les inconnues sont des matrices possédant certaines propriétés de symétrie. Nous avons d'abord montré que la correction au premier ordre du courant ne dépend pas de la taille du système. Ensuite, nous avons montré que la première correction au profil de température est linéaire lorsque la partie harmonique du potentiel d'accrochage est nulle. Le signe du gradient de température est opposé au signe de celui de la différence de températures entre les deux bains de chaleur.

Conduction de la chaleur et collisions entre phonons.

Au cours du siècle passé, de nombreuses méthodes ont été développées pour permettre un calcul théorique de quantités telles que la conductivité thermique. La plus connue est sans doute celle de la réponse linéaire permettant de décrire des situations proches de l'équilibre; elle lie la réponse à un forçage hors équilibre aux fluctuations du même système à l'équilibre thermique. En revanche, cette méthode n'aborde pas la question de la détermination de l'effet des nonlinéarités sur les propriétés de transport de la chaleur. Une autre théorie permettant quant à elle de comprendre dynamiquement l'approche (ou retour) à l'équilibre pour des gaz très dilués est basée sur l'équation de Boltzmann dont la validité repose sur des hypothèses portant sur les conditions initiales du système que l'on souhaite étudier. Cette approche est ce qu'on appelle la théorie cinétique. Elle peut être envisagée pour toutes sortes de situations hors équilibre pour des systèmes dont les composantes interagissent faiblement. Elle permet elle aussi de calculer certains coefficients de réponse. En particulier, pour le système décrit ci-dessus, modélisant les solides cristallins dont les atomes interagissent entre eux et avec un substrat externe par l'intermédiaire d'interactions faiblement anharmoniques. C'est l'approche qu'a initiée Peierls [80] en écrivant une équation correspondant à l'équation de Boltzmann pour l'évolution des nombres d'occupation des phonons dans un contexte quantique. On peut reformuler le problème dans un cadre classique et obtenir une équation analogue pour l'évolution des fonctions de corrélations correspondant aux modes propres de vibration d'une chaîne d'oscillateurs. Les interactions anharmoniques (faibles) entre les modes propres de la chaîne sont prises en compte sous une forme analogue aux collisions entre atomes d'un gaz dilué. Pour évaluer concrètement des quantités telles que la conductivité thermique dans le cadre de la réponse linéaire, il faut alors analyser le noyau

de collisions entre les modes propres de la chaîne. Techniquement, cela se résume à localiser explicitement certaines résonances entre les phonons. C'est ce que nous avons réalisé en collaboration avec Alain Schenkel [60]. La validité de notre calcul théorique de la conductivité thermique a été vérifiée à deux reprises par des simulations numériques [2, 62]. De manière surprenante vu l'ancienneté du problème, ce calcul était le premier reliant la conductivité thermique aux paramètres microscopiques du modèle. Il a également permis de mettre un terme à une certaine confusion entourant l'explication des mécanismes donnant lieu à une conductivité finie dans les solides cristallins en termes de processus "Umklapp".

Grandes déviations et caractérisation variationelle des états hors équilibre.

Une autre approche, plus globale, des phénomènes hors équilibre qui a connu une activité considérable ces dernières années est l'étude des fluctuations et des grandes déviations dans les systèmes hors équilibre de grande taille [5, 6, 7, 9]. Cette approche est reliée à une autre ancienne tentative de caractériser les états hors équilibre par un principe variationnel, c'est à dire le principe de minimum de production d'entropie [82]. Bien que ses déficiences loin de l'équilibre soient bien connues, il s'agit là d'une description potentiellement universelle et analogue à la caractérisation des états d'équilibre en termes d'un principe variationel. Récemment, Maes et Netočný [66] ont observé que dans les systèmes aléatoires hors équilibre la théorie des grandes déviations fournit naturellement une caractérisation variationelle des états stationnaires et que celle-ci est reliée au principe de minimum de production d'entropie. La théorie des grandes déviations étudie les fluctuations exponentiellement rares de la dynamique. L'objet central décrivant ces fluctuations est le taux de décroissance exponentielle dans le temps d'une fluctuation de la dynamique décrite par une statistique différente de l'état stationnaire. Une formule explicite a été donnée par Donsker et Varadhan [24, 25] pour cette fonctionnelle de grandes déviations. Lorsque la dynamique aléatoire possède de bonnes propriétés ergodiques, la mesure minimisant la fonctionelle de grande déviations est l'état stationnaire du système. D'un point de vue physique, l'aspect intéressant est que ceci peut être relié au principe du minimum de production d'entropie. Ceci a été mis en évidence par Maes et Netočný pour des processus de sauts Markoviens. En collaboration avec Thierry Bodineau [8], nous avons étudié comment le formalisme de Donsker-Varadhan s'applique aux réseaux d'oscillateurs hamiltoniens couplés à des thermostats stochastiques. Bien qu'en général ces systèmes soient non réversibles, ils possèdent certaines propriétés de symmétrie sous renversement du temps. Nous avons utilisé ces propriétés pour démontrer une formule générale pour la fonctionnelle de Donsker-Varadhan. Cette formule généralise la formule habituelle pour les dynamiques réversibles. Nous avons aussi établi précisément la relation qui existe entre le principe variationnel pour les mesures invariantes fourni par la fonctionnelle de Donsker-Varadhan et le principe de minimum d'entropie. Nous avons calculé explicitement la fonctionnelle de grande déviations du courant dans le cas d'une chaîne harmonique couplée à des bains de chaleur.

1.3 Dynamiques de collisions et leurs description stochastiques.

Dynamiques de collisions.

En collaboration avec Thomas Gilbert, nous avons introduit une classe de modèles [43] obtenus comme limites de chaines d'oscillateurs lorsque l'on prend des interactions en un site et entre plus proches voisins de plus en plus anharmoniques. Typiquement, dans ces modèles, les particules sont confinées dans des boîtes disposées sur un réseau régulier et interagissent avec les particules des boites voisines par des interactions de cœur dur, c'est-à-dire de manière analogue aux particules d'un gaz ordinaire. Pour fixer les idées, considérons les modèles d'échange complet sur un réseau unidimensionel ou encore les modèles "carré-corde" introduits en [43]. Les premiers sont obtenus comme limites de modèles de chaines d'oscillateurs disposés sur un réseau et décrits par un Hamiltonien H de la forme,

$$H(\underline{p},\underline{q}) = \sum_{i=1}^{N} \frac{p_i^2}{2} + V(q_i) + U(q_i - q_{i+1}) \tag{21}$$

dans lequel les interactions deviennent de plus en plus anharmoniques, jusqu'à se transformer en puits de potentiel infini. C'est -à -dire que l'on prend

$$V_k(x) = f_k(\frac{x}{b}), \qquad U_k(x) = f_k(\frac{x}{a}), \tag{22}$$

avec $f_k(x) = x^{2k}/2k$ et k tendant vers l'infini. La dynamique consiste alors en des particules piégées et se mouvant librement dans des boîtes de taille $2b$ disposées sur un réseau uni-dimensionel et échangeant leur vitesse avec leur plus proche voisin lorsque leur distance par rapport à celui-ci devient supérieure à un certain paramètre a. Dans les modèle "carré-corde", les particules se meuvent dans des boîtes de forme carrée et interagissent lorsqu'une "corde"reliant deux particules voisines se tend. La dynamique peut être visualisée aisément sur les figures suivantes. Lorsque l'on réalise une analyse numérique de ces deux

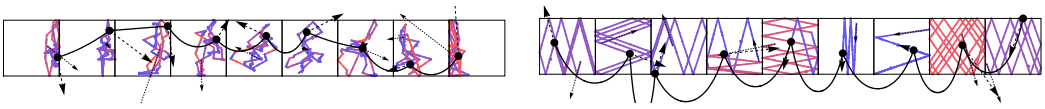

Figure 1.1: Trajectoires typiques du modèle carré-corde pour deux valeurs de la longueur maximale de la corde, colorées du bleu au rouge en fonction de leur énergie. Les petites et grandes flèches indiquent respectivement les vitesses initiales et finales.

modèles, on observe dans les deux cas que la loi de Fourier est vérifiée et que la conductivité est finie. Cependant, on observe aussi que l'approche de type Boltzmann n'est valide que dans le cas des modèles "carré-corde". La différence de comportement entre les deux modèles est évidemment intéressante en elle-même et mériterait une étude plus approfondie. Nous verrons plus bas que certains modèles stochastiques que nous avons introduit avec Lorenzo Zambotti [61] permettent de rendre compte de la différence entre ces modèles.

D'un point de vue théorique, ces modèles ont l'avantage de posséder à la fois la structure d'ordre spatial caractérisant les solides et des interactions se faisant par l'intermédaire de collisions, typiques des gaz. Ceci les rend aussi particulièrement utiles pour étudier la conduction de la chaleur dans les aérogels, gels conservant une matrice solide et dont les composants liquides ont été retirés et remplacés par des atomes de gaz. On peut représenter les atomes comme des petites boules piégées dans leur cellule (nanopore) et entrant en collision avec leurs voisines par l'intermédiaire de trous dans la paroi des cellules. Considérant un régime où les interactions sont rares et le nombre de particules grand, nous avons appliqué une approche de type Boltzmann pour calculer théoriquement la conductivité thermique en fonction des paramètres microscopiques du modèle. Nous avons validé cette approche avec une très grande précision en comparant le résultat prédit théoriquement à la mesure directe de la conductivité thermique des modèles au moyen de simulations numériques. Ces modèles sont intéressants à la fois d'un point de vue théorique et en vue de possibles applications à l'étude des aérogels. Nous allons donner ci-dessous une description stochastique de ces dynamiques. Afin de justifier l'aléa introduit dans les modèles, il est important de comprendre comment il émerge dans les modèles déterministes. Les dynamiques décrites par des interactions régulières et les dynamiques de collisions possèdent des différences qualitatives et certaines similarités que nous discutons maintenant. Dans les deux cas, les interactions entre les composants se font exclusivement entre plus proches vosins sur le réseau et l'évolution de l'énergie locale peut donc s'écrire :

$$E_n(t) - E_n(0) = J_{n-1\to n}([0,t]) - J_{n\to n+1}([0,t]). \tag{23}$$

Dans le cas de potentiels d'interaction réguliers le courant d'énergie intégré entre les site n et $n+1$ prend la forme

$$J_{n\to n+1}([0,t]) = \int_0^t \tfrac{1}{2}(\mathbf{p}_n(s) + \mathbf{p}_{n+1}(s)) \cdot \nabla U(\mathbf{q}_n(s) - \mathbf{q}_{n+1}(s))ds$$

tandis que dans le cas des dynamiques de collisions

$$J_{n\to n+1}([0,t]) \;=\; \tfrac{1}{2} \sum_{0\le k\le N_t} \left[p_n^\perp (S_n^k)^2 - p_{n+1}^\perp (S_n^k)^2\right], \tag{24}$$

où la composante du vecteur $\mathbf{p}_n$ dans la direction du vecteur unité $\widehat{\mathbf{n}} = ||q_i - q_{i+1}||^{-1}(q_i - q_{i+1})$ à l'instant de la collision est noté $p_n^\perp = \mathbf{p}_n \cdot \widehat{\mathbf{n}}$. N_t compte le nombre de collision jusqu'au temps t et $(S_n^k)_k$ est la suite des temps de collision. Notons que dans les modèles d'échange complet, $p_n^\perp = p_n$ et le courant intégré entre les deux voisins est simplement la somme de tous les échanges d'énergie cinétique entre les particules. Supposons à présent qu'un tel système soit thermalisé à des températures différentes à ses extrémités. Pour comprendre le transfert d'énergie d'un bout à l'autre du système, on s'intéresse au comportement ergodique du courant et on veut calculer $\lim_{t\to+\infty} t^{-1} J_{n\to n+1}([0,t])$ qui donne le courant moyen d'énergie dans l'état stationnaire. A cause de la forme particulière du courant intégré (24), il est naturel de supposer que l'équilibre local s'instaure et que la limite est donnée par

$$\lim_{t\to+\infty} \frac{1}{t} J_{n\to n+1}([0,t]) = \nu\,(T_n - T_{n+1}) \tag{25}$$

où $\nu = \lim_{t\to\infty} t^{-1}N_t$ est la fréquence de collisions entre les voisins sous des conditions d'équilibre local. $T_n = \frac{1}{2}\langle p_n^2\rangle$ est l'énergie cinétique moyenne. La conductivité est donc donnée par la fréquence de collisions. Typiquemment, les collisions se produisent quand les particules sont proches des frontières de leur cellule et par conséquent la fréquence de collisions est proportionnelle au nombre moyen de visites aux frontières par unité de temps. La particule se déplaçant librement dans sa cellule, la fréquence est proportionnelle à $\sqrt{T_n}$. Une fois cette relation établie, le profil de température peut être calculé parce que, par conservation de l'énergie, le courant est constant à travers le système:

$$\lim_{t\to+\infty} \frac{1}{t} J_{(n-1)\to n}([0,t]) = \lim_{t\to+\infty} \frac{1}{t} J_{n\to n+1}([0,t]).$$

Ceci est équivalent à une équation aux différences finies pour l'ensemble des températures de la distribution d'équilibre local. Les études numériques ont montré que l'identification de la conductivité à la fréquence de collisions est valide avec un très haut degré de précision pour une grande classe de dynamique de collisions, lorsque les particules entrent en collision rarement. Un élément important de notre analyse [43] est que cette identification ne dépend pas des propriétés de chaos local de la dynamique.

Bien qu'il n'y ait pas de manière aussi directe de deviner la conductivité dans les systèmes faiblement anharmoniques, il existe des similarités entre les deux types de dynamique lorsqu'on les considère dans un régime d'interaction faible et qu'on décrit le systèmes dans les coordonnées les mieux adaptées. Dans les deux cas, une équation de Boltzmann linéarisée décrit correctement les propriétés thermiques des systèmes. Selon le contexte, chaque mode ou particule se comporte comme s'il était couplé à un bain de chaleur idéal et l'intensité du couplage fournit la conductivité thermique. Cette quantité est aussi identifiée avec la fréquence de collisions entre les composants (phonons ou particules) à l'équilibre. Plus précisément, dans le cas de dynamique de collisions, chaque particule se déplace librement dans sa cellule et interagit avec ses voisines comme si elles faisaient partie d'un bain de chaleur infini.

Traceurs et diffuseurs chauds pour la conduction de la chaleur dans les dynamiques de collisions.

Avec Lorenzo Zambotti [61], nous avons introduit et étudié de nouveaux modèles stochastiques pour la conduction de la chaleur dans les dynamiques de collisions décrites ci-dessus. Un aspect important des modèles de collisions est que l'évolution de l'énergie se produit à des temps discrets et consiste en un échange d'énergie cinétique entre les voisins. La longueur de l'intervalle de temps entre deux collisions successives dépend de l'énergie cinétique de la particule, ce qui fixe la dépendance en $\sqrt{T}$ de la fréquence de collisions. L'idée initiale est donc de construire et d'analyser des modèles qui sont stochastiques au départ et possèdent la structure générale donnée par la description de la dynamique en termes d'équation de Boltzmann.

Par conséquent, on considère des dynamiques qui consistent en un mélange de dynamique Hamiltonienne intégrable et de collisions avec des bains de chaleur stochastiques. Les modèles que nous avons construits sont fait de diffuseurs décrits comme des bains de chaleur et de traceurs qui transfèrent de l'énergie entre ces diffuseurs. Chaque traceur se déplace dans un intervalle

unidimensionnel à l'intérieur duquel les diffuseurs se trouvent situés sur un réseau. Le mouvement d'un traceur est balisitique sauf quand il rencontre un diffuseur. A cet instant, sa vitesse est mise à jour aléatoirement selon une loi qui dépend de la température du diffuseur. La température des diffuseurs est finalement fixée par la condition qu'en moyenne, dans l'état stationnaire, aucune énergie ne soit échangée entre les diffuseurs et les traceurs. Conceptuellement, cette condition est similaire à celle utilisée dans la chaîne d'oscillateurs "auto-consistants"[10, 13, 14], mais dans notre cas elle peut être interprétée naturellement comme imposant la condition que le transfert d'énergie par unité de temps entre les diffuseurs soit constant tout le long du système.

Géométriquement, les systèmes que nous étudions sont analogues à ceux introduits et étudiés par [33, 34, 76]. Les diffuseurs de nos modèles sont similaires aux "energy storing devices" de ces modèles. Cependant, dans notre cas, la dynamique est stochastique depuis le début et l'action d'un diffuseur est supposée modéliser l'action d'un très grand système. Comme dans ces modèles, nous pouvons distinguer deux types de dynamique. Selon que les particules sont libres ou confinées entre les diffuseurs, nous montrons que le profil de température des diffuseurs doit être linéaire ou non. Ces deux types de comportements semblent être universels pour les systèmes décrits par une dynamique de collision à l'échelle microscopique [33, 34, 76, 42, 43, 83].

En tant que processus stochastiques, nos modèles sont naturellement décrits comme des processus de renouvellement Markoviens. La dynamique la plus simple que l'on peut imaginer est celle d'une particule dans une boîte : la particule frappe la paroi de la boîte et sa vitesse est mise à jour selon une certaine distribution de probabilité. Nous avons d'abord calculé la mesure invariante de ce processus. Cela a permis de justifier rigoureusement la règle de mise à jour utilisée dans les simulations numériques [97]. Ensuite, nous avons calculé la mesure invariante pour les dynamiques décrites ci-dessus et nous avons démontré que selon que les particules sont libres ou confinées entre les diffuseurs le profile auto-consistant des températures des diffuseurs est linéaire ou non. L'identité de la conductivité thermique et de la fréquence de collisions apparaît comme une conséquence naturelle du théorème de renouvellement pour les processus de renouvellement Markoviens. Nous avons aussi étudié la fonction génératrice des cumulants du courant d'énergie intégré. Nous avons donné une formule permettant de calculer explicitement les dérivées de tout ordre de la fonction génératrice. Ceci permet d'établir la formule de Green-Kubo pour ces modèles. Un aspect frappant de ce modèle que nous avons pu mettre en évidence est le manque d'analyticité de la fonction génératrice dès que l'on veut décrire une situation hors équilibre. L'origine de ce phénomène peut être attribuée à la présence de particules de vitesse arbitrairement petite.

1.4 Organisation du mémoire.

Chaque chapitre de ce mémoire consiste en un résumé cohérent, mis à jour et contextualisé des résultats obtenus dans un ou plusieurs articles. Les parties les plus techniques des preuves sont systématiquement omises.

Chapter 2

Ergodicity of the stochastic Navier-Stokes equations in 2D.

I give here some background and summary of the research works I pursued during my first postdoctoral years. This corresponds to references [16, 17, 18]. In those works, in collaboration with Jean Bricmont and Antti Kupiainen we showed the ergodicity of the Navier-Stokes equations with a stochastic external forcing.

2.1 Turbulence.

I give some general background that may be found in [50]. The understanding and control of turbulence in fluids remains one of the major unsolved problems of classical physics and it is easy to understand why physicists, mathematicians and enginneers continue to study it intensively. On the one hand it has enormous practical consequences ranging form airplane and ship design to weather forecasts. On the other hand, it is believed to be a property of solutions of a relatively simple partial differential equation, the Navier-Stokes (NS) equation. The simplicity of the equation stands in contrast with the complexity of the phenomena. The main problem resides in the mathematical treatment of the non-linear term in the equations.

Let us consider a fluid (i.e. a gas or a liquid) confined in a region $\Omega \subset \mathbb{R}^d$ where the spatial dimension d is in applications usually 3 or 2. Denoting the velocity of the fluid at a point $\mathbf{x}$ and at time t by $\mathbf{u}(t, \mathbf{x}) \in \mathbb{R}^d$, the NS equation is

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} - \nu \nabla^2 \mathbf{u} = \tfrac{1}{\rho}(\mathbf{f} - \nabla p)\,, \tag{1}$$

where ν is the viscosity of the fluid, ρ its density, $\mathbf{f}$ is the external force acting on the fluid and p is the pressure. We will restrict the discussion to the case of *incompressible* fluids wich means that ρ is constant and that $\mathbf{u}$ is divergence free $\nabla \cdot \mathbf{u} = 0$. It follows then by taking the divergence of both sides of (1) that $\nabla^2 p = -\nabla \cdot (\mathbf{u} \cdot \nabla)\mathbf{u}$ so the pressure becomes a function of the velocity field $\mathbf{u}$.

Eq. (1) is a nonlinear parabolic PDE (actually an integrodifferential equation due to the pressure term). The $\nu \nabla^2 \mathbf{u}$ term in the NS equation represents

the effect of friction and tends to smoothen and drive down the motion of the fluid. The motion is maintained by the external force $\mathbf{f}$, whereas the action of the nonlinear term is much more complicated and is of course crucial for the turbulent behaviour of fluids. However difficult to understand might be its effect on the dynamics, it has the property of conserving the energy (the L^2-norm of the velocity field) in any dimension and the enstrophy (the L^2 norm of the rotational of the velocity field) in 2D.

As we will see below, a series of progresses have been made concerning the ergodicity of the Navier-Stokes when the external force becomes stochastic. A important issue to settle is what kind of force is physically relevant to the problem of turbulence. In experimental situations the forcing may be produced by boundary conditions like in the case of a flow in a pipe or around an obstacle (e.g. airplane wing) where the velocity field vanishes at the boundary and takes a characteristic value far enough away from it (the relative velocity of the air and the plane or the velocity with which the fluid enters the pipe). Alternatively, one may use an explicit stirring mechanism : an external force is then applied on a characteristic lengthscale: L. In the equation (1) we could e.g. consider $\mathbf{f}$ whose Fourier transform in $\mathbf{x}$, $\widehat{\mathbf{f}}(t,\xi)$ has compact support near $|\xi| = L^{-1}$.

It is intuitively clear that the relative sizes of ν and $\mathbf{f}$ contribute to the strength of the nonlinearity: $\mathbf{f}$ tends to increase $\mathbf{u}$ and ν drive it down. A more precise formulation of this intuition involves the *Reynolds number*, a measure of the strength of the nonlinear effects that takes into account two symmetries of (1): scale and Galilean invariance.

A scale invariant measure of the relative strength of the forcing vs viscosity is given by the Reynolds number

$$Re = \frac{L\delta u}{\nu}, \tag{2}$$

where δu is a characteristic size of velocity differences produced by the force. The reason why velocity differences and not absolute velocities matter is that the NS equation is invariant (modulo boundary conditions) under Galilean transformation $\mathbf{u}(t,\mathbf{x}) \to \mathbf{u}(t,\mathbf{x}+\mathbf{v}t) - \mathbf{v}$ where $\mathbf{v}$ is a constant velocity. For the flow in the pipe or around the wing we may take δu as the difference of the velocity at the boundary (zero actually) and far away from it.

The basic phenomenological facts about hydrodynamic flows are as follows. If $Re \ll 1$, one encounters regular (" laminar") flows. For Re between ~ 1 and $\sim 10^2$, a series of bifurcations occur leading to ever more complicated flows ("transition to chaos"). Finally, for $Re \gg 10^2$, a peculiar chaotic state, turbulence, is reached that seems to exhibit for very large Re ("*developed turbulence*") universal features, i.e. features that are independent on the detailed nature of the forcing. In particular for large Re another length scale η seems to emerge in the problem in addition to the forcing scale L and the invariant measure seems to possess universal features for scales between η and L. As $Re \to \infty$ the scale $\eta \to 0$ and in this limit the so called *inertial range* $[\eta, L]$ extends all the way to zero. The so-called *cascade picture* of turbulence describes the system as follows : the stationary state is an energy flux state where energy is injected to the system at large scales and transported in the

inertial range by the nonlinearity to small scales where it is dissipated by the viscous forces. The repartition of the energy among the modes of the system is described by the so-called Kolmogorov spectrum. It is given by a polynomial decay with a specific exponent.

2.2 Probabilistic estimates.

In this section we consider the Navier-Stokes equation with a random force, white noise in time and large scale in space and prove probabilistic estimates for the long time behaviour of the solutions. These estimates imply that the solution of the stochastic equation remains analytic for all times and bounds on the energy spectrum, i.e the repartition of energy per mode. Our analysis was inspired by a paper of Mattingly and Sinai [75] who gave a simple proof of the analyticity of the solutions of the 2d Navier-Stokes equation. We extended their analysis to the random case.

We consider the stochastic Navier-Stokes equation for the velocity field $\mathbf{U}(t,\mathbf{x})$ defined on the torus $\mathbf{T}_L = (\mathbb{R}/2\pi L\mathbf{Z})^2$:

$$d\mathbf{U} + ((\mathbf{U}\cdot\nabla)\mathbf{U} - \nu\nabla^2\mathbf{U} + \nabla p)dt = d\mathbf{F} \tag{3}$$

where $\mathbf{F}(t,\mathbf{x})$ is a Wiener process with covariance

$$\mathbb{E}F_\alpha(s,\mathbf{x})F_\beta(t,\mathbf{y}) = \min\{s,t\}C_{\alpha\beta}(\tfrac{\mathbf{x}-\mathbf{y}}{L}) \tag{4}$$

and $C_{\alpha\beta}$ is a smooth function defined on the unit torus and satisfying $\partial_\alpha C_{\alpha\beta} = 0$. (4) represents large scale forcing, the scale being the size of the box. (3) is supplemented with the incompressibility condition $\nabla\cdot\mathbf{U} = 0 = \nabla\cdot\mathbf{F}$ and we will also assume the vanishing averages over the torus: $\int_{\mathbf{T}_L}\mathbf{U}(0,\mathbf{x}) = 0 = \int_{\mathbf{T}_L}\mathbf{F}(t,\mathbf{x})$ which imply that $\int_{\mathbf{T}_L}\mathbf{U}(t,\mathbf{x}) = 0$ for all times t.

(3) implies the transport equation for the vorticity $\Omega = \partial_1 U_2 - \partial_2 U_1$:

$$d\Omega + ((\mathbf{U}\cdot\nabla)\Omega - \nu\nabla^2\Omega)dt = dG, \tag{5}$$

where $G = \partial_1 F_2 - \partial_2 F_1$ has the covariance

$$\mathbb{E}G(t,\mathbf{x})G(s,\mathbf{y}) = L^{-2}\min\{s,t\}\Gamma(\tfrac{\mathbf{x}-\mathbf{y}}{L})$$

with $\Gamma = -\Delta\mathrm{tr}C$.

It is convenient to change to dimensionless variables s.t. ν and L become one. This is achieved by setting

$$\mathbf{U}(t,\mathbf{x}) = \tfrac{\nu}{L}\mathbf{u}(\tfrac{\nu}{L^2}t, \tfrac{1}{L}\mathbf{x})\,,\ \Omega(t,\mathbf{x}) = \tfrac{\nu}{L^2}\omega(\tfrac{\nu}{L^2}t, \tfrac{1}{L}\mathbf{x}).$$

Then $\mathbf{u}$ and ω live on the unit torus and satisfy (3) and (5) with ν and L replaced by 1, and C and Γ replaced by

$$c = \tfrac{L^4}{\nu^3}C\,,\ \gamma = \tfrac{L^4}{\nu^3}\Gamma\,.$$

Going to the Fourier transform $\omega_{\mathbf{k}}(t) = (2\pi)^{-2}\int_{\mathbf{T}_1} e^{i\mathbf{k}\cdot\mathbf{x}}\omega(t,\mathbf{x})d\mathbf{x}$ with $\mathbf{k}\in\mathbf{Z}^2$ we may write the enstrophy equation as

$$d\omega_{\mathbf{k}} = (-\mathbf{k}^2\omega_{\mathbf{k}} + \sum_{\mathbf{l}\in\mathbf{Z}^2\setminus\{\mathbf{0},\mathbf{k}\}}(\mathbf{k}\times\mathbf{l})|\mathbf{l}|^{-2}\omega_{\mathbf{k}-\mathbf{l}}\omega_{\mathbf{l}})dt + df_{\mathbf{k}} \tag{6}$$

where $\mathbf{k} \times \mathbf{l} = k_1 l_2 - l_1 k_2$ and $\{f_{\mathbf{k}}\}$ are Brownian motions with $\bar{f_{\mathbf{k}}} = f_{-\mathbf{k}}$ and

$$\mathbb{E} f_{\mathbf{k}}(s) f_{\mathbf{l}}(t) = \min\{s,t\} \delta_{\mathbf{k},-\mathbf{l}} \gamma_{\mathbf{k}}$$

and we have used the relation $\mathbf{u_k} = i\frac{(-k_2,k_1)}{\mathbf{k}^2}\omega_{\mathbf{k}}$.

The dimensionless control parameter is the ω injection rate,

$$R = \frac{1}{2}\sum_{\mathbf{k}\in\mathbf{Z}^2} \gamma_{\mathbf{k}} = \frac{1}{2}\gamma(0) = \frac{1}{2}\frac{L^4}{\nu^3}\Gamma(0),$$

which is proportional to the third power of the Reynolds number $Re = L^{\frac{4}{3}}\epsilon^{\frac{1}{3}}\nu^{-1}$ ($\epsilon = \frac{1}{2}\mathrm{tr}\, C(0)$ is the energy injection rate) in our model. Ultimately, one is interested in the turbulent region $R \to \infty$. We make the following assumption on the noise covariance:

$$\gamma_{\mathbf{k}} \le CRe^{-|\mathbf{k}|}. \tag{7}$$

The coefficient of $|\mathbf{k}|$ is arbitrary, but we require exponential decay. The physically relevant case is the one with $\gamma_{\mathbf{k}} \neq 0$ only for a finite number of $\mathbf{k}$ with $|\mathbf{k}|$ of the order of unity.

To state the main result of this section, define the enstrophy

$$\Phi = \frac{1}{2}\sum_{\mathbf{k}} |\omega_{\mathbf{k}}|^2 \tag{8}$$

and fix numbers $r > 1$, $\alpha > 1 + r$. Consider, for positive D, the norm

$$||\omega||_D = \sup_{\mathbf{k}} |\omega_{\mathbf{k}}||\mathbf{k}|^r e^{D^{-\alpha}|\mathbf{k}|}. \tag{9}$$

D will vary below, but r and α are fixed.

Theorem. *Let $||\omega(0)||_{D_0} \le D_0^\alpha < \infty$ and $\Phi(0) = K < \infty$. Then, there exists a random function D_t , $D_t < \infty$ for all t, such that with probability* 1, *$||\omega(t)||_{D_t} < D_t^\alpha$. For any $t > C(\log D_0 + \log K)$, and for $D^2 > CR\log R$,*

$$\mathrm{Prob}\{||\omega(t)||_D \le D^\alpha \ \ \& \ \ \Phi(t) \le D^2\} \ge 1 - Ce^{-c\frac{D^2}{R}}. \tag{10}$$

Remark. Here and below, C (and c) are sufficiently large (small) constants, which may vary from place to place but that are uniformly bounded as $R \to \infty$. The theorem says that with probability one $\omega(t, \mathbf{x})$ is analytic for all times, the dissipation scale is (up to a logarithm) $> R^{-\frac{1}{2}\alpha}$ and the energy spectrum

$$e(k) \equiv k^{-1}\int_{S^1} d\widehat{\mathbf{k}} E|\omega_{\widehat{\mathbf{k}}k}|^2 \le CR^{\widetilde{\alpha}}k^{-(2r+1)}$$

with $k = |\mathbf{k}|$, where r can be taken arbitrary close to 1 and $\widetilde{\alpha}$ arbitrary close to $1 + r$. These bounds hold for any fixed time and also for the average of these quantities over any fixed time interval. For example, using Jensen's and Chebyshev's inequalities, one derives from (10)

$$\mathrm{Prob}\{\frac{1}{T}\int_t^{t+T} |\omega_{\mathbf{k}}(s)|^2 ds > D^{2\alpha}k^{-2r}e^{-2D^{-\alpha}k}\} \le Ce^{-c\frac{D^2}{R}}.$$

(10) also implies that all correlation functions of the type

$$E\prod_i \nabla^{n_i}\omega(t,x_i)$$

exist. Such assumptions were used eg. in [36] to to derive some physical consequences concerning 2d turbulence.
What is the relationship of these results with the standard 2d turbulence picture [53, 4]? One considers (3) in infinite volume with the forcing as we do at spatial scale L, but *not periodic*, rather, for instance, having a smooth Fourier transform with compact support around L^{-1}. Then it is expected that a stationary state for Ω emerges for which the energy spectrum $e(k) = k^{-1}\int_{S^1} d\widehat{\mathbf{k}}\int d\mathbf{x}e^{ik\widehat{\mathbf{k}}\cdot\mathbf{x}}\mathbb{E}\Omega(\mathbf{x})\Omega(0)$ has two scaling regimes

$$e(k) \propto \left\{ \begin{array}{cc} k^{-3} & \eta^{-1} >> k >> L^{-1} \\ k^{-\frac{5}{3}} & k << L^{-1} \end{array} \right\} \tag{11}$$

refered to as the direct (enstrophy) cascade regime and the inverse (energy) cascade regime respectively. The scale η is the "viscous scale" beyond which the $e(k)$ decays more rapidly and it scales like $\nu^{\frac{1}{2}}$. In particular, the total energy density $\int_0^\infty e(k)dk$ is infinite in the stationary state. This means that starting with say vanishing $\mathbf{u}$ at time zero, the energy density increases linearly with time and for the ensuing stationary state only the vorticity remains a well defined random field. One can also work in finite volume like in this paper by forcing the system in an intermediate scale $\eta << \ell << L$, provided the energy is absorbed by friction acting on the $|\mathbf{k}| \sim L^{-1}$ regime. This indeed is what one does in experimental approaches, see for instance [78].

In our case the absence of the friction forces the energy to dissipate in the short scales too and the spectrum should be different from (11). Our bound above is certainly far from realistic, but one would expect the $e(k)$ to diverge as $R \to \infty$. It would be very interesting to get hold of the direct and inverse cascade regimes, but certainly much more sophisticated ideas are needed than what are used in the present paper.

2.3 Force acting at discrete time.

As we explained above, a convenient mathematical model for the study of homogenous isotropic turbulence is to consider the Navier-Stokes equation subject to a random stationary (in space and time) forcing. The turbulent situation is modelled by a smooth force, i.e. one whose Fourier transform decays fast for large wave numbers. One is then interested in various properties of the correlation functions of the velocity field in a stationary state of the ensuing stochastic process. An obvious first question concerns the large time convergence to such a stationary state starting from an arbitrary initial condition of the velocity field, i.e. the uniqueness of the stationary state. In this section I state the first result that I obtained with J.Bricmont and A. Kupiainen regarding the existence, uniqueness and exponential mixing of the stationary state in the case of two dimensional turbulence.

We consider the Navier-Stokes equation for an incompressible velocity field $\mathbf{u}(t,\mathbf{x})$ defined on the torus $\mathbf{T} = (\mathbb{R}/2\pi\mathbf{Z})^2$:

$$\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nu\Delta\mathbf{u} = \mathbf{f} - \nabla p \tag{12}$$

supplemented with the incompressibility condition

$$\nabla\cdot\mathbf{u} = 0. \tag{13}$$

The external force $\mathbf{f}(t,\mathbf{x})$ consists of random kicks at discrete times

$$\mathbf{f}(t,\mathbf{x}) = \sum_{\mathbf{k}\in\mathbf{Z}^2} e^{-2\pi i\mathbf{x}\cdot\mathbf{k}}\mathbf{f}_{\mathbf{k}}(t) \tag{14}$$

with

$$\mathbf{f}_{\mathbf{k}}(t) = \sum_{n\in\mathbf{Z}} \delta(t-n)\mathbf{f}_{\mathbf{k},n}. \tag{15}$$

The random variables $\mathbf{f}_{\mathbf{k},n}$ will be taken Gaussian, with mean zero, $\bar{\mathbf{f}_{\mathbf{k}}} = \mathbf{f}_{-\mathbf{k}}$ and covariance

$$\mathbb{E} f^{\alpha}_{\mathbf{k}}(m) f^{\beta}_{\mathbf{l}}(n) = \delta_{\mathbf{k},-\mathbf{l}}\delta_{m,n}\delta^{\alpha\beta}\,\phi_{\mathbf{k}}.$$

Furthermore, we will assume $\phi_0 = 0$, which implies the vanishing of the average force over the torus: $\int_{\mathbf{T}} \mathbf{f}(t,\mathbf{x}) = 0$. Assuming also zero average initial velocity $\int_{\mathbf{T}} \mathbf{u}(0,\mathbf{x}) = 0$ we conclude that $\int_{\mathbf{T}} \mathbf{u}(t,\mathbf{x}) = 0$ for all times t.

It is convenient to solve the incompressibility condition (13) by expressing the Navier-Stokes equation (12) in terms of the vorticity $\omega = \partial_1 u_2 - \partial_2 u_1$ which satisfies the transport equation

$$\partial_t\omega + (\mathbf{u}\cdot\nabla)\omega - \nu\Delta\omega = g, \tag{16}$$

where $g = \partial_1 f_2 - \partial_2 f_1$.

Going to the Fourier transform $\omega_{\mathbf{k}}(t) = (2\pi)^{-2}\int_{\mathbf{T}} e^{i\mathbf{k}\cdot\mathbf{x}}\omega(t,\mathbf{x})d\mathbf{x}$ with $\mathbf{k}\in\mathbf{Z}^2$, we may solve the velocity in terms of the vorticity as

$$\mathbf{u}_{\mathbf{k}} = i\tfrac{(-k_2,k_1)}{\mathbf{k}^2}\omega_{\mathbf{k}}$$

and write the vorticity equation as

$$\partial_t\omega_{\mathbf{k}} = -\nu\mathbf{k}^2\omega_{\mathbf{k}} + \sum_{\mathbf{l}\in\mathbf{Z}^2\setminus\{\mathbf{0},\mathbf{k}\}} (\mathbf{k}\times\mathbf{l})|\mathbf{l}|^{-2}\omega_{\mathbf{k}-\mathbf{l}}\omega_{\mathbf{l}} + \sum_{n\in\mathbf{Z}}\delta(t-n)g_{\mathbf{k}}(n) \tag{17}$$

where $\mathbf{k}\times\mathbf{l} = k_1 l_2 - l_1 k_2$ and $g_{\mathbf{k}}(n)$ are Gaussian with mean zero, $\bar{g_{\mathbf{k}}} = g_{-\mathbf{k}}$ and covariance

$$E g_{\mathbf{k}}(m) g_{\mathbf{l}}(n) = \delta_{\mathbf{k},-\mathbf{l}}\delta_{m,n}\,\gamma_{\mathbf{k}}.$$

with

$$\gamma_{\mathbf{k}} = \mathbf{k}^2\phi_{\mathbf{k}}.$$

We assume

$$b^{-1}e^{-\kappa_\gamma^{-1}|\mathbf{k}|} \le \gamma_{\mathbf{k}} \le b e^{-\kappa_\gamma^{-1}|\mathbf{k}|} \tag{18}$$

where $\kappa_\gamma > 0$, and we think of b as being large. We will be interested in the turbulent region $\nu \to 0$; therefore, when it is convenient, *we will always assume below that ν is small enough*, although our results hold for all ν.

Before stating our result, we need some definitions. First, we define the enstrophy as (a multiple of) the square of the L^2 norm

$$\Phi = \frac{1}{2}\sum_{\mathbf{k}} |\omega_{\mathbf{k}}|^2 = \frac{1}{2}||\omega||^2_{L^2}. \tag{19}$$

Next, we fix a number $r > 1$ and consider the Banach space

$$\Omega = \{\omega \mid \|\omega\| \equiv \sup_{\mathbf{k}} |\omega_{\mathbf{k}}||\mathbf{k}|^r < \infty\}$$

as our probability space, with $\mathcal{B}$ the product σ-algebra. Note that Ω is a subspace of L^2.

Finally, due to the analyticity (with probability one) of the noise, $\omega(t)$ also will turn out to be analytic with probability one and it will be useful to introduce norms capturing this property. For any positive number κ, we define a norm (that we shall call the κ-norm),

$$||\omega||_\kappa = \sup_{\mathbf{k}} |\omega_{\mathbf{k}}||\mathbf{k}|^r e^{\kappa^{-1}|\mathbf{k}|}. \tag{20}$$

Functions with $||\omega||_\kappa < \infty$ are analytic in a κ^{-1} neighbourhood of the torus. The factor $|\mathbf{k}|^r$ is useful technically (and was already used in [75]).

The stochastic equation (17) gives rise to a Markov chain $\omega(n)$, $n \in \mathbf{N}$ defined by

$$\omega(n+1) = F(\omega(n)) + g(n+1) \tag{21}$$

where F is the map at time 1 of the Navier-Stokes flow (17) without the forcing. We denote by $P(\omega, E)$ the transition probability of this chain.
Our main result is the

Theorem 1 *The Markov chain (21) is defined on $(\Omega, \mathcal{B})$ and has a unique invariant measure μ there. It satisfies*

$$\int 1_{(||\omega||_\kappa \geq \nu\kappa)} \mu(d\omega) \leq C \exp(-c\nu^4 \kappa^{\frac{2}{\alpha}}) \tag{22}$$

for any $\alpha > 1 + r$, and $C, c < \infty$, depending on α. Moreover, $\forall \omega \in \Omega$ and $\forall E \in \mathcal{B}$, we have,

$$|P^t(\omega, E) - \mu(E)| \leq C(\omega) e^{-mt} \tag{23}$$

where $m = m(\nu) > 0$ for all ν, and $C(\omega) \leq C(\frac{\|\omega\|+1}{\nu})^C$.

Remark 2 *Since $||\cdot||_{\kappa'} < ||\cdot||_\kappa$ for $\kappa' > \kappa$, (22) holds for all κ'-norms with $\kappa' > \kappa$ too, including the norm $||\cdot||$ defining Ω, which corresponds to $\kappa' = \infty$. Estimate (22) means that with high probability ω is analytic in a $\nu^{2\alpha}$-neighbourhood of the torus and bounded there by $\nu^{1-2\alpha}$. By taking r close to 1, α can be taken close to 2.*

Remark 3 *Here and below, we denote by C or c a "generic" constant that can vary from place to place, even in the same equation.*

Remark 4 *We obtain a lower bound on m in (23) of the form $m \geq \exp(-C\nu^{-3}(\log \nu^{-1})^c)$ (see Proposition 2 and Lemma 4 below), which means, however, that our estimate on the rate of convergence is unphysically small for ν small.*

The proof of Theorem 1 is based on probabilistic estimates and on properties of the deterministic Navier-Stokes equation, which we discuss now.

2.3.1 Properties of the deterministic flow : analyticity improving.

In this section we derive some properties of the flow of the deterministic Navier-Stokes equation, i.e. (17) without the forcing term $g_{\mathbf{k}}(t)$. Let us define a family of subsets of Ω that impose constraints on the size of the L^2-norm and of the κ-norm:

$$U(\kappa, \phi, A) = \{\omega | \Phi \leq \phi, \ ||\omega||_\kappa \leq A\}. \tag{24}$$

Then, we introduce a one-parameter subfamily of $U(\kappa, \phi, A)$:

$$U_\kappa \equiv U(\kappa, \phi(\kappa), A(\kappa)) \tag{25}$$

where, $\phi(\kappa) = \nu^2 \varphi \kappa^{\frac{2}{\alpha}}$ and $A(\kappa) = \nu a \kappa$. This family is useful because, as we shall see, the flow maps one U_κ in that family into another one with a smaller κ. The parameter α will be taken to satisfy $\alpha > 1 + r$ and φ and a will be chosen small depending on some "geometric" constants that will appear in the course of the proof. Thus, if $\omega \in U_\kappa$, then for all $\mathbf{k}$ we have

$$|\omega_{\mathbf{k}}| \leq \nu a \kappa |\mathbf{k}|^{-r} e^{-\kappa^{-1}|\mathbf{k}|} \tag{26}$$

and

$$\Phi \leq \nu^2 \varphi \kappa^{\frac{2}{\alpha}} \tag{27}$$

Let now

$$\kappa(t) = \frac{\kappa}{1 + \eta \nu t \min(1, \kappa)} \tag{28}$$

where η will be chosen suitably small below, and denote also by $\omega(t)$ the solution of (17) without the forcing term $g_{\mathbf{k}}(t)$.

Proposition 5 *(a) Let $\omega(0) \in U_\kappa$, then for all $0 \leq t \leq 1$, $\omega(t) \in U_{\kappa(t)}$.*
(b) Suppose $\omega(0) \in \Omega$ with $\|\omega(0)\| \leq D\nu$. Then $\omega(1) \in U_\kappa$ for $\kappa = C(D^\alpha + \frac{1}{\nu})$.

The point of part (a) of this Proposition is that the domain of analyticity of the solution of the unforced Navier-Stokes equation increases with time and its L^2 and κ-norms decrease with time. Part (b) says that, even if $\omega(0)$ is not analytic, but belongs to Ω, the solution after time 1 is analytic and its L^2 and κ-norms are bounded in terms of the norm of the initial data in Ω. Our proof of Proposition 1 is inspired by [75] (see also [16]).

2.3.2 Confinement of the stochastic dynamics.

We define a region $U \equiv U_{\nu^{-p}}$, where $p > \frac{7}{2}\alpha$, and in which the solution of (17) is confined with high probability. Let us divide the transition probability into a likely and unlikely part:

$$P(\omega, E) = Q(\omega, E) + R(\omega, E) \tag{29}$$

where

$$Q(\omega, E) = \chi_U(\omega) P(\omega, U \cap E). \tag{30}$$

The following Proposition about the dynamics in U and the unprobability of excursions outside U will play a central role in the proof of our uniqueness result[1].

Proposition 6 *(a) There exist constants $c, C < \infty$, $c' > 0$, such that for all $\omega \in U$, $E \in \mathcal{B}$,*

$$|Q^t(\omega, E) - Q^t(0, E)| \leq 4e^{-mt} \tag{31}$$

where $m \geq \exp(-C\nu^{-3}(\log \nu^{-1})^c)$ and $t \leq c' m^{-1} \nu^{-q}$, with $q \equiv \frac{2p}{\alpha} - 4 > 3$.
(b) There exists $\zeta < 1$, $c > 0$, $C < \infty$, such that $\forall \kappa \geq 0$, for all $\omega \in U_\kappa$ and for $\kappa' \geq \zeta\kappa$,

$$P(\omega, U^c_{\kappa'}) \leq C \exp(-c\nu^4 {\kappa'}^{\frac{2}{\alpha}}) \tag{32}$$

The proof of (31) is based on a standard argument for exponential convergence of Markov chains (given in Doob [26]), and the idea is fairly simple. If Q was a genuine transition probability, it would be enough, in order to prove the Proposition, to show that Q has good mixing properties. The precise properties are stated in the Lemmas below.

First, Lemma 7 says that, for any point in U there is a nonzero probability to go in a finite time to a smaller region $\bar{U} \subset U$ determined by the covariance of the noise and thus by κ_γ:

$$\bar{U} \equiv U_{2\kappa_\gamma + \rho\nu}. \tag{33}$$

where $\rho > 0$ will be chosen below (sufficiently small)[2]. This is an easy consequence of Proposition 5. On each time interval, the solution increases its domain of analyticity (which is determined by κ, i.e. κ decreases); then, if the "kicks" of the noise are sufficiently small (but not too small, so that this event is not too unprobable), the solution reaches $\bar{U}$ in a finite time (of order $\nu^{-1} \log \nu^{-1}$).

[1] Here and below, the kernel $AB(\omega, E)$ is defined in the obvious way by $\int A(\omega, d\omega') B(\omega', E)$.

[2] Similar ideas were used by Kuksin and Shirikyan in [49].

Secondly, we show in Lemma 8 that, in the region $\bar{U}$, the stochastic dynamics is sufficiently mixing; this is again due to the fact that the deterministic Navier-Stokes evolution increases the domain of analyticity of the solution.

Third, the fact that Q is not a bona fide transition probability is what limits the Proposition to finite times. For longer times, we will need to have some estimate on the probability of escaping the region U, which follows from part (b) of the Proposition. Indeed, the latter implies, using (29, 30) and taking $\kappa = \kappa' = \nu^{-p}$ that, for all $\omega \in U$,

$$P(\omega, U^c) = R(\omega, \Omega) \leq e^{-c\nu^{-q}}, \tag{34}$$

with $q = \frac{2p}{\alpha} - 4 > 3$ (remember that $p > \frac{7}{2}\alpha$ and that ν is small).

Lemma 7 *There exist constants $c, C < \infty$, such that $\forall \omega \in U$,*

$$P^{T_1}(\omega, \bar{U}) \geq \exp(-C\nu^{-3}(\log \nu^{-1})^c) \tag{35}$$

with $T_1 = C\nu^{-1} \log \nu^{-1}$.

Lemma 8 *There exist constants $c, C < \infty$, such that, $\forall \omega, \omega' \in \bar{U}$, $\forall B \subset \bar{U}$,*

$$P(\omega, B) + P(\omega', \bar{U} \backslash B) \geq \exp(-C\nu^{-2}(\log \nu^{-1})^c) \tag{36}$$

Lemmas 7, 8 imply that there exist

$$\delta(\nu) \equiv \exp(-C\nu^{-3}(\log \nu^{-1})^c)$$

and

$$T \equiv T(\nu) = C\nu^{-1} \log \nu^{-1}$$

with $C, c < \infty$, such that $\forall \omega, \omega' \in U$ and $\forall B \subset \bar{U}$,

$$P^T(\omega, B) + P^T(\omega', \bar{U} \backslash B) \geq \delta(\nu) \tag{37}$$

which implies in turn, since $\bar{U} \subset U$, that $\forall \omega, \omega' \in U$ and $\forall B \subset U$,

$$P^T(\omega, B) + P^T(\omega', U \backslash B) \geq \delta(\nu) \tag{38}$$

This the main inequality that is used in the proof of Proposition 6.

2.4 Force acting up to the dissipative scale.

In this section, I explain how we extended the analysis of previous section to the case where only finitely many modes are excited, and the forcing is white noise in time. An essential ingredient in this analysis is the Lyapunov-Schmidt type reduction introduced in [49], that allows to transform the original Markov process with infinite dimensional state space to a non-Markovian process with finite dimensional state space. We apply standard ideas of statistical mechanics

(high temperature expansions) to this process to deduce mixing properties of the dynamics.

We consider the stochastic Navier-Stokes equation for the velocity field $u(t,x) \in \mathbb{R}^2$ defined on the torus $\mathbf{T} = (\mathbb{R}/2\pi\mathbf{Z})^2$:

$$du + ((u \cdot \nabla)u - \nu\nabla^2 u + \nabla p)dt = df \tag{39}$$

where $f(t,x)$ is a Wiener process with covariance

$$Ef_\alpha(t,x)f_\beta(t',y) = \min\{t,t'\}C_{\alpha\beta}(x-y) \tag{40}$$

and $C_{\alpha\beta}$ is a smooth function satisfying $\sum_\alpha \partial_\alpha C_{\alpha\beta} = 0$. Equation (39) is supplemented with the incompressibility condition $\nabla \cdot u = 0 = \nabla \cdot f$, and we will also assume that the averages over the torus vanish: $\int_{\mathbf{T}} u(0,x) = 0 = \int_{\mathbf{T}} f(t,x)$, which imply that $\int_{\mathbf{T}} u(t,x) = 0$ for all times t.

It is convenient to change to dimensionless variables so that ν becomes equal to one. This is achieved by setting $u(t,x) = \nu u'(\nu t, x)$. Then u' satisfies (39), (40) with ν replaced by 1, and C by

$$C' = \nu^{-3}C.$$

From now on, we work with such variables and drop the primes. The dimensionless control parameter in the problem is the (rescaled) energy injection rate $\frac{1}{2}\mathrm{tr}\, C'(0)$, customarily written as $(\mathrm{Re})^3$ where Re is the Reynolds number:

$$\mathrm{Re} = \epsilon^{\frac{1}{3}}\nu^{-1},$$

and $\epsilon = \frac{1}{2}\mathrm{tr}\, C(0)$ is the energy injection rate in the original units (for explanations of the terminology see [39]).

In two dimensions, the incompressibility condition can be conveniently solved by expressing the velocity field in terms of the vorticity $\omega = \partial_1 u_2 - \partial_2 u_1$. First (39) implies the transport equation

$$d\omega + ((u \cdot \nabla)\omega - \nabla^2\omega)dt = db, \tag{41}$$

where $b = \partial_1 f_2 - \partial_2 f_1$ has the covariance

$$Eb(t,x)b(t',y) = \min\{t,t'\}(2\pi)^{-1}\gamma(x-y)$$

with $\gamma = -2\pi\nu^{-3}\Delta\mathrm{tr}C$.

Next, going to the Fourier transform, $\omega_k(t) = \frac{1}{2\pi}\int_{\mathbf{T}} e^{ik\cdot x}\omega(t,x)dx$, with $k \in \mathbf{Z}^2$; we may express u as $u_k = i\frac{(-k_2,k_1)}{k^2}\omega_k$, and write the vorticity equation as

$$d\omega(t) = F(\omega(t))dt + db(t), \tag{42}$$

where the drift is given by

$$F(\omega)_k = -k^2\omega_k + \frac{1}{2\pi}\sum_{l\in\mathbf{Z}^2\setminus\{0,k\}} \frac{k_1 l_2 - l_1 k_2}{|l|^2}\omega_{k-l}\omega_l \tag{43}$$

and $\{b_k\}$ are Brownian motions with $\bar{b}_k = b_{-k}$ and

$$Eb_k(t)b_l(t') = \min\{t, t'\}\delta_{k,-l}\,\gamma_k.$$

The dimensionless control parameter for the vorticity equation is

$$R = \sum_{k\in\mathbf{Z}^2} \gamma_k = 2\pi\gamma(0) \tag{44}$$

which is proportional to the ω injection rate, and also to the third power of the Reynolds number. We will be interested in the turbulent region $R \to \infty$; therefore, we will always assume below, when it is convenient, that R is sufficiently large.

As I explained above, one is interested in the properties of stationary state of the stochastic equation (42) in the case of *smooth* forcing (see [16] for some discussion of this issue) and, ideally, one would like to consider the case where one excites only a finite number of modes,

$$\gamma_k \neq 0\ ,\ k^2 \leq N,$$

with N of order of one. In this paper we assume that N scales as

$$N = \kappa R, \tag{45}$$

with κ an absolute constant fixed below. We take all the other $\gamma_k = 0$, although this condition can easily be relaxed. Let us denote the minimum of the covariance by

$$\rho = \min\{|\gamma_k| \mid |k|^2 \leq N\}.$$

Before stating our result, we need some definitions. Let P be the orthogonal projection in $H = L^2(\mathbf{T})$ to the subspace H_s of functions having zero Fourier components for $|k|^2 > N$. We will write

$$\omega = s + l$$

with $s = P\omega$, $l = (1-P)\omega$ (respectively, the small k and large k parts of ω). Denote also by H_l the complementary subspace (containing the nonzero components of l). H is our probability space, equipped with $\mathcal{B}$, the Borel σ-algebra.

The stochastic equation (42) gives rise to a Markov process $\omega(t)$ and we denote by $P^t(\omega, E)$ the transition probability of this process.

Our main result is the

Theorem. *The stochastic Navier-Stokes equation* (42) *defines a Markov process with state space* $(H, \mathcal{B})$ *and for all* $R < \infty$, $\rho > 0$ *it has a unique invariant measure* μ *there. Moreover,* $\forall \omega \in H$, *for all Borel sets* $E \in H_s$ *and for all bounded Hölder continuous functions* F *on* H_l, *we have,*

$$\left|\int P^t(\omega, d\omega')1_E(s')F(l') - \int \mu(d\omega')1_E(s')F(l'))\right| \leq C(\omega)||F||_\alpha e^{-mt} \tag{46}$$

where $m = m(R, \rho, \alpha) > 0$, $||F||_\alpha$ *is the Hölder norm of exponent* α, *and* $C(\omega)$ *is a.s. finite.*

We have shown above that, with probability 1, the functions on the support of such a measure as constructed here are real analytic. In particular all correlation functions of the form

$$\int \mu(d\omega) \prod_i \nabla^{n_i} u(x_i)$$

exist.

We close this section by giving the outline of the proof and explain its connection to ideas coming from Statistical Mechanics.

Let us start by observing that, if we neglect the nonlinear term in (42-43), we expect $\|\omega\|$ to be of order $R^{\frac{1}{2}}$, for typical realizations of the noise ($R^{\frac{1}{2}}$ is the typical size of the noise, and the $-k^2\omega_k$ term will dominate in eq. (6) for larger values of $\|\omega\|$). It turns out that similar probabilistic estimates hold for the full equation (6) as shown in Section 3. Now, if $\|\omega\|$ is of size $R^{\frac{1}{2}}$, the $-k^2\omega_k$ term will dominate the nonlinear term (which is roughly of size $\|\omega\|^2$) in eq. (6), for $|k| \geq \kappa R^{\frac{1}{2}}$, and one can expect that those modes (corresponding to l above) will behave somewhat like the solution of the heat equation and, in particular, that they will converge to a stationary state.

Thus, the first step is to express the l-modes in terms of the s-modes at previous times. This produces a process for the s-modes that is no longer Markovian but has an infinite memory. In Statistical Mechanics, this would correspond to a system of unbounded spins (the s-modes) with infinite range interactions, with the added complications that, here, the measure is not given in a Gibbsian form, but only through a Girsanov formula, and that time is continuous. Hence, one must solve several problems: the possibility that ω is atypically large, the long range "interactions", and finally, showing that a version of the s-process with a suitable cutoff is ergodic and mixing.

The large ω problem is treated using probabilistic estimates developped in [16], which, in Statistical Mechanics, would be called stability estimates. The infinite memory problem is treated by methods inspired "high temperature expansion" in Statistical Mechanics, namely writing the Gibbs measure or, here, the Girsanov factor, as sum of products of factors having a finite range memory and which become smaller as that range increases. However, in the situation considered here, carrying out this expansion requires a careful and non standard partition of the phase space. The problem is that, even though for typical noise, hence for typical ω's, the l-modes depend exponentially weakly on their past, thus producing, typically, "interactions" that decay exponentially fast, they may depend sensitively on their past when the noise is large. In the language of Statistical Mechanices, atypically large noise produces long range correlations.

This problem of sensitive dependence is coupled to the last problem, that of the convergence of the s-process with finite memory to a stationary state. We have to get lower bounds on transition probabilities and we can prove those only when the s-modes remain for a sufficiently long time in a suitable region of the phase space; thus, if we did not control the sensitive dependence, we would not be able to carry out that last step.

2.5 Brief litterature overview.

There is by now a long history of proofs of the ergodicity of the 2D Navier-Stokes equation. The first ones treated the cases cases that do not correspond to the turbulence problem. Either the forcing was taken to decay very slowly for large $|\mathbf{k}|$, i.e. with a lower bound of the form $|\mathbf{k}|^{-p}$ (see [38] and references therein), or the viscosity is taken large [72]. The first proof of uniqueness in the case of a force exciting only a finite number of modes was given by Kuksin and Shirikyan in [49] where the authors consider a model like the one of section 1.3, the force is acting at discrete time but with bounded noise (each $g_{\mathbf{k}}$ has compact support). Simultaneously to our paper on the ergodicity and exponential mixing of the stochastic Navier-Stokes dynamics, E, Mattingly and Sinai published a paper [27] containing the proof of the uniqueness of the invariant measure. Their proof was more probabilistic in nature than ours which used a statistical mechanics approach. Mattingly then proved the exponential mixing in time of the dynamics [73]. In all those works, the number of modes excited by the external force was finite but increasing with the Reynolds number. A first step in the direction of taking a number of modes independent of R was taken by E and Mattingly in [28] where they showed that finite dimensional Galerkin approximations coupled to a stochastic force exciting only three modes are hypoelliptic diffusions. The optimal result was finally obtained by Hairer and Mattingly [44] following a first application of Malliavin calculus to the stochastic Navier-Stokes equations by Mattingly and Pardoux [74].

Chapter 3

Invariant measures of Hamiltonian dynamics out thermal equilibrium.

In this chapter, I present the results obtained in [59, 60].
A frequently used model to describe the transfer of heat in crystalline solids is given by coupled Hamiltonian oscillators located on a lattice and whose boundaries are thermalized at different temperatures. Namely, in one dimension, the set-up is as follows. At each site i of a lattice $\{1, \ldots, N\}$ is attached a particle of momentum p_i and position q_i. The dynamics is Hamiltonian in the bulk and stochastic through the Langevin coupling to heat baths at the boundaries. The Hamiltonian is of the form,

$$H(\underline{p}, \underline{q}) = \sum_{i=1}^{N} \Big(\tfrac{1}{2} p_i^2 + V(q_i) \Big) + \sum_{i=2}^{N} U(q_i - q_{i-1}) + U(q_1) + U(q_N). \tag{1}$$

The equations of motions are given by,

$$\begin{aligned} dq_i &= p_i dt, \quad i = 1, \ldots, N, \\ dp_i &= -\frac{\partial H}{\partial q_i}(\underline{p}, \underline{q}) dt, \quad i = 2, \ldots, N-1, \end{aligned} \tag{2}$$

and,

$$\begin{aligned} dp_1 &= -\frac{\partial H}{\partial q_1}(\underline{p}, \underline{q}) dt - \gamma p_1 dt + \sqrt{2\gamma k T_L}\, dw_l\,, \\ dp_N &= -\frac{\partial H}{\partial q_N}(\underline{p}, \underline{q}) dt - \gamma p_N dt + \sqrt{2\gamma k T_R}\, dw_r\,. \end{aligned} \tag{3}$$

T_L and T_R stand for the temperature of the left and right reservoirs, respectively, whereas w_l and w_r are two independent standard Wiener processes.

It is an easy fact to check that when $T_L = T_R = T = \beta^{-1}$, the equilibrium measure on the configuration space $\mathbf{R}^{2N}$ whose density with respect to the Lebesgue measure is given by

$$\rho(\underline{p}, \underline{q}) = Z^{-1} e^{-\beta H(\underline{p}, \underline{q})} \tag{4}$$

is invariant (stationary) for the stochastic dynamics defined above. In the case of two different temperatures, existence, uniqueness and exponential convergence to an unique invariant state has been established under fairly general conditions on the potentials U and V [31, 29, 87]. In the case of harmonic coupling, the covariance of the stationary state has been exactly computed in [77, 90].

The Gibbs-Boltzmann distribution allows in principle to analyze all the macroscopic properties of the system one wishes to study. WHen the temperatures on the boundaries are different, there does not exist such an explicit formula for the stationary state. The system is crossed by a flow of energy going from the high-temperature region to the low-temperature one. The lack of knowledge of the invariant measure makes difficult the computation of such a simple quantityt as the the thermal conductivity of the system. This is defined as the ratio of the heat flow and local temperature gradient. This quantity is analogous the equilibrium response functions such as the magnetic susceptibility in ferrmoganets. Over the past century various methods have been devised to allow theoretical computations of such quantities. One of these is the linear response theory which relates the response of the system to an small external constraint out of equilibrium to fluctuations of the system in equilibrium. Another theory which allows to understand the approach (or return) to equilibrium of dilute gases is based on Boltzmann equation. The same type of analysis maybe applied to different systems out of equilibrium when the components interact weakly. This kinetic theory approach has been initiated by Peierls in quantum mechanical context [80]. He established an equation for the occupation numbers of the phonons analogous to the Boltzmann equation One may reformulate the problem in classical set-up and obtain an analogous equation for the evolution of the correlation functions of the stationary waves of the harmonic oscillators chain perturbed by a small anharmonic term. The weak anharmonic interactions between the modes are taken into account under a collision term analogous to the one describing the collisions between the atoms in a dilute gas. To evaluate quantities such as the thermal conductivity, one must then analyze the collision kernel. Technically, this boils down to localize resonnances between phonons. That was achieved in a paper written in collaboration with Alain Schenkel [60]. The validity of our theoretical computation has been checked twice in numerical simulations [2, 62]. Maybe surprisingly, given the fact that the problem is an old one, this computation was the first to connect the value of the thermal conductivity to the microscopic parameters of the model. It also allowed to clarify some confusion in the litterature surrounding the mechanism giving rise to a finite conductivity in solid crystals and the role of what the physicists call the "Umklapp" processes. Before giving in section 3.3 a Boltzmann analysis outlined above, we explain the perturbative analysis that we begun for the stationary state of coupled anharmonic oscillators.

3.1 Perturbative analysis.

The goal of this section is to begin a perturbative analysis of invariant probability measures arising as stationary states of chains of weakly anharmonic

oscillators. The dynamics is as in previous section. As a model at hand, we will consider a hamiltonian chain of N harmonic oscillators interacting through nearest-neighbour harmonic interactions, coupled at its boundaries to stochastic heat baths of different temperatures, and that we will perturb by a small anharmonic (quartic) on-site interaction. The covariance of the stationary state in the purely harmonic case has been computed in [90, 77]. For other cases, i.e. anharmonic cases, almost nothing is known about the physical content of the stationary state, except results about the positivity of entropy production and validity of linear response theory [32]. The main obstacle to developing a perturbative expansion of SNS's is that, in contrast to the equilibrium case, no explicit formula for the invariant density is known. Moreover, the fact that the relevant models are degenerate in a stochastic sense makes it laborious to obtain a systematic perturbative expansion starting from the equations of motion. We circumvent this difficulty by deriving a formula for the two-point correlation functions of invariant states, which holds under the assumption of L^1-convergence of the finite-time correlation functions to those of the (unique) invariant measure. We emphasize that the validity of the formula is not restricted to the concrete problem of the anharmonic chain considered here. It may prove useful whenever the invariant measure is not explicitely known, in particular in the context of transport phenomena modelized by hypoelliptic stochastic processes. We also remark that the form of the formula for the covariance is very similar to, and provides a lower bound on, the expectation of the Malliavin matrix.

Our main result concerning the heat current is that its first-order correction remains uniformly bounded as the number of oscillators goes to infinity. In particular, perturbative analysis does not, at first order, reveal any sign that Fourier law holds in such anharmonic models as numerical studies suggest. Furthermore, we find that the first-order correction to the temperature profile is exponentially decaying in the bulk of the chain, with a decay rate that depends on the strength of the harmonic part of the on-site potential. When this strength vanishes, the correction to the temperature profile is linear. However, the sign is "wrong", in the sense that the linear profile has the *lowest* temperature near the *hottest* bath and the *highest* temperature near the *coldest* bath. This is analogous to the result of [90], where the temperature profile is also oriented in the "wrong" direction. The main difference is of course that in [90], the temperature profile is exponentially decaying. It would be interesting to examine the perturbation theory of the harmonic model with other couplings to heat baths. The Langevin coupling is probably not the optimal one and it might be responsible for the awkward orientation of the temperature profile. Another feature of our solution is that the temperature profile is shifted downwards, in the sense that the temperature at the middle point of the chain is lower than the arithmetic mean of the temperatures of the heat baths.

3.1.1 The Malliavin matrix and the covariance matrix of the stationary measure

We consider now a general system of stochastic equations. Denote by $x_t \in \mathbf{R}^d$ the solution of the stochastic differential equation,

$$dx_t = X_0(x_t)\, dt + \sum_{k=1}^{n} X_k(x_t)\, dw_k(t) \tag{5}$$

with initial condition $x_0 = x$, where the w_k's are n independent one-dimensional brownian motions and X_l, $l = 0, \ldots, n$, are $\mathcal{C}^\infty$ vector fields over $\mathbf{R}^d$ satisfying for any multi-index α,

$$||\partial^\alpha X_l(x)|| \leq C(1 + ||x||^{K_\alpha}) \tag{6}$$

for some $K_\alpha > 0$. We note that solutions to such equations are in general not ensured to exist globally. In the sequel, we restrict ourselves to the following situations.

Hypothesis 9 *For all $x \in \mathbb{R}^d$, equation (5) has a unique strong solution x_t, $t > 0$. This solution has finite moments of all order: for all $p \geq 1$, $T < \infty$, and $x \in \mathbb{R}^d$, there exists a constant $C = C(x, p, T) < \infty$ such that for $0 \leq t \leq T$,*

$$\mathbb{E}_x(||x_t||^p) \leq C. \tag{7}$$

When in need of emphasizing the dependence of the solution to (5) on the initial condition x and the realization of the d-dimensional Brownian motion w in the interval $[0, t]$, we shall write it as $x_t(x, w([0, t]))$. We denote by $\mathcal{P}^t$ the associated semigroup,

$$\mathcal{P}^t f(x) = \mathbb{E}_x(f(x_t)) \equiv \int f(x_t(x, w([0, t])))\, \mathbf{dP}(w([0, t]), \tag{8}$$

where $\mathbf{P}$ is the d-dimensional Wiener measure, by $\mathcal{A}$ the generator of the semigroup, and by L the associated second order differential operator,

$$L = \sum_{i=1}^{d} X_0^i\, \partial_i + \sum_{i,j=1}^{d} a_{ij}\, \partial_i \partial_j\,, \tag{9}$$

where, with $\otimes$ denoting the tensor product,

$$a = \tfrac{1}{2} \sum_{k=1}^{n} X_k \otimes X_k\,. \tag{10}$$

From Assumption 3.1 on the process solution x_t and the bounds (6) for the vector fields X_l, it follows that for each t and $w[0, t]$, the map $x \mapsto x_t(x, w[0, t])$ is $\mathcal{C}^\infty$ on $\mathbb{R}^d$ with derivatives of all orders satisfying the stochastic differential equation obtained from (5) by formal differentation. Furthermore, for all multi-index α, $p \geq 1$, and $t \geq 0$,

$$\mathbb{E}(||\partial^\alpha x_t(x, \cdot)||^p) < \infty. \tag{11}$$

In the sequel, we will denote $U_t(x, w[0,t]) = Dx_t(x, w[0,t])$, where DX denotes the Jacobian matrix of a vector field X on $\mathbb{R}^d$. The matrix U_t is the linearized flow and it solves the equation, with initial condition $U_0 = \mathbf{1}$,

$$dU_t = DX_0(x_t)U_t\,dt + \sum_{k=1}^{n} DX_k(x_t)U_t\,dw_k(t)\,. \tag{12}$$

Below, $\mathbb{E}_x U_t$ denotes $\int U_t(x, w[0,t])\,\mathbf{dP}(w[0,t])$.

Let us now assume the existence of an invariant probability measure μ for the process solution x_t of (5) and consider the covariance matrix at time t,

$$C_t(x) \equiv \mathbb{E}_x(x_t \otimes x_t) - \mathbb{E}_x\, x_t \otimes \mathbb{E}_x\, x_t. \tag{13}$$

The following result is the starting point of the perturbative analysis performed in subsequent sections. It provides an expression for $\mu(C_t)$ in terms of the linearized flow U_t, where $\mu(f)$ is a shorthand notation for $\int_{\mathbb{R}^d} f(x)\,d\mu(x)$.

Proposition 10 *Suppose that the bounds (6) and Hypothesis 9 are satisfied. Suppose in addition that the invariant measure μ for the process solution x_t of (5) is such that the functions $x \mapsto \mathbb{E}_x\, x_s^i$, $x \mapsto L\mathbb{E}_x\, x_s^i$, and $x \mapsto a_{ij}(x)\mathbb{E}_x\, U_s^{jl}$, belong to $L^2(\mathbb{R}^d, d\mu)$ for all i, j, l, and $s \le t$. Then,*

$$\mu(C_t) = \int_0^t ds \sum_{k=1}^{n} \mu(\mathbb{E}_\cdot U_s X_k(\cdot) \otimes \mathbb{E}_\cdot U_s X_k(\cdot))\,. \tag{14}$$

Proof. We will show below that the map $s \mapsto \mu(\mathbb{E}_\cdot x_s \otimes \mathbb{E}_\cdot x_s)$ is differentiable, with

$$\frac{d}{ds}\mu(\mathbb{E}_\cdot x_s \otimes \mathbb{E}_\cdot x_s) = -\sum_{k=1}^{n} \mu(\mathbb{E}_\cdot U_s X_k(\cdot) \otimes \mathbb{E}_\cdot U_s X_k(\cdot))\,. \tag{15}$$

Identity (14) thus follows from the invariance of the measure μ, since

$$\begin{aligned} \mu(C_t) &= \mu(\mathbb{E}_\cdot(x_t \otimes x_t)) - \mu(\mathbb{E}_\cdot x_t \otimes \mathbb{E}_\cdot x_t) && (16)\\ &= \mu(x \otimes x) - \mu(\mathbb{E}_\cdot x_t \otimes \mathbb{E}_\cdot x_t) && (17)\\ &= -\int_0^t ds \frac{d}{ds}\mu(\mathbb{E}_\cdot x_s \otimes \mathbb{E}_\cdot x_s). && (18) \end{aligned}$$

To obtain (15), we first note that (7) implies that any function $f \in \mathcal{C}^2(\mathbb{R}^d)$ with first derivatives of at most polynomial growth is in the domain of the generator $\mathcal{A}$ with $\mathcal{A}f = Lf$. Similarly, one easily checks that for such f, (11) implies $\mathcal{A}(\mathcal{P}_t f) = L(\mathcal{P}_t f)$. Therefore, Kolmogorov equation yields $\frac{d}{ds}(\mathbb{E}_x\, x_s \otimes \mathbb{E}_x\, x_s) = L\mathbb{E}_x\, x_s \otimes \mathbb{E}_x\, x_s + \mathbb{E}_x\, x_s \otimes L\mathbb{E}_x\, x_s$, which, by Hölder inequality and our assumptions, belongs to $L^1(\mathbb{R}^d, d\mu)$. Thus,

$$\frac{d}{ds}\mu(\mathbb{E}_\cdot x_s \otimes \mathbb{E}_\cdot x_s) = \mu(L\mathbb{E}_\cdot x_s \otimes \mathbb{E}_\cdot x_s + \mathbb{E}_\cdot x_s \otimes L\mathbb{E}_\cdot x_s). \tag{19}$$

Let us next define for $f, g \in \mathcal{C}^2(\mathbb{R}^d)$,

$$\Gamma(f, g) \equiv L(fg) - fLg - gLf\,, \tag{20}$$

which reads

$$\Gamma(f,g) = 2\sum_{i,j=1}^{d} a_{ij}\,\partial_i f\,\partial_j g\,. \tag{21}$$

Since it follows from (11) that $\partial_i \mathbb{E}_x x_s^j = \mathbb{E}_x U_s^{ji}$, our assumptions imply as above that $\Gamma(\mathbb{E}_\cdot x_s^i, \mathbb{E}_\cdot x_s^j) \in L^1(\mathbb{R}^d, d\mu)$ for all i,j. It follows in particular that $L(\mathbb{E}_\cdot x_s \otimes \mathbb{E}_\cdot x_s) \in L^1(\mathbb{R}^d, d\mu)$. Because of the invariance of μ (which implies $\mu(Lf) = 0$), we are thus free to substract from the μ-expectation on the right hand side of (19) a term $L(\mathbb{E}_\cdot x_s \otimes \mathbb{E}_\cdot x_s)$, so that

$$\frac{d}{ds}\mu\Big((\mathbb{E}_\cdot x_s \otimes \mathbb{E}_\cdot x_s)_{ij}\Big) = -\mu(\Gamma(\mathbb{E}_\cdot x_s^i\,, \mathbb{E}_\cdot x_s^j)). \tag{22}$$

Formula (15) finally follows from the computation, recalling (10),

$$\Gamma(\mathbb{E}_\cdot x_s^i, \mathbb{E}_\cdot x_s^j)(x) = \sum_{k=1}^{n}\Big(\mathbb{E}_x U_s X_k(x) \otimes \mathbb{E}_x U_s X_k(x)\Big)_{ij}\,. \tag{23}$$

This concludes the proof of Proposition 3.2.

Proposition 3.2 immediately implies the

Corollary 11 *Suppose that the hypothesis of Proposition 3.2 are satisfied for all $t \geq 0$. Suppose in addition that*

$$\lim_{t\to\infty} C_t = \mu(x\otimes x) - \mu(x)\otimes\mu(x) \equiv \Phi\,, \tag{24}$$

in $L^1(\mathbb{R}^d, d\mu)$. Then,

$$\Phi = \int_0^\infty ds \sum_{k=1}^{n} \mu(\mathbb{E}_\cdot U_s X_k(.) \otimes \mathbb{E}_\cdot U_s X_k(.)). \tag{25}$$

The expression (25) for the covariance matrix of a stationary state is the basic formula that we shall use to develop a perturbation expansion in the next section. Since both sides of (25) involve an averaging with respect to μ, it is not clear at first sight how informations on μ can be extracted from (25). We observe, however, that in the case of a linear drift X_0 and constant vector fields X_k, $k = 1,\ldots,n$, all expectations may be dropped and (25) becomes

$$\Phi_{\rm linear} = \int_0^\infty ds\, U_s\Big(\sum_{k=1}^{n} X_k \otimes X_k\Big)U_s^{\rm T}. \tag{26}$$

One thus recovers the standard formula for the covariance of the stationary state of a linear stochastic equation with constant diffusion coefficients. As we shall see in the next section, it is possible to iterate this simple observation in order to begin a perturbation expansion.

Another feature of formula (14) is to provide a link between the covariance matrix C_t and the so-called Malliavin matrix. The Malliavin matrix associated to equation (5) at time t reads, in the normalization of [47],

$$M_t = \int_0^t ds \sum_{k=1}^{n} U_t V_s X_k(x_s) \otimes U_t V_s X_k(x_s)\,, \tag{27}$$

where V_s is the inverse matrix of U_s. An easy computation reveals that $\mu(\mathbb{E}_\cdot M_t)$ can be expressed in a form closely related to (14), namely,

$$\mu(\mathbb{E}_\cdot M_t) = \int_0^t ds \sum_{k=1}^n \mu(\mathbb{E}_\cdot(U_s X_k(.) \otimes U_s X_k(.))). \tag{28}$$

Indeed, we first observe that for $s \geq 0$ fixed, $Y_s^t \equiv U_t V_s$ satisfies $Y_s^s = \mathbf{1}$ and

$$dY_s^t = DX_0(x_t)Y_s^t\, dt + \sum_{k=1}^n DX_k(x_t)Y_s^t\, dw_k(t) \tag{29}$$

for $t \geq s$. Comparing with (12) yields that $Y_s^t = Y_s^t(x_s(x, w[0,s]), w[s,t])$ has the same $\mathbf{P}$-distributions as $U_{t-s}(x_s(x, w[0,s]), \bar{w}[s,t])$, where $\bar{w}(\tau) = w(\tau) - w(s)$ for $\tau \geq s$. Furthermore, for x fixed the map $w \mapsto Y_s^t(x, w[s,t])$ is $w[0,s]$-independent. Therefore, since $(x,w) \mapsto Y_s^t(x,w)X_k(x) \otimes Y_s^t(x,w)X_k(x)$ is measurable, one may use the Markov property of x_t to write,

$$\mathbb{E}_x(Y_s^t(x_s)X_k(x_s) \otimes Y_s^t(x_s)X_k(x_s)) = \mathbb{E}_x(\mathbb{E}_{y=x_s}(U_{t-s}(y)X_k(y) \otimes U_{t-s}(y)X_k(y))). \tag{30}$$

Identity (28) then follows by using the invariance of the measure μ and changing variables in the integral over s in (27). As a consequence, Proposition 3.2 provides a lower bound on the expectation of the Malliavin matrix.[1]

Corollary 12 *One has*

$$\mu(C_t) \leq \mu(\mathbb{E}_\cdot M_t). \tag{31}$$

Proof. The inequality simply follows from (14), (28), and the matrix

$$\mathbb{E}_x\Big[\Big(U_s X_k(x) - \mathbb{E}_x U_s X_k(x)\Big) \otimes \Big(U_s X_k(x) - \mathbb{E}_x U_s X_k(x)\Big)\Big] \tag{32}$$

being positive definite.

3.2 Perturbative analysis of the non-equilibrium anharmonic chain

We shall analyse the effect of adding an anharmonic perturbation to a modification of the model treated by Rieder, Lebowitz and Lieb [90]. We consider the case of a harmonic chain with fixed ends to which one adds an anharmonic on-site potential, i.e. in (1), we set

$$U(x) = \tfrac{1}{2}\omega^2 x^2 \quad \text{and} \quad V = \tfrac{1}{2}\omega^2\kappa x^2 + \frac{1}{4}\lambda x^4. \tag{33}$$

The model considered in [90] has $\kappa = 0$ but the computation of the covariance of the stationary state is very similar and the result is given below. We write the equations of motions (2)-(3) under the matrix form,

$$\begin{pmatrix} d\underline{q} \\ d\underline{p} \end{pmatrix} = \mathbf{b}\begin{pmatrix} \underline{q} \\ \underline{p} \end{pmatrix} dt - \lambda \begin{pmatrix} \mathbf{0} \\ \mathcal{N}(\underline{q}) \end{pmatrix} dt + \begin{pmatrix} \mathbf{0} \\ \mathbf{dw} \end{pmatrix} \tag{34}$$

[1] The order relation is defined in the following way. For two matrices X_1, X_2, we say that $X_1 \geq X_2$ whenever $X_1 - X_2$ is a positive definite matrix.

with $\mathcal{N}(\underline{q})$ and $\mathbf{dw}$ the vectors in $\mathbf{R}^N$ given by $\mathcal{N}_i(\underline{q}) = q_i^3$ and $\mathbf{dw}_i = \delta_{1i}\sqrt{2\gamma k T_1}\, dw_l + \delta_{Ni}\sqrt{2\gamma k T_N}\, dw_r$, and

$$\mathbf{b} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{g}_\kappa & -\mathbf{a} \end{pmatrix} \tag{35}$$

where $\mathbf{g}_\kappa$ and $\mathbf{a}$ are $N \times N$ matrices given by $(\mathbf{g}_\kappa)_{ij} = \omega^2((2+\kappa)\delta_{ij} - \delta_{ij+1} - \delta_{ij-1})$ and $\mathbf{a}_{ij} = \gamma\delta_{ij}(\delta_{1j} + \delta_{Nj})$. Above, $\mathbf{1}$ denotes the unit matrix and $\mathbf{0}$ the zero matrix or vector, as is clear from the context. We note that the stochastic terms in (34) are given by constant vector fields, namely, in the notation of Section 3,

$$X_k = \begin{pmatrix} \mathbf{0} \\ \mathbf{d}_k \end{pmatrix} \quad \text{where} \quad (\mathbf{d}_k)_j = \delta_{kj}\sqrt{2\gamma k T_k}\,, \tag{36}$$

for $k = 1, N$. In particular, the coefficients a_{ij} involved in the generator L are constant. They are given by

$$\sum_{k=1,N} X_k \otimes X_k = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \Delta \end{pmatrix}, \tag{37}$$

where $\Delta_{ij} = 2\gamma k \delta_{ij}(T_1\delta_{1j} + T_N\delta_{Nj})$. Furthermore, the linearized flow U_t^λ of (34) is given by

$$dU_t^\lambda = \mathbf{b}U_t^\lambda\, dt - 3\lambda C^\lambda(t)U_t^\lambda\, dt\,, \tag{38}$$

where

$$C^\lambda(t) = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{v}^\lambda(t) & \mathbf{0} \end{pmatrix}, \tag{39}$$

with $\mathbf{v}_{ij}^\lambda(t) = \delta_{ij}q_i^2(t)$ and $q_i(t)$ the q_i-component of the solution of (34) at time t. Finally, we note that the matrix $\mathbf{b}$ in (34) has the property that all its eigenvalues have strictly negative real part. A proof of this fact can be found in [77] modulo obvious modifications.

In order to study perturbatively the SNS of our chain, we would like to use the identity (25). However, some of the hypothesis of Corollary 3.3 related to the invariant measure are not known to hold for equation (34) when $\lambda > 0$. (The case $\lambda = 0$ has been covered in [90].) Although from a mathematical point of view, this is not a mere technical problem, but since the main goal of this paper is to illustrate the use of formula (25) for perturbative analysis on a specific example, we will assume that these hypothesis hold, see Assumption 4.1 below and the remark that follows. On the other hand, Assumption 3.1, i.e., the existence of strong solutions and their moments, follows from standard techniques and we briefly discuss it now. We first note that for $\lambda > 0$, the function $\widetilde{H}(\underline{q}, \underline{p}) = 2N + H(\underline{q}, \underline{p})$, with H the Hamiltonian given by (1) and (33), satisfies

$$\widetilde{H}(\underline{q}, \underline{p}) \geq C(1 + ||\underline{q}||^2 + ||\underline{p}||^2), \tag{40}$$

for some $C > 0$ and all $(\underline{q}, \underline{p}) \in \mathbb{R}^{2N}$. Thus, $\widetilde{H}$ is a $\mathcal{C}^2(\mathbb{R}^{2N})$ confining function. Furthermore, one computes

$$(L\widetilde{H})(\underline{q}, \underline{p}) = -\gamma(p_1^2 + p_N^2) + 2\gamma k(T_1 + T_N), \tag{41}$$

which implies that $L\widetilde{H}$ is uniformly bounded by above. A classical result, see e.g. [45], Thm 4.1, then ensures for all initial conditions $(\underline{q},\underline{p}) \in \mathbb{R}^{2N}$ the existence of a unique global strong solution to (34). Regarding the bounds (7), they are an immediate consequence of the following a priori bound. For any $\theta \leq (2k\max\{T_1,T_N\})^{-1}$, one has

$$\mathbb{E}_{(\underline{q},\underline{p})}\left[e^{\theta H(\underline{q}_t,\underline{p}_t)}\right] \leq e^{2\gamma k\theta(T_1+T_N)t}\, e^{\theta H(\underline{q},\underline{p})}\,. \tag{42}$$

Bound (42) can be obtained in a similar way as in the proof of Lemma 3.5 in [88]. However, the existence of a unique invariant measure for (34) is still an open problem. We thus introduce the following

Assumption 13 *The finite time truncated two-point correlation function of the process defined by (34) converges to the covariance matrix of a unique stationary measure μ^λ in $L^1(\mathbb{R}^{2N}, d\mu^\lambda)$-norm. Furthermore, the decay properties of μ^λ are such that $\mathbb{E}_{(\underline{q},\underline{p})}[(\underline{q}_t,\underline{p}_t)]$, $L\mathbb{E}_{(\underline{q},\underline{p})}[(\underline{q}_t,\underline{p}_t)]$, and $\mathbb{E}_{(\underline{q},\underline{p})}[U_t^\lambda]$ belong to $L^2(\mathbb{R}^{2N}, d\mu^\lambda)$.*

Remark. The uniqueness of the invariant measure is proved in [29, 88] for a large class of anharmonic chains. The invariant measure has a smooth density with exponential decay and is shown to be mixing [2]. An important restriction is that the potential U must not grow asymptotically slower than V, and thus equation (34) does not fall into the class covered in [29, 88]. However, as is argued in [88], the fact that the on-site potential grows faster than the nearest-neighbour interaction should not affect the ergodic properties of the measure but only the rate of convergence. Although we could consider a similar anharmonic chain with an additional quartic term in the nearest-neighbour interaction, the equations that one then needs to solve, see below, are computionally more involved. Furthermore, restricting to (34) will allow us to compare our results to the usual $\lambda\phi^4$ expansion when the temperatures of the two baths are equal.

Provided Assumption 4.1 holds, let Φ^λ denote the covariance matrix of the unique stationary state of equation (34) and express it according to (25) as

$$\Phi^\lambda = \int_0^\infty dt \sum_{k=1,N} \mu^\lambda(\mathbb{E}_\cdot U_t^\lambda X_k \otimes \mathbb{E}_\cdot U_t^\lambda X_k)\,. \tag{43}$$

We first briefely review the harmonic case $\lambda = 0$. As mentioned at the end of the previous section, one obtains from (43)

$$\Phi^0 = \int_0^\infty dt\, e^{\mathbf{b}t}\,\mathbf{D}\, e^{\mathbf{b}^{\mathrm{T}}t}\,, \tag{44}$$

where

$$\mathbf{D} = \sum_{k=1,N} X_k \otimes X_k = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \Delta \end{pmatrix}\,, \tag{45}$$

[2] In [88], the result is actually stronger. The convergence to the unique invariant measure is shown to be exponential.

with $\Delta_{ij} = 2\gamma k\delta_{ij}(T_1\delta_{1j} + T_N\delta_{Nj})$. Since the eigenvalues of $\mathbf{b}$ have strictly negative real part, the integral in (44) is convergent and it follows from integrating by parts in $\mathbf{b}\Phi^0$ that Φ^0 must satisfy the equation

$$\mathbf{b}\Phi^0 + \Phi^0\mathbf{b}^{\mathrm{T}} = -\mathbf{D}\,. \tag{46}$$

The unique solution of this equation has been explicitely derived in [90]. It is given by

$$\Phi^0 = \begin{pmatrix} \Phi^0_x & \Phi^0_z \\ -\Phi^0_z & \Phi^0_y \end{pmatrix} \tag{47}$$

where, denoting $T = \frac{T_1+T_N}{2}$, $\eta = \frac{T_1-T_N}{2T}$, and $\mathbf{G}_\kappa = \omega^{-2}\mathbf{g}_\kappa$,

$$\Phi^0_x = \frac{kT}{\omega^2}(\mathbf{G}_\kappa^{-1} + \eta\mathbf{X}^0), \tag{48}$$

$$\Phi^0_y = kT(\mathbf{1} + \eta\mathbf{Y}^0), \tag{49}$$

$$\Phi^0_z = \frac{kT}{\gamma}\eta\mathbf{Z}^0, \tag{50}$$

and

$$\mathbf{X}^0 = \begin{pmatrix} \phi_1 & \phi_2 & & \phi_{N-2} & \phi_{N-1} & 0 \\ \phi_2 & \ddots & \ddots & \ddots & \ddots & -\phi_{N-1} \\ \phi_3 & \ddots & \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \\ \phi_{N-1} & & & \ddots & \ddots & -\phi_2 \\ 0 & -\phi_{N-1} & & & -\phi_2 & -\phi_1 \end{pmatrix}, \tag{51}$$

$$\mathbf{Y}^0_{ij} = \delta_{ij}(\delta_{i1} - \delta_{iN}) - \nu\mathbf{X}^0_{ij}\,, \tag{52}$$

$$\mathbf{Z}^0 = \begin{pmatrix} 0 & \phi_1 & \phi_2 & & \phi_{N-2} & \phi_{N-1} \\ -\phi_1 & \ddots & \ddots & \ddots & & \phi_{N-2} \\ -\phi_2 & \ddots & \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \phi_2 \\ & & & \ddots & \ddots & \phi_1 \\ -\phi_{N-1} & & & -\phi_2 & -\phi_1 & 0 \end{pmatrix}. \tag{53}$$

Above, $\nu = \frac{\omega^2}{\gamma^2}$ and the quantities ϕ_j, $1 \le j \le N-1$, satisfy the equation

$$\sum_{j=1}^{N-1}(\mathbf{G}^{(N-1)}_{\nu+\kappa})_{ij}\phi_j = \delta_{1i}\,, \tag{54}$$

where $\mathbf{G}^{(k)}_{\nu+\kappa}$ denotes the k-square matrix given by $(\mathbf{G}^{(k)}_{\nu+\kappa})_{ij} = (2+\nu+\kappa)\delta_{ij} - \delta_{i,j+1} - \delta_{i,j-1}$. The solution of (54) is given by

$$\phi_j = \frac{\sinh(N-j)\alpha}{\sinh N\alpha}\,, \tag{55}$$

with α defined by $\cosh\alpha = 1 + (\nu+\kappa)/2$. Hence, one has for large N and fixed j the asymptotic formula $\phi_j = e^{-\alpha j}$. In the context of SNS, one usually defines the temperature to be the average kinetic energy, i.e. in our case,

$$T_i = (\Phi_y^0)_{ii}. \tag{56}$$

It is easy to see that the above solution yields an exponentially flat profile in the bulk of the chain.

We now turn to the first-order perturbation of the anharmonic chain. We first introduce our second assumption on the process solution of (34).

Assumption 14 *The measure μ^λ is absolutely continuous with respect to the Lebesgue measure and as a function of λ its density $\rho^\lambda(x)$ is C^∞ in a neighbourhood of 0. For all x, all derivatives are bounded in a neighbourhood of 0.*

Remark. The proof of this fact should follow from an analysis similar to the ones developped in [30] or [99] to prove the smoothness of the probability transitions in a parameter of the related stochastic differential equations.

To derive an expression for $\Phi^1 \equiv \frac{d}{d\lambda}\Phi^\lambda|_{\lambda=0}$, we compute from (43)

$$\begin{aligned}
\Phi^1 &= \frac{d}{d\lambda}\Phi^\lambda|_{\lambda=0} &(57)\\
&= \mu^1\Big(\int_0^\infty dt \sum_{i=1,N} \mathbb{E}_\cdot U_t^0 X_i(\cdot)\otimes \mathbb{E}_\cdot U_t^0 X_i(\cdot)\Big)\\
&\quad + \mu^0\Big(\int_0^\infty dt \sum_{i=1,N} \mathbb{E}_\cdot \frac{d}{d\lambda}U_t^\lambda|_{\lambda=0} X_i(\cdot)\otimes \mathbb{E}_\cdot U_t^0 X_i(\cdot)\Big) + \text{tr.}\,, &(58)
\end{aligned}$$

and observe that the first term vanishes because $\mu^1 \equiv \frac{d}{d\lambda}\mu^\lambda|_{\lambda=0}$ integrates constants to zero. In order to compute the last terms, we first evaluate $W_t \equiv \frac{d}{d\lambda}U_t^\lambda|_{\lambda=0}$. Deriving with respect to λ on both sides of equation (38), we get

$$dW_t = \mathbf{b}\, W_t\, dt - 3\, C^0(t)\, U_t^0\, dt, \tag{59}$$

from which it follows that, since $W_0 = 0$,

$$W_t = -3\int_0^t ds\, e^{\mathbf{b}(t-s)} C^0(s)\, e^{\mathbf{b}s}\,. \tag{60}$$

Inserting (60) in (58), we obtain, using in addition the invariance of μ^0,

$$\begin{aligned}
\Phi^1 &= -3\int_0^\infty dt \int_0^t ds \sum_{i=1,N} e^{\mathbf{b}(t-s)}\mathbf{N}\, e^{\mathbf{b}s} X_i \otimes e^{\mathbf{b}t} X_i + \text{tr.}\,, &(61)\\
&= -3\int_0^\infty dt \int_0^t ds\; e^{\mathbf{b}(t-s)}\,\mathbf{N}\, e^{\mathbf{b}s}\,\mathbf{D}\, e^{\mathbf{b}^{\mathrm{T}}t} + \text{tr.}\,, &(62)
\end{aligned}$$

where $\mathbf{D}$ is given by (45) and

$$\mathbf{N} = \mu^0(C^0(0)) = \begin{pmatrix} 0 & 0 \\ \mathrm{diag}(\Phi_x^0) & 0 \end{pmatrix}. \tag{63}$$

Exchanging the integrations over t and s and changing variables leads to

$$\Phi^1 = -3\int_0^\infty dt\, e^{\mathbf{b}t}\mathbf{N}\Big(\int_0^\infty ds\, e^{\mathbf{b}s}\,\mathbf{D}\, e^{\mathbf{b}^{\mathrm{T}}s}\Big)e^{\mathbf{b}^{\mathrm{T}}t} + \mathrm{tr.}\,, \tag{64}$$

which, with (44), finally yields,

$$\Phi^1 = -3\int_0^\infty dt\, e^{\mathbf{b}t}(\mathbf{N}\Phi^0 + \Phi^0\mathbf{N}^{\mathrm{T}})e^{\mathbf{b}^{\mathrm{T}}t}\,. \tag{65}$$

The method used to derive the above equation will also provide the equations for the next orders of the perturbative expansion. However, obtaining them concretely requires some more work and we reserve that part and the general Feynman rules for a further publication. We note that integrating by parts in (65) yields the equation for Φ^1

$$\mathbf{b}\Phi^1 + \Phi^1\mathbf{b}^{\mathrm{T}} = 3(\mathbf{N}\Phi^0 + \Phi^0\mathbf{N}^{\mathrm{T}}). \tag{66}$$

In Section 6, we will derive an explicit expression for Φ^1 and thus for the first order correction to the heat current and temperature profile. It turns out to be easier to do so by solving equation (66) rather than by using (65). We write :

$$\Phi^1 = \begin{pmatrix} \frac{1}{\omega^2}\mathbf{X}^1 & \frac{1}{\gamma}\mathbf{Z}^1 \\ -\frac{1}{\gamma}\mathbf{Z}^1 & \mathbf{Y}^1 \end{pmatrix}, \tag{67}$$

Heavy computations involving a systematic way to solve general matrix equations of the form (66) were developped in [59] and we obtained an exact solution Φ^1 as a function of Φ^0. One is mainly interested in the contribution to the temperature profile given by the diagonal elements of $\mathbf{Y}^1$ and the correction to the current given by the elements of $\mathbf{Z}^1$ of the form $(\mathbf{Z}^1)_{i,i+1}$, $1 \le i \le N-1$. We find that the part corresponding to the heat current is uniformly bounded in N. In particular, a first-order perturbation does not reveal any sign that Fourier law might hold in such anharmonic models, as numerical studies indicate, see e.g. [46]. Indeed, if Fourier law holds whenever λ is finite, one might expect the derivatives of the heat current to develop a singularity at $\lambda = 0$ when $N \to \infty$.

Regarding the temperature profile, the part of the solution proportional to η is exponentially decaying in the bulk of the chain whenever $\kappa > 0$. The decay rate is slower than in the purely harmonic case. For $\kappa = 0$, the profile proportional to η is linear in the bulk of the chain and we compute its slope explicitely. However as explained in the introduction, the sign is "wrong", in the sense that the linear profile has the *lowest* temperature close to the *hottest* bath and the *highest* temperature close to the *coldest* bath. The same type of phenomenon is present for $\kappa > 0$, see fig. 1. Moreover, we observe that the part proportional to η^2 gives a significant contribution, which results in a shift of the temperature at the middle point of the chain. The temperature at this point is no more the arithmetic mean of the baths temperatures. Although surprising, this is a phenomenon which seems to be observed in numerical studies of certain anharmonic chains, see [46].

$$\begin{aligned}(\mathbf{Y}^1)_{ii} = \; & - \; \frac{2\nu}{(\nu+\kappa)(2+\nu+\kappa)(4+\nu+\kappa)} \\ & - \; \frac{\nu(2+\kappa)(\rho_1-\rho_0)}{(4+\nu+2\kappa)}\frac{\sinh(N+1-2i)\bar{\alpha}}{\sinh(N+1)\bar{\alpha}} + \mathcal{O}(e^{-2\alpha i}).\end{aligned} \tag{68}$$

for $1 \leq i < [N/2]+1$. The elements corresponding to $[N/2]+1 \leq i \leq N$ are determined by symmetry considerations. In the limit $N \to \infty$, it is possible to compute that for $\kappa = 0$, the temperature profile is given by

$$(\mathbf{Y}^1)_{ii} = -\frac{2\nu}{\nu(2+\nu)(4+\nu)} + \frac{2\nu}{(4+\nu)^2}\Big(\frac{2i}{N+1} - 1\Big) + \mathcal{O}(e^{-2\alpha i}). \tag{69}$$

The temperature profile is linear, but oriented in the "wrong" direction. The correction to the current only brings about exponential corrections, uniformly bounded in N.

3.3 Phonons collisions.

3.3.1 Translation-invariant non-equilibrium dynamics.

In contrast to equilibrium states for which the explicit Gibbs formula may be used, the effective computation of correlation functions of the stationary states out of equilibrium remains a challenging problem. Conceptually, one may distinguish two different reasons for that. The first one is common with the equilibrium situation and has to do with the difficulty of dealing with nonlinear interactions between the components of the system. The second one has to do with the lack of translation invariance which is, in a sense built-in in the non-equilibrium set-up. Those difficulties are especially obvious when one tries to identify the physical mechanism giving rise to a finite thermal conductivity in non-linear Hamiltonian systems and compute its dependance on the microscopic interactions. The conductivity is a local property of the system that relates local quantities like the current and the local temperature gradient. In the next chapter we outline a method which, by dealing with the lack of translation invariance of the system, allows to focus on the effect of nonlinearities on the non-equilibrium steady states and perform concrete computations of their correlation functions. In order to study the local non-equilibrium dynamics, we will consider a spatially homogeneous Hamiltonian chain of oscillators coupled to a stochastic thermostat at a fixed temperature T and, in order to recover the time-reversal symmetry breaking induced locally by the heat baths located at the boundaries, we include an additional non-Hamiltonian term in the deterministic part of the dynamics. The force is designed in such way that, locally, the two dynamics satisfy a generalized detailed balance with respect to the same Hamiltonian and energy current. The method is a priori independent of any approximation scheme and apply to any local Hamiltonian lattice system out of equilibrium. For a justification of the dynamics (70) below, see my paper [58] where it was originally introduced or the next chapter where I summarize my paper with Thierry Bodineau [8].

3.3.2 Anharmonic oscillators and closure approximation on the stationary state.

Our goal in this section is to analyze the stationary state of the dynamics defined by

$$dq_i = p_i dt \tag{70}$$

$$dp_i = -\gamma p_i dt - \frac{\partial H}{\partial q_i}dt - \frac{\tau}{2T}(U'(q_{i-1}-q_i)+U'(q_i-q_{i+1}))dt + \sqrt{2\gamma T}dw_i\,,$$

with,

$$H(\underline{q},\underline{p}) = \sum_{i=1}^{N}[\frac{p_i^2}{2} + \omega^2\mu^2\frac{q_i^2}{2} + \frac{\lambda}{4}q_i^4 + \frac{\omega^2}{2}(q_i-q_{i-1})^2],\ \lambda > 0 \tag{71}$$

and $U(x) = \frac{\omega^2}{2}x^2$.

Proposition 15 *For all $\gamma, T > 0$, there exists a unique invariant measure for the stochastic process defined by (70,71).*

Outline of the Proof. We note that the hypoellipticity of the process defined (70) may be shown by checking the Hörmander condition on the generator as in [88]. For this particular system chain, no coupling between nearest-neighbour is even required because the noise acts on every particle. Hypoellipticity of the process implies the smoothness of the probability transition and thus that the stationary state, whenever it exists, is described by a smooth density. Irreducibility properties of the process may be checked by a control argument and Stroock-Varadhan support theorem [96] as explained in [20, 88]. Hypoellipticity and irreducibility imply together that there is at most one stationary measure. The existence of a (unique) stationary measure follows from those two properties and the existence of a Lyapunov function as in [8] in the appendix (see for instance Theorem 8.7 of [84]).

We first consider the harmonic case $\lambda = 0$. We introduce the Fourier coordinates for the periodic linear chain by $Q_k = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} e^{i\frac{2\pi}{N}kj}q_j$,with $-N/2+1 \leq k \leq N/2$. The P_k coordinates are defined in a similar fashion. We recall for further purposes that $Q_k^* = Q_{-k}$ and $P_k^* = P_{-k}$. In the complex coordinates,

$$A_k^{\pm} = \frac{1}{\sqrt{2\omega_k}}(P_k \pm i\omega_k Q_k), \tag{72}$$

with $\omega_k^2 = \omega^2(\mu^2 + 4\sin^2(\frac{\pi k}{N}))$, the Hamilton equations for the linear periodic chain read

$$dA_k^{\pm} = \pm i\omega_k A_k^{\pm} dt. \tag{73}$$

Those equations give the temporal evolution of the amplitudes of the waves with wave number k traveling through the chain in the positive or negative direction. Our (non-equilibrium) model is defined in the linear case by the system of stochastic equations

$$\begin{aligned} dA_k^{\pm} &= \pm i\omega_k A_k^{\pm} dt - \frac{\gamma}{2}(A_k^+ + A_k^-)dt - \frac{i\lambda}{N}R_k \\ &+ \frac{\tau}{T}\frac{\omega^2}{\sqrt{2\omega_k}}\sin(\frac{2\pi k}{N})(A_k^+ - A_k^-) + dW_k^{\pm} \end{aligned} \tag{74}$$

where the Wiener processes $W_k^{\pm}$ satisfy the relations

$$d(W_k^s W_{k'}^{s'}) \equiv I_{k,k'}^{s,s'}dt \equiv \frac{2\gamma T}{\omega_k}\delta(k+k')dt. \tag{75}$$

and

$$R_k = \sum_{k_1,k_2,k_3} \sum_{s_1,s_2,s_3} \delta(k-k_1-k_2-k_3)\, s_1 s_2 s_3\, L_{kk_1k_2k_3}\, A^{s_1}_{k_1} A^{s_2}_{k_2} A^{s_3}_{k_3}\,, \qquad (76)$$

and $L_{kk_1k_2k_3} = (16\,\omega_k\omega_{k_1}\omega_{k_2}\omega_{k_3})^{-1/2}$. Here and below, unless otherwise specified, the sums are over the k_i such that $-N/2+1 \leq k_i \leq N/2$ and $s_i = \pm 1$.

From (74), the equations for the n-point correlation functions in the stationary state,

$$(\Phi^{(n)})^{s_1,\ldots,s_n}_{k_1,\ldots,k_n} \equiv \left\langle A^{s_1}_{k_1} \ldots A^{s_n}_{k_n} \right\rangle, \qquad (77)$$

read

$$i\bar{\omega}^{(n)}\Phi^{(n)} = \gamma\Gamma^{(n)}(\Phi^{(n)}) + i\frac{\lambda}{N}M^{(n)}(\Phi^{(n+2)}) + \frac{\tau\omega^2}{T}F(\Phi^{(n)} - \tfrac{1}{2}I^{(n)}(\Phi^{(n-2)}), \qquad (78)$$

where $\bar{\omega}^{(n)}$ is the combination of frequencies,

$$(\bar{\omega}^{(n)})^{s_1,\ldots,s_n}_{k_1,\ldots,k_n} = \sum_{i=1}^{n} s_i\omega_{k_i}\,, \qquad (79)$$

and

$$(\Gamma^{(n)}(\Phi^{(n)}))^{s_1,\ldots,s_n}_{k_1,\ldots,k_n} = \frac{n}{2}(\Phi^{(n)})^{s_1,\ldots,s_n}_{k_1,\ldots,k_n} + \frac{1}{2}\sum_{i=1}^{n}(\Phi^{(n)})^{s_1,\ldots-s_i,\ldots,s_n}_{k_1,\ldots,k_n}. \qquad (80)$$

$I^{(n)}$ gathers the effects of the random forcing, the special case $I^{(2)}$ being given in (75).

$$F(\Phi^{(n)} = \sum_{i=1}^{n}\sum_{s_i=\pm 1}\frac{s_i\sin(\frac{2\pi k_i}{N})}{\sqrt{2\omega_{k_i}}}(\Phi^{(n)})^{s_1,\ldots,s_n}_{k_1,\ldots,k_n} \qquad (81)$$

The explicit expression of $M^{(n)}$ will be given below in the relevant cases. We are mainly interested in the contribution to the current of the correlation functions $\Phi^{s,s'}_{k,k'}$. The total current is given by

$$J = \frac{\omega^2}{2N}\sum_{k=-N/2+1}^{N/2}\sin(2\pi k/N)\, J_k, \qquad (82)$$

where $J_k = (\Phi^{+-}_{k,-k} - \Phi^{-+}_{k,-k})$. For $n=2$ and $k_1 = -k_2 = k$, one gets from (78) the balance equation in the stationary state,

$$\gamma J_k + \frac{i\lambda}{N}\left[(M^{(2)}(\Phi^{(4)}))^{+-}_{k,-k} - (M^{(2)}(\Phi^{(4)}))^{-+}_{k,-k}\right] = -\frac{2\tau}{T}\frac{\omega^2}{\sqrt{2\omega_k}}\sin(\frac{2\pi k}{N})\langle|A^+_k - A^-_k|^2\rangle \qquad (83)$$

where,

$$\begin{aligned}&(M^{(2)}(\Phi^{(4)}))^{+-}_{k,-k} - (M^{(2)}(\Phi^{(4)}))^{-+}_{k,-k}\\ =\;& 2i\sum_{k_1,k_2,k_3}\sum_{s_1,s_2,s_3}\delta(k+k_1+k_2+k_3)\, s_1s_2s_3\, L_{kk_1k_2k_3}\,\Im[(\Phi^{(4+)})^{+s_1s_2s_3}_{k,k_1,k_2,k_3}] \qquad (84)\end{aligned}$$

with

$$(\Phi^{(n\pm)})^{s_1,\ldots,s_n}_{k_1,\ldots,k_n} \equiv (\Phi^{(n)})^{s_1,\ldots,s_n}_{k_1,\ldots,k_n} \pm (\Phi^{(n)})^{-s_1,\ldots,-s_n}_{k_1,\ldots,k_n}. \qquad (85)$$

3.3.3 Closure and Linearization.

The assumption that we use is a Boltzmann-type assumption but at the level of the correlation functions in the stationary state of the system. Proving rigorously this assumption is expected to be a very difficult task.

Conjecture 16 Closure assumption.
$\exists \epsilon_0 > 0, \exists N_0 > \epsilon_0^{-1}$ *such that* $\forall N > N_0$ *and* $\forall \lambda, \omega \in \mathbb{R}^+$ *satisfying* $\frac{1}{N_0} < \frac{\lambda^2}{\omega^4} < \epsilon_0$

$$\Phi^{(2n)} = \mathcal{W}^{(2n)}(\Phi^{(2)}) + O(\frac{\lambda}{\omega^2}).$$

$\mathcal{W}^{(2n)}(\Phi^{(2)})$ *is the Wick formula expressing the* $2n$*-points correlation functions of Gaussian random variables as a sum of product of 2-points correlation functions.*

This assumption allows to obtain a closed system of equation for the $\Phi^{(2)}$ which may be solved. The closed equation is a non-linear one, but one can show that Φ^2 is an analytic function of τ. The case $\tau = 0$ being the equilibrium case. Linearizing the equation, one obtains an equation for the lowest order correction proportionnal to τ. The part contributing to the currents per mode J_k does not contain any equilibrium part and we keep the same notation J_k for the first-order correction (proportionnal to τ). In particular, one gets, for large pinning interaction μ, the equation for J_k is (83) with,

$$\begin{aligned}(M^{(2)}(\Phi^{(4)}))^{+-}_{k,-k} \quad - \quad & (M^{(2)}(\Phi^{(4)}))^{-+}_{k,-k} = \\ & -\frac{c\,T^2}{\omega^6\mu^6}\frac{i\lambda}{N}\sum_{l,n}(\Omega_\gamma)^{++--}_{k,l,n,k+l+n}[J_k + J_l + J_n - J_{k+l+n}] \end{aligned} \quad (86)$$

where,

$$(\Omega_\gamma)^{s_1s_2s_3s_4}_{k_1,k_2,k_3,k_4} = \frac{2\gamma}{4\gamma^2 + (s_1\omega_{k_1} + s_2\omega_{k_2} + s_3\omega_{k_3} + s_4\omega_{k_4})^2}\,.$$

We will estimate (86) in the limit of large N and for small γ, more precisely, $1 \gg \gamma/\omega \gg 1/N$. We first observe that the main contributions to the sum will arise from the resonances in Ω_γ, i.e., for lattice points (l, n) near the zeros of the function $f_x : [-\frac{\pi}{2}, \frac{\pi}{2}]^2 \to \mathbf{R}$,

$$\begin{aligned} f_x(y,z) \quad = \quad & \sqrt{\mu^2 + 4\sin^2(x)} + \sqrt{\mu^2 + 4\sin^2(y)} \\ & - \sqrt{\mu^2 + 4\sin^2(z)} - \sqrt{\mu^2 + 4\sin^2(x+y+z)}. \end{aligned} \quad (87)$$

A careful analysis reveals that for $\mu^2 > 0$, the zeros of f_x form three smooth curves. Two of these curves are obvious and given by $x+z = 0$, and $y+z = 0$. These resonances do not contribute to the sum, however, since the combination of J's in (86) vanishes for $k + n = 0$ or $l + n = 0$. This corresponds to the so-called *normal* processes. The third curve, corresponding to the *umklapp* processes, depends on μ and is difficult to localize explicitly. For large μ, it is given by $x + y = \frac{\pi}{2} + \mathcal{O}(1/\mu^2)$. Performing the sum over l in (86) in the

above-mentioned parameter regimes thus yields at lowest order in γ and $1/\mu$ (resonances are at $l = -k + N/2$),

$$(M^{(2)}(\Phi^{(4)}))^{+-}_{k,-k} \;-\; (M^{(2)}(\Phi^{(4)}))^{-+}_{k,-k} \tag{88}$$

$$= -i\lambda \frac{c\,T^2}{\omega^7\mu^5} \sum_n \frac{J^-_k + J^-_n}{|\sin(\frac{\pi(k+n)}{N})\cos(\frac{\pi(k-n)}{N})|}\,, \tag{89}$$

where we have defined $J^-_k \equiv \frac{1}{2}(J_k - J_{k+N/2})$. Before proceeding to solving equation (83), we note that any vector J can be decomposed as $J = J^+ + J^-$ where J^- as above and $J^+_k \equiv \frac{1}{2}(J_k + J_{k+N/2})$ have the symmetry properties $J^\pm_{k+N/2} = \pm J^\pm_k$. It then follows from (89) that J^+ does not contribute to Ψ, and that $\Psi = \Psi^-$.

3.3.4 Solution to the Current Equation.

Recall that J is odd and periodic of period N. We first observe that J^+ does not contribute to the average current $\langle J\rangle$ given by (82). This follows from $\sum_k \sin(2\pi k/N)J^+_k = 0$. Since, in addition, J is mapped by (89) into a vector Ψ with $\Psi = \Psi^-$ and since J^+ does not contribute to Ψ, we need only to consider in equation (83) odd forcings α and odd currents J satisfying $\alpha(\frac{\pi k}{N} + \frac{\pi}{2}) = -\alpha(\frac{\pi k}{N})$ and $J = J^-$. We denote by $\mathcal{S}^-$ the subspace of such vectors J, in which equation (83) becomes

$$\gamma J_k + c\,\frac{\lambda^2 T^2}{\omega^7\mu^5}\mathcal{L}(J)_k = -\frac{2\tau}{T}\frac{\omega^2}{\sqrt{2\omega_k}}\sin(\frac{2\pi k}{N})\langle|A^+_k - A^-_k|^2\rangle_{\tau=0}\,, \tag{90}$$

where $\mathcal{L} : \mathcal{S}^- \to \mathcal{S}^-$ is given by

$$\mathcal{L}(J)_k = \frac{1}{N}\sum_{k'} \frac{J_k + J_{k'}}{|\sin(\frac{\pi(k+k')}{N})\cos(\frac{\pi(k-k')}{N})|}\,. \tag{91}$$

We now proceed to analyze the linear operator $\mathcal{L}$. The subspace $\mathcal{S}^-$ has dimension $N/4$, and a basis for $\mathcal{S}^-$ is given by $\mathcal{J}^n_k = \sin(2\pi(2n+1)\frac{k}{N})$, $n = 0,\ldots,N/4-1$. We let $\mathcal{A}^n \equiv \mathcal{L}(\mathcal{J}^n)$. An explicit computation shows that the set of $\mathcal{A}^n$, $n = 0,\ldots,N/4-1$, also forms a basis of $\mathcal{S}^-$ and that $\mathcal{L}$ is uniformly invertible (in N). This implies that the first term on the LHS of (90) is negligible for γ small. Furthermore, it follows from $\sum_k \sin(\frac{2\pi k}{N})\mathcal{J}^n_k = 0$ for $n \neq 0$ that only $\mathcal{J}^0_k$ contribute to the current (82). Therefore, the only contribution of the noise α to the current is the component of α along $\mathcal{A}^0$, say α^0, where

$$\mathcal{A}^0_k \equiv \mathcal{L}(\mathcal{J}^0)_k = 2\,\mathrm{sign}(k)\Big(\frac{1}{4} - \Big|\mathrm{sign}(k)\frac{k}{N} - \frac{1}{4}\Big|\Big). \tag{92}$$

One thus finally obtains from (82),

$$\langle J\rangle \sim \frac{\omega^9\mu^5}{\lambda^2 T^2}\,\alpha^0\,\tau\,, \tag{93}$$

As mentioned in the introduction, the result of [94] shows that the local gradient of temperature imposes the choice $\alpha(k) \sim \omega^{-1}(k)\nabla\omega(k)$, that is,

$\mu^{-2}\sin(2\pi k/N)$ for large μ. It has a non-zero component along $\mathcal{A}^0$ and the corresponding conductivity is thus given by $\kappa \equiv \langle J \rangle / \tau \sim \frac{\omega^9 \mu^3}{\lambda^2 T^2}$. Our explicit treatment of the resonances and the inversion of the linearized Boltzmann operator allows to justify rigorously the physical picture that these are the four-body *umklapp* collisions between phonons which are responsible for a normal conductivity in pinned anharmonic chains. Indeed, considering a cubic instead of a quartic interaction in the Hamiltonian would yield an expression analogous to (87) but with a combination of only three frequencies. The latter is always non-zero when $\mu \neq 0$, leading to an infinite conductivity. We finally point out that when the pinning goes to zero, the localization of the resonances and the inversion of the linearized collision operator are more difficult and there is no reason for expression (93) to be valid.

Chapter 4

Large deviations of lattice Hamiltonian dynamics coupled to stochastic thermostats.

In this chapter, I present the results obtained in [8].
We discuss the Donsker-Varadhan theory of large deviations in the framework of Hamiltonian systems thermostated by a Gaussian stochastic coupling. We derive a general formula for the Donsker-Varadhan large deviation functional for dynamics which satisfy natural properties under time reversal. Next, we discuss the characterization of the stationary states as the solution of a variational principle and its relation to the minimum entropy production principle.
In the recent years, several studies of large systems out of equilibrium through fluctuation theory have been made [5, 6, 7, 9, 35, 40, 41, 48]. In a recent series of papers [66, 67, 68, 69, 70], it has been understood that in random systems driven out of equilibrium, the theory of large deviations provides naturally a variational characterization of the steady states which is related to the minimum entropy production principle. In [8], we pursued this approach in the framework of thermostated lattices of Hamiltonian oscillators and investigated in this setting the Donsker-Varadhan large deviation theory [24, 25].

4.1 Models

We will first recall the general framework of Hamiltonian dynamics and define the relevant physical quantities in this context. In section 4.1.2, the notion of *generalized* detailed balance is introduced. It will be an important feature of the Hamiltonian systems with a stochastic forcing considered in this chapter (see sections 4.1.3, 4.1.4 and 4.1.5).

4.1.1 Hamiltonian dynamics

We consider a one-dimensional lattice of N particles $(\underline{q}, \underline{p}) = (q_i, p_i)_{1 \leq i \leq N}$, each one moving around an equilibrium position, the position of the i-th particle is denoted by q_i and its momentum by p_i. The systems we have in mind are

described by a Hamiltonian, which is the energy function of the set of particles,

$$H(\underline{q},\underline{p}) = \sum_{i=1}^{N} \left[\frac{p_i^2}{2} + V(q_i) + \tfrac{1}{2}(U(q_{i+1}-q_i) + U(q_i - q_{i-1})) \right]. \tag{1}$$

We will consider either periodic boundary conditions (with the convention $q_{N+1} = q_1$ and $q_0 = q_N$) or open systems with the convention $q_0 = q_{N+1} = 0$. V is the potential energy corresponding to an interaction with an external substrate. U describes the potential energy of the interaction between nearest-neighbours. Precise assumptions on the growth of the potentials will be detailed in Section 4.2.1 along with the mathematical statements.

The positions q_i and momenta p_i of the particles obey the Hamilton's equations,

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{2}$$

The generator of the Hamiltonian dynamics is given by

$$L_H = \sum_{i=1}^{N} -\frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i} + \frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i}. \tag{3}$$

In order to describe the propagation of heat in the lattice, one defines a local energy function,

$$h_i(\underline{p},\underline{q}) = \frac{p_i^2}{2} + V(q_i) + \tfrac{1}{2}(U(q_i - q_{i+1}) + U(q_{i-1} - q_i)), \tag{4}$$

such that $H = \sum_{i=1}^{N} h_i$. The local energy transfer is identified with the transfer of mechanical energy between nearest-neighbours. The energy current is therefore defined through the time evolution of the local energy,

$$\frac{dh_i}{dt} = L_H h_i = j_i - j_{i-1} \tag{5}$$

with j_i the microscopic current of energy or heat between oscillator i and $i+1$

$$j_i = -\tfrac{1}{2}U'(q_i - q_{i+1})(p_i + p_{i+1}). \tag{6}$$

In section [8], we have also investigated the large deviations of the spatial average of the current defined by

$$J(\underline{q},\underline{p}) = \frac{1}{N}\sum_{i=1}^{N} j_i. \tag{7}$$

When such a Hamiltonian system is in thermal equilibrium at a temperature $T = \beta^{-1}$, its statistical properties are described by the Boltzmann-Gibbs probability distribution over the phase space $\mathbb{R}^{2N}$,

$$\rho(\underline{p},\underline{q}) = \frac{1}{Z}\exp\left(-\frac{1}{T}H(\underline{p},\underline{q})\right). \tag{8}$$

Remark that with respect to that distribution, $\langle p_i^2 \rangle = T$ and the averaged current is null $\langle j_i \rangle = 0$. This last identity is straightforward because the equilibrium distribution is even under the reversal of momenta $\underline{p} \to -\underline{p}$ while the current is odd.

4.1.2 The generalized detailed balance

We now recall the notion of reversibility in the framework of lattices of coupled oscillators. Then, we introduce the notion of *generalized detailed balance* which will apply when the chain of oscillators is forced out of equilibrium by stochastic heat baths (sections 4.1.3 and 4.1.4) or a driving force (section 4.1.5).

In Hamiltonian dynamics, the variables $\underline{p}$ basically describe the velocities of the particles and are therefore odd functions under time reversal. When isolated, those systems are reversible in the sense that if one lets evolve the particles from some initial conditions at time 0 up to some time T and then reverse all momenta, Hamilton's dynamics will take back the particles through the same trajectory but with reverse momenta. Thus in the case of Hamiltonian dynamics (with possibly a stochastic forcing), the standard notion of detailed balance has to take into account the reversal of momenta. We denote by Π the operator which reverses momenta

$$\Pi(\underline{q},\underline{p}) = (\underline{q},-\underline{p})\,. \tag{9}$$

Let $P_t\left((\underline{q},\underline{p}),(\underline{q}',\underline{p}')\right)$ be the semi-group associated to an Hamiltonian dynamics with a stochastic perturbation (for a precise definition see sections 4.1.3 and 4.1.4) with initial data $(\underline{q},\underline{p})$ and final data $(\underline{q}',\underline{p}')$ at time t. We consider a probability measure with density $\rho(\underline{q},\underline{p})$ symmetric wrt to time reversal $\Pi\rho = \rho$. The dynamics is reversible wrt to the density $\rho(\underline{q},\underline{p})$ if for any time t

$$\rho\left(\underline{q},\underline{p}\right)\; P_t\left((\underline{q},\underline{p}),(\underline{q}',\underline{p}')\right) = \rho\left(\underline{q}',\underline{p}'\right)\; P_t\left(\Pi(\underline{q}',\underline{p}'),\Pi(\underline{q},\underline{p})\right)\,. \tag{10}$$

Let L be the generator of this dynamics and let $L^\dagger$ denote the adjoint with respect to the Lebesgue measure. The adjoint L^*_ρ of the operator L with respect to the measure with density $\rho(\underline{q},\underline{p})$ is defined by

$$L^*_\rho f(\underline{q},\underline{p}) = \rho^{-1}(\underline{q},\underline{p})\; L^\dagger(\rho(\underline{q},\underline{p})f(\underline{q},\underline{p})) \tag{11}$$

for any regular function $f(\underline{q},\underline{p})$. Alternatively, L^*_ρ satisfies

$$\langle fLg\rangle_\rho = \left\langle gL^*_\rho f\right\rangle_\rho\,.$$

L^*_ρ is therefore interpreted as the generator of the time reversed dynamics sampled with initial data distributed according to ρ. Applying (10) for an infinitesimal amount of time, the equivalent form of the detailed balance relation can be obtained

$$L^*_\rho = \Pi L \Pi\,, \tag{12}$$

where we used that the density ρ satisfies $\Pi\rho = \rho$. For stochastic dynamics, the usual detailed balance relation does not involve the time reversal operator, however we keep the same terminology for simplicity.

For general Hamiltonian systems coupled to stochastic thermostats, the reversibility may not hold and (12) has to be replaced by the *generalized detailed balance relation* (see for example [32]) which can be defined as follows

Definition 17 *We consider an evolution with generator L and $\rho(\underline{q},\underline{p})$ a reference measure such that $\Pi\rho = \rho$. If there exists a function $\sigma(\underline{q},\underline{p})$ such that*

$$L_\rho^* = \Pi L \Pi + \sigma, \qquad \text{and} \qquad \Pi\sigma = -\sigma\,, \tag{13}$$

then the triplet (L,ρ,σ) is said to satisfy a generalized detailed balance relation. By convention in (13), σ acts as a multiplication operator.

This definition will be illustrated in the examples introduced in sections 4.1.3, 4.1.4 and 4.1.5. In equilibrium dynamics (when $\sigma = 0$) and when sampled with initial conditions distributed according to the equilibrium measure, the dynamics is equivalent to its time-reverse, this is the detailed balance principle. When the system is subject to some non-equilibrium dynamics forcing a heat current through the system, the stationary state looses its invariance under time-reversal ($\sigma \neq 0$). In Markovian systems, the generalized detailed balance is a central feature of the Gallavotti-Cohen symmetry [64, 35, 40, 51, 57, 88, 89] for the large deviation functional of the function σ.

Typically σ is a function of the microscopic currents of energy in the lattice and the reference measure is an equilibrium or a local equilibrium distribution. A given dynamics may satisfy a generalized detailed balance relation with respect to different reference measures and different functions σ (see section 4.1.4).

4.1.3 Heat in the bulk

The simplest perturbation of the Hamiltonian dynamics (2) is to couple each oscillator to a heat bath. The boundary conditions are fixed $q_0 = q_{N+1} = 0$ and each oscillator $i = 1,\dots,N$ evolves according to

$$\begin{aligned} dq_i &= p_i dt \\ dp_i &= -\gamma_i p_i dt - \frac{\partial H}{\partial q_i} dt + \sqrt{2\gamma_i T_i} dw_i\,, \end{aligned} \tag{14}$$

where the w_i are standard independent Brownian motions, $T_i = \beta_i^{-1}$ is the temperature of each heat bath and $\gamma_i > 0$ is the friction. The generator of the dynamics is given by

$$L = L_S + L_H \tag{15}$$

where the Hamiltonian part L_H was introduced in (3) and the symmetric part is

$$L_S = \sum_{i=1}^{N} -\gamma_i p_i \frac{\partial}{\partial p_i} + \gamma_i T_i \frac{\partial^2}{\partial p_i^2}\,. \tag{16}$$

When the temperatures $\{T_i\}_i$ are not equal, the reversibility is lost and the invariant measure unknown. The self-consistent chain [11], for which the temperatures $\{T_i\}_i$ are tuned in order to maintain a constant average microscopic current along the chain, falls in the framework of the dynamics (14).

We check now that this dynamics satisfies the generalized detailed balance (see definition 17). Given a collection of inverse temperatures $\underline{\beta} = (\beta_1, \dots, \beta_N)$, we take as a reference measure the following density

$$\rho_{\underline{\beta}}(\underline{p}, \underline{q}) = \frac{1}{Z} \exp\left(-\widehat{H}(\underline{p}, \underline{q})\right), \quad \text{with} \quad \widehat{H}(\underline{p}, \underline{q}) = \sum_{i=1}^{N} \beta_i \, h_i(\underline{p}, \underline{q}), \tag{17}$$

where h_i are the local energies introduced in (4) and $\beta_i^{-1} = T_i$ is the temperature of the heat bath at site i. We compute now $L^*_{\rho_{\underline{\beta}}}$ the adjoint of L with respect to the measure $\rho_{\underline{\beta}}$. Since $L_S = \Pi L_S \Pi$ and the stochastic part of the dynamics is reversible with respect to the measure $\rho_{\underline{\beta}}$, one has for any function f

$$L_S f(\underline{q}, \underline{p}) = \rho_{\underline{\beta}}^{-1}(\underline{q}, \underline{p}) L_S^\dagger(\rho_{\underline{\beta}}(\underline{q}, \underline{p}) f(\underline{q}, \underline{p})). \tag{18}$$

We turn now to the Hamiltonian part. Thanks to the relation $L_H^\dagger = -L_H$, we get

$$\rho_{\underline{\beta}}^{-1} L_H^\dagger \rho_{\underline{\beta}} = \sum_{i=1}^{N} \beta_i L_H h_i \,. \tag{19}$$

From (5), one has $L_H h_i = j_i - j_{i-1}$ with the convention $j_0 = j_N = 0$, thus

$$\rho_{\underline{\beta}}^{-1} L_H^\dagger \rho_{\underline{\beta}} = \sum_{i=1}^{N} \beta_i (j_i - j_{i-1}) = -\sum_{i=1}^{N-1} (\beta_{i+1} - \beta_i) j_i \,. \tag{20}$$

Since $\Pi L_H \Pi = -L_H = L_H^\dagger$, this implies that

$$L^*_{\rho_{\underline{\beta}}} = \Pi L \Pi + \sigma_{\underline{\beta}}, \qquad \text{with} \quad \sigma_{\underline{\beta}} = -\sum_{i=1}^{N-1} (\beta_{i+1} - \beta_i) j_i \,. \tag{21}$$

Thus the triplet $(L, \rho_{\underline{\beta}}, \sigma_{\underline{\beta}})$ satisfies a generalized detailed balance relation and $\sigma_{\underline{\beta}}$ is a linear combination of the local currents.

4.1.4 Heat at the boundary

If there are no heat baths in the bulk ($\gamma_i = 0$ for $i = 2, \dots, N-1$), the dynamics (14) represents a crystal of atoms heated at two different temperatures at its boundaries. The equations of motion are given by,

$$\begin{aligned} dq_i &= p_i dt, \quad i = 1, \dots, N, \\ dp_i &= -\frac{\partial H}{\partial q_i}(\underline{p}, \underline{q}) dt, \quad i = 2, \dots, N-1, \end{aligned} \tag{22}$$

and,

$$\begin{aligned} dp_1 &= -\frac{\partial H}{\partial q_1}(\underline{p}, \underline{q}) dt - \gamma p_1 dt + \sqrt{2\gamma T_1}\, dw_1 \,, \\ dp_N &= -\frac{\partial H}{\partial q_N}(\underline{p}, \underline{q}) dt - \gamma p_N dt + \sqrt{2\gamma T_N}\, dw_N \,, \end{aligned} \tag{23}$$

where T_1 and T_N stand for the temperature of the left and right reservoirs, respectively, whereas w_1 and w_N are two independent standard Wiener processes.

When $T_1 = T_N = T = \beta^{-1}$, the Gibbs measure (8) is invariant (stationary) for the stochastic dynamics defined above. For two different temperatures, existence, uniqueness and exponential convergence to an unique invariant state has been established under fairly general conditions on the potentials U and V [20, 31, 29, 88].

A computation similar to the case of heat baths in the bulk (21) shows that the dynamics (22) satisfies the generalized detailed balance (see definition 17) for any reference measure $\rho_{\underline{\beta}}$ of the form (17)

$$L^*_{\rho_{\underline{\beta}}} = \Pi L \Pi + \sigma_{\underline{\beta}}, \qquad \text{with} \quad \sigma_{\underline{\beta}} = -\sum_{i=1}^{N-1} (\beta_{i+1} - \beta_i) j_i \,, \tag{24}$$

provided the collection of inverse temperatures $\underline{\beta} = (\beta_1, \ldots, \beta_N)$ is such that $\beta_1^{-1} = T_1$ and $\beta_N^{-1} = T_N$. Thus any $\sigma_{\underline{\beta}}$ such that $\beta_1^{-1} = T_1$ and $\beta_N^{-1} = T_N$ will satisfy the Gallavotti-Cohen symmetry relation. This was already observed in [32, 88].

4.1.5 Asymmetric periodic chain

Building on a previous work [58], we introduce new dynamics by adding a mechanical force which creates a current through the system. On a periodic lattice, these dynamics lead to non-equilibrium systems with non-vanishing currents and in this sense, they are reminiscent of the asymmetric processes in lattice gas dynamics [93].

We start with an heuristic discussion before giving the definition of the dynamics. If the heat baths are at different temperatures, the dynamics (22) is no longer reversible with respect to the Gibbs measure or any "local equilibrium" measure $\rho_{\underline{\beta}}$. As observed in (24), the function σ which breaks the reversibility is a linear combination of the local energy currents. We show that adding an appropriate mechanical force allows to modify at will the coefficients of this linear combination. In particular, the reversibility may be restored in (22) by tuning the intensity of the additional mechanical force. From the point of view of the generalized detailed balance, the action of the mechanical force is equivalent to the action of the local temperature gradient.

Let us first show that one may choose a (non-Hamiltonian) force which modifies the coefficients of the combination of local currents of energy in σ. Take as generator of the dynamics,

$$L = L_S + L_H + L_{\underline{\theta}} \,, \tag{25}$$

where L_H is the generator of the Hamiltonian dynamics (3), L_S the generator of the two stochastic reservoirs (23)

$$L_S = -\gamma p_1 \frac{\partial}{\partial p_1} + \gamma T_1 \frac{\partial^2}{\partial p_1^2} - \gamma p_N \frac{\partial}{\partial p_N} + \gamma T_N \frac{\partial^2}{\partial p_N^2} \,,$$

and the contribution of the mechanical drift is given by the antisymmetric operator

$$L_{\underline{\theta}} = -\sum_{i=1}^{N} \tfrac{1}{2} T_i(\theta_{i-1} U'(q_{i-1} - q_i) + \theta_i U'(q_i - q_{i+1})) \frac{\partial}{\partial p_i}\,, \tag{26}$$

To study the reversibility (12) properties of this dynamics, we first compute,

$$\begin{aligned} \rho_{\underline{\beta}}^{-1} L_{\underline{\theta}}^T \rho_{\underline{\beta}} &= -\sum_{i=1}^{N} \tfrac{1}{2}(\theta_{i-1} U'(q_{i-1} - q_i) + \theta_i U'(q_i - q_{i+1})) p_i \\ &= -\sum_{i=1}^{N-1} \theta_i \tfrac{1}{2}(p_i + p_{i+1}) U'(q_i - q_{i+1}) = \sum_{i=1}^{N-1} \theta_i j_i\,. \end{aligned}$$

Since the operator $L_S + L_H$ satisfies a generalized detailed balance relation wrt $\sigma_{\underline{\beta}} = -\sum_{i=1}^{N-1}(\beta_{i+1} - \beta_i) j_i$ (24), we see that the dynamics (25) satisfies now the generalized detailed balance (see definition 17) for the measure $\rho_{\underline{\beta}}$ (17) with respect to $\sigma_{\underline{\beta},\underline{\theta}}$

$$L^*_{\rho_{\underline{\beta}}} = \Pi L \Pi + \sigma_{\underline{\beta},\underline{\theta}}, \qquad \text{with} \quad \sigma_{\underline{\beta},\underline{\theta}} = \sum_{i=1}^{N-1} (\beta_i - \beta_{i+1} + \theta_i) j_i\,. \tag{27}$$

When the relation $\theta_i \neq (\beta_{i+1} - \beta_i)$ for some i, then the system is driven out of equilibrium. However, with the choice $\theta_0 = \theta_N = 0$ and $\theta_i = (\beta_{i+1} - \beta_i)$ reversibility is restored. This is the key point which allows to identify the strength of the mechanical force with the action of the local gradient of temperature.

For $\theta_i = (\beta_{i+1} - \beta_i)$ and slowly varying temperatures of the form $\beta_i^{-1} = T_i = T(\frac{i}{N})$ where T is a smooth function, the generator $L_{\underline{\theta}}$ becomes at lowest order in $\frac{1}{N}$,

$$L_{\underline{\theta}} = \sum_{i=1}^{N} \frac{1}{N} \frac{\nabla T(\frac{i}{N})}{2T(\frac{i}{N})} (U'(q_{i-1} - q_i) + U'(q_i - q_{i+1})) \frac{\partial}{\partial p_i}\,. \tag{28}$$

Note that in the sum over i, the prefactors depending on the temperature and its gradient are basically constant when i varies over distances much smaller than N.

The asymmetric periodic chain [58], described below, is a chain with periodic boundary conditions and a dynamics made of three parts. The first one corresponds to a usual Langevin dynamics for each oscillator, the second one to the Hamiltonian dynamics on the lattice and the third one is the previous generator (28) with constant prefactors (but arbitrary values). Namely, it is defined as

$$L = L_S + L_H + L_\tau\,, \tag{29}$$

with,

$$L_S = \sum_i -\gamma p_i \frac{\partial}{\partial p_i} + \gamma T \frac{\partial^2}{\partial p_i^2}\,. \tag{30}$$

L_H is defined in (3) and the part driving the system out of equilibrium is,

$$L_\tau = -\frac{\tau}{2T}\sum_i (U'(q_{i-1}-q_i)+U'(q_i-q_{i+1}))\frac{\partial}{\partial p_i}\,. \tag{31}$$

In terms of equations of motion the dynamics is described as follows,

$$\begin{aligned} dq_i &= p_i dt \\ dp_i &= -\gamma p_i dt - \frac{\partial H}{\partial q_i}dt - \frac{\tau}{2T}(U'(q_{i-1}-q_i)+U'(q_i-q_{i+1}))dt + \sqrt{2\gamma T}dw_i\,, \end{aligned} \tag{32}$$

where $\tau \in \mathbf{R}$ is the new parameter regulating the strength of the non-equilibrium forcing and the w_i are standard independent Brownian motion $i = 1, \ldots, N$. Periodic boundary conditions means $q_0 = q_N$ and $q_{N+1} = q_1$. Compared to the dynamics (14), the new term proportional to τ is the non-equilibrium part of the dynamics. As should be clear from the above argument it is responsible for the breaking of the time-reversal symmetry of the equilibrium dynamics ($\tau = 0$). Indeed, for the dynamics (32), taking the Gibbs measure (8) at constant temperature T as the reference measure, the generalized detailed balance holds with a function σ proportional to the total current (7)

$$\sigma = \frac{\tau}{T^2}\sum_{i=1}^{N} j_i = \frac{\tau\, N}{T^2}J. \tag{33}$$

One can show [8] that when $\tau \neq 0$, $\tau\langle J\rangle_{\widehat{\rho}} > 0$ for a stationary measure $\widehat{\rho}$. Thus, the dynamics ensures the existence of an average non-vanishing energy current in the stationary state.

4.2 The large deviation functional

The goal of this section is to rephrase the Donsker-Varadhan theory [24, 25] in the framework of the Hamiltonian systems coupled to Gaussian stochastic thermostats and to discuss the relation with entropy production.

4.2.1 The Donsker-Varadhan functional

In order to cover all the examples introduced in sections 4.1.3 and 4.1.5, we consider the general dynamics defined by

$$\begin{aligned} dq_i &= p_i dt \\ dp_i &= -\gamma_i p_i dt - \frac{\partial H}{\partial q_i}dt - \tfrac{1}{2}T_i(\theta_{i-1}U'(q_i-q_{i-1})+\theta_i U'(q_{i+1}-q_i))dt + \sqrt{2\gamma_i T_i}dw_i\,, \end{aligned} \tag{34}$$

with $\gamma_i > 0, T_i > 0$ for $i = 1, \ldots, N$. We stress the fact that the noise acts at each site i. To simplify notation, we restrict to open systems (with the convention $q_0 = q_{N+1} = 0$, $\theta_0 = \theta_N = 0$), but similar results hold with periodic boundary conditions (with the convention $q_{N+1} = q_1$ and $q_0 = q_N$). We denote by P the probability of the evolution (34) starting from a given initial data (which will play no role in the large t asymptotic).

Typically, we shall be interested in the deviations over time of some physical quantities like the heat current (7). Let the empirical distribution ν_t be defined by,

$$\nu_t(A) = \frac{1}{t}\int_0^t \mathbf{1}_A((\underline{p}(s),\underline{q}(s)))ds\,,$$

where $\mathbf{1}_A$ is the indicator function of a set $A \subset \mathbf{R}^{2N}$. If the dynamics is ergodic ν_t converges to the ergodic invariant measure. We now look at the asymptotic probability $P[\nu_t \simeq \mu]$ that the empirical distribution is close to the distribution of a given measure μ (in the sense of the weak convergence topology [100]) for large t. Under suitable hypothesis (see Proposition 18), the dynamics obeys a large deviation principle with rate function I and asymptotically in t

$$P[\nu_t \simeq \mu] \sim \exp\left(-tI(\mu)\right). \tag{35}$$

Furthermore, from the Donsker-Varadhan theory [24, 25, 100] the functional is given by

$$I(\mu) = \sup_g \left\{ -\left\langle \frac{Lg}{g} \right\rangle_\mu \;\middle|\; g \in C_b^\infty(\mathbf{R}^{2N};[1,\infty[) \right\}, \tag{36}$$

where $C_b^\infty(\mathbf{R}^{2N};[1,\infty[)$ is the set of bounded infinitely differentiable functions in $\mathbf{R}^{2N}$ taking values larger or equal to 1. We refer to Lemma 6.3.7 of [23] for the variational expression of I in the case of hypoelliptic diffusions.

The following Proposition justifies the validity of the large deviation principle (35).

Proposition 18 *Suppose that the potentials V and U of the Hamiltonian (1) are convex, twice differentiable and satisfy*

$$V''(q) \geq \delta \quad \text{and} \quad \sum_{i=1}^N V(q_i) + \frac{U(q_i - q_{i+1}) + U(q_{i+1} - q_i)}{2} \geq \delta \sum_{i=1}^N \left(U'(q_i - q_{i+1})\right)^2, \tag{37}$$

for some constant $\delta > 0$.

The dynamics (34) (with $\forall i, \gamma_i > 0$) obeys a large deviation principle with a functional I given by the Donsker-Varadhan theory (36) provided $\max_i |\theta_i| \leq \tau_0$ and $\max_i |T_i - T_{i+1}| \leq \Delta_0$, where Δ_0 and τ_0 are two constants depending only on $\delta, \{\gamma_i, T_i\}_i$. Furthermore, the previous assumptions on the potentials (37) ensure that the current (7) is exponentially integrable: for any λ small enough

$$\limsup_{t\to\infty} \frac{1}{t} \log P\left(\exp\left(\lambda \int_0^t dsJ(\underline{p}(s),\underline{q}(s))\right)\right) < \infty\,. \tag{38}$$

The proof heavily relies on previous results in the paper [100] and it is postponed to the Appendix. The assumptions of Proposition 18 on the potentials V and U are not optimal, but they are sufficient to cover a wide class of physical examples. In particular, similar statements hold also for any local modifications of the potentials V and U. Remark that when the reservoirs act

only at the boundary ($\gamma_i = 0, i \in \{2, \dots, N-1\}$), the large deviation principle for the current has been justified in [89] (for a different class of Hamiltonians).

We are going to rewrite the functional I (36) in a more explicit form. The generator of the dynamics (34) can be decomposed as $L = L_S + L_A$, with a symmetric part L_S (16) due to the noise and an antisymmetric part $L_A = \frac{1}{2}(L - \Pi L \Pi)$. We introduce the notation,

$$\Gamma(f, g) = 2 \sum_{i=1}^{N} \gamma_i T_i \left(\partial_{p_i} f\right) \left(\partial_{p_i} g\right), \tag{39}$$

for any smooth functions f, g.

Proposition 19 *Let ρ be a measure and $\sigma(\underline{q}, \underline{p})$ a function such that*

$$L_\rho^* = \Pi L \Pi + \sigma \,. \tag{40}$$

Let μ be a measure absolutely continuous with respect to the measure ρ, with $f = d\mu/d\rho \in C^\infty(\mathbf{R}^{2N}; \mathbf{R})$ such that $\left\langle \|\nabla_{\underline{p}} \sqrt{f}\|_2 \right\rangle_\rho < \infty$. Then the functional I (36) is given by

$$I(\mu) = -\left\langle f^{\frac{1}{2}} L_S f^{\frac{1}{2}} \right\rangle_\rho + K(\mu) - \tfrac{1}{2} \langle \sigma \rangle_\mu \,, \tag{41}$$

with

$$K(\mu) = -\inf_W \left(\frac{1}{8} \langle \Gamma(W, W) \rangle_\mu + \tfrac{1}{2} \langle L_A W \rangle_\mu \right) \geq 0 \,, \tag{42}$$

where the infimum is taken over the smooth functions $W \in C^\infty(\mathbf{R}^{2N}; \mathbf{R})$ such that $W \in L^2(\mu)$ and $|\nabla_{\underline{p}} W| \in L^2(\mu)$.

From (27), we see that the dynamics (34) satisfies the generalized detailed balance for the measure $\rho_{\underline{\beta}}$ (17), the assumption (40) of Proposition 19 is satisfied with $\rho_{\underline{\beta}}$ and $\sigma_{\underline{\beta},\underline{\theta}}$

$$L_{\rho_{\underline{\beta}}}^* = \Pi L \Pi + \sigma_{\underline{\beta},\underline{\theta}}, \qquad \text{with} \quad \sigma_{\underline{\beta},\underline{\theta}} = \sum_{i=1}^{N-1} (\beta_i - \beta_{i+1} + \theta_i) j_i \,.$$

Remark that the generalized detailed balance requires symmetry assumptions on the reference measure and on σ which are not necessary for the Proposition 19 to hold.

One of the important features of the representation (41) for $I(\mu)$ is the presence of $K(\mu)$. One can check using Proposition 20 and that it is in general neither infinite or zero even in the case of dynamics satisfying detailed balance, i.e for equilibrium dynamics. $K(\mu)$ gathers the thermalizing effect of the noise which is transmitted from the $\underline{p}$ variables to $\underline{q}$ variables. It corresponds to the "traffic" in the terminology of [68]. It is invariant under reversal of the sign of the momenta (i.e $K(\mu) = K(\Pi\mu)$) and when non-equilibrium forces are included it is invariant under a change of sign of the non-equilibrium parameter

as we shall see in the gaussian systems of the last section. It measures the dynamical "activity" in the Hamiltonian system irrespective of the sign of the non-equilibrium parameter. We shall see its role in the variational characterization of stationary states in section 4.3. We now compute a more explicit form for $K(\mu)$.

Proposition 20 *Let μ be a measure on $\mathbf{R}^{2N}$ with smooth density wrt the Lebesgue measure $d\mu(\underline{p},\underline{q}) = \exp(-\Phi)d\underline{p}d\underline{q}$. If $\overline{W} \in L^2(\mu)$ is a solution of*

$$\sum_{i=1}^{N} -\gamma_i T_i \partial_{p_i}^2 W + \gamma_i T_i \, \partial_{p_i}\Phi \partial_{p_i} W = -L_A \Phi \,, \tag{43}$$

with $|\nabla_{\underline{p}} \overline{W}| \in L^2(\mu)$ then

$$K(\mu) = \frac{1}{8} \left\langle \Gamma(\overline{W},\overline{W}) \right\rangle_\mu = -\frac{1}{4} \left\langle L_A \overline{W} \right\rangle_\mu \,. \tag{44}$$

Moreover, $\left\langle \Gamma(\overline{W},\overline{W}) \right\rangle_\mu$ is independent from the solution of (43). Finally, K is symmetric wrt time reversal $K(\Pi\mu) = K(\mu)$.

4.3 Entropy production

In this section, we show that the minimum entropy production principle does not apply for Hamiltonian dynamics and that the large deviation functional (41) is a natural extension for a variational characterization of the steady state. Connections between large deviation functionals in stochastic systems and entropy production were initiated in [66]. In order to identify the average entropy production of a dynamics in a given measure, we proceed as in [93] in the context of interacting particle systems. Namely, we define the entropy production as the difference between the variation of the Gibbs (Shannon) entropy and the transfer of heat by unit time due to the action of the thermostats. A similar computation was performed in [65] for heat conduction networks and the identification of the average entropy production with the Dirichlet form of the process was obtained there and in [32].

We consider the dynamics (34) for which the generator is given by $L = L_S + L_A$ with a symmetric part given by

$$L_S = -\sum_{i=1}^{N} -\gamma_i p_i \frac{\partial}{\partial p_i} + \gamma_i T_i \frac{\partial^2}{\partial p_i^2} \,.$$

We first introduce the entropy production. In thermodynamics, the entropy variation rate, or entropy production is the transfer of energy per unit time divided by the temperature at which the transfer takes place. Therefore, it is natural to define the average (with respect to a given measure μ) entropy flux associated with the exchange of energy with the external heat baths as

$$\sigma_{ext}(\mu) = \left\langle \widetilde{L}_S H \right\rangle_\mu \,,$$

where

$$\widetilde{L}_S = \sum_{i=1}^{N} \gamma_i T_i^{-1} p_i \frac{\partial}{\partial p_i} + \sum_{i=1}^{N} \gamma_i \frac{\partial^2}{\partial p_i^2}. \tag{45}$$

We have simply divided the contribution of each bath by its temperature T_i: when the temperatures are all equal to T then $\widetilde{L}_S = \frac{1}{T} L_S$. Computation yields,

$$\widetilde{L}_S H = \sum_{i=1}^{N} \gamma_i (1 - \frac{p_i^2}{T_i}) \,,$$

and thus the average entropy flux due to the coupling to the heat baths in the measure μ is,

$$\sigma_{ext}(\mu) = \sum_{i=1}^{N} \gamma_i \left\langle (1 - \frac{p_i^2}{T_i}) \right\rangle_{\mu} . \tag{46}$$

The Gibbs (or Shannon) entropy for any measure μ is,

$$S(\mu) = -\int dx f \log f. \tag{47}$$

We define the entropy production in the chain as

$$s(\mu) \equiv \frac{d}{dt} S(\mu_t)|_{\mu_t = \mu} - \sigma_{ext}(\mu) \,. \tag{48}$$

We show now that with this definition, the entropy production is always positive. Note that,

$$\frac{d}{dt} S(\mu_t) = -\int dx f_t L \log f_t \,.$$

As $L = L_S + L_A$ and L_A is a first-order differential operator such that $L_A^\dagger = -L_A$, we see that

$$\frac{d}{dt} S(\mu_t) = -\int dx f_t (L_S + L_A) \log f_t = -\int dx f_t L_S \log f_t,$$

Comparing the density f_t with the reference measure $\rho_{\underline{\beta}}$ (see (17))

$$\rho_{\underline{\beta}} = \frac{1}{Z_{\underline{\beta}}} \exp\left(-\sum_{i=1}^{N} \beta_i h_i \right) , \tag{49}$$

where $\beta_i = T_i^{-1}$ for every i such that $\gamma_i \neq 0$ (other β_i are arbitrary), we get,

$$\begin{aligned} \frac{d}{dt} S(\mu_t) &= -\int dx f_t L_S \log \frac{f_t}{\rho_{\underline{\beta}}} + \int dx f_t L_S \left(\sum_{i=1}^{N} \beta_i h_i \right) \\ &= -\int dx f_t L_S \log \frac{f_t}{\rho_{\underline{\beta}}} + \sum_{i=1}^{N} \gamma_i \int f_t (1 - \frac{p_i^2}{T_i}). \end{aligned} \tag{50}$$

We recall that $\Gamma(f,g) = 2\sum_{i=1}^N \gamma_i T_i\, \partial_{p_i} f \partial_{p_i} g$. For the first term, we note the identity,

$$L_S(\log h) = h^{-1} L_S h - \tfrac{1}{2} h^{-2} \Gamma(h,h)\,.$$

Combining (46), (50) and using the fact that $(L_S)^\dagger \rho_{\underline{\beta}} = 0$ (because $\beta_i = T_i^{-1}$ for every i such that $\gamma_i \neq 0$), with (48), this yields

$$s(\mu) = \tfrac{1}{2} \int dx \rho_{\underline{\beta}} (\frac{\rho_{\underline{\beta}}}{f}) \Gamma\left(\frac{f}{\rho_{\underline{\beta}}}, \frac{f}{\rho_{\underline{\beta}}}\right) = 2 \int dx \rho_{\underline{\beta}} \Gamma\left(\sqrt{\frac{f}{\rho_{\underline{\beta}}}}\,,\, \sqrt{\frac{f}{\rho_{\underline{\beta}}}}\right)\,, \qquad (51)$$

with f the density of the measure μ. Since $\Gamma(f,f) \geq 0$, it is easy to see that $s(\mu) \geq 0$ and that the infimum is reached when $f = \rho_{\underline{\beta}}$. As already observed in [65], it is also obvious that, as Γ only involves derivatives with respect to the variables $\underline{p}$, one can add any function of $\underline{q}$ in the exponential defining $\rho_{\underline{\beta}}$. Therefore, even in the case of an equilibrium dynamics, when $T_i = T$, $\forall i$, such that $\gamma_i \neq 0$ in L_S, the minimum entropy production principle does not single out the equilibrium measure $\rho_{\underline{\beta}}$. This comes from (49) which expresses the fact that the Gibbs entropy is invariant under the Hamiltonian evolution. Entropy is produced solely by the action of the thermostats which act only on the $\underline{p}$ variables.

As observed in [66], the large deviation functional I provides a natural variational characterization of the stationary measure, which as we will see below, generalizes the minimum production entropy principle. As far as the variational principle is concerned, the key observation is that $I(\mu) \geq 0$ and $I(\mu) = 0$ if and only if μ is a stationary measure for the process associated to the generator L (Theorem 4.2.39 of [23]). We apply now Proposition 19 to the dynamics (34) which satisfies a generalized detailed balance (27) wrt the reference measure $\rho = \rho_{\underline{\beta}}$ (49) and $\sigma_{\underline{\beta},\underline{\theta}} = \sum_{i=1}^{N-1} (\beta_i - \beta_{i+1} + \theta_i) j_i$. Thus (41) reads

$$I(\mu) = \frac{1}{4} s(\mu) + K(\mu) - \tfrac{1}{2} \left\langle \sigma_{\underline{\beta},\underline{\theta}} \right\rangle_\mu\,, \qquad (52)$$

where we have used the following identity obtained by integration by parts from (51)

$$\frac{1}{4} s(\mu) = -\left\langle f^{\frac{1}{2}} L_S f^{\frac{1}{2}} \right\rangle_{\rho_{\underline{\beta}}}\,, \qquad (53)$$

for the reference measure $\rho_{\underline{\beta}}$. The first term in (52) is identified with the entropy production s of the measure μ, and as we have seen in the previous section, the second one K records the coupling between the positions and momenta. The last term in (52) is the time-reversal breaking term given by combination of the microscopic currents. For equilibrium dynamics, by definition, the term σ is absent, and the presence of K ensures that the minimization of the sum of the first two terms in (52) yields the stationary measure univocally. Indeed, as we have explained above, minimizing entropy production alone is not sufficient to determine the equilibrium distribution.

Chapter 5

Transfer of heat in lattice collisional dynamics.

In this chapter, I present the results of [43, 61].

5.1 Boltzmann approach to the transfer of heat in lattice collisional dynamics.

As a generic model of heat transfer in insulating crystalline solids, one often considers a lattice of coupled particles with nearest-neighbor interactions whose motion obeys Hamilton's equations. Thus consider N particles of unit masses located on a one-dimensional lattice with positions and momenta $(\underline{\mathbf{q}}, \underline{\mathbf{p}}) \equiv \{(\mathbf{q}_i, \mathbf{p}_i)\}_{1 \leq i \leq N}$, with $\mathbf{q}_i, \mathbf{p}_i \in \mathbb{R}^d$. The Hamiltonian H takes the form

$$H(\underline{\mathbf{p}}, \underline{\mathbf{q}}) = \sum_{i=1}^{N} \left[\frac{p_i^2}{2} + V(\mathbf{q}_i) + U(\mathbf{q}_i - \mathbf{q}_{i+1}) \right], \tag{1}$$

where V represents the interaction with the external substrate and U the nearest-neighbor interactions [1].

After Peierls' work [80], all attempts to give a satisfactory derivation of Fourier's law in mechanical systems have focused on the study of weakly anharmonic dynamics. Using the Peierls-Boltzmann equation, recent works have studied the effects of phonon collisions on the heat conductivity [15, 81, 95, 60, 2]. In this context, the conductivity may be interpreted as a collision frequency between phonons.

In this letter, we focus on the opposite limit, namely extremely anharmonic interactions, and, under minimal assumptions on the chaotic nature of the dynamics, identify a class of models which display a universal response to non-equilibrium thermal constraints. The motivation for this study is twofold: First, the heat conductivity can be computed from first principles and takes a simple form; Second, as pointed out in [42], such systems of locally confined particles in interaction find concrete applications in the study of aerogels, materials in which gas particles are trapped in nano-size pores and rarely interact

[1] It is understood here that the positions $\mathbf{q}_i$ are measured with respect to a local referential at site i.

among themselves. Assuming the validity of a Boltzmann-like equation to describe such systems of rarely interacting particles when they become large, we show that the heat conductivity of such systems is generically equal to the average frequency of interaction between the systems' components, *i.e.* irrespective of the detailed geometric properties of the confinement mechanism. This will be checked in detail by numerical simulations, showing the universality and power of the Boltzmann approach to analyze the transfer of heat in the mechanical systems we study.

To be specific, we consider the case of interaction potentials which take only the values zero inside a region $\Omega_U \subset \mathbb{R}^d$ with smooth boundary Λ of dimension $d-1$, and infinity outside. Likewise, the pinning potential V is assumed to be zero inside a bounded region Ω_V and infinity outside, implying that the motion of a single particle remains confined for all times. The regions Ω_U and Ω_V being specified, the dynamics is equivalent to a billiard in higher dimension. An important quantity in such models is the average rate of collisions between nearest-neighbors under equilibrium conditions. We will be specifically concerned with the limit of rare collision events.

The shape of the region Ω_V determines the nature of the local dynamics. In ref. [42], Ω_V was chosen to be a semi-dispersive billiard with bounded horizon, thus ensuring strong chaotic properties of the dynamics. In particular the fast decay of correlations of the local dynamics was invoked to set up a stochastic equation describing the energy exchange dynamics. It is our purpose to show that this assumption can be relaxed: local ergodicity is enough to warrant the identity between heat conductivity and frequency of energy exchanges. We regard this as an important result which further validates the analogy between this class of models and aerogels whose nanopores need not have dispersing properties.

Examples of the simplest type of billiards we may consider are periodic arrays of square boxes in two dimensions in each of which a single hard disk particle moves freely, but can still perform collisions with neighboring disks by interacting through the confining walls, for instance, provided we let the cells overlap a bit. The specific nature of the interaction mechanism at play is however not relevant in our formalism. We will instead consider point particles moving freely in two-dimensional square boxes of unit sides and interacting among nearest neighbors when the Euclidean distance between them becomes equal to a parameter which we denote by a. At that point, they exchange their longitudinal velocities, *i.e.* the velocity components in the direction of their relative motion. We refer to this model as the *square-strings model*. The interaction may be depicted by attaching strings of lengths a separating neighboring particles, as shown in Fig. 5.1. In this case, we take $\Omega_V = [-1/2, 1/2]^2$, and $\Omega_U = \mathbb{D}^2_{(-1,0)}(a)$, the disk of radius a with center at $(-1, 0)$ [2]. We note that, in the absence of interactions, the dynamics of the individual particles is pseudo-integrable; it is ergodic on the configuration space for most values of the velocity directions, but is known to be non-mixing. We will consider this model in some details below and provide numerical evidence that the analysis which follows applies to it.

[2]The origin of the disk is shifted because the positions of the particles are measured with respect to the center of the cell Ω_V.

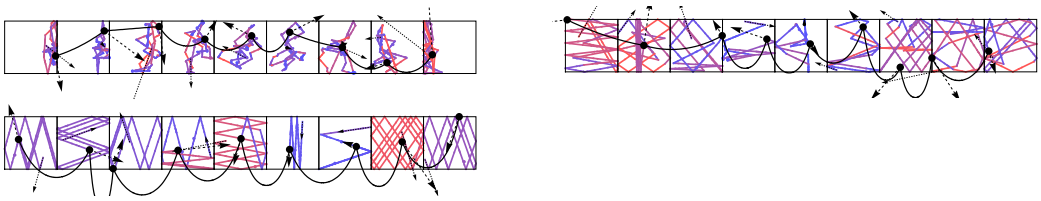

Figure 5.1: Typical trajectories of the square-strings model, displayed for increasing values of a, color-coded from blue to red according to their energies. Small and large arrows indicate initial and final velocities respectively. For large a, the system appears to be near-integrable, reflecting the rarity of interactions, but is nevertheless fully chaotic.

This model can be compared to a simpler class of *complete exchange models*, specified by square well potentials, obtained from Eq. (1) with $d = 1$, as a limit of models with smooth interaction potentials. In this case, $\Omega_V = [-b, b]$ and $\Omega_U = [-a, a]$. Each particle on the lattice moves freely on a one-dimensional cell of size $2b$, changing directions at the boundaries. The interaction between a pair of particles acts when the difference between the positions of the two particles reaches the value a, at which point they exchange their velocities.

In the general d-dimensional set-up, the particles move freely inside their respective cells, bouncing off the walls elastically, until the vector $\mathbf{q}_i - \mathbf{q}_{i+1}$ (resp. $\mathbf{q}_{i-1} - \mathbf{q}_i$) reaches the boundary Λ. The corresponding particles then exchange the components of their velocities in the direction normal to the boundary Λ, *i.e.* longitudinal to the direction of their relative motion.

The Hamiltonian (1) may be written as a sum of local terms,

$$h_i(\underline{\mathbf{p}}, \underline{\mathbf{q}}) = p_i^2/2 + V(\mathbf{q}_i) + 1/2\left[U(\mathbf{q}_{i-1} - \mathbf{q}_i) + U(\mathbf{q}_i - \mathbf{q}_{i+1})\right].$$

This allows one to define a function describing the local transfer of energy by computing the variation in time of the local energy h_i along the solutions of the equations of motion, $\frac{d}{dt}h_i(\underline{\mathbf{p}}, \underline{\mathbf{q}}) = j_{i-1} - j_i$, where the local energy current between sites i and $i+1$ is defined as, $j_i \equiv \frac{1}{2}(\mathbf{p}_i + \mathbf{p}_{i+1}) \cdot \nabla U(\mathbf{q}_i - \mathbf{q}_{i+1})$, which, for hard core interactions, becomes

$$j_i = -hf\delta_\Lambda(\mathbf{q}_i - \mathbf{q}_{i+1})|p_{i+1}^\perp - p_i^\perp|^+ \left[(p_{i+1}^\perp)^2 - (p_i^\perp)^2\right], \tag{2}$$

where $|x|^+ = x$, if $x \geq 0$, and 0 otherwise, $p_i^\perp = \mathbf{p}_i \cdot \widehat{\mathbf{n}}$ is the component of the vector $\mathbf{p}_i$ in the direction of the unit vector $\widehat{\mathbf{n}}$, normal to the boundary Λ, and δ_Λ denotes the delta function concentrated on this boundary. The first factor corresponds to the localization of the collisions in configuration space, the second one gives the rate at which collisions occur and the last one corresponds to the exchange of longitudinal components of the kinetic energies.

Starting from the Liouville equation for the evolution of probability densities on phase space, it is straightforward to derive an equation for the evolution of the probability density of a single particle in a given cell. It involves the probability distribution of the pairs of particles which consist of the particle itself and either of its nearest-neighbors on the lattice. The Boltzmann approximation simply amounts to assuming that this two-particle distribution factorizes in terms of the one-particle distributions f_i at each site. To justify

this assumption, one needs to show that a version of molecular chaos holds in our models. Namely, that the dynamical variables involved in the successive collisions between two neighbors are independent at the times of collisions. For that purpose, we require two ingredients: First, local correlations are typically destroyed after a collision between neighboring particles; Second, the number of particles must be very large, so that in the long run, the whole system plays the role of a reservoir for the specified pair of nearest neighbors. How these conditions are realized in the models we consider and, in particular, in the square-strings model which we test numerically, is not yet fully elucidated. We interpret the first condition as requiring interactions to be rare compared to the collisions within a single cell. In the square-strings model, it amounts to taking the maximal separation close to the length of the diagonal joining opposite corners of neighboring boxes ($\equiv \sqrt{5}$), as in the third panel of Fig. 5.1.

We denote by $\underline{f} = \{f_i(\mathbf{p}, \mathbf{q}, t)\}_{1 \leq i \leq N}$, the set of the marginal probability distributions of each particle in each cell. The Boltzmann equation for this set of probability densities is

$$\frac{d}{dt} f_i(\mathbf{p}, \mathbf{q}, t) = -\mathbf{p} \cdot \nabla_{\mathbf{q}} f_i + L^{\mathrm{w}} f_i + L^{\mathrm{c}}_{i,i+1}(\underline{f}) + L^{\mathrm{c}}_{i,i-1}(\underline{f}). \tag{3}$$

Here L^{w} accounts for the collisions of the particles with the walls of their respective cells, and $L^{\mathrm{c}}_{i,i\pm1}$ for the collisions of the i-th particle with the $i\pm1$th, *viz.*

$$\begin{aligned} L^{\mathrm{c}}_{i,i\pm1}(\underline{f}) = \int \mathrm{d}\ \mathbf{p}_a \mathrm{d}\ \mathbf{q}' \delta_\Lambda(\mathbf{q} - \mathbf{q}') |p^\perp - p_a^\perp|^+ \\ \times [f_{i\pm1}(\mathbf{p}_b, \mathbf{q}') f_i(\mathbf{p}_c, \mathbf{q}) - f_i(\mathbf{p}, \mathbf{q}) f_{i\pm1}(\mathbf{p}_a, \mathbf{q}')], \end{aligned} \tag{4}$$

with $p_b^\perp = p^\perp$, $p_c^\perp = p_a^\perp$, $\mathbf{p}_c - p_c^\perp \widehat{\mathbf{n}} = \mathbf{p} - p^\perp \widehat{\mathbf{n}}$, and $\mathbf{p}_b - p_b^\perp \widehat{\mathbf{n}} = \mathbf{p}_a - p_a^\perp \widehat{\mathbf{n}}$. One can check that the distribution

$$\mu_{\mathrm{eq}} \equiv \prod_{i=1}^{N} f_i(\mathbf{p}_i, \mathbf{q}_i) = Z^{-1} \prod_{i=1}^{N} e^{-\beta p_i^2/2} \mathbf{1}_{\Omega_V}(\mathbf{q}_i) \tag{5}$$

is stationary for any inverse temperature β. Applied to this distribution, the advection term in Eq. (3) is zero except on the cell borders where it cancels with $L^{\mathrm{w}} f_i$. β may be fixed by imposing identical thermal boundary conditions at both ends of the lattice.

When the system is set out of equilibrium by imposing different temperatures at its boundaries, we proceed with a standard Chapman-Enskog expansion around a local equilibrium distribution,

$$\mu_{\mathrm{leq}} \equiv \prod_{k=1}^{N} f_k(\mathbf{p}_k, \mathbf{q}_k) = Z^{-1} \prod_{k=1}^{N} e^{-\beta_k p_k^2/2} \mathbf{1}_{\Omega_V}(\mathbf{q}_k), \tag{6}$$

with $\beta_k = \widehat{\beta}(k/N)$ for some smooth function $\widehat{\beta}$, taking as a small parameter the local temperature gradient. Plugging Eq. (6) into (3), we observe that only terms of second-order in the temperature gradient survive. This is in contrast with the case of an ordinary gas of colliding particles. This simplification occurs because the advection term of the Boltzmann equation (3) acts only

on the position variable within each cell and therefore not as a gradient on the lattice dependent variables. This means that local averages with respect to the distribution (6) are identical to local averages with respect to the true non-equilibrium stationary state, denoted $\langle\cdot\rangle_{\rm neq}$, up to $1/N^2$ corrections.

In particular, one may compute the average current (2) with respect to the measure (6) and get (with $\beta_i = T_i^{-1}$),

$$\langle j_i\rangle_{\rm neq} = -\nu(T_i)(T_{i+1} - T_i) + \mathcal{O}(1/N^2), \tag{7}$$

where, $\nu(T_i) = \langle\delta_\Lambda(q_i - q_{i+1})|p_i^\perp - p_{i+1}^\perp|^+\rangle_{T_i}$ is readily interpreted as the average collision frequency between the neighbors i and $i+1$, with respect to a global equilibrium measure at temperature T_i, Eq. (5). This computation therefore shows that the conductivity $\kappa(T_i)$, defined as

$$\kappa(T_i) \equiv \lim_{N\to\infty} -\frac{\langle j_i\rangle_{\rm neq}}{T_{i+1} - T_i}, \tag{8}$$

is identical to $\nu(T_i)$. Furthermore a simple scaling argument shows that $\kappa(T_i) = \nu(T_i) = \sqrt{T_i}\nu$, where ν denotes the collision frequency computed at unit temperature. Being the result of an equilibrium integration, the frequency may be computed with arbitrary precision.

In order to get a better picture of the process that is described by the Boltzmann equation (3), we linearize the equation around the global equilibrium solution (5). Doing so, we obtain an equation similar to (3), but with the collision operators $L^{\rm c}_{i,i\pm1}$ now replaced by $L^{\rm lin}_i$,

$$\frac{d}{dt}f_i(\mathbf{p},\mathbf{q},t) = -\mathbf{p}\cdot\nabla_{\mathbf{q}}f_i + L^{\rm w}f_i + 2L^{\rm lin}_i f, \tag{9}$$

where the linearized collision operator $L^{\rm lin}_i$ is obtained from Eq. (4) by replacing $f_{i\pm1}$ by equilibrium distributions at common inverse temperature β.

The interpretation of the stochastic process described by the linearized collision operator is straightforward: when collisions take place, the particles velocities are updated as though they collided with stochastic thermal walls at inverse temperature β [56]. At each collision, the new velocities are independent from the previous ones.

With this prescription, we now compute the conductivity using the Green-Kubo formula, which is derived as follows. Integrated over time, the energy current between sites i and $i+1$ takes the form

$$J_i([0,t]) = \int_0^t j_i(s)ds = \tfrac{1}{2}\sum_{0\le s_i^k\le t}\left[p_i^\perp(s_i^k)^2 - p_{i+1}^\perp(s_i^k)^2\right], \tag{10}$$

where the $(s_i^k)_{k\in\mathbb{N}}$ are the successive collision times between particles i and $i+1$. The Green-Kubo formula, reads in our case,

$$\kappa_{\rm GK}(T) = \frac{1}{2NT^2}\lim_{t\to\infty}\frac{1}{t}\sum_{i,k=1}^{N}\Big\langle J_i([0,t])J_k([0,t])\Big\rangle_T. \tag{11}$$

Using the expression (10), (2), translation-invariance and the independence of the transfer of energy at each collision, we get, after some calculations,

$$\kappa_{\mathrm{GK}}(T) = \frac{1}{8T^2}\left\langle \delta_\Lambda(\mathbf{q}_0-\mathbf{q}_1)|p_0^\perp - p_1^\perp|^+ \left[(p_0^\perp)^2-(p_1^\perp)^2\right]^2\right\rangle_T, \tag{12}$$

which, after further computations turns out to be equal to the collision frequency, $\kappa_{\mathrm{GK}}(T) = \nu(T)$.

The square-strings model displayed in Fig. 5.1 lends itself to a detailed study of the dependence of the ratio κ/ν on the parameter values a.

To this end we consider systems of varying sizes N with both ends in contact with stochastic thermal baths at respective temperatures $T_- = 1/2$ and $T_+ = 3/2$. This gives rise to non-equilibrium stationary states with temperature profiles such as displayed in Fig. 5.2, which, as N increases, approach the corresponding solution of the heat equation, $\partial_x[\kappa(T(x))\partial_x T(x)] = 0$, with $\kappa(T(x)) \propto \sqrt{T(x)}$. The ratio κ/ν is obtained by linearly extrapolating to $N \to \infty$ finite N measurements of the spatial averages of $\kappa(T_i)/\nu(T_i)$, with $\kappa(T_i)$ defined by Eq. (8) and $\nu(T_i)$ the collision frequency at the local temperature, as functions of $1/N$.

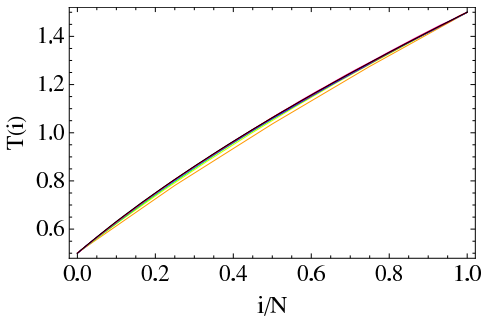

Figure 5.2: Non-equilibrium temperature profiles of the square-strings model with $a = 2.08$, for increasing values of $N = 5, 10, \ldots, 50$. The black curve is the stationary solution of the heat equation. The inset displays the corresponding measurements of $\langle \kappa(T_i)/\nu(T_i)\rangle$. The infinite N extrapolation, $\kappa/\nu = 1.0037$, is the approximate heat conductivity reported in Table 5.1.

These values are reported in Table 5.1. Notice the excellent agreement with the prediction $\kappa = \nu$, Eq. (12), as the value of the parameter a gets closer to its maximal allowed value, the limit of rare collisions, in close agreement with the results presented in [42] for a class of coupled semi-dispersing billiards. In particular we underline that the parameter range of validity of our result is very similar to that observed in [42], which further validates that it is independent of the detailed nature of the local dynamics.

To summarize, we have showed that the derivation of Fourier's law in a large class of locally confined particle systems with hard-core interactions can be achieved from a Boltzmann-type approach with the main result that, in the appropriate limits, the heat conductivity is identified with the collision frequency.

The same identity was derived in [42] in the context of semi-dispersing billiards. The comparison is interesting since, in contrast, chaos in the square-strings model results from a defocusing mechanism which takes place after

$\sqrt{5}-a$	κ/ν	$\sqrt{5}-a$	κ/ν	$\sqrt{5}-a$	κ/ν
1.029	6.000	0.618	1.892	0.322	1.320
0.870	3.159	0.511	1.632	0.236	1.0718
0.736	2.336	0.413	1.452	0.155	1.0037

Table 5.1: Measurements of κ/ν for selected values of a, obtained from data similar to Fig. 5.2. Our results indicate that $\kappa/\nu \to 1$ as $a \to \sqrt{5}$, in agreement with Eq. (12).

particles interact. The identity between conductivity and collision frequency therefore proves to be more general as it accounts for the transport properties of systems lacking the local mixing property. In fact, the only dynamical property which is a priori necessary in our derivation is ergodicity of the local dynamics, *i.e.* in the absence of interactions. This property guarantees that two neighbors always interact provided the coupling is switched on, and that the fraction of time during which they interact is proportional to a fixed geometrical factor which can be adjusted by tuning the systems' parameters.

The square-strings model is a perfect example of a system which lends itself with ease to a precise and reliable numerical analysis, while retaining the molecular chaos property. The square-strings model is actually a kind of higher dimensional fully chaotic stadium and displays a very rich structure of dynamical properties.

We regard the proof of the molecular chaos hypothesis upon which our computation relies as a promising and realistic way to eventually obtain a clear picture of the different mechanisms responsible for the origin of Fourier's law in a large class of mechanical systems.

5.2 Stochastic models for the transfer of heat in collisional dynamics.

An important feature of the collisional models is that the evolution of energy occurs at discrete (collision) times and amounts to an exchange of kinetic energy between neighbors. The length of the interval of time between two successive collisions depends itself on the kinetic energy of the particle, which fixes the $\sqrt{T}$ dependance of the collision frequency. Our idea is to build and analyze models which are stochastic from the start and share the general structure described by the Boltzmann description sketched above.

Thus, we want to consider dynamics which consists of a mixture of integrable Hamiltonian dynamics and collisions with stochastic heat baths. The models are made of scatterers described as heat baths and tracer particles transferring energy between those "hot" scatterers. The tracers move in a one-dimensional interval in which the scatterers are located on a lattice. The motion of a tracer is ballistic except when it encounters a scatterer. At that point its velocity is randomly updated according to a law which depends on the temperature of the scatterer. The temperature of the scatterers is fixed by the condition that in the stationary state, no energy is exchanged between the scatterers and the tracers. In spirit, this is similar to the so-called self-

consistent chain of (an-)harmonic oscillators [10, 13, 14], but in our case it may be naturally interpreted as a condition ensuring that the energy transfer per unit time between scatterers is constant throughout the system.

Geometrically, the systems we study are analogous to the ones introduced and studied in [33, 34, 76]. The scatterers of our models are similar to the energy storing devices of those models. However, in our case, the dynamics is stochastic from the start and the action of the scatterer models the one of a very large system. As in those models we distinguish two types of dynamics. Depending on whether the particles are confined or not between the scatterers, we derive a non-linear or linear profile of temperatures for the scatterers. Those two types of behaviours described by *wandering* or *confined* tracers seem to be universal in systems described by a collisional dynamics at a microscopic level [33, 34, 76, 42, 43, 83]. Among the collisional dynamics described above, two typical examples are given in [83] and [42, 43]. In [83], a detailed numerical analysis of the complete exchange model is provided. Fourier's law holds and the temperature profile is linear. In our framework this may be understood as an instance of wandering tracer dynamics. Indeed, in the complete exchange dynamics, it is not only the energy that is exchanged between neighbors but also the momenta of the particles. Thus, the dynamics is more similar to the one of particles traveling through the whole system. In [42, 43], models where the particles are confined and exchange only a fraction of their energy are considered. They display a temperature profile identical to the ones of the confined tracers.

As stochastic processes, our models are naturally described by *Markov renewal processes*. In section 5.3, we define the tracers and scatterers models in full generality and provide an explicit formula for the stationary measure out of equilibrium. In section 5.3.1, we describe and analyze the properties of the *wandering tracer* model in its simplest version, i.e. when a tracer encounters a scatterer it is deterministically transmitted on the other side of the scatter. We find that when the temperatures are fixed and the temperatures in the bulk chosen such that the transfer of energy is constant throughout the system, then the temperature profile of the scatterers is linear. The identity between thermal conductivity and frequency of collisions between tracers and scatterers appears as a natural consequence of the renewal theorem for Markov renewal processes. Next, we study the cumulant generating function of the time-integrated current of energy. We give a rather explicit formula allowing to compute derivatives of any order. A striking feature is the lack of analyticity of the the generating function. The origin of this phenomenon may traced back to the presence of particles with arbitrarily low speed. Nevertheless, we are able to show the validity of the Green-Kubo formula for the conductivity. The final section 5.3.3 is devoted to the analysis of the dynamics of confined tracers. In that case, we find that the condition that there are no exchange of energy between the scatterers and the particles imposes a non-linear profile of temperature.

5.3 Tracers and hot scatterers

We consider a gas of M non-interacting tracer particles moving through a one-dimensional lattice of scatterers w_n, $n = 1, \ldots, N$. In between the scatterers,

the tracers move with constant speed in the boxes I_i,

$$I_n = [n-1, n]\,, \qquad n = 1, \ldots, N \tag{13}$$

When a tracer encounters the scatterer n, it is absorbed and re-emitted on either side according to a certain probability distribution with a random velocity p distributed according to the law

$$\phi^{\pm}_{\beta_n}(p) = p^{\pm}\, \beta_n\, e^{-\beta_n \frac{p^2}{2}}, \tag{14}$$

The state space describing the motion of the particle is thus the cartesian product of the positions space $I = [0, N]$ and velocity space $\mathbb{R}^* = \mathbb{R}\backslash\{0\}$, $\Omega = I \times \mathbb{R}^*$. At the extremities of the system the sign of the velocity is reversed but the particle bounces back with a random velocity distributed according to the same law with parameter β_L and β_R. This dynamics defines a Markov renewal process which we describe now more formally using the same notations as above.

For notational simplicity, we define the dynamics for a single tracer particle, the extension to M particles is straightforward. The particle moves in the interval $I := [0, N]$, which is split into N subintervals of equal length: $I_n := [n-1, n]$, $n = 1, \ldots, N$. At time $t = 0$, the particle starts at position $q_0 \in]0, N[$ with speed $p_0 \in \mathbb{R}^* := \mathbb{R}\backslash\{0\}$ and we define $(n_0, \sigma_0) \in E$ as follows: $n_0 := \lfloor q + (\mathrm{sign}(p_0) + 1)/2 \rfloor \in \{0, 1, \ldots, N\}$, where $\lfloor \cdot \rfloor$ denotes the integer part; in other words n_0 is such that

$$\begin{cases} n_0 - 1 < q_0 \leq n_0 & \text{if} \quad \mathrm{sign}(p_0) = +1, \\ n_0 \leq q_0 < n_0 + 1 & \text{if} \quad \mathrm{sign}(p_0) = -1. \end{cases}$$

and denotes the first scatterer the particle hits. We define moreover

$$\sigma_0 := \begin{cases} \mathrm{sign}(p_0), & \text{if} \quad n_0 \in \{1, \ldots, N-1\}, \\ -\mathrm{sign}(p_0), & \text{if} \quad n_0 \in \{0, N\}. \end{cases}$$

In other words, if the first scatterer the particle hits is at the boundary $\{0, N\}$ of the system, then the particle will be reflected at the first hitting.

We suppose that the sequence $X_k = (n_k, \sigma_k)$ of scatterers visited by the particle and signs of the velocity is a Markov chain on

$$E := \{(n, \sigma),\ n = 1, \ldots, N-1,\ \sigma = \pm 1\} \cup \{(0, +1), (N, -1)\},$$

with initial state (n_0, σ_0) and with an irreducible probability transition matrix on E such that

$$q_{(n,\sigma),(n',\sigma')} = \begin{cases} 1 & \text{if} \quad (n, \sigma) = (1, -1) \text{ and } (n', \sigma') = (0, +1) \\ 1 & \text{if} \quad (n, \sigma) = (N-1, +1) \text{ and } (n', \sigma') = (N, -1) \\ 0 & \text{if} \quad n \in \{1, \ldots, N-1\} \quad \text{and} \quad n' - n \neq \sigma'. \end{cases}$$

The first two conditions mean that the tracer is always reflected at $n = 0$ and $n = N$. The last condition means that the new sign σ' gives the next scatterer n' visited: if $\sigma' = +1$ then $n' = n + 1$, if $\sigma' = -1$ then $n' = n - 1$. The irreducibility assumption gives the existence of a unique invariant probability measure that we call $(\nu_\alpha)_{\alpha \in E}$.

We now define the time the particle takes between two subsequent visits to the scatterers. Conditionally on $\mathcal{H} = \sigma((X_k)_{k\geq 0})$, the sequence $(\tau_k)_{k\geq 1}$ is independent with distribution defined by

$$\mathbb{P}(\tau_k \in d\tau \,|\, \mathcal{H}) = \mathbb{P}(\tau_k \in d\tau \,|\, X_{k-1}) = \frac{\beta_n}{\tau^3} \exp\left(-\frac{\beta_n}{2\tau^2}\right) \mathbb{1}_{(\tau>0)}\, d\tau =: \psi_n(d\tau) \tag{15}$$

on the event $\{X_{k-1} = (n, \sigma)\}$, where $\beta_0, \ldots, \beta_N \in \mathbb{R}_+$. We consider now the Markov chain $(X_k)_{k\geq 0}$ with initial state $X_0 = (n, \sigma)$ and the associated sequence $(\tau_k)_{k\geq 1}$. The time of the first collision with a wall is

$$S_0 = S_0(q_0, p_0) := \frac{n_0 - q_0}{p_0} > 0,$$

and the time of the k-th collision with one of the scatterers is

$$S_k := S_0 + \tau_1 + \cdots + \tau_k, \qquad k \geq 1.$$

Before time S_0, the particle moves with uniform velocity p. Between time S_{k-1} and time S_k, the particle moves with uniform velocity $\frac{\sigma_k}{\tau_k}$ and $(S_k)_{k\geq 0}$ is the sequence of times when $q_t \in \{0, \ldots, N\}$. In particular we define the sequence of incoming velocity v_k at time S_k

$$v_0 := p_0, \qquad v_k := \frac{\sigma_k}{\tau_k}, \quad k \geq 1. \tag{16}$$

We define precisely the stochastic process $(q_t, p_t)_{t\geq 0}$ with values in $[0, N] \times \mathbb{R}^*$

$$(q_t, p_t) := \begin{cases} (q_0 + p_0 t, p_0) & \text{if} \quad t < S_0, \\ \left(n_{k-1} + \frac{\sigma_k}{\tau_k}(t - S_{k-1}), \frac{\sigma_k}{\tau_k}\right) & \text{if} \quad S_{k-1} \leq t < S_k,\ k \geq 1, \end{cases} \tag{17}$$

and we use the notation $X_k = (n_k, \sigma_k)$, $X_{k-1} = (n_{k-1}, \sigma_{k-1})$. The invariant measure of the process is given explicitely in the following proposition.

Proposition 21 *The process $(q_t, p_t)_{t\geq 0}$ is Markov and its only invariant measure on $[0, 1] \times \mathbb{R}^*$ is given by*

$$\gamma(dq, dp) = \frac{1}{Z_N} \sum_{n=1}^{N} \mathbb{1}_{I_n}(q) \sum_{\sigma=\pm 1} \Big(\nu_{(n-1,\sigma)}\, q_{(n-1,\sigma),(n,+1)}\, \mathbb{1}_{(p>0)}\, \beta_{n-1}\, e^{-\beta_{n-1}\frac{p^2}{2}} \tag{18}$$

$$+ \nu_{(n,\sigma)}\, q_{(n,\sigma),(n-1,-1)}\, \mathbb{1}_{(p<0)}\, \beta_n\, e^{-\beta_n \frac{p^2}{2}} \Big)\, dq\, dp \tag{19}$$

where $Z_N = \sqrt{\frac{\pi}{2}} \sum_{(n,\sigma)\in E} \nu_{(n,\sigma)} \sqrt{\beta_n}$.

5.3.1 Wandering tracers

In the first model that we study, when a tracer reaches a scatterer $n \in \{1, \ldots, N-1\}$, it is absorbed on one side and re-emitted on the other side with a random velocity distributed according to a law determined by the temperature of the scatterers. The sign of the velocity changes when and only

when the tracer reaches the scatterers 0 or N. The transition matrix of the underlying Markov chain is

$$q_{(n,\sigma),(n',\sigma')} = \begin{cases} 1 & \text{if} \quad n' = n + \sigma \notin \{0, N\} \text{ and } \sigma = \sigma' \\ 1 & \text{if} \quad (n, \sigma) = (1, -1) \text{ and } (n', \sigma') = (0, +1) \\ 1 & \text{if} \quad (n, \sigma) = (N-1, +1) \text{ and } (n', \sigma') = (N, -1) \\ 0 & \text{otherwise.} \end{cases}$$

The associated invariant probability measure given is the uniform distribution on E. In fact, in this case the Markov chain moves deterministically as follows: $X_k = (n_k, \sigma_k)$ where

$$\begin{cases} n_k &= f\left(|n_0 + \sigma_0 k| \bmod 2N\right), \qquad f(i) := N - |N - i|, \quad i = 0, \ldots, 2N \\ \sigma_k &= \sigma_0 \, (-1)^{\lfloor (n + \sigma_0 (n_0 - N) + N)/N \rfloor}, \qquad k \geq 1. \end{cases} \tag{20}$$

In particular, we have the following periodicity

$$(X_k)_{k \geq 0} \stackrel{d}{=} (X_{k+2N})_{k \geq 0} \quad \text{under} \quad \mathbb{P}_{(n_0, \sigma_0)} \tag{21}$$

where $\stackrel{d}{=}$ denotes equality in distribution. Proposition 21 becomes

Proposition 22 *The process $(q_t, p_t)_{t \geq 0}$ is Markov and its only invariant measure on $[0, 1] \times \mathbb{R}^*$ is given by*

$$\gamma(dq, dp) = \frac{1}{Z_N} \sum_{n=1}^{N} \mathbb{1}_{I_n}(q) \left(\mathbb{1}_{(p>0)} \, \beta_{n-1} \, e^{-\beta_{n-1} \frac{p^2}{2}} + \mathbb{1}_{(p<0)} \, \beta_n \, e^{-\beta_n \frac{p^2}{2}} \right) dq \, dp \tag{22}$$

where $Z_N = \sqrt{\frac{\pi}{2}} \sum_{n=1}^{N} \left(\sqrt{\beta_{n-1}} + \sqrt{\beta_n} \right)$.

The first useful result is the computation of the asymptotic frequency of collision of a tracer with a fixed scatterer.

Proposition 23 *For $n \in \{0, \ldots, N\}$ set $\phi_{n,0} := \inf\{\ell \geq 0 : \, n_\ell = n\}$,*

$$\phi_{n,k+1} := \inf\{\ell > \phi_{n,k} : \, n_\ell = n\}, \qquad k \geq 0$$

and

$$N_t^n := \sum_{k=1}^{\infty} \mathbb{1}_{(S_{\phi_{n,k}} \leq t)}, \qquad \widehat{N}_t^n := \sum_{k=1}^{\infty} 2 \, \mathbb{1}_{(S_{\phi_{n,2k}} \leq t)}, \qquad t \geq 0. \tag{23}$$

Then for any initial condition (q_0, p_0), $\mathbb{P}_{(q_0,p_0)}$-a.s.

$$\lim_{t \to +\infty} \frac{N_t^n}{t} = \lim_{t \to +\infty} \frac{\widehat{N}_t^n}{t} = \frac{2}{Z_N}, \quad \text{if} \quad n \in \{1, \ldots, N-1\}, \tag{24}$$

$$\lim_{t \to +\infty} \frac{N_t^n}{t} = \frac{1}{Z_N}, \quad \text{if} \quad n \in \{0, N\}. \tag{25}$$

We next identify the physical quantities of interest. The energy exchanged between the scatterer n and a particle during a time interval $[0,t]$ is given by

$$E_n([0,t]) := \tfrac{1}{2} \sum_{k\geq 0:\, S_k \leq t} \left(v_{k+1}^2 - v_k^2\right) \mathbb{1}_{(n_k=n)},$$

recall that, by (16) and (17), v_k and v_{k+1} are respectively the incoming and the outcoming velocity at time S_k. The total entropy flow due to the exchange of energy between the scatterers and a particle is given by

$$S_n([0,t]) := -\frac{E_n([0,t])}{T_n}, \qquad S([0,t]) := \sum_{n=0}^{N} S_n([0,t]). \tag{26}$$

The energy exchanged between scatterers n and $(n+1)$ during a time interval $[0,t]$ is

$$J_{n\to n+1}([0,t]) := \tfrac{1}{2} \sum_{k\geq 1:\, S_k \leq t} v_k^2 \left(\mathbb{1}_{(n_{k-1}=n,\ \sigma_{k-1}=1)} - \mathbb{1}_{(n_{k-1}=n+1,\ \sigma_{k-1}=-1)}\right).$$

We define the energy flow per unit time in the stationary state by

$$\mathcal{E}_n := \lim_{t\to+\infty} \frac{1}{t}\, E_n([0,t]). \tag{27}$$

Similarly, the entropy flow per unit time is given by

$$\mathcal{S}_n := \lim_{t\to+\infty} \frac{1}{t}\, S_n([0,t]), \qquad \mathcal{S} := \sum_{n=0}^{N} \mathcal{S}_n \tag{28}$$

and the current of energy between scatterers w_n and w_{n+1} is given by the transfer of energy per unit time,

$$\mathcal{J}_n := \lim_{t\to+\infty} \frac{1}{t}\, J_{n\to n+1}([0,t]). \tag{29}$$

Proposition 24 *The limits in (27), (28) and (29) exist $\mathbb{P}_{(q_0,p_0)}$ a.s. and for all $n = 1,\dots,N-1$,*

$$\mathcal{E}_n = \frac{2T_n - T_{n-1} - T_{n+1}}{Z_N} \quad \text{and} \quad \mathcal{E}_0 = \frac{T_0 - T_1}{Z_N}, \quad \mathcal{E}_N = \frac{T_N - T_{N-1}}{Z_N}, \tag{30}$$

$$\mathcal{J}_n = \frac{T_n - T_{n+1}}{Z_N}, \qquad \mathcal{S} = \frac{1}{Z_N} \sum_{n=0}^{N-1} \frac{(T_n - T_{n+1})^2}{T_n T_{n+1}} \geq 0. \tag{31}$$

From (30) and (31), we have the obvious result

Proposition 25 (Self-consistency condition) *The only collection $(T_n)_{n=0,\dots,N}$ such that*

$$\mathcal{E}_n = 0,\ n = 1,\dots,N-1$$

with $T_0 = T_L$ and $T_N = T_R$ is

$$T_n = T_L + \frac{n}{N}(T_R - T_L), \qquad n = 0,\dots,N. \tag{32}$$

The entropy flow per unit time $\mathcal{S}$ is equal to 0 if and only if $T_L = T_R$.

Note that the condition on the exchange of energy is imposed only for the scatterers. In contrast, when $T_L \neq T_R$ the tracer will always exchange energy with the boundary walls.
Let us consider now M_N (to be fixed) non-interacting tracer particles described by their momenta and positions $(\underline{p}, \underline{q}) = (p_i, q_i)_{1 \leq i \leq M_N}$ and moving through the array of scatterers. As the motions of the tracers are independent, the generalization is straightforward. The corresponding stationary measure is given by

$$\gamma^{M_N}(d\underline{q}, d\underline{p}) = \prod_{i=1}^{M_N} \gamma(dq_i, dp_i) \tag{33}$$

and the total average current between scatterers w_n and w_{n+1} is the sum of the contribution of each particle in (31)

$$\mathcal{J}_n^{M_N} = M_N \, \frac{T_n - T_{n+1}}{Z_N}. \tag{34}$$

The total rate of energy exchanged between the scatterer w_n and the tracers in the stationary state is given by

$$\mathcal{E}_n^{M_N} = M_N \, \frac{2T_n - T_{n-1} - T_{n+1}}{Z_N}. \tag{35}$$

Thus, if the the self-consistency condition is imposed and the temperatures of the scatterers is given by (32), then, by (34), one has

$$\mathcal{J}_n^{M_N} = -\frac{M_N}{N Z_N} \, (T_R - T_L). \tag{36}$$

The local conductivity is defined as the ratio of the average current of energy to the local temperature gradient, namely,

$$\kappa_n \equiv \lim_{N \to \infty} \frac{\mathcal{J}_n^{M_N}}{T_n - T_{n+1}} = \lim_{N \to \infty} \frac{M_N}{Z_N}. \tag{37}$$

If the temperature profile is given by (32), then one may compute the explicit asymptotic behavior of Z_N in the large N limit

$$\lim_{N \to \infty} \frac{Z_N}{N} = \sqrt{2\pi} \int_0^1 \frac{dx}{(T_L + x(T_R - T_L))^{\frac{1}{2}}} = \frac{2\sqrt{2\pi}}{T_R^{\frac{1}{2}} + T_L^{\frac{1}{2}}}. \tag{38}$$

Thus for a number of tracers $M_N = o(N)$, we have $\kappa_n = 0$. This is because when the number of scatterers increases, the proportion of time that a given tracer spends carrying energy from scatterer w_n to w_{n+1} goes to zero simply because the tracer must go back and forth in a larger and larger system. However, we see that if we take as many tracer particles as scatterers, namely $M_N = N$, then Fourier's law holds, i.e the conductivity is finite. Its value is given by

$$\kappa_n = \frac{T_R^{\frac{1}{2}} + T_L^{\frac{1}{2}}}{2\sqrt{2\pi}}. \tag{39}$$

Notice that κ_n does not depend on n. In particular, if $T_L = T_R = T$

$$\kappa_n = \sqrt{\frac{T}{2\pi}}. \tag{40}$$

5.3.2 Cumulant generating function and the Gallavotti-Cohen symmetry relation

We denote $\mathcal{B} = (\beta_0, \ldots, \beta_N) \in \mathbb{R}_+^{N+1}$. We do not need in this section to assume that $T_i := \beta_i^{-1}$ satisfy (32). Fix $n \in \{0, \ldots, N-1\}$. We are going to compute and study the properties of the cumulant generating function,

$$f_n(\lambda, \mathcal{B}) := \lim_{t \to +\infty} \frac{1}{t} \log \mathbb{E}\left(\exp\left(-\lambda J_n([0,t])\right)\right), \qquad \forall\, \lambda \in]-\beta_n, \beta_{n+1}[. \quad (41)$$

We define $\Delta_n(\alpha) := \left(\mathbb{1}_{(i=n,\ \sigma=1)} - \mathbb{1}_{(i=n+1,\ \sigma=-1)}\right)$ for $\alpha = (i,\sigma) \in E$. For $\lambda \in]-\beta_n, \beta_{n+1}[$ and $\epsilon \geq 0$, we define

$$C_n(\alpha, \lambda, \epsilon) := \beta_i \int_0^{+\infty} v\, e^{-\frac{\epsilon}{v} - (\beta_i + \lambda\, \Delta_n(\alpha))\, \frac{v^2}{2}}\, dv, \qquad \alpha = (i,\sigma) \in E. \quad (42)$$

and the function F_n, which is crucial in the computation of $f_n(\lambda, \mathcal{B})$,

$$F_n(\lambda, \epsilon, \mathcal{B}) := \prod_{\alpha \in E} C_n(\alpha, \lambda, \epsilon).$$

F_n will be identified with the spectral radius of some matrix.

We anticipate a striking feature of our model: for $\beta_n \neq \beta_{n+1}$, the cumulant generating function $f_n(\cdot, \mathcal{B})$ is *not* analytic around $\lambda = 0$. In particular, $f_n(\cdot, \mathcal{B}) > 0$ for λ in a left neighborhood of 0, while $f_n(\cdot, \mathcal{B}) = 0$ in a right neighborhood of 0.

Proposition 26 *If $\beta_n \leq \beta_{n+1}$ then $\forall\, \lambda \in]-\beta_n, 0[\cup]\beta_{n+1} - \beta_n, \beta_{n+1}[$, $f_n(\lambda, \mathcal{B})$ is given by the unique solution $\epsilon_0 > 0$ to the equation*

$$F_n(\lambda, \epsilon_0, \mathcal{B}) = 1.$$

If $\lambda \in [0, \beta_{n+1} - \beta_n]$, then $f_n(\lambda, \mathcal{B}) = 0$. The function $f_n(\cdot, \mathcal{B})$ is convex and continuous over $]-\beta_n, \beta_{n+1}[$ and satisfies the Gallavotti-Cohen symmetry relation

$$f_n(\lambda, \mathcal{B}) = f_n(\beta_{n+1} - \beta_n - \lambda, \mathcal{B}). \quad (43)$$

5.3.3 Confined tracers

In this section, we introduce a model which gives rise to a qualitatively different behavior for the self-consistent temperature profile. The self-consistent temperature profile of the scatterers in the wandering tracers model was linear. We will see that in the case of confined tracers, the temperature profile becomes non-linear. A major difference between the two models is the dependence of the thermal conductivity on the set of temperatures of the scatterers. For an arbitrary temperature distribution of the scatterers, we have seen that in the case of wandering tracers, the conductivity was identified with a frequency of collisions of a tracer with two neighboring scatterers. As such and because the wandering tracer travels through the whole system, it was dependent on the temperature of every scatterer. In the case of confined tracers, the conductivity is a purely local function of the set of temperatures.

The general structure of the process is again one of a Markov renewal process, the notations and proofs are strictly analogous to the case of wandering tracers. In this model, the disposition of the scatterers is the same but there are exactly N tracer particles locked in between the scatterers, including the ones on the boundaries. The n-th particle moves in between the scatterers, in the interval $I_n = [n-1, n]$, being reflected at the scatterers w_{n-1} and w_n with a random velocity p distributed according to

$$\phi^{\pm}_{\beta_n}(p) = p^{\pm}\beta_n e^{-\beta_n \frac{p^2}{2}}. \tag{44}$$

Because the particle is reflected, the sign in the distribution is the opposite of the sign of the incoming velocity. Those models are described by N independent Markov renewal processes. Each scatterer exchange energy with its two adjacent tracer particles and in order to express the self-consistency condition, we must introduce notations to describe the motion of each tracer. We describe now the process describing the motion of the n-th particle traveling between scatterers w_n and w_{n+1}. The state space of the Markov chain is $E = \{-1, +1\}$, with transition probability defined by $q_{1,-1} = q_{-1,1} = 0$.

Let $(q_{n,0}, p_{n,0})$ the initial data and velocity of the n-th particle. We define $\sigma_{n,0} = \text{sign}(p_{n,0})$. We consider now the Markov chain $(\sigma_{n,k})_{k\geq 0}$ in E with initial state $X_0 = \sigma_{n,0}$. In fact, the Markov chain has a deterministic evolution $\sigma_{n,k} = (-1)^k \sigma_{n,0}$, $k \geq 0$.

For each $\sigma \in E$, we write $\widehat{\sigma} = \frac{1}{2}(\sigma + 1)$. Then the time of the first collision with a scatterer is

$$S_{n,0} = S_{n,0}(q_{n,0}, p_{n,0}) := \frac{n + \widehat{\sigma}_{n,0} - q_{n,0}}{p_{n,0}} > 0,$$

We now define the time the particle takes between two subsequent visits to the scatterers. Conditionally on the σ-algebra generated by $(\sigma_{n,k})_{k\geq 0}$ the sequence $(\tau_{n,k})_{k\geq 1}$ is independent with distribution defined by

$$\mathbb{P}(\tau_{n,k} \in d\tau \,|\, \sigma_{n,k-1}) = \frac{\beta_{n+\widehat{\sigma}_{n,k-1}}}{\tau^3} \exp\left(-\frac{\beta_{n+\widehat{\sigma}_{n,k-1}}}{2\tau^2}\right) \mathbb{1}_{(\tau>0)}\, d\tau. \tag{45}$$

The time of the k-th collision with one of the two scatterers w_n and w_{n+1} is

$$S_{n,k} := S_{n,0} + \tau_{n,1} + \cdots + \tau_{n,k}, \qquad k \geq 1.$$

Before time $S_{n,0}$, the particle moves with uniform velocity $p_{n,0}$. Between time $S_{n,k-1}$ and time $S_{n,k}$, the particle moves with uniform velocity $\frac{\sigma_{n,k}}{\tau_{n,k}}$ and $(S_{n,k})_{k\geq 0}$ is the sequence of times when $q_{n,t} \in \{n, n+1\}$. In particular we define the sequence of incoming velocities $v_{n,k}$ at time $S_{n,k}$

$$v_{n,0} := p_{n,0}, \qquad v_{n,k} := \frac{\sigma_{n,k}}{\tau_{n,k}}, \quad k \geq 1. \tag{46}$$

We define the stochastic process $(q_{n,t}, p_{n,t})_{t\geq 0}$ with values in $[n, n+1] \times \mathbb{R}^*$

$$(q_t, p_t) := \begin{cases} (q_{n,0} + p_{n,0}t, p_{n,0}) & \text{if} \quad t < S_{n,0}, \\ \\ \left(n + \widehat{\sigma}_{n,k-1} + \frac{\sigma_{n,k}}{\tau_{n,k}}(t - S_{n,k-1}), \frac{\sigma_{n,k}}{\tau_{n,k}}\right) & \text{if} \quad S_{n,k-1} \leq t < S_{n,k},\ k \geq 1, \end{cases} \tag{47}$$

Then, we have the result,

Proposition 27 *The process* $((q_{n,t}, p_{n,t})_{t>0})_{0\le n\le N-1}$ *is Markov and its only invariant measure is given by*

$$\mu(\underline{p},\underline{q}) = \frac{1}{\widehat{Z}_N}\prod_{n=0}^{N-1}\mathbb{1}_{I_n}(q_n)\left[\mathbb{1}_{(p_n>0)}\,\beta_n\,e^{-\beta_n\frac{p_n^2}{2}} + \mathbb{1}_{(p_n<0)}\,\beta_{n+1}\,e^{-\beta_{n+1}\frac{p_n^2}{2}}\right] \tag{48}$$

where $\beta_0 = \beta_L$ *and* $\beta_N = \beta_R$ *and* Z_N *is the normalization constant,*

$$\widehat{Z}_N := \prod_{n=0}^{N-1} Z_n, \qquad Z_n := \left(\frac{\pi\beta_n}{2}\right)^{\frac12} + \left(\frac{\pi\beta_{n+1}}{2}\right)^{\frac12}. \tag{49}$$

We next identify the physical quantities of interest. The energy exchanged between the scatterer n and its two neighboring particles during a time interval $[0,t]$ is given by

$$\begin{aligned} E_n([0,t]) := \quad & \tfrac12 \sum_{k\ge 0:\, S_{n,k}\le t} \left(v_{n,k+1}^2 - v_{n,k}^2\right)\mathbb{1}_{(\widehat\sigma_{n,k}=0)} \\ + \quad & \tfrac12 \sum_{k\ge 0:\, S_{n-1,k}\le t} \left(v_{n-1,k+1}^2 - v_{n-1,k}^2\right)\mathbb{1}_{(\widehat\sigma_{n-1,k}=1)}, \end{aligned}$$

recall that, by (46) and (47), $v_{n,k}$ and $v_{n,k+1}$ are respectively the incoming and the outcoming velocity of the n-th particle at time $S_{n,k}$. The energy exchanged between scatterers n and $(n+1)$ during a time interval $[0,t]$ is given by

$$J_{n\to n+1}([0,t]) := \tfrac12 \sum_{k\ge 1:\, S_{n,k}\le t} v_{n,k}^2\,\sigma_{n,k}$$

The total entropy flow $S_n([0,t])$ and $S([0,t])$ due to the exchange of energy between the scatterers and a particle can be defined as in (26). The energy flow per unit time $\mathcal{E}_n$ in the stationary state, the entropy flow per unit time $\mathcal{S}_n$ and $\mathcal{S}$, and the average current of energy per unit time $\mathcal{J}_n$ between w_n and w_{n+1}, can be defined as in, respectively, (27), (28) and (29).

As in the case of wandering tracers (Proposition 24), we may study the above limits defining the physical properties of the model. As compared to Proposition 24, the main difference resides in the expression of the energy exchanged $\mathcal{E}_n$ with the system. This is the origin of the difference of shapes of the temperature profiles of the two models.

Proposition 28 *For all* $n = 1,\dots,N-1$,

$$\mathcal{E}_n = \frac{T_n - T_{n-1}}{Z_{n-1}} + \frac{T_n - T_{n+1}}{Z_n} \quad \text{and} \quad \mathcal{E}_0 = \frac{T_0 - T_1}{Z_0}, \quad \mathcal{E}_N = \frac{T_N - T_{N-1}}{Z_{N-1}}, \tag{50}$$

$$\mathcal{J}_n = \frac{T_n - T_{n+1}}{Z_n}, \qquad \mathcal{S} = \sum_{n=0}^{N-1}\frac{(T_n - T_{n+1})^2}{Z_n T_n T_{n+1}} \ge 0. \tag{51}$$

The proof is completely analogous to that of Proposition (24) and we do not repeat it. The main feature of the proof is again that by using the renewal theorem, the conductivity

$$\kappa_n = \frac{\mathcal{J}_n}{T_n - T_{n+1}} = \frac{1}{Z_n}$$

appears as a frequency of collision of the tracer with the walls of the box to which it is confined.

5.3.4 Self-consistency condition, temperature profile and Fourier's law.

We now derive the consequence of the self-consistency condition $\mathcal{E}_n = 0$, $n = 1, \dots, N-1$ on the shape of the temperature profile.
We set

$$g_N(x) := \sum_{i=0}^{N-1} \mathbb{1}_{\left[\frac{i}{N}, \frac{i+1}{N}\right[}(x)\, N(T_{i+1} - T_i)$$

and

$$h_N(x) := T_L + \int_0^x g_N(t)\, dt.$$

Notice that $h_N(i/N) = T_i$ and that h_N linearly interpolates between these values.

Proposition 29 (Self-consistency condition) *The only collection $(T_n)_{n=0,\dots,N}$ such that*

$$\mathcal{E}_n = 0,\ n = 1, \dots, N-1$$

with $T_0 = T_L$ and $T_N = T_R$, is the solution of

$$\left(\frac{(T_n - T_{n+1})}{(T_n)^{-\frac{1}{2}} + (T_{n+1})^{-\frac{1}{2}}} + \frac{(T_n - T_{n-1})}{(T_n)^{-\frac{1}{2}} + (T_{n-1})^{-\frac{1}{2}}} \right) = 0, \qquad 1 \le n \le N-1. \quad (52)$$

In this case, when $N \to +\infty$, h_N converges uniformly to the function

$$h(x) := \left(T_L^{\frac{3}{2}} + x(T_R^{\frac{3}{2}} - T_L^{\frac{3}{2}}) \right)^{\frac{2}{3}}, \qquad x \in [0,1], \quad (53)$$

unique solution of the equation

$$\begin{cases} \left(h^{\frac{1}{2}}\, h' \right)' = 0, \quad x \in]0,1[, \\ \\ h(0) = T_L,\ h(1) = T_R \end{cases}$$

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