Commun. Math. Phys. 293, 361–398 (2010)
Digital Object Identifier (DOI) 10.1007/s00220-009-0924-z

Communications in **Mathematical Physics**

Quantum Brownian Motion in a Simple Model System

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Received: 1 December 2008 / Accepted: 29 June 2009
Published online: 23 September 2009 –

Abstract: We consider a quantum particle coupled (with strength λ) to a spatial array of independent non-interacting reservoirs in thermal states (heat baths). Under the assumption that the reservoir correlations decay exponentially in time, we prove that the motion of the particle is diffusive at large times for small, but finite λ. Our proof relies on an expansion around the kinetic scaling limit ($\lambda \searrow 0$, while time and space scale as λ^{-2}) in which the particle satisfies a Boltzmann equation. We also show an equipartition theorem: the distribution of the kinetic energy of the particle tends to a Maxwell-Boltzmann distribution, up to a correction of $O(\lambda^2)$.

1. Introduction

1.1. Diffusion. Diffusion and Brownian motion are among the most fundamental phenomena described by transport theory. They refer to the apparent random motion of a particle or, for that matter, any degree of freedom, interacting with many other, mutually independent degrees of freedom in a thermal state. The interactions produce an erratic macroscopic motion that we perceive as diffusive or as Brownian motion. From a mathematical point of view, we may attempt to understand diffusive motion by invoking a central limit theorem: N interactions produce an effect δx, which is given by $\delta x \sim \sqrt{N}$. Since the number of interactions is proportional to the time lapse δt, we can write $(\delta x)^2 = D\delta t$, where the proportionality constant D is called the diffusion constant. Via the Einstein relation, the diffusion constant determines quantities such as the thermal or electric conductivity.

The model of a particle (quantum or classical) coupled to a thermal reservoir of free particles is a natural starting point for an analysis of diffusion. We assume the particle to be quantum mechanical. By $\langle \cdot \rangle_\beta$ we denote the expectation value in a state where the

⋆ Postdoctoral Fellow FWO-Flanders at K.U. Leuven, Belgium reservoir has an inverse temperature $\beta < \infty$. Then

$$\langle(\delta x)^2\rangle_\beta = \langle(x(t) - x(0))^2\rangle_\beta = \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \langle \dot{x}(t_1)\dot{x}(t_2)\rangle_\beta, \tag{1.1}$$

where $x(t)$ is the position of the particle at time t and $\dot{x}(t) = \mathrm{i}[H, x(t)]$, where H is the Hamiltonian of the system, is the velocity. We expect that, because of interactions with the reservoir, $\dot{x}(t_1)$ and $\dot{x}(t_2)$ become de-correlated rapidly, as $|t_1 - t_2|$ grows. Thus, the quantity $|\langle \dot{x}(t_1)\dot{x}(t_2)\rangle_\beta|$ is expected to be integrable in the variable $t_2 - t_1$. Combining this with isotropy, i.e., $\langle \dot{x}(t)\rangle_\beta \to 0$ rapidly, as $t \to \infty$, for $\beta < \infty$, one concludes that, asymptotically as t tends to ∞,

$$\langle(x(t) - x(0))^2\rangle_\beta = D(\beta)|t|, \tag{1.2}$$

for some positive, finite constant $0 < D(\beta) < \infty$, given by

$$D(\beta) = \int_{\mathbb{R}} \mathrm{d}t \langle \dot{x}(0)\dot{x}(t)\rangle_\beta. \tag{1.3}$$

Because of the equipartition theorem, one expects that

$$\langle \dot{x}(t)^2\rangle_\beta \to \frac{1}{Z(\beta)} \int_{\mathbb{R}^d} \mathrm{d}v\, v^2 \mathrm{e}^{-\beta E(v)}, \qquad \text{as } t \nearrow \infty, \tag{1.4}$$

where $E(v)$ is the kinetic energy of a particle with velocity v and $Z(\beta)$ is a normalization constant. Obviously, (1.4) is strictly positive for finite β. Likewise, we expect that $D(\beta)$ is strictly positive, for $\beta < \infty$.

Equations (1.2) and (1.4) suggest that, at very large times, the motion of a particle interacting with a reservoir or heat bath at strictly positive temperature has universal features: The mean value of its speed is strictly positive and finite, and its mean displacement is proportional to the square root of time. In contrast, at zero temperature ($\beta = \infty$), the nature of the particle's motion depends on properties of the reservoir and the dispersion law, $\varepsilon(k)$, of the particle; ($k \in \mathbb{R}^d$ is its momentum). If, for a particle momentum k,

$$\varepsilon(k - q) + \omega(q) > \varepsilon(k), \qquad \text{for all}\, q \neq 0, \tag{1.5}$$

where $\omega(q)$ is the dispersion law of a mode (particle) of the reservoir with momentum q, then the particle cannot lower its energy and reduce its speed by exciting a reservoir mode, i.e., by spontaneously emitting a reservoir particle. Its motion will therefore be ballistic. The only effect of the reservoir is a renormalization of the effective mass (the dispersion law ε) of the particle. If, however, (1.5) is not satisfied, then the particle can excite reservoir modes (emit reservoir particles). This process reduces its kinetic energy and speed, i.e., it leads to friction. Friction takes place at all momenta k if, e.g., $\omega(q) \propto |q|^2$ (reservoir particles are non-relativistic). If $\omega(q) = c|q|$, i.e., the reservoir particles are low-energetic phonons or photons, friction only takes place at momenta k of the particle where $|\nabla\varepsilon(k)| > c$. The radiation corresponding to the reservoir particles emitted in the process of friction is called Cerenkov radiation.

Despite the importance of diffusion and its conceptual simplicity, there has, so far, not existed any rigorous proof that it occurs in a model as described above. In the present paper, we establish diffusion for models where the particle is coupled to a spatial array of independent heat baths.

1.2. Informal description of the model and main results. We consider a quantum particle hopping on the lattice $\mathbb{Z}^d$. With each lattice point, we associate an independent thermal reservoir consisting of a free bosonic quantum field describing phonons or photons at temperature β^{-1}. (In this section, we present a description of the system appropriate at zero temperature; it is formal when $\beta < \infty$.) The total Hilbert space, $\mathscr{H}$, of the coupled system is a tensor product of the system space, $\mathscr{H}_{\mathrm{S}}$, with a reservoir space, $\mathscr{H}_{\mathrm{R}}$, which is a (separable) subspace of the infinite tensor product of reservoir spaces $\mathscr{H}_{\mathrm{R}_x}$, $x \in \mathbb{Z}^d$, at all sites. Thus

$$\mathscr{H} := \mathscr{H}_{\mathrm{S}} \otimes \mathscr{H}_{\mathrm{R}}. \tag{1.6}$$

The system space $\mathscr{H}_{\mathrm{S}}$ is given by $l^2(\mathbb{Z}^d)$, and the particle Hamiltonian is given by the finite-difference Laplacian Δ. Each reservoir is described by a boson field; creation and annihilation operators creating/annihilating bosons with momentum $q \in \mathbb{R}^d$ at site x are written as $a_x^*(q)$, $a_x(q)$ respectively, and satisfy the canonical commutation relations

$$[a_x^{\#}(q), a_{x'}^{\#}(q')] = 0, \qquad [a_x(q), a_{x'}^*(q')] = \delta_{x,x'}\delta(q-q'), \tag{1.7}$$

where $a^{\#}$ stands for either a or a^*.

The total Hamiltonian of the system is taken to be

$$\begin{aligned} H_\lambda := -\Delta + \sum_{x\in\mathbb{Z}^d} \int_{\mathbb{R}^d} \mathrm{d}q\, \omega(q) a_x^*(q) a_x(q) \\ +\lambda \sum_{x\in\mathbb{Z}^d} \int_{\mathbb{R}^d} \mathrm{d}q\, |x\rangle\langle x| \otimes \left\{\phi(q) a_x^*(q) + \text{h.c.}\right\}, \end{aligned} \tag{1.8}$$

where $\phi(q)$ is a form factor and $\lambda \in \mathbb{R}$ is the coupling strength. We are writing Δ instead of $\Delta \otimes 1$ and $a_x(q)$ instead of $1 \otimes a_x(q)$

The independence of the reservoirs has far-reaching consequences. Consider the lattice translation $\mathcal{T}_z$, $z \in \mathbb{Z}^d$, acting on operators on $\mathscr{H}$ by

$$\mathcal{T}_z(|x\rangle\langle y|) := |x+z\rangle\langle y+z|, \tag{1.9}$$

$$\mathcal{T}_z(a_x^{\#}(q)) := a_{x+z}^{\#}(q). \tag{1.10}$$

It is easily seen that

$$\mathcal{T}_z(H_\lambda) = H_\lambda. \tag{1.11}$$

Notice that this transformation does not involve the momentum coordinates q inside the reservoirs. It is the existence of this translation symmetry that allows us to obtain results on diffusion without very hard work. Assume we had started from a model with only one reservoir, with Hamiltonian given by

$$\begin{aligned} H_\lambda := -\Delta + \int_{\mathbb{R}^d} \mathrm{d}q\, \omega(q) a^*(q) a(q) \\ +\lambda \sum_{x\in\mathbb{Z}^d} \int_{\mathbb{R}^d} \mathrm{d}q\, |x\rangle\langle x| \otimes \left\{a^*(q)\phi(q)\mathrm{e}^{-\mathrm{i}(x,q)} + \text{h.c.}\right\}, \end{aligned} \tag{1.12}$$

where, now, the operators $a(q), a^*(q)$ do not carry an index x and $(\cdot,\cdot)$ is the scalar product on $\mathbb{C}^d$. This model still exhibits translation symmetry, but this symmetry maps $a^*(q) \to a^*(q)\mathrm{e}^{-\mathrm{i}(z,q)}$, $a(q) \to \mathrm{e}^{\mathrm{i}(z,q)}a(q)$, which is the reason for the factor $\mathrm{e}^{-\mathrm{i}(x,q)}$ in the interaction Hamiltonian of (1.12) and leads to bad decay properties of the reservoir correlation functions.

The initial state for the reservoirs is chosen to be $\rho_{\mathrm{R}}^{\beta} := \otimes_{x\in\mathbb{Z}^d}\rho_{\mathrm{R}_x}^{\beta}$, where each $\rho_{\mathrm{R}_x}^{\beta}$ is an equilibrium state at inverse temperature β for the reservoir at site x. For mathematical details on the construction of infinite reservoirs, see [1,3,7]. In Lemma 2.3, we define the reduced Heisenberg-picture dynamics (i.e., the particle dynamics obtained by tracing out the reservoir degrees of freedom)

$$S \mapsto \mathcal{Z}_t^{\lambda,*}(S) := \rho_{\mathrm{R}}^{\beta}\left[\mathrm{e}^{itH_\lambda}(S\otimes 1)\mathrm{e}^{-itH_\lambda}\right], \qquad S\in\mathscr{B}(\mathscr{H}_{\mathrm{S}}). \tag{1.13}$$

Placing the particle initially at site 0, that is, in the vector $|0\rangle$, we study the distribution function

$$\mu_t^{\lambda}(x) := \langle 0|\mathcal{Z}_t^{\lambda,*}(|x\rangle\langle x|)|0\rangle. \tag{1.14}$$

The quantity $\mu_t^{\lambda}(x) \geq 0$ is the probability to find the particle at site x at time t. One easily checks that

$$\sum_{x\in\mathbb{Z}^d}\mu_t^{\lambda}(x) = 1, \tag{1.15}$$

and hence it is justified to think of $\mu_t^{\lambda}(\cdot)$ as a probability density on $\mathbb{Z}^d$. By diffusion, we mean that, for large t,

$$\mu_t^{\lambda}(x) \sim \left(\frac{2\pi}{t}\right)^{d/2}(\det D_\lambda)^{-1}\exp\left\{-\frac{1}{2}\left(\frac{x}{\sqrt{t}}, D_\lambda^{-1}\frac{x}{\sqrt{t}}\right)\right\}, \tag{1.16}$$

where $D_\lambda \equiv D_\lambda(\beta)$ is a positive-definite matrix with the interpretation of a diffusion tensor. (Actually, if the particle Hamiltonian is given by $-\Delta$ (as in this section), the tensor D_λ is isotropic and hence a scalar). We now move towards quantifying (1.16). Let us fix a time t. Since $\mu_t^{\lambda}(x)$ is a probability measure, one can think of x_t as a random variable such that

$$\mathrm{Prob}_\lambda(x_t = x) := \mu_t^{\lambda}(x). \tag{1.17}$$

The claim that the random variable $\frac{x_t}{\sqrt{t}}$ converges in distribution, as $t\nearrow\infty$, to a Gaussian random variable with mean 0 and variance D_λ^{-1} is called a Central Limit Theorem (CLT). It is equivalent to pointwise convergence of the characteristic function, i.e.,

$$\sum_{x\in\mathbb{Z}^d}\mathrm{e}^{-\frac{\mathrm{i}}{\sqrt{t}}(x,q)}\mu_t^{\lambda}(x) \underset{t\uparrow\infty}{\longrightarrow} \mathrm{e}^{-\frac{1}{2}(q,D_\lambda q)}, \quad \text{for all } q\in\mathbb{R}^d, \tag{1.18}$$

and it is this statement which is our main result, Theorem 3.2.

Let $X := \sum_{x\in\mathbb{Z}^d} x\,|x\rangle\langle x|$ be the position operator on the lattice and write $X_t := \mathcal{Z}_t^{\lambda,*}(X)$. Then a slightly stronger version of (1.18) implies that

$$\left\langle 0|\frac{X_t}{t}|0\right\rangle \underset{t\uparrow\infty}{\longrightarrow} 0, \qquad \left\langle 0|\frac{X_t^2}{t}|0\right\rangle \underset{t\uparrow\infty}{\longrightarrow} D_\lambda, \tag{1.19}$$

and this will also follow from our results; see Remark 3.3.

Our second result concerns the asymptotic expectation value of the kinetic energy of the particle. Let $E_t := \mathcal{Z}_t^{\lambda,*}(-\Delta)$ be the kinetic energy at time t. We prove that, for all bounded functions θ,

$$\langle 0|\theta(E_t)|0\rangle \underset{t\uparrow\infty}{\longrightarrow} \frac{\int_{\mathbb{T}^d} \mathrm{d}k\, \theta(\varepsilon(k))\mathrm{e}^{-\beta\varepsilon(k)}}{\int_{\mathbb{T}^d} \mathrm{d}k\, \mathrm{e}^{-\beta\varepsilon(k)}} + O(\lambda^2), \qquad \lambda \downarrow 0, \tag{1.20}$$

where $\varepsilon(k) = \sum_{j=1}^d (2 - 2\cos k^j)$ is the dispersion law of the particle. This is stated in Theorem 3.1.

1.3. Related results. In the physics literature, the model with Hamiltonian (1.12) and with reservoir particles being phonons is referred to as the polaron model. We refer to [21,23] and references therein for a discussion. The first rigorous result on this model at positive temperature is probably in [22] and the best result up to date is in [9]; (see also Sect. 4.3).

To describe some related results, we first introduce a different model, which, however, will turn out to be closely related to ours.

Assume that the quantum particle interacts with random time-dependent impurities. That is, let $V(x,t)$ be a real-valued random variable, for $x \in \mathbb{Z}^d$, $t \in \mathbb{R}$, with mean zero

$$\mathbb{E}[V(x,t)] = 0, \tag{1.21}$$

satisfying the Gaussian property

$$\mathbb{E}[V(x_{2n},t_{2n})\dots V(x_1,t_1)] = \sum_{\text{pairings } \pi} \prod_{(r,s)\in\pi} \mathbb{E}[V(x_s,t_s)V(x_r,t_r)], \tag{1.22}$$

$$\mathbb{E}[V(x_{2n+1},t_{2n+1})\dots V(x_1,t_1)] = 0, \tag{1.23}$$

where a pairing π is a partition of $\{1,\dots,2n\}$ into n pairs and the product is over these pairs (r,s). In addition, we assume that the correlation functions are invariant under translations in time and space,

$$\mathbb{E}\left[V(x,t)V(x',t')\right] = \mathbb{E}\left[V(x-x',t-t')V(0,0)\right]. \tag{1.24}$$

A time-dependent Hamiltonian is given by

$$H_\lambda(t) := -\Delta + \lambda \sum_{x\in\mathbb{Z}^d} V(x,t)|x\rangle\langle x|, \tag{1.25}$$

and the dynamics U_t^λ is defined (almost surely) by

$$\frac{\mathrm{d}}{\mathrm{d}t}U_t^\lambda = -\mathrm{i}H_\lambda(t)U_t^\lambda, \qquad U_0^\lambda = 1. \tag{1.26}$$

One can check that if we choose

$$\mathbb{E}\left[V(x,t)V(0,0)\right] := \delta_{x,0} \int_{\mathbb{R}^d} \mathrm{d}q\, |\phi(q)|^2 \left(\rho_{\mathrm{R}}^{\beta}\left[a_0(q)a_0^*(q)\right] \mathrm{e}^{-\mathrm{i}t\omega(q)} + \rho_{\mathrm{R}}^{\beta}\left[a_0^*(q)a_0(q)\right] \mathrm{e}^{\mathrm{i}t\omega(q)} \right), \tag{1.27}$$

(the RHS will be motivated in Sect. 2.3.2), then we have that

$$\mathbb{E}\left[U_t^{\lambda}\rho(U_t^{\lambda})^*\right] = \mathcal{Z}_t^{\lambda}(\rho). \tag{1.28}$$

The reason for this equivalence is that both models share a “quasi-free”, or, “Gaussian property”. (In the Hamiltonian model, this is a consequence of the fact that the free reservoir Hamiltonian is quadratic in the creation and annihilation operators). Of course, it is not clear that the definition (1.27) makes sense. For example, the RHS could have an imaginary part, whereas the LHS is real. However, upon inspection of our proof, it becomes clear that whenever

$$\left|\mathbb{E}\left[V(x',t')V(x,t)\right]\right| \leq \delta_{x,x'} c\mathrm{e}^{-g_{\mathrm{R}}|t-t'|}, \qquad c<\infty, g_{\mathrm{R}}<\infty, \tag{1.29}$$

then our proof (which assumes the same bound for the RHS of (1.27)) carries over, and we can establish diffusive behavior for the averaged dynamics $\mathbb{E}\left[U_t^{\lambda}\rho(U_t^{\lambda})^*\right]$. In fact, the locality in space (expressed by $\delta_{x,x'}$) is not crucial, at all, but we do not pursue this generalization here.

The case $\mathbb{E}\left[V(x',t')V(x,t)\right] = \delta_{x,x'}\delta(t-t')$ has been treated in [16]. While we were completing this paper, a preprint [15] appeared where diffusion is proven under the assumption that $V(x,t)$ is an exponentially ergodic Markov process (not necessarily Gaussian) for each x. Preliminary results were obtained in [17 and 24]. One of the ultimate goals of these projects is to treat the case where $V(x,t) = V(x)$ is time-independent and $d=3$, i.e., $\mathbb{E}\left[V(x')V(x)\right] = \delta_{x,x'}$. This is the well-known Anderson model.

Models in which the particle is coupled to a thermal reservoir are expected to be easier than the Anderson model, mainly because one expects that diffusion persists for large values of the coupling constant λ, whereas the Anderson model has a phase transition, and the particle gets localized at large values of $|\lambda|$.

However, even for a particle coupled to a thermal reservoir in $d=3$, our techniques fail, since this model would essentially correspond to one with $\mathbb{E}\left[V(x',t')V(x,t)\right] \sim \frac{1}{|x-x'|}\chi[|x-x'| \geq c|t-t'|]$, (for reservoir particles with dispersion relation $\omega(q) = c|q|$).

There are however results that establish diffusive behavior up to times of order $\lambda^{-(2+\delta)}$, for some $\delta>0$, even for the Anderson model, see [10,11] (a resulting lower bound for the localization length is proven in [5]). In fact, our technique employs results of the type proven in these references as an ingredient of the proof; see Sect. 4.3.

We might add that we expect that the model treated in the present paper can also be analyzed using operator-theoretic techniques introduced for the study of return to equilibrium in open quantum systems, see e.g. [2,14], and we are currently working on such a formulation. The technique used in the present paper is largely based on [20].

1.4. Outline. In Sect. 2, we introduce our model, making precise the description in the Introduction. Then, in Sect. 3, we state our assumptions and main results with as few divagations as possible. Section 4 contains the main ideas of the paper and the plan of the proof. The technical parts of the proof are postponed to Sect. 5, which contains the proof of Theorem 4.4, and Sect. 6, where one finds the proof of Theorem 4.5.

2. Model

2.1. Conventions and notation. Given a Hilbert space $\mathscr{E}$, we use the standard notation

$$\mathscr{B}_p(\mathscr{E}) := \left\{ S \in \mathscr{B}(\mathscr{E}), \operatorname{Tr}\left[(S^*S)^{p/2}\right] < \infty \right\}, \qquad 1 \le p \le \infty, \tag{2.1}$$

with $\mathscr{B}_\infty(\mathscr{E}) \equiv \mathscr{B}(\mathscr{E})$ the bounded operators on $\mathscr{E}$, and

$$\|S\|_p := \left(\operatorname{Tr}\left[(S^*S)^{p/2}\right]\right)^{1/p}, \qquad \|S\| := \|S\|_\infty. \tag{2.2}$$

For bounded operators acting on $\mathscr{B}_p(\mathscr{E})$, i.e. elements of $\mathscr{B}(\mathscr{B}_p(\mathscr{E}))$, we use in general the calligraphic font: $\mathcal{V}, \mathcal{W}, \mathcal{T}, \ldots$. An operator $X \in \mathscr{B}(\mathscr{E})$ determines an operator $\operatorname{ad}(X) \in \mathscr{B}(\mathscr{B}_p(\mathscr{E}))$ by

$$\operatorname{ad}(X)S := [X, S] = XS - SX, \qquad S \in \mathscr{B}_p(\mathscr{E}). \tag{2.3}$$

We will mainly use the case $p = 2$. The norm of operators in $\mathscr{B}(\mathscr{B}_2(\mathscr{E}))$ is defined by

$$\|\mathcal{W}\| := \sup_{S \in \mathscr{B}_2(\mathscr{E})} \frac{\|\mathcal{W}(S)\|_2}{\|S\|_2}. \tag{2.4}$$

For vectors $\kappa \in \mathbb{C}^d$, we let $\Re\kappa, \Im\kappa$ denote the vectors $(\Re\kappa^1, \ldots, \Re\kappa^d)$ and $(\Im\kappa^1, \ldots, \Im\kappa^d)$, respectively. The scalar product on $\mathbb{C}^d$ is written as $(\cdot, \cdot)$ and the norm as $|\kappa| := \sqrt{(\kappa, \kappa)}$. The scalar product on an infinite-dimensional Hilbert space $\mathscr{E}$ is written as $\langle \cdot, \cdot \rangle$, or, occasionally, as $\langle \cdot, \cdot \rangle_{\mathscr{E}}$. All scalar products are defined to be linear in the second argument and anti-linear in the first one.

We write $\Gamma_{\mathrm{s}}(\mathscr{E})$ for the symmetric (bosonic) Fock space over the Hilbert space $\mathscr{E}$ and we refer to [7] for definitions and discussion. If ω is a self-adjoint operator on $\mathscr{E}$, then its (self-adjoint) second quantization, $\mathrm{d}\Gamma_{\mathrm{s}}(\omega)$, is defined by

$$\mathrm{d}\Gamma_{\mathrm{s}}(\omega)\operatorname{Sym}(\phi_1 \otimes \cdots \otimes \phi_n) := \sum_{i=1}^n \operatorname{Sym}(\phi_1 \otimes \cdots \otimes \omega\phi_i \otimes \cdots \otimes \phi_n), \tag{2.5}$$

where Sym projects on the symmetric subspace and $\phi_1, \ldots, \phi_n \in \mathscr{E}$.

2.2. The particle. We set $\mathscr{H}_{\mathrm{S}} = l^2(\mathbb{Z}^d)$ (the subscript S refers to 'system', as is customary in system-reservoir models). We define the one-dimensional projector 1_x on $\mathscr{H}_{\mathrm{S}}$ by

$$(1_x f)(x') := \delta_{x,x'} f(x'), \qquad x, x' \in \mathbb{Z}^d, \ f \in l^2(\mathbb{Z}^d). \tag{2.6}$$

We will often consider the space $\mathscr{H}_{\mathrm{S}}$ in its dual representation, i.e. as $L^2(\mathbb{T}^d, \mathrm{d}k)$, where $\mathbb{T}^d$ is the d-dimensional torus, which is identified with $L^2([-\pi, \pi]^d)$. We define the 'momentum' operator P as multiplication by $k \in \mathbb{T}^d$, i.e.,

$$(P\theta)(k) := k\theta(k), \qquad \theta \in L^2(\mathbb{T}^d, \mathrm{d}k). \tag{2.7}$$

Although P is well-defined as a bounded operator, it does not have nice properties; e.g., it is not true that $[X^i, P^j] = \mathrm{i}\delta_{i,j}$. Throughout the paper, we only use operators $f(P)$, where f is periodic on $\mathbb{R}^d$ with period 2π, i.e. a function on $\mathbb{T}^d$. We choose a periodic function ε to be the dispersion law of the system. Although this is not essential, we require ε to have inversion symmetry, i.e.,

$$\varepsilon(k) = \varepsilon(-k), \qquad k \in \mathbb{T}^d. \tag{2.8}$$

The Hamiltonian of our particle is given by

$$H_{\mathrm{S}} := \varepsilon(P). \tag{2.9}$$

Our first assumption ensures that H_{S} is sufficiently regular.

Assumption 2.1 (Analyticity of system dynamics). The function ε, defined originally on $\mathbb{T}^d$, extends to an analytic function in a strip of width $\delta_\varepsilon > 0$. That is, when viewed as a periodic function on $\mathbb{R}^d$, ε is analytic in $(\mathbb{R} + \mathrm{i}[-\delta_\varepsilon, \delta_\varepsilon])^d$. Moreover, we assume that the function $\mathbb{T}^d \ni k \mapsto (\upsilon, \nabla\varepsilon(k))$ does not vanish identically for any vector $\upsilon \in \mathbb{R}^d$, $\upsilon \neq 0$.

The most natural choice for ε satisfying Assumption 2.1 is $\varepsilon(k) = \sum_{j=1}^d (2 - 2\cos(k^j))$, which corresponds to $-H_{\mathrm{S}}$ being the discrete Laplacian.

2.3. The reservoirs.

2.3.1. Reservoir spaces. We consider an array of independent reservoirs. With each site $x \in \mathbb{Z}^d$ we associate a one-particle Hilbert space $\mathfrak{h}_x$ (one can imagine that $\mathfrak{h}_x = L^2(\mathbb{R}^d)$) with a positive one-particle Hamiltonian ω_x. The reservoir at x is now described by the Fock space $\Gamma_{\mathrm{s}}(\mathfrak{h}_x)$ with Hamiltonian $\mathrm{d}\Gamma_{\mathrm{s}}(\omega_x)$. The full reservoir space is

$$\mathscr{H}_{\mathrm{R}} := \Gamma_{\mathrm{s}}(\oplus_{x\in\mathbb{Z}^d}\mathfrak{h}_x) \quad \text{with Hamiltonian} \quad H_{\mathrm{R}} := \sum_{x\in\mathbb{Z}^d} \mathrm{d}\Gamma_{\mathrm{s}}(\omega_x). \tag{2.10}$$

We choose the different reservoir one-particle spaces to be isomorphic copies of a fixed space $\mathfrak{h}$ so that $\varphi \in \mathfrak{h}_x$ is naturally identified with an element of $\mathfrak{h}_{x'}$ that is also denoted by φ without further warning. Likewise, ω_x is naturally identified with $\omega_{x'}$. Hence, if no confusion is possible we simply write $\mathfrak{h}$ and ω to denote the (one-particle) one-site space and the Hamiltonian, respectively.

For $\varphi \in \mathfrak{h}$, the operators $a_x^*(\varphi)/a_x(\varphi)$ stand for the creation/annihilation operators on the Fock space $\Gamma_{\mathrm{s}}(\mathfrak{h}_x)$. By the embedding of $\mathfrak{h}_x$ into $\oplus_{y\in\mathbb{Z}^d}\mathfrak{h}_y$, these creation/annihilation operators act on $\mathscr{H}_{\mathrm{R}}$ in a natural way. They satisfy the commutation relations

$$[a_x(\varphi), a_{x'}^*(\varphi')] = \delta_{x,x'}\langle\varphi, \varphi'\rangle_{\mathfrak{h}}, \qquad [a_x^\#(\varphi), a_{x'}^\#(\varphi')] = 0, \tag{2.11}$$

where $a^\#$ stands for either a^* or a.

2.3.2. Interaction and initial reservoir state. We pick a 'structure factor' $\phi \in \mathfrak{h}$ and we choose the interaction between the system and the reservoir at site x to be given by

$$1_x \otimes \Psi_x(\phi), \quad \text{where} \quad \Psi_x(\phi) = a_x(\phi) + a_x^*(\phi). \tag{2.12}$$

So far, we have not made any assumptions concerning ω and ϕ, but their form will be restricted by Assumption 2.2 in (2.20). The particle interacts with all reservoirs in a translation invariant way. Hence the total interaction Hamiltonian is given by

$$H_{\mathrm{SR}} := \sum_{x \in \mathbb{Z}^d} 1_x \otimes \Psi_x(\phi) \quad \text{on} \quad \mathscr{H}_{\mathrm{S}} \otimes \mathscr{H}_{\mathrm{R}}. \tag{2.13}$$

Next, we put the tools in place to describe the positive temperature reservoirs. Let $\mathscr{C}$ be the $*$-algebra consisting of polynomials in $a_x(\varphi), a^*_{x'}(\varphi')$, with $\varphi, \varphi' \in \mathfrak{h}$, $x, x' \in \mathbb{Z}^d$. We introduce the positive operator $T_\beta = (\mathrm{e}^{\beta\omega} - 1)^{-1}$ on $\mathfrak{h}$; β should be thought of as the inverse temperature.

We let ρ_{R}^β be a quasi-free state defined on $\mathscr{C}$. It is fully specified[1] by

1) Gauge-invariance

$$\rho_{\mathrm{R}}^\beta\left[a_x^*(\varphi)\right] = \rho_{\mathrm{R}}^\beta\left[a_x(\varphi)\right] = 0. \tag{2.14}$$

2) Two-point correlation functions

$$\begin{pmatrix} \rho_{\mathrm{R}}^\beta\left[a_x^*(\varphi)a_{x'}(\varphi')\right] & \rho_{\mathrm{R}}^\beta\left[a_x^*(\varphi)a_{x'}^*(\varphi')\right] \\ \rho_{\mathrm{R}}^\beta\left[a_x(\varphi)a_{x'}(\varphi')\right] & \rho_{\mathrm{R}}^\beta\left[a_x(\varphi)a_{x'}^*(\varphi')\right] \end{pmatrix} = \delta_{x,x'} \begin{pmatrix} \langle \varphi' | T_\beta \varphi \rangle & 0 \\ 0 & \langle \varphi | (1+T_\beta)\varphi') \rangle \end{pmatrix}. \tag{2.15}$$

3) Quasi-freeness, i.e. , the higher-point correlation functions are expressed in terms of the two-point function by

$$\rho_{\mathrm{R}}^\beta\left[a_{x_1}^\#(\varphi_1)\dots a_{x_{2n}}^\#(\varphi_{2n})\right] = \sum_{\text{pairings}\,\pi} \prod_{(r,s)\in\pi} \rho_{\mathrm{R}}^\beta\left[a_{x_r}^\#(\varphi_r)a_{x_s}^\#(\varphi_s)\right], \tag{2.16}$$

$$\rho_{\mathrm{R}}^\beta\left[a_{x_1}^\#(\varphi_1)\dots a_{2n+1}^\#(\varphi_{2n+1})\right] = 0, \tag{2.17}$$

where a pairing π is a partition of $\{1,\dots,2n\}$ into n pairs and the product is over these pairs (r,s).

A quantity that will play an important role in our analysis is the on-site-reservoir correlation function defined by

$$\hat\psi(t) := \rho_{\mathrm{R}}^\beta\left[\Psi_x(\mathrm{e}^{\mathrm{i}t\omega}\phi)\Psi_x(\phi)\right] = \langle \phi, T_\beta \mathrm{e}^{\mathrm{i}t\omega}\phi\rangle + \langle \phi, (1+T_\beta)\mathrm{e}^{-\mathrm{i}t\omega}\phi\rangle. \tag{2.18}$$

[1] The reason why, in models like ours, it is enough to know the state on $\mathscr{C}$, has been explained in many places, e.g. [1,3,8,13].

It is useful to introduce ψ, the inverse Fourier transform of $\hat{\psi}$,

$$\hat{\psi}(t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}\xi \, \mathrm{e}^{\mathrm{i}\xi t} \psi(\xi). \tag{2.19}$$

As is explained in Appendix A, ψ is the (squared norm of) the *effective structure factor*. In particular, $\psi(\xi) \geq 0$.

The following assumption requires the reservoir to have exponential decay of correlations.

Assumption 2.2. There is a decay rate $g_{\mathrm{R}} > 0$ such that

$$\sup_{t \in \mathbb{R}} \left(|\hat{\psi}(t)| \mathrm{e}^{g_{\mathrm{R}}|t|} \right) < \infty. \tag{2.20}$$

We assume that $\hat{\psi} \not\equiv 0$, or equivalently $\psi \not\equiv 0$.

The assumption that $\hat{\psi} \not\equiv 0$ ensures that the particle interacts effectively with the fields describing the reservoirs. In Appendix A, we discuss examples of reservoirs that satisfy Assumption 2.2, provided that $\beta < \infty$.

2.4. The dynamics. Consider the zero-temperature Hilbert space $\mathscr{H}_{\mathrm{S}} \otimes \mathscr{H}_{\mathrm{R}}$. The Hamiltonian (with coupling constant λ) is formally defined by

$$H_{\lambda} := H_{\mathrm{S}} + H_{\mathrm{R}} + \lambda H_{\mathrm{SR}}. \tag{2.21}$$

This operator generates the zero-temperature dynamics. However, we need to consider the dynamics at positive temperature. In particular, we must understand the reduced positive-temperature dynamics of the system S after the reservoir degrees of freedom have been traced out.

By a slight abuse of notation, we use $\rho_{\mathrm{R}}^{\beta}$ to denote the conditional expectation from $\mathscr{B}(\mathscr{H}_{\mathrm{S}} \otimes \mathscr{C})$ to $\mathscr{B}(\mathscr{H}_{\mathrm{S}})$ given by

$$\rho_{\mathrm{R}}^{\beta}(S \otimes R) := S \rho_{\mathrm{R}}^{\beta}(R), \qquad S \in \mathscr{B}(\mathscr{H}_{\mathrm{S}}),\, R \in \mathscr{C}, \tag{2.22}$$

where $\rho_{\mathrm{R}}^{\beta}(R)$ is defined through (2.15–2.17).

Formally, the reduced dynamics in the Heisenberg picture is given by

$$\mathcal{Z}_t^{\lambda,*}(S) := \rho_{\mathrm{R}}^{\beta} \left[\mathrm{e}^{\mathrm{i}tH_{\lambda}} (S \otimes 1) \, \mathrm{e}^{-\mathrm{i}tH_{\lambda}} \right] \tag{2.23}$$

whenever the RHS is well-defined.

A mathematically precise definition of the reduced dynamics is the subject of the next lemma.

Lemma 2.3. *Suppose that Assumption 2.2 (see (2.20)) holds and define*

$$H_{\mathrm{SR}}(t) := \sum_{x \in \mathbb{Z}^d} 1_x(t) \otimes \Psi_x(\mathrm{e}^{\mathrm{i}t\omega}\phi) \quad \textit{with} \quad 1_x(t) := \mathrm{e}^{\mathrm{i}tH_{\mathrm{S}}} 1_x \mathrm{e}^{-\mathrm{i}tH_{\mathrm{S}}}. \tag{2.24}$$

The series[2]

$$\mathcal{Z}_t^{\lambda,*}(S) := \sum_{n\in\mathbb{Z}^+} (\mathrm{i}\lambda)^n \int_{0\le t_1\le\cdots\le t_n\le t} \mathrm{d}t_1\ldots\mathrm{d}t_n\, \rho_{\mathrm{R}}^{\beta} \left[\mathrm{ad}(H_{\mathrm{SR}}(t_1))\ldots\mathrm{ad}(H_{\mathrm{SR}}(t_n))\,\mathrm{e}^{\mathrm{i}t\,\mathrm{ad}(H_{\mathrm{S}})}(S\otimes 1)\right] \tag{2.25}$$

is well-defined for any $\lambda, t \in \mathbb{R}$ *and arbitrary* $S \in \mathscr{B}(\mathscr{H}_{\mathrm{S}})$*, i.e., the RHS converges absolutely in the norm of* $\mathscr{B}(\mathscr{H}_{\mathrm{S}})$*, and* $\mathcal{Z}_t^{\lambda,*}$ *has the expected properties, namely*

$$\mathcal{Z}_t^{\lambda,*}(1) = 1, \qquad \|\mathcal{Z}_t^{\lambda,*}(S)\| \le \|S\|. \tag{2.26}$$

One can prove this lemma (under less restrictive conditions than those in Assumption 2.2) by direct estimates of the RHS of (2.25). For this purpose, the estimates given in the present paper amply suffice. However, one can also define the system-reservoir dynamics as a dynamical system on a Von Neumann algebra through the Araki-Woods representation. This is the usual approach in the mathematical physics literature; see e.g. [8,13,14].

Finally, we define $\mathcal{Z}_t^{\lambda} : \mathscr{B}_1(\mathscr{H}_{\mathrm{S}}) \to \mathscr{B}_1(\mathscr{H}_{\mathrm{S}})$, the reduced dynamics in the Schrödinger picture, by duality, i.e.,

$$\mathrm{Tr}[\rho_{\mathrm{S}}\mathcal{Z}_t^{\lambda,*}(S)] = \mathrm{Tr}[\mathcal{Z}_t^{\lambda}(\rho_{\mathrm{S}})S], \qquad S \in \mathscr{B}(\mathscr{H}_{\mathrm{S}}),\ \rho_{\mathrm{S}} \in \mathscr{B}_1(\mathscr{H}_{\mathrm{S}}). \tag{2.27}$$

We could also have started by defining the full initial state ρ_{SR} of the total system consisting of the particle and reservoirs as the positive, normalized functional

$$\rho_{\mathrm{SR}} := \rho_{\mathrm{S}} \otimes \rho_{\mathrm{R}}^{\beta} \qquad \text{on} \quad \mathscr{B}(\mathscr{H}_{\mathrm{S}}) \otimes \mathscr{C}, \tag{2.28}$$

where we abuse notation by employing the same symbol ρ_{S} for both the density operator (a positive element of $\mathscr{B}_1(\mathscr{H}_{\mathrm{S}})$) and the state it determines on $\mathscr{B}(\mathscr{H}_{\mathrm{S}})$, i.e.,

$$\rho_{\mathrm{S}}[S] := \mathrm{Tr}[\rho_{\mathrm{S}}S], \qquad S \in \mathscr{B}(\mathscr{H}_{\mathrm{S}}). \tag{2.29}$$

Then,

$$\rho_{\mathrm{SR}}\left[\mathrm{e}^{\mathrm{i}tH_\lambda}\,(S\otimes 1)\,\mathrm{e}^{-\mathrm{i}tH_\lambda}\right] = \mathrm{Tr}[\mathcal{Z}_t^{\lambda}(\rho_{\mathrm{S}})S]. \tag{2.30}$$

In what follows, we simply write ρ for ρ_{S}. For convenience, we treat ρ as an element of the Hilbert space $\mathscr{B}_2(\mathscr{H}_{\mathrm{S}})$, which is justified since $\mathscr{B}_1(\mathscr{H}_{\mathrm{S}}) \subset \mathscr{B}_2(\mathscr{H}_{\mathrm{S}})$.

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[2] In fact, one needs to do things more carefully, since $H_{\mathrm{SR}}(t) \notin \mathscr{C}$. A possible solution is to define the cut-off interaction $H_{\mathrm{S-R},\Lambda}(t) = \sum_{x\in\Lambda} 1_x(t)\otimes\Psi_x(\mathrm{e}^{\mathrm{i}t\omega}\phi)$, for some finite subset $\Lambda \subset \mathbb{Z}^d$, and to show that one can take the limit $\Lambda \nearrow \mathbb{Z}^d$ in the expression analogous to (2.25).

3. Result

We now state our main results. Recall that the position operator X on $l^2(\mathbb{Z}^d)$ is given by

$$(Xf)(x) = xf(x), \qquad x \in \mathbb{Z}^d,\ f \in l^2(\mathbb{Z}^d). \tag{3.1}$$

For $\kappa \in \mathbb{C}^d$, we define

$$\mathcal{J}_\kappa S := \mathrm{e}^{-\frac{\mathrm{i}}{2}(\kappa,X)}\, S\, \mathrm{e}^{-\frac{\mathrm{i}}{2}(\kappa,X)}, \qquad S \in \mathscr{B}(\mathscr{H}_\mathrm{S}). \tag{3.2}$$

Note that $\mathcal{J}_\kappa$ is unbounded if $\kappa \notin \mathbb{R}^d$. We choose an initial state $\rho \in \mathscr{B}_1(\mathscr{H}_\mathrm{S})$ satisfying

$$\rho > 0, \qquad \mathrm{Tr}[\rho] = 1 \qquad \|\mathcal{J}_\kappa \rho\|_2 < \infty, \tag{3.3}$$

for κ in some open neighborhood of $0 \in \mathbb{C}^d$.

Our first result says that the momentum distribution of the particle tends to a stationary distribution exponentially fast.

Theorem 3.1 [Equipartition Theorem]. *Suppose that Assumption 2.1 (see Sect. 2.2) and Assumption 2.2 (see (2.20)) hold, and let ρ satisfy condition (3.3). There are positive constants $\lambda_0 > 0$ and $g > 0$ such that for $0 < |\lambda| \leq \lambda_0$, there is a function $\zeta_\lambda^0 \in L^2(\mathbb{T}^d)$ satisfying*

$$\mathrm{Tr}[\theta(P)\mathcal{Z}_t^\lambda(\rho)] = \langle \theta, \zeta_\lambda^0 \rangle_{L^2(\mathbb{T}^d)} + O(\|\theta\|_2 \mathrm{e}^{-\lambda^2 g t}), \qquad \text{as } t \nearrow \infty,$$
$$\text{for any } \theta = \overline{\theta} \in L^\infty(\mathbb{T}^d), \tag{3.4}$$

and

$$\zeta_\lambda^0(k) = \frac{\mathrm{e}^{-\beta\varepsilon(k)}}{\int_{\mathbb{T}^d} \mathrm{d}k\, \mathrm{e}^{-\beta\varepsilon(k)}} + O(\lambda^2), \qquad \lambda \searrow 0. \tag{3.5}$$

The decay rate $\lambda^2 g$ is strictly smaller than g_R, introduced in (2.20).

Define a probability density μ_t^λ depending on the initial state $\rho \in \mathscr{B}_1(\mathscr{H}_\mathrm{S})$ by

$$\mu_t^\lambda(x) := \mathrm{Tr}\left[1_x \mathcal{Z}_t^\lambda(\rho)\right]. \tag{3.6}$$

It is easy to see that

$$\mu_t^\lambda(x) \geq 0, \qquad \sum_{x \in \mathbb{Z}^d} \mu_t^\lambda(x) = \mathrm{Tr}[\rho] = 1. \tag{3.7}$$

We claim that the particle exhibits a diffusive motion. This is the content of the next result.

Theorem 3.2 [Diffusion] *Under the same assumptions as in Theorem 3.1, the following holds. Let the initial state ρ satisfy condition (3.3) and let μ_t^λ be as defined in (3.6). There is a positive constant λ_0 such that, for $0 < |\lambda| \leq \lambda_0$,*

$$\sum_{x \in \mathbb{Z}^d} \mu_t^\lambda(x) \mathrm{e}^{-\frac{\mathrm{i}}{\sqrt{t}}(q,x)} \underset{t \nearrow \infty}{\longrightarrow} \mathrm{e}^{-\frac{1}{2}(q, D_\lambda q)}, \qquad q \in \mathbb{R}^d, \tag{3.8}$$

where the **diffusion matrix** *D_λ is positive-definite (i.e., has strictly positive eigenvalues), and*

$$D_\lambda = \lambda^{-2}\left(D_{\mathrm{kin}} + O(\lambda^2)\right), \qquad \lambda \searrow 0, \tag{3.9}$$

with D_{kin} a λ-independent positive-definite matrix introduced in Sect. 4.3.

We refer to Sect. 1 for an explanation of the connection between this result and diffusion in the physicists' sense. We close this section with some remarks concerning possible extensions of our results.

Remark 3.3. Our proof of Theorem 3.2 actually gives a stronger result. Assume the n^{th} moments of the initial distribution are bounded, or, equivalently,

$$q \mapsto \sum_{x \in \mathbb{Z}^d} \mu_0^\lambda(x) \mathrm{e}^{-\mathrm{i}(q,x)} \quad \text{is } n \text{ times differentiable.} \tag{3.10}$$

Then the rescaled n^{th} moments converge to the n^{th} moments of the limiting distribution, or equivalently, the derivatives of n^{th} order of

$$q \mapsto \sum_{x \in \mathbb{Z}^d} \mu_t^\lambda(x) \mathrm{e}^{-\frac{\mathrm{i}}{\sqrt{t}}(q,x)} \tag{3.11}$$

converge, as $t \nearrow \infty$, to the derivatives of $\mathrm{e}^{-(q,D_\lambda q)}$. For $n = 2$, this implies (1.19). Note that the condition (3.10) is a weaker assumption than (3.3); in fact, (3.3) implies that (3.10) is a real-analytic function.

Remark 3.4. By the same technique as employed in our proofs, one can show that correlations decay rapidly in time. As explained in the Introduction, this rapid decay provides an intuitive explanation why the particle motion is diffusive.

Define the particle velocity operator by

$$V(t) := \mathrm{i}\mathrm{e}^{\mathrm{i}tH_\lambda}[H_\lambda, X]\mathrm{e}^{-\mathrm{i}tH_\lambda}, \tag{3.12}$$

and observe that

$$V(0) = \mathrm{i}[H_\lambda, X] = \mathrm{i}[H_\mathrm{S}, X] = (\nabla\varepsilon)(P). \tag{3.13}$$

Suppose that Assumptions 2.1 and 2.2 hold and let $\rho = \rho_\mathrm{S}$ satisfy condition (3.3).

By reasoning similar to that in Lemma 2.3, one can define the velocity-velocity correlation function $\rho_\mathrm{SR}\,[V(t_1)V(t_2)]$. Let the coupling strength λ and the positive constant g be as in Theorem 3.1. Then, for all $0 \le t_1, t_2 < \infty$,

$$|\rho_\mathrm{SR}\,[V(t_1)V(t_2)]| \le c\,\mathrm{e}^{-\lambda^2 g|t_2-t_1|}, \qquad \text{for some } c < \infty. \tag{3.14}$$

Remark 3.5. The condition that the particle dispersion satisfies $\varepsilon(k) = \varepsilon(-k)$ is not really necessary for our results to hold. If one did not impose this condition, the particle could have a drift velocity v_dr given by

$$v_\mathrm{dr} := \langle \nabla\varepsilon, \zeta_\lambda^0 \rangle, \tag{3.15}$$

and the particle motion would still be diffusive, but one would now consider the "random variable" $\frac{1}{\sqrt{t}}(x_t - v_\mathrm{dr}t)$, instead of $\frac{1}{\sqrt{t}}x_t$. In other words, in (3.8), one would have to replace

$$\sum_{x \in \mathbb{Z}^d} \mu_t^\lambda(x)\mathrm{e}^{-\frac{\mathrm{i}}{\sqrt{t}}(q,x)} \quad \text{by} \quad \sum_{x \in \mathbb{Z}^d} \mu_t^\lambda(x)\mathrm{e}^{-\frac{\mathrm{i}}{\sqrt{t}}(q,(x-v_\mathrm{dr}t))}. \tag{3.16}$$

Similarly, in Eq. (3.14), one would have to replace $V(t)$ by $V(t) - v_\mathrm{dr}$.

4. Discussion and Outline of the Proof

4.1. Translation invariance. Consider the space of Hilbert-Schmidt operators $\mathscr{B}_2(\mathscr{H}_{\mathrm{S}}) \sim \mathscr{B}_2(l^2(\mathbb{Z}^d)) \sim L^2(\mathbb{T}^d \times \mathbb{T}^d, \mathrm{d}k_1 \mathrm{d}k_2)$, and define

$$\hat{S}(k_1, k_2) := \frac{1}{(2\pi)^d} \sum_{x_1, x_2 \in \mathbb{Z}^d} S(x_1, x_2) \mathrm{e}^{-\mathrm{i}(x_1, k_1) + \mathrm{i}(x_2, k_2)}, \qquad S \in \mathscr{B}_2(l^2(\mathbb{Z}^d)). \quad (4.1)$$

In what follows, we simply write S for $\hat{S}$. To deal conveniently with the translation invariance in our model, we make the change of variables

$$k = \frac{k_1 + k_2}{2}, \qquad p = k_1 - k_2, \quad (4.2)$$

and, for a.e. $p \in \mathbb{T}^d$, we obtain a well-defined function $S_p \in L^2(\mathbb{T}^d)$ by putting

$$(S_p)(k) := S(k + \frac{p}{2}, k - \frac{p}{2}). \quad (4.3)$$

This follows from the fact that the Hilbert space $\mathscr{B}_2(\mathscr{H}_{\mathrm{S}}) \sim L^2(\mathbb{T}^d \times \mathbb{T}^d, \mathrm{d}k_1 \mathrm{d}k_2)$ can be represented as a direct integral

$$\mathscr{B}_2(\mathscr{H}_{\mathrm{S}}) = \int_{\oplus \mathbb{T}^d} \mathrm{d}p \, \mathscr{H}^p, \qquad S = \int_{\oplus \mathbb{T}^d} \mathrm{d}p \, S_p, \quad (4.4)$$

where each 'fiber space' $\mathscr{H}^p$ is naturally identified with $L^2(\mathbb{T}^d)$. Let $\mathcal{T}_z$, $z \in \mathbb{Z}^d$, be the lattice translation

$$(\mathcal{T}_z S)(x_1, x_2) := S(x_1 + z, x_2 + z), \qquad S \in \mathscr{B}(\mathscr{H}_{\mathrm{S}}), \quad (4.5)$$

or, equivalently,

$$(\mathcal{T}_z S)_p(k) = \mathrm{e}^{\mathrm{i}(p,z)} S_p, \qquad S \in \mathscr{B}(\mathscr{H}_{\mathrm{S}}). \quad (4.6)$$

Since H_λ and ρ_{R}^β are translation invariant, it follows that

$$\mathcal{T}_{-z} \mathcal{Z}_t^\lambda \mathcal{T}_z = \mathcal{Z}_t^\lambda. \quad (4.7)$$

Let $\mathcal{W} \in \mathscr{B}(\mathscr{B}_2(\mathscr{H}_{\mathrm{S}}))$ be translation invariant in the sense of Eq. (4.7), i.e., $\mathcal{T}_{-z} \mathcal{W} \mathcal{T}_z = \mathcal{W}$. Then it follows that, in the representation defined by (4.4), $\mathcal{W}$ acts diagonally in p, i.e. $(\mathcal{W}S)_p$ depends only on S_p, and we define $\mathcal{W}_p$ by

$$(\mathcal{W}S)_p = \mathcal{W}_p S_p. \quad (4.8)$$

For the sake of clarity, we give an explicit expression for $\mathcal{W}_p$. Define the kernel $\mathcal{W}(x, y; x', y')$ by

$$(\mathcal{W}S)(x', y') = \sum_{x, y \in \mathbb{Z}^d} \mathcal{W}(x, y; x', y') S(x, y), \qquad x', y' \in \mathbb{Z}^d. \quad (4.9)$$

Translation invariance is expressed by

$$\mathcal{W}(x, y; x', y') = \mathcal{W}(x + z, y + z; x' + z, y' + z), \qquad z \in \mathbb{Z}^d, \quad (4.10)$$

and, as an integral kernel, $\mathcal{W}_p \in \mathscr{B}(L^2(\mathbb{T}^d))$ is given by

$$\mathcal{W}_p(k',k) = \sum_{\substack{x,y,x',y' \in \mathbb{Z}^d \\ x=0}} \mathrm{e}^{\mathrm{i}(k,x-y)-\mathrm{i}(k',x'-y')} \mathrm{e}^{\frac{\mathrm{i}}{2}(p,(x'+y')-(x+y))} \mathcal{W}(x,y;x',y'). \tag{4.11}$$

Next, we state an easy lemma.

Lemma 4.1. *Let $S \in \mathscr{B}_1(\mathscr{H}_{\mathrm{S}})$. Then, S_p, as defined in (4.3), is well-defined as a function in $L^1(\mathbb{T}^d)$ for every p, and*

$$\mathrm{Tr}[\mathcal{J}_p S] = \sum_{x\in\mathbb{Z}^d} \mathrm{e}^{-\mathrm{i}px} S(x,x) = \langle 1, S_p \rangle, \tag{4.12}$$

where $1 \in L^2(\mathbb{T}^d) \cap L^\infty(\mathbb{T}^d)$ is the constant function with value $1(k) = 1$. Assume, moreover, that there is a constant $\delta > 0$ such that

$$\|\mathcal{J}_\kappa S\|_2 < \infty \quad \text{for} \quad |\Im\kappa| < \delta, \tag{4.13}$$

then the function $p \mapsto S_p \in L^2(\mathbb{T}^d)$ has a bounded-analytic extension to the strip $|\Im p| < \delta$.

The first statement of the lemma follows from the singular-value decomposition for trace-class operators and standard properties of the Fourier transform. In fact, the correct statement asserts that one can *choose* S_p such that (4.12) holds. Indeed, one can change the value of the kernel $S(k_1,k_2)$ on the line $k_1 - k_2 = p$ without changing the operator S, and hence S_p in (4.12) can not be defined via (4.3) for all p, but only for almost all p.

The second statement of Lemma 4.1 is the well-known relation between exponential decay of functions and analyticity of their Fourier transforms. Since we will always demand the initial density matrix ρ_0 to be such that $\|\mathcal{J}_\kappa \rho_0\|_2$ is finite for κ in a complex domain, we will mainly need the second statement of Lemma 4.1.

4.2. Return to equilibrium inside the fibers. The main idea of our proof is that the reduced evolution in the 'low momentum fibers', $(\mathcal{Z}_t^\lambda)_p$, for p near 0, has an invariant state to which every well-localized initial state relaxes exponentially fast.

Recalling that $H_{\mathrm{S}} = \varepsilon(P)$ and that the system is weakly coupled to a heat bath at inverse temperature β, we expect that, in an appropriate sense, and for arbitrary initial states $\rho \in \mathscr{B}_1(\mathcal{H}_{\mathrm{S}})$,

$$\mathcal{Z}_t^\lambda(\rho) \text{``}\underset{t\uparrow\infty}{\longrightarrow}\text{''} \frac{1}{Z(\beta)} \mathrm{e}^{-\beta\varepsilon(P)} + o(\lambda^0), \qquad \lambda \searrow 0. \tag{4.14}$$

We observe that $\mathrm{e}^{-\beta\varepsilon(P)} \notin \mathscr{B}_1(\mathcal{H}_{\mathrm{S}})$, hence (4.14) cannot hold in norm (in other words, $Z(\beta) = \infty$). One way to interpret (4.14) is that it gives the correct asymptotic expectation value of functions of the momentum, and that is exactly what Theorem 3.1 states.

For every ρ satisfying (3.3), we have that

$$\mathrm{Tr}[\overline{\theta}(P)\mathcal{Z}_t^\lambda(\rho)] = \langle \theta, (\mathcal{Z}_t^\lambda \rho)_0 \rangle, \qquad \theta \in L^\infty(\mathbb{T}^d), \tag{4.15}$$

by applying Lemma 4.1 with $S := \overline{\theta}(P)\mathcal{Z}_t^\lambda(\rho)$. Hence, we should apparently attempt to prove 'return to equilibrium' for the evolution $(\mathcal{Z}_t^\lambda)_0$ on $L^2(\mathbb{T}^d)$.

The dynamics in the fibers corresponding to small values of p provides information on the diffusive character of the system. The probability density $\mu_t^\lambda(x)$ corresponding to some initial state ρ is defined as in (3.6). By Lemma 4.1,

$$\sum_{x\in\mathbb{Z}^d} \mu_t^\lambda(x)\mathrm{e}^{-\mathrm{i}(p,x)} = \sum_{x\in\mathbb{Z}^d} (\mathcal{Z}_t^\lambda \rho)(x,x)\mathrm{e}^{-\mathrm{i}(p,x)} = \int_{\mathbb{T}^d} \mathrm{d}k(\mathcal{Z}_t^\lambda \rho)(k+\frac{p}{2}, k-\frac{p}{2}) = \langle 1, (\mathcal{Z}_t^\lambda \rho)_p\rangle. \tag{4.16}$$

To establish diffusion, it suffices to show that, for λ fixed and for p in a neighborhood of $0 \in \mathbb{T}^d$,

$$\langle 1, (\mathcal{Z}_t^\lambda \rho)_p\rangle = \mathrm{e}^{t(-\frac{1}{2}(p,D_\lambda p)+o(p^2))}(1+o(t^0)+o(p^0)), \qquad t\nearrow\infty, p\searrow 0, \tag{4.17}$$

for some positive-definite matrix D_λ. Indeed, by (4.16), Theorem 3.2 follows from (4.17) by taking $p = \frac{q}{\sqrt{t}}$. Thus, in order to prove Theorem 3.2, we are led to study the long-time asymptotics of the evolution $(\mathcal{Z}_t^\lambda)_p$, for small p.

However, as our approach is perturbative in λ, expression (4.17) is not a good starting point, since $(p, D_\lambda p) = O(\lambda^{-2})$, for fixed p (as can be seen from the statement of Theorem 3.2), and hence one cannot perturb around $(p, D_\lambda p)\big|_{\lambda=0}$. The way out of this difficulty is to set up the perturbation on a scale where the diffusion constant is finite (this will turn out to be the kinetic scale), or, in other words, to take the p-neighborhood in (4.17) to shrink, as $\lambda\searrow 0$. Since λ approaches 0, one must wait a time of order λ^{-2}, before one sees the effect of the interaction. Since, between collisions, the velocity of the free particle is unaffected, it travels a distance of order λ^{-2}. This means that when both space and time are measured in units of λ^{-2};

$$x = \lambda^{-2}\tilde{x}_\lambda, \qquad t = \lambda^{-2}\tilde{t}_\lambda, \tag{4.18}$$

we expect a diffusion constant $\tilde{D}_\lambda \sim \frac{(\tilde{x}_\lambda)^2}{\tilde{t}_\lambda}$ of order $O(1)$. This is consistent with the fact that $D_\lambda \sim \frac{x^2}{t}$ is of order λ^{-2}. The limit $\tilde{D}_{\lambda\searrow 0}$ is the diffusion constant in the kinetic limit, as outlined in the next section.

4.3. The kinetic limit. To control the asymptotics of the effective time-evolution $(\mathcal{Z}_t^\lambda)_p$, we compare it with the corresponding evolution in the *kinetic limit*, which is the limit approached when microscopic space and time are taken to be $\lambda^{-2}x$, $\lambda^{-2}t$, respectively, and the coupling strength $\lambda\to 0$; as announced in the previous section. It has been proven in [9] (for models with only one thermal reservoir) that, in this limit, the dynamics is described by a linear Boltzmann equation.

Our variant of this result is described below.

4.3.1. Convergence to a linear Boltzmann equation. The effective reservoir structure factor ψ has been defined in (2.18–2.19). For convenience, we introduce a positive function $r(\cdot,\cdot)$, with

$$r(k,k') := \psi[\varepsilon(k') - \varepsilon(k)] \geq 0. \tag{4.19}$$

For $\kappa \in \mathbb{R}^d$, we define a bounded linear operator, M^κ, on $L^2(\mathbb{T}^d)$ by

$$(M^\kappa \theta)(k) := \mathrm{i}(\kappa, \nabla\varepsilon)(k)\theta(k) + \int_{\mathbb{T}^d} \mathrm{d}k' \left[r(k', k)\theta(k') - r(k, k')\theta(k) \right], \qquad \theta \in L^2(\mathbb{T}^d), \quad (4.20)$$

where $(\kappa, \nabla\varepsilon)(k)$ stands for the scalar product in $\mathbb{C}^d$ of κ and $\nabla\varepsilon(k)$. The operator M^κ has a straightforward interpretation: Consider a classical particle whose states are specified by a position $x \in \mathbb{R}^d$ and a 'momentum' $k \in \mathbb{T}^d$. The momentum k evolves according to a Poisson process with a rate $r(k, k')$ for the transition from state k to k'. Between two momentum jumps, the particle moves freely, with speed given by $(\nabla\varepsilon)(k)$. The translation of this picture into a mathematical statement is as follows: The state-space distribution of the classical particle at time t is given by a probability density $\nu_t(\cdot, \cdot)$ on $\mathbb{R}^d \times \mathbb{T}^d$; ($\nu(x, k) \geq 0$ and $\int \mathrm{d}x\mathrm{d}k \, \nu_t(x, k) = 1$). Then

$$\frac{\partial}{\partial t} \nu_t(x, k) = (\nabla_k \varepsilon, \nabla_x \nu_t)(x, k) + \int_{\mathbb{T}^d} \mathrm{d}k' \left[r(k', k)\nu_t(x, k') - r(k, k')\nu_t(x, k) \right]. \quad (4.21)$$

One checks that

$$\hat{\nu}_t^\kappa(k) := (2\pi)^{-d/2} \int_{\mathbb{R}^d} \mathrm{d}x \, \mathrm{e}^{-\mathrm{i}(\kappa, x)} \nu_t(x, k) \quad (4.22)$$

satisfies an evolution equation generated by M^κ;

$$\frac{\partial}{\partial t} \hat{\nu}_t^\kappa = M^\kappa \hat{\nu}_t^\kappa. \quad (4.23)$$

We claim that the rates $r(k, k')$ satisfy the identity

$$r(k, k') = r(k', k)\mathrm{e}^{-\beta(\varepsilon(k') - \varepsilon(k))}, \quad (4.24)$$

known as the *detailed balance condition* in the context of Markov processes. It is a direct consequence of the KMS-condition for the reservoirs. In our context, it is easily derived from (2.15). The detailed balance condition implies that

$$M^0 \zeta^0_{\mathrm{kin}} = 0, \qquad \text{where} \quad \zeta^0_{\mathrm{kin}}(k) = \frac{\mathrm{e}^{-\beta\varepsilon(k)}}{\int_{\mathbb{T}^d} \mathrm{d}k \mathrm{e}^{-\beta\varepsilon(k)}}. \quad (4.25)$$

In the language of Markov processes, ζ^0_{kin} is a stationary state.

The relevance of M^κ is that it describes the evolution $\mathcal{Z}^\lambda_{\lambda^{-2}t}$ in the fiber indexed by $\lambda^2\kappa$ in the limit $\lambda \searrow 0$. Moreover, the convergence of the fiber dynamics $(\mathcal{Z}^\lambda_{\lambda^{-2}t})_{\lambda^2\kappa}$ holds even after analytic continuation to complex κ. One can prove the following result

Proposition 4.2. *Assume Assumptions 2.1 and 2.2. Then, for $|\Im\kappa|$ sufficiently small and $0 < t < \infty$,*

$$\left\| (\mathcal{Z}^\lambda_{\lambda^{-2}t})_{\lambda^2\kappa} - \mathrm{e}^{tM^\kappa} \right\| \underset{\lambda \searrow 0}{\longrightarrow} 0, \quad (4.26)$$

where the norm is the operator norm on $L^2(\mathbb{T}^d)$.

We do not prove this proposition (which is not needed for the proof of our results). In fact, the proof is based on the same reasoning as in Sect. 6. Of course, one can also express Proposition 4.2 in terms of the rescaled Wigner function, as is done in [9,12]. Indeed, setting

$$\hat{\alpha}_t^{\kappa}(k) := \lim_{\lambda\searrow 0} \left(\mathcal{Z}^{\lambda}_{\lambda^{-2}t}\rho\right)(k+\lambda^2\frac{\kappa}{2}, k-\lambda^2\frac{\kappa}{2}) = \lim_{\lambda\searrow 0}(\mathcal{Z}^{\lambda}_{\lambda^{-2}t}\rho)_{\lambda^2\kappa}(k), \tag{4.27}$$

one obtains from Proposition 4.2 that $\hat{\alpha}_t^{\kappa}(k)$ satisfies the evolution equation (4.23). (It would thus be justified to call $\hat{\alpha}_t^{\kappa}(k)$ simply $\hat{\nu}_t^{\kappa}(k)$). Its inverse Fourier transform

$$\alpha_t(x,k) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \mathrm{d}\kappa\, \mathrm{e}^{\mathrm{i}(\kappa,x)} \hat{\alpha}_t^{\kappa}(k) \tag{4.28}$$

is a probability density on $\mathbb{R}^d \times \mathbb{T}^d$ and satisfies (4.21) with initial condition $\alpha_0(x,k) = \delta(x)\rho(k,k)$.

We state another useful consequence of Proposition 4.2. Recall that the probability density $\mu_t(\cdot)$ has been defined in (3.6), for any initial state ρ. Taking the scalar product with $1 \in L^2(\mathbb{T}^d)$ on both sides of (4.27) and using (4.16), we obtain that

$$\sum_{x\in\mathbb{Z}^d} \mathrm{e}^{-\mathrm{i}\lambda^2(\kappa,x)} \mu^{\lambda}_{\lambda^{-2}t}(x) \underset{\lambda\searrow 0}{\longrightarrow} \int_{\mathbb{T}^d} \mathrm{d}k\, \hat{\alpha}_t^{\kappa}(k). \tag{4.29}$$

As outlined in Sect. 4.2, the $t \nearrow \infty$ asymptotics of the LHS of (4.29) contains information on the diffusive behavior of the particle. In the next section we discuss the $t \nearrow \infty$ asymptotics of the RHS of (4.29).

4.3.2. Diffusive behavior of solutions of the Boltzmann equation. To realize that the Boltzmann equation describes diffusion, one studies the spectral properties of M^{κ}, for small κ. We state a crucial result, Theorem 4.3, and we refer the reader to [6] for complete proofs and a more extended discussion of quantum dissipative evolutions.

Theorem 4.3. *Suppose that Assumptions 2.1 and 2.2 hold, and let $M^{\kappa} \in \mathscr{B}(L^2(\mathbb{T}^d))$ be defined as in (4.20).*

Then there is a positive constant δ_{kin} such that the operator M^{κ}, with $|\kappa| \leq \delta_{\mathrm{kin}}$, has a simple eigenvalue, $f_{\mathrm{kin}}(\kappa)$, separated from the rest of the spectrum by a gap,

$$\mathrm{dist}(\Re f_{\mathrm{kin}}(\kappa), \Re\Omega) =: g_{\mathrm{kin}} > 0, \tag{4.30}$$

where

$$\Omega := \cup_{|\kappa|<\delta_{\mathrm{kin}}} \left(\mathrm{sp} M^{\kappa} \setminus \{f_{\mathrm{kin}}(\kappa)\}\right), \qquad \text{and} \quad \Re\Omega < 0. \tag{4.31}$$

The eigenvalue f_{kin} and its associated eigenvector $\zeta^{\kappa}_{\mathrm{kin}}$ and spectral projection $P^{\kappa}_{\mathrm{kin}}$ are analytic in κ and

$$f_{\mathrm{kin}}(\kappa) = \left\langle 1, \left(\kappa, \nabla\varepsilon\right) \left(M^0\right)^{-1} \left(\kappa, \nabla\varepsilon\right)\zeta^0_{\mathrm{kin}} \right\rangle + O\left(\kappa^3\right), \qquad \kappa \searrow 0, \tag{4.32}$$

where $\nabla\varepsilon$ denotes the operator that acts by multiplication with the function $\nabla\varepsilon$ on $\mathbb{T}^d$. The diffusion matrix, D_{kin}, defined by

$$(D_{\mathrm{kin}})^{i,j} := -\frac{\partial^2}{\partial\kappa^i \partial\kappa^j} f_{\mathrm{kin}}(\kappa)\Big|_{\kappa=0}, \qquad i,j = 1,\ldots d, \tag{4.33}$$

has real entries and is positive-definite.

Sketch of proof. We write $M^0 = K + T$ with

$$(K\theta)(k) = \int_{\mathbb{T}^d} \mathrm{d}k' r(k',k)\theta(k'),$$
$$(T\theta)(k) = -\left(\int_{\mathbb{T}^d} \mathrm{d}k' r(k,k')\right)\theta(k), \qquad \theta \in L^2(\mathbb{T}^d, \mathrm{d}k). \tag{4.34}$$

Notice that T is a multiplication operator with spectrum

$$\mathrm{sp}T = \left\{ -\int_{\mathbb{T}^d} \mathrm{d}k' r(k,k') \,\middle|\, k \in \mathbb{T}^d \right\}, \qquad r(k,k') \geq 0. \tag{4.35}$$

The operators K and T are sometimes referred to as the *gain* and *loss* terms in the Boltzmann equation. Assumptions 2.1 and 2.2 imply that the functions ψ and ε are real-analytic in k, and hence $r(\cdot,\cdot)$ is real-analytic in both variables. It follows that K is a compact operator on $L^2(\mathbb{T}^d)$ and, since we assumed that $\psi \not\equiv 0$, we have that $\sup \Re \mathrm{sp}T < 0$. By Weyl's theorem on the stability of the essential spectrum (see e.g. p. 101 of [18]), we deduce that the spectrum of M^0 in the region $\Re z > \sup \Re \mathrm{sp} T$ consists of isolated eigenvalues of finite multiplicity. From the pointwise positivity of $r(\cdot,\cdot)$, the Perron-Frobenius theorem and from the fact that M^0 generates a contractive semigroup on $L^1(\mathbb{T}^d)$ we then conclude that the eigenvalue 0 of M^0 is simple and that it is separated by a gap from the rest of the spectrum. The spectral projection P^0_{kin} is explicitly given by

$$P^0_{\mathrm{kin}}\theta = \langle 1, \theta\rangle \zeta^0_{\mathrm{kin}}, \qquad \theta \in L^2(\mathbb{T}^d) \tag{4.36}$$

with ζ^0_{kin} as in (4.25). The analyticity of $f_{\mathrm{kin}}(\kappa)$ and $\zeta^\kappa_{\mathrm{kin}}$ is proven with the help of analytic perturbation theory. Using the assumption that $\varepsilon(k) = \varepsilon(-k)$, we check that

$$P^0_{\mathrm{kin}} \nabla\varepsilon P^0_{\mathrm{kin}} = 0. \tag{4.37}$$

Employing explicit expressions of second order perturbation theory, we obtain formula (4.32) as a consequence of the fact that $M^\kappa - M^0 = \mathrm{i}(\kappa, \nabla\varepsilon)$ and (4.37).

Since $\overline{f_{\mathrm{kin}}(\kappa)} = f_{\mathrm{kin}}(-\overline{\kappa})$, it follows that the matrix D_{kin} has real entries. The positive-definiteness of D_{kin} is established as follows. Consider the bounded operator

$$(W\theta)(k) = \mathrm{e}^{\frac{1}{2}\beta\varepsilon(k)}\theta(k), \qquad \theta \in L^2(\mathbb{T}^d), \tag{4.38}$$

and notice that $\tilde{M} := W^{-1}M^0 W$ is a self-adjoint operator on $L^2(\mathbb{T}^d)$, in particular $\tilde{\zeta} := W\zeta^0_{\mathrm{kin}} = W^{-1}1$, (i.e., the left and right eigenvector corresponding to the eigenvalue 0 are identical). For $\kappa \in \mathbb{R}^d$, we can rewrite (4.33) as

$$\left(\kappa, D_{\mathrm{kin}}\kappa\right) = -\left\langle \left(\kappa, \nabla\varepsilon\right)\tilde{\zeta}, \left(\tilde{M}\right)^{-1} \left(\kappa, \nabla\varepsilon\right)\tilde{\zeta} \right\rangle. \tag{4.39}$$

By Assumption 2.1, the function $k \mapsto (\kappa, \nabla\varepsilon(k))$ does not vanish identically on $\mathbb{T}^d$ (for $\kappa \neq 0$). Hence, by the spectral theorem applied to $\tilde{M}$, expression (4.39) is strictly positive. □

Let $\hat{\nu}_t^{\kappa}(k)$ be a solution of the evolution equation (4.23) for κ in some neighborhood of 0 in $\mathbb{C}^d$. Using Theorem 4.3 and reasoning similar to that in Sect. 4.2, it follows that

$$\int_{\mathbb{T}^d} \mathrm{d}k \, \hat{\nu}_t^{\kappa}(k) \quad \underset{\kappa=\frac{q}{\sqrt{t}},\, t\nearrow\infty}{\longrightarrow} \quad \mathrm{e}^{-\frac{1}{2}(q, D_{\mathrm{kin}} q)}, \qquad q \in \mathbb{R}^d. \tag{4.40}$$

Hence a solution $\nu_t(x,k)$ of the Boltzmann equation (4.21) behaves diffusively, with diffusion tensor D_{kin}.

4.4. Perturbation around the kinetic limit. Up to now, we have seen that, in the kinetic limit, the particle motion is described by a linear Boltzmann equation. Since solutions of the linear Boltzmann equation behave diffusively for large times (as is essentially stated in Theorem 4.3), we can associate a diffusion constant to our model. Indeed, by (4.29) and (4.40),

$$\lim_{t\nearrow\infty} \lim_{\lambda\searrow 0} \sum_{x\in\mathbb{Z}^d} \mu^{\lambda}_{\lambda^{-2}t}(x) \mathrm{e}^{-\mathrm{i}\frac{\lambda^2}{\sqrt{t}}(q,x)} = \mathrm{e}^{-\frac{1}{2}(q, D_{\mathrm{kin}} q)}. \tag{4.41}$$

However, (4.41) does not give information on the long-time asymptotics of our system for small, but fixed $|\lambda| > 0$. The least one would wish for is to be able to exchange the order of limits in (4.41), and, indeed, Theorem 3.2 states that one can do so without affecting the RHS. We stress this point, because it is an improvement of our paper when compared to most earlier results on diffusion.

Since we have learned that $(\mathcal{Z}^{\lambda}_{\lambda^{-2}t})_{\lambda^2\kappa}$ has a well-defined limit, $\mathrm{e}^{tM^{\kappa}}$, as $\lambda \searrow 0$, (see Proposition 4.2), it is natural to expand $(\mathcal{Z}^{\lambda}_{\lambda^{-2}t})_{\lambda^2\kappa}$ around this limit, in such a way that we can take $t \nearrow \infty$. We perform the expansion on the Laplace transform of $\mathcal{Z}^{\lambda}_t$,

$$\mathcal{R}_{\lambda}(z) := \int_{\mathbb{R}^+} \mathrm{d}t \, \mathrm{e}^{-tz} \mathcal{Z}^{\lambda}_t. \tag{4.42}$$

Theorem 4.4 below summarizes the result of our expansion. Loosely speaking, a key consequence of this theorem is the fact that, in the fibers indexed by $\lambda^2\kappa$, one has that

$$(\mathcal{R}_{\lambda}(z))_{\lambda^2\kappa} = (z - \lambda^2 M^{\kappa} - A(z,\lambda,\kappa))^{-1}, \tag{4.43}$$

where the operator $A(z,\lambda,\kappa)$ is "small" compared to $\lambda^2 M^{\kappa}$.

Theorem 4.4. *Suppose that Assumptions 2.1 and 2.2 in Sect. 2 hold. Then, there are operators $\mathcal{L}(z)$ and $\mathcal{R}^{\mathrm{ex}}_{\lambda}(z)$ in $\mathscr{B}(\mathscr{B}_2(\mathscr{H}_{\mathrm{S}}))$ such that the following statements hold:*

1) *For $(z,\lambda) \in \mathbb{C}\times\mathbb{R}$ satisfying $\Re z > \|\lambda^2\mathcal{L}(z) + \mathcal{R}^{\mathrm{ex}}_{\lambda}(z)\|$,*

$$\mathcal{R}_{\lambda}(z) = (z - \mathrm{ad}(\mathrm{i}H_{\mathrm{S}}) - \lambda^2\mathcal{L}(z) - \mathcal{R}^{\mathrm{ex}}_{\lambda}(z))^{-1}. \tag{4.44}$$

2) *The operators $\mathcal{L}(z)$ and $\mathcal{R}^{\mathrm{ex}}_{\lambda}(z)$ have the following properties: There are positive constants $\delta_1', \delta_2', g' > 0$ such that*

$$\mathcal{J}_{\kappa}\mathcal{L}(z)\mathcal{J}_{-\kappa}, \qquad \mathcal{J}_{\kappa}\mathcal{R}^{\mathrm{ex}}_{\lambda}(z)\mathcal{J}_{-\kappa} \tag{4.45}$$

are analytic in the variables $(z, \kappa) \in \mathbb{C} \times \mathbb{C}^d$ *in the region defined by* $|\kappa| \leq \delta_1'$, $\Re z > -g'$, $|\lambda| \leq \delta_2'$. *Moreover,*

$$\sup_{|\kappa| \leq \delta_1', \Re z > -g'} \| \mathcal{J}_\kappa \mathcal{L}(z) \mathcal{J}_{-\kappa} \| = O(1), \qquad \lambda \searrow 0, \tag{4.46}$$

$$\sup_{|\kappa| \leq \delta_1', \Re z > -g'} \| \mathcal{J}_\kappa \mathcal{R}^{\mathrm{ex}}_\lambda(z) \mathcal{J}_{-\kappa} \| = O(\lambda^4), \qquad \lambda \searrow 0, \tag{4.47}$$

where $\| \cdot \|$ *refers to the operator norm on* $\mathscr{B}(\mathscr{B}_2(\mathscr{H}_{\mathrm{S}}))$ *(as in (2.4)).*

3) *Let* M^κ *be defined as in Sect. 4.3. Then*

$$\| \left(\mathrm{ad}(\mathrm{i}H_{\mathrm{S}}) + \lambda^2 \mathcal{L}(0) \right)_{\lambda^2 \kappa} - \lambda^2 M^\kappa \| = O(\lambda^4 \kappa^2) + O(\lambda^4 \kappa), \qquad \lambda^2 \kappa \searrow 0, \lambda \searrow 0. \tag{4.48}$$

The proof of Theorem 4.4 is the subject of Sect. 5. From that proof, it becomes clear that g' can be chosen to be any fraction of g_{R} by making δ_1' and δ_2' small enough.

From Theorem 4.4, one obtains our main result by using Theorem 4.3 and standard analytic perturbation theory. More precisely, we prove the following theorem.

Theorem 4.5. *Suppose that Assumptions 2.1 and 2.2 in Sect. 2 hold. Then, there are positive constants* $\delta_1, \delta_2, g > 0$ *such that, for* $(\lambda, \kappa) \in \mathbb{R} \times \mathbb{C}^d$ *and* $|\kappa| \leq \delta_1$, $0 < |\lambda| \leq \delta_2$, *there is a rank* 1 *operator* $P^{\lambda,\kappa}$ *and a function* $f(\lambda, \kappa)$ *satisfying*

$$\| (\mathcal{Z}^\lambda_t)_{\lambda^2 \kappa} - \mathrm{e}^{t f(\lambda,\kappa)} P^{\lambda,\kappa} \| = O(\mathrm{e}^{t(f(\lambda,\kappa) - \lambda^2 g)}), \qquad t \nearrow \infty \tag{4.49}$$

and

$$\| P^{\lambda,\kappa} - P^\kappa_{\mathrm{kin}} \| = O(\lambda^2), \qquad |f(\lambda,\kappa) - \lambda^2 f_{\mathrm{kin}}(\kappa)| = O(\lambda^4), \qquad \lambda \searrow 0 \tag{4.50}$$

Moreover, $P^{\lambda,\kappa}$ *and* $f(\lambda, \kappa)$ *are analytic in* $\kappa \in \mathbb{C}^d$ *in the region defined by* $|\kappa| \leq \delta_1$, $|\lambda| \leq \delta_2$.

By making δ_2 small enough, the constant g can be chosen to be any fraction of g_{kin} and δ_1 can be chosen to be given by δ_{kin}, with $g_{\mathrm{kin}}, \delta_{\mathrm{kin}}$ as in Theorem 4.3.

Theorems 3.1 (Equipartition Theorem) and 3.2 (Diffusion) then follow as discussed in Sect. 4.2. We briefly recapitulate our reasoning.

Proof of Theorems 3.1 and 3.2. We first prove Theorem 3.1. Using (4.15) and Theorem 4.5, we write, for $\theta = \overline{\theta} \in L^\infty(\mathbb{T}^d)$,

$$\mathrm{Tr}[\theta(P) \mathcal{Z}^\lambda_t \rho] = \langle \theta, (\mathcal{Z}^\lambda_t \rho)_0 \rangle = \langle \theta, \mathrm{e}^{t f(\lambda,0)} P^{\lambda,0} \rho_0 \rangle + O(\mathrm{e}^{t(f(\lambda,0) - \lambda^2 g)}). \tag{4.51}$$

Since $\mathcal{Z}^\lambda_t \rho$ has trace 1 (it is a density matrix) for all $t \geq 0$, we deduce that $f(\lambda, 0) = 0$ and, setting $\theta = 1$,

$$\langle 1, P^{\lambda,0} \rho_0 \rangle = 1. \tag{4.52}$$

The fact that $P^{\lambda,0}$ is a rank 1 operator (by Theorem 4.5) implies, together with (4.52), that,

$$P^{\lambda,0} \eta = \zeta^0_\lambda \langle 1, \eta \rangle, \qquad \text{for any } \eta \in L^2(\mathbb{T}^d), \tag{4.53}$$

for some $\zeta^0_\lambda \in L^2(\mathbb{T}^d)$ which satisfies $\langle 1, \zeta^0_\lambda \rangle = 1$. Theorem 3.1 follows.

We define the diffusion matrix by

$$(D_\lambda)^{i,j} := -\lambda^{-4} \frac{\partial^2}{\partial\kappa^i \partial\kappa^j} f(\lambda,\kappa)\big|_{\kappa=0}, \qquad i,j = 1,\dots d. \tag{4.54}$$

From (4.12), with $S := \mathcal{Z}_t^\lambda \rho$, we conclude that $\overline{f(\lambda,\kappa)} = f(\lambda,-\overline{\kappa})$, and hence the matrix D_λ has real entries. Positive-definiteness of D_λ follows then from positive-definiteness of D_{kin}, for λ small enough. Using Theorem 4.5, we find that

$$\begin{aligned}
\sum_{x\in\mathbb{Z}^d} \mathrm{e}^{-\frac{\mathrm{i}}{\sqrt{t}}(q,x)} \mu_t^\lambda(x) &= \langle 1, (\mathcal{Z}_t^\lambda \rho)_{\frac{q}{\sqrt{t}}} \rangle \qquad (4.55)\\
&= \langle 1, (\mathcal{Z}_t^\lambda \rho)_{\lambda^2\kappa} \rangle, \qquad \text{with}\, \kappa = \lambda^{-2}\frac{q}{\sqrt{t}},\ q\in\mathbb{R}^d\\
&= \langle 1, \mathrm{e}^{tf(\lambda,\kappa)} P^{\lambda,\kappa} \rho_{\lambda^2\kappa} \rangle (1+O(\mathrm{e}^{-gt})), \qquad \text{as}\, t \nearrow \infty\\
&= \langle 1, \mathrm{e}^{-t(\lambda^4 \frac{1}{2}(\kappa, D_\lambda \kappa)+O(\kappa^3))} P^{\lambda,0} \rho_0 \rangle (1+O(\kappa))(1+O(\mathrm{e}^{-gt})),\\
&\qquad \text{as}\, \kappa \searrow 0\\
&= \langle 1, \mathrm{e}^{-\frac{1}{2}(q,D_\lambda q)+O(t\kappa^3)} P^{\lambda,0} \rho_0 \rangle (1+O(\kappa))(1+O(\mathrm{e}^{-gt})),
\end{aligned}$$

which proves Theorem 3.2 upon using $\langle 1, P^{\lambda,0}\rho_0\rangle = 1$ and $\kappa = \lambda^{-2}\frac{q}{\sqrt{t}}$. □

Remark 3.3 follows by standard reasoning, using the following facts:

1) The family of operators

$$(\mathcal{Z}_t^\lambda)_{\lambda^2\kappa} - \mathrm{e}^{tf(\lambda,\kappa)} P^{\lambda,\kappa} \tag{4.56}$$

is analytic in κ in a neighborhood of $0 \in \mathbb{C}^d$ and bounded by a constant independent of κ and t.

2) The function $f(\lambda,\kappa)$ and the rank 1 operator $P^{\lambda,\kappa}$ are analytic in κ in a neighborhood of $0 \in \mathbb{C}^d$.

This is related to the general fact that the central limit theorem follows from the existence and analyticity of the large deviation generating function, as described in [4]. Indeed, $\kappa \mapsto f(\lambda,\kappa)$ can be viewed as the large deviation generating function corresponding to the family of random variables x_t, $t>0$, as defined in (1.17).

5. Dyson Expansion and Proof of Theorem 4.4

To construct a "polymer model", we first write a Dyson expansion for $\mathcal{Z}_t^\lambda$.

5.1. Dyson expansion. In this section, we set up a convenient notation to handle the Dyson expansion, which has been introduced in Lemma 2.3. Define the unitary group $\mathcal{U}_t$ on $\mathscr{B}_2(\mathscr{H}_{\mathrm{S}})$ by

$$\mathcal{U}_t S := \mathrm{e}^{-\mathrm{i}tH_{\mathrm{S}}} S \mathrm{e}^{\mathrm{i}tH_{\mathrm{S}}}, \qquad S \in \mathscr{B}_2(\mathscr{H}_{\mathrm{S}}), \tag{5.1}$$

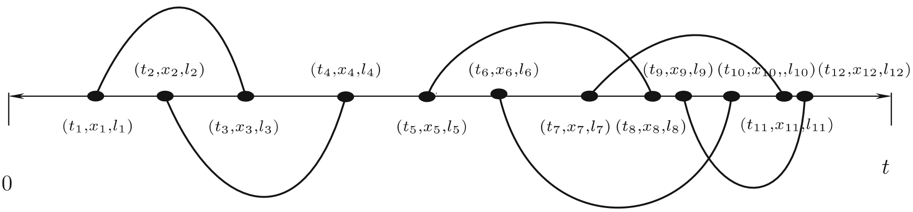

Fig. 5.1. Graphical representation of a term contributing to the RHS of (5.3) with $\pi = \{(1,3),(2,4),(5,8),(6,10),(7,11),(9,12)\} \in \mathcal{P}_6$. The times t_i correspond to the position of the points on the horizontal axis

Starting from this graphical representation, we can reconstruct the corresponding term in (5.3) - an operator on $\mathscr{B}_2(\mathscr{H}_S)$)- as follows:

- To each straight line between the points (t_i, x_i, l_i) and $(t_{i+1}, x_{i+1}, l_{i+1})$, one associates the operators $\mathcal{U}_{t_{i+1}-t_i}$.
- To each point (t_i, x_i, l_i), one associates the operator $\lambda^2 \mathcal{I}_{x_i,l_i}$, defined in (5.2).
- To each curved line between the points (t_r, x_r, l_r) and (t_s, x_s, l_s), with $r < s$, we associate the factor

$$\delta_{x_r,x_s} \begin{cases} \hat{\psi}(t_s - t_r) & l_r = L \\ \hat{\psi}(-(t_s - t_r)) & l_r = R. \end{cases}$$

Rules like these are commonly called “Feynman rules” by physicists.

and the operators $\mathcal{I}_{x,l}$, with $x \in \mathbb{Z}^d$ and $l \in \{L, R\}$ (L, R stand for “*left*” and “*right*”), as

$$\mathcal{I}_{x,l} S := \begin{cases} \mathrm{i}\, 1_x S & \text{if } \; l = L \\ -\mathrm{i}\, S 1_x & \text{if } \; l = R. \end{cases} \tag{5.2}$$

Let $\mathcal{P}_n$ be the set of partitions π of the integers $1, \ldots, 2n$ into n pairs. We write $(r, s) \in \pi$ if (r, s) is one of these pairs, with the convention that $r < s$. Note that the same notation was already used in (1.22) and in (2.16). Elements in $\mathbb{R}^{2n}$, $(\mathbb{Z}^d)^{2n}$, $\{L, R\}^{2n}$ are denoted by $\underline{t}, \underline{x}, \underline{l}$, with t_i, x_i, l_i their respective components, for $i = 1, \ldots, 2n$. We evaluate (2.25) by using (2.15) and (2.16)-(2.17):

$$\mathcal{Z}_t^\lambda = \sum_{n \in \mathbb{Z}^+} \lambda^{2n} \int_{0 \le t_1 \ldots \le t_{2n} \le t} (\prod_{i=1}^{2n} \mathrm{d}t_i) \sum_{\underline{x},\underline{l}} \sum_{\pi \in \mathcal{P}_n} \zeta_\pi(\underline{t}, \underline{x}, \underline{l}) \mathcal{U}_{t-t_{2n}} \mathcal{I}_{x_{2n},l_{2n}} \ldots \mathcal{I}_{x_2,l_2} \mathcal{U}_{t_2-t_1} \mathcal{I}_{x_1,l_1} \mathcal{U}_{t_1}, \tag{5.3}$$

where

$$\zeta_\pi(\underline{t}, \underline{x}, \underline{l}) := \prod_{(r,s)\in\pi} \delta_{x_r,x_s} \begin{cases} \hat{\psi}(t_s - t_r) & l_r = L, \\ \hat{\psi}(-(t_s - t_r)) & l_r = R, \end{cases} \tag{5.4}$$

and, for $n = 0$, the integral in (5.3) is meant to be equal to $\mathcal{U}_t$.

We introduce some more terminology, extending the above definition of pairings. It will be helpful in classifying the pairings.

Definition 5.1. 1) *Let Σ_n be the set of sets of n pairs of (distinct) natural numbers. More concretely, for each $\sigma \in \Sigma_n$, we can write*

$$\sigma = \{(r_1, s_1), \ldots, (r_n, s_n)\}, r_i, s_i \in \mathbb{N}, \tag{5.5}$$

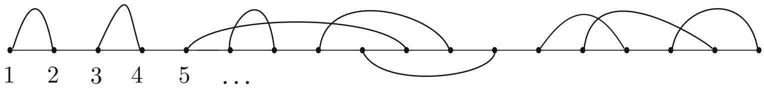

Fig. 5.2. Graphical representation of a pairing $\pi \in \mathcal{P}_9$. The pair (r, s) belongs to π whenever the natural numbers r, s are connected by an arc. This type of diagrams differs from those of Fig. 5.1 in that we don't keep track of the t_i-coordinates, but only of the topological structure of the pairings. Below is the decomposition of π into irreducible components

for natural numbers $r_i, s_i, i = 1, \dots, n$ which are all distinct. By convention, $r_i < s_i, i = 1, \dots, n$ and $r_i < r_{i+1}, i = 1, \dots, n-1$. If $\sigma_1 \in \Sigma_{n_1}$ and $\sigma_2 \in \Sigma_{n_2}$, we write $\sigma_1 < \sigma_2$ whenever all elements of the pairs (r_i^1, s_i^1) in σ_1 are smaller than all elements of the pairs (r_j^2, s_j^2) in σ_2, i.e.,

$$s_i^1 < r_j^2, \qquad i = 1, \dots, n_1, j = 1, \dots, n_2. \tag{5.6}$$

2) *Recall the definition of $\mathcal{P}_n$, the set of pairings with n pairs. Obviously $\mathcal{P}_n \subset \Sigma_n$, and $\sigma \in \Sigma_n$ belongs to $\mathcal{P}_n$ whenever $\cup_{i=1}^n \{r_i, s_i\} = \{1, \dots, 2n\}$. Further, with any $\sigma \in \Sigma_n$, we associate the unique pairing $\pi \in \mathcal{P}_n$ for which there is a monotone increasing function q on $\{1, \dots, 2n\}$ such that*

$$(i, j) \in \pi \Leftrightarrow (q(i), q(j)) \in \sigma. \tag{5.7}$$

3) *We set $\mathcal{P} := \cup_{n \geq 1} \mathcal{P}_n$ and write $|\pi| = n$ whenever $\pi \in \mathcal{P}_n$.*
4) *We call $\sigma \in \Sigma_n$ irreducible (Notation:* irr. *) whenever there are no two sets $\sigma_1 \in \Sigma_{n_1}, \sigma_2 \in \Sigma_{n_2}, n_1 + n_2 = n$ such that $\sigma = \sigma_1 \cup \sigma_2$ and $\sigma_1 < \sigma_2$. For any $\sigma \in \Sigma_n$ that is not irreducible, we can thus find partitioning subsets $\sigma_1, \dots, \sigma_m$ ($\cup_{i=1}^m \sigma_i = \sigma$) such that $\sigma_{i=1,\dots,m}$ are irreducible and $\sigma_i < \sigma_{i+1}$ for $i = 1, \dots, m-1$.*
5) *Consider some $\pi \in \mathcal{P}$ and its partitioning into irreducible subsets $\sigma_1, \dots, \sigma_m$, as defined above. By (5.7), we can associate to each of the σ_i a unique π_i in $\mathcal{P}$. We call the set $(\pi_1, \dots, \pi_m)$ of pairings, obtained in this way the decomposition of π into irreducible components.*
6) *For each $n \in \mathbb{N}$, we define a distinguished pairing $\pi \in \mathcal{P}_n$, which is called the* **minimally irreducible** *pairing (Notation:* min.irr. *). For $n > 2$, this minimally irreducible pairing is given by*

$$(r_1, s_1) = (1, 3), \quad (r_n, s_n) = (2n-2, 2n), \quad (r_{i+1}, s_{i+1}) = (2i, 2i+3), \\ \textit{for} \quad i = 1, \dots, n-2. \tag{5.8}$$

For $n = 1$ and $n = 2$, the minimally irreducible pairing is defined to be $(1, 2)$ and $\{(1, 3), (2, 4)\}$ respectively. Intuitively, the minimally irreducible pairing in $\mathcal{P}_n$ is characterized by the fact that if one removes any pair, other than the pair with $r = 1$ or $s = 2n$, the resulting pairing is no longer irreducible.

For an irreducible pairing $\pi \in \mathcal{P}_n$, we introduce (using the same conventions as in (5.3), (5.4)),

$$\mathcal{V}_t(\pi) := \int_{0=t_1 \leq \dots \leq t_{2n}=t} (\prod_{i=2}^{2n-1} \mathrm{d}t_i) \sum_{\underline{x}, \underline{l}} \zeta_\pi(\underline{t}, \underline{x}, \underline{l}) \mathcal{I}_{x_{2n}, l_{2n}} \mathcal{U}_{t-t_{2n-1}} \dots \mathcal{I}_{x_2, l_2} \mathcal{U}_{t_2 - t_1} \mathcal{I}_{x_1, l_1}. \tag{5.9}$$

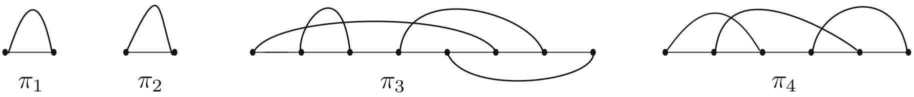

Fig. 5.3. The irreducible components $\pi_1, \pi_2, \pi_3, \pi_4$. Explicitly, $\pi_1 = \pi_2 = \{(1,2)\}$, $\pi_3 = \{(1,6),(2,3),(4,7),(5,8)\}$ and $\pi_4 = \{(1,3),(2,5),(4,6)\}$. The pairings π_1, π_2 and π_4 are minimally irreducible, whereas π_3 is not. Indeed, one can remove the pair $(4,7)$ from π_3 without destroying the irreducibility

We can now rewrite (5.3) as a sum over collections of irreducible pairings;

$$\mathcal{Z}_t^\lambda = \sum_{m \in \mathbb{Z}^+} \int_{0 \le t_1 \ldots \le t_{2m} \le t} \mathrm{d}t_1 \ldots \mathrm{d}t_{2m}$$

$$\sum_{\substack{\pi_1,\ldots,\pi_m \in \mathcal{P} \\ \pi_1,\ldots,\pi_m \text{ irr.}}} \lambda^{(2\sum_{i=1}^m |\pi_i|)} \mathcal{U}_{t-t_{2m}} \mathcal{V}_{t_{2m}-t_{2m-1}}(\pi_m) \ldots \mathcal{U}_{t_3-t_2} \mathcal{V}_{t_2-t_1}(\pi_1) \mathcal{U}_{t_1}. \tag{5.10}$$

To obtain this last expression, we decompose each pairing π in (5.3) into its irreducible components $\pi_1, \ldots, \pi_m$, and we made use of a simple factorization property of (5.3). The term on the RHS of (5.10) corresponding to $m = 0$ is understood to be equal to $\mathcal{U}_t$.

In expression (5.10), we view the pairings π_i with $|\pi_i| \ge 2$ as excitations. If $|\pi_i| = 1$, for all $i = 1, \ldots, m$, the corresponding term in (5.10) is called a *ladder* diagram. These ladder diagrams provide the leading contribution to the dynamics, and they are the only terms that survive in the kinetic limit. We define separately the Laplace transforms of the irreducible "excitation" diagrams ($\mathcal{R}_\lambda^{\text{ex}}$) and the irreducible "ladder" diagram ($\mathcal{L}$):

$$\mathcal{R}_\lambda^{\text{ex}}(z) := \int_{\mathbb{R}^+} \mathrm{d}t\, \mathrm{e}^{-tz} \sum_{\substack{|\pi| \ge 2 \\ \pi \text{ irr.}}} \lambda^{2|\pi|} \mathcal{V}_t(\pi), \tag{5.11}$$

$$\mathcal{L}(z) := \int_{\mathbb{R}^+} \mathrm{d}t\, \mathrm{e}^{-tz} \sum_{|\pi|=1} \mathcal{V}_t(\pi) = \int_{\mathbb{R}^+} \mathrm{d}t\, \mathrm{e}^{-tz} \mathcal{V}_t(\{(1,2)\}). \tag{5.12}$$

Here and in what follows, we omit the specification $\pi \in \mathcal{P}$ under the summation symbol. We observe that, in (5.12), the only element of $\mathcal{P}_1$ is the set containing the single pair $(1,2)$. The operators $\mathcal{R}_\lambda^{\text{ex}}(z)$ and $\mathcal{L}(z)$ have already appeared in Theorem 4.4. We will prove Theorem 4.4 in Sect. 5.3. First, we establish some helpful estimates.

5.2. Estimates on the Dyson expansion.

5.2.1. A priori estimates. The following Lemma 5.1 is a useful a-priori estimate. Its main assertion, Statement 2), i.e., Eq. (5.14), gives a bound on $\mathcal{V}_t(\pi)$, the contribution of the irreducible pairing π to the dynamics, in terms of the temporal coordinates $\underline{t}$. In particular, the sum over the other coordinates, $\underline{x}$ and $\underline{l}$ is already performed. This is possible because the matrix elements of the free dynamics $(\mathrm{e}^{-\mathrm{i}tH_{\mathrm{S}}})(0,x)$ decay exponentially in space, for fixed t; (see Statement 1 of Lemma 5.1, or Eq. (5.17)). Equation (5.18) tells us that one can sum over x at the cost of introducing an exponential growth in time. This exponential growth in time is also visible in (5.14), in the factor $\mathrm{e}^{2tc_\varepsilon(\gamma_1)}$. However, this exponential growth is harmless, because the reservoir correlation functions $\hat{\psi}$ on the

RHS of (5.14) are exponentially decaying in time, by Assumption 2.2, and the growth constant $c_\varepsilon(\gamma_1)$ can be chosen arbitrarily small. In particular, it can be chosen smaller than the reservoir decay rate g_{R}, and this fact will be exploited in Sect. 5.3.2.

Lemma 5.1. *Suppose that Assumption 2.1 holds (with some $\delta_\varepsilon > 0$) and define*

$$c_\varepsilon(\delta) := \sup_{k\in\mathbb{T}^d} \sup_{|\Im\kappa|\le\delta} |\Im\varepsilon(k+\kappa)|, \; (c_\varepsilon(\delta) < \infty, \quad \text{for} \quad 0<\delta<\delta_\varepsilon),$$
$$b_d(\delta) := \sum_{x\in\mathbb{Z}^d} \mathrm{e}^{-\delta|x|}, \qquad (b_d(\delta) < \infty, \quad \text{for} \quad 0<\delta).$$

Then the following statements hold true:

1) *For any $\kappa \in \mathbb{C}^d$ with $|\Im\kappa| \le \gamma_1$, for some $\gamma_1 < \delta_\varepsilon$,*

$$\|\mathrm{e}^{\mathrm{i}(\kappa,X)}\mathrm{e}^{-\mathrm{i}t\varepsilon(P)}\mathrm{e}^{-\mathrm{i}(\kappa,X)}\| \le \mathrm{e}^{tc_\varepsilon(\gamma_1)}, \qquad t\ge 0. \tag{5.13}$$

2) *Let $\pi \in \mathcal{P}_n$, and choose constants $0<\gamma<\gamma_1<\delta_\varepsilon$. For any $\kappa\in\mathbb{C}^d$ satisfying $|\Im\kappa| \le \gamma_1-\gamma$,*

$$\|\mathcal{J}_\kappa\, \mathcal{V}_t(\pi)\, \mathcal{J}_{-\kappa}\| \le \begin{cases} b_d(2\gamma)\,[b_d(\gamma_1-\gamma-|\Im\kappa|)]^{2n}\, 2^{2n}\,\mathrm{e}^{2tc_\varepsilon(\gamma_1)} \\ \times \displaystyle\int_{0=t_1\le\ldots\le t_{2n}=t} \left(\prod_{i=2}^{2n-1} \mathrm{d}t_i\right) \prod_{(r,s)\in\pi} |\psi(t_s-t_r)|. \end{cases} \tag{5.14}$$

We recall that $\|\cdot\|$ in (5.14) refers to the operator norm on $\mathscr{B}(\mathscr{B}_2(\mathscr{H}_{\mathrm{S}}))$.

Proof. Statement 1). Recall that $H_{\mathrm{S}} = \varepsilon(P)$. By analytic continuation from $\Im\kappa = 0$ to $|\Im\kappa| \le \delta_\varepsilon$, one has that

$$\mathrm{e}^{\mathrm{i}(\kappa,X)}\mathrm{e}^{-\mathrm{i}t\varepsilon(P)}\mathrm{e}^{-\mathrm{i}(\kappa,X)} = \mathrm{e}^{-\mathrm{i}t\varepsilon(P-\kappa)}. \tag{5.15}$$

Since, for $|\Im\kappa| \le \gamma_1$,

$$\|\mathrm{e}^{-\mathrm{i}t\varepsilon(P-\kappa)}\| \le \mathrm{e}^{t\|\Im\varepsilon(P-\kappa)\|} \le \mathrm{e}^{tc_\varepsilon(\gamma_1)}, \qquad t\ge 0, \tag{5.16}$$

the claim (5.13) is proven. We observe that (5.13) implies

$$|(\mathrm{e}^{-\mathrm{i}tH_{\mathrm{S}}})(x,x')| \le \mathrm{e}^{tc_\varepsilon(\gamma_1)}\mathrm{e}^{-\gamma_1|x'-x|}, \qquad \text{for any } 0<\gamma_1<\delta_\varepsilon, \qquad t\ge 0, \tag{5.17}$$

and hence

$$\sum_{x'\in\mathbb{Z}^d} \mathrm{e}^{\gamma|x'-x|}|(\mathrm{e}^{-\mathrm{i}tH_{\mathrm{S}}})(x,x')| \le \mathrm{e}^{tc_\varepsilon(\gamma_1)} b_d(\gamma_1-\gamma), \quad \text{for any } 0<\gamma<\gamma_1<\delta_\varepsilon,$$
$$t\ge 0. \tag{5.18}$$

Statement 2). To estimate the integrand in (5.9), we choose $0<\gamma'<\gamma_1<\delta_\varepsilon$ and find that

$$\sum_{y',z'} \left| \mathrm{e}^{\gamma'(|y'-y|+|z'-z|)} \left(\sum_{\underline{x},\underline{l}} \zeta_\pi(\underline{t},\underline{x},\underline{l}) \mathcal{I}_{x_{2n},l_{2n}} \ldots \mathcal{I}_{x_2,l_2} \mathcal{U}_{t_2-t_1} \mathcal{I}_{x_1,l_1} \right)(y,z;y',z') \right|$$
$$\le (\sup_{\underline{x},\underline{l}} |\zeta_\pi(\underline{t},\underline{x},\underline{l})|) \sum_{\underline{l}} \mathrm{e}^{2tc_\varepsilon(\gamma_1)} (b_d(\gamma_1-\gamma'))^{2n}, \tag{5.19}$$

where we can replace "$\sum_{\underline{l}}$" by 2^{2n}, the number of terms in the sum. The bound (5.19) is obtained by applying (5.18) $2n$ times.

For clarity, we illustrate this with an example: Take $n = 4$ and $(l_1, l_2, l_3, l_4, l_5, l_6, l_7, l_8) = (L, R, L, L, R, L, R, R)$. First, we notice that

$$\left|\left(\mathcal{I}_{x_8,l_8}\ldots\mathcal{I}_{x_2,l_2}\mathcal{U}_{t_2-t_1}\mathcal{I}_{x_1,l_1}\right)(y,z;y',z')\right| \tag{5.20}$$

vanishes unless $x_1 = y$ and $x_8 = z'$, and that it is bounded by

$$\begin{cases} w(t_3-t_1, x_3-x_1)\times w(t_4-t_3, x_4-x_3)\times w(t_6-t_4, x_6-x_4)\times w(t-t_6, y'-x_6) \\ \times\, w(t_2-0, x_2-z)\times w(t_5-t_2, x_5-x_2)\times w(t_7-t_5, x_7-x_5)\times w(t_8-t_7, x_8-x_7), \end{cases} \tag{5.21}$$

where $w(u,x) := |(\mathrm{e}^{-\mathrm{i}uH_S})(0,x)|$, $t_1 = 0$, $t_8 = t$.

We use the decomposition (recall that $x_1 = y$ and $x_8 = z$)

$$|y'-y| \le |x_3-x_1| + |x_4-x_3| + |x_6-x_4| + |y'-x_6|,$$
$$|z'-z| \le |x_2-z| + |x_5-x_2| + |x_7-x_5| + |x_8-x_7|,$$

and (5.21) to factorize the sum over $y', z', \underline{x}$ on the LHS of (5.19). Those sums can then be carried out with the help of (5.18), yielding the bound

$$(b_d(\gamma_1-\gamma'))^8 \begin{Bmatrix} \exp\left(c_\varepsilon(\gamma_1)\left[(t_8-t_6)+(t_6-t_4)+(t_4-t_3)+(t_3-t_1)\right]\right) \\ \times\exp\left(c_\varepsilon(\gamma_1)\left[(t_8-t_7)+(t_7-t_5)+(t_5-t_2)+(t_2-0)\right]\right) \end{Bmatrix}$$
$$= (b_d(\gamma_1-\gamma'))^8\, \mathrm{e}^{2tc_\varepsilon(\gamma_1)}. \tag{5.22}$$

Note that this bound only depends on $|\pi|$ and t, and not on $\underline{t}$, $\underline{l}$, or π. Hence it can be applied for all $\underline{l}$, which yields the factor 2^{2n} in (5.19).

For a linear operator $\mathcal{W}$ on $l^2(\mathbb{Z}^d \times \mathbb{Z}^d)$, a straightforward application of the Cauchy-Schwarz inequality yields

$$\|\mathcal{W}\| \le b_d(2\delta)\left(\sup_{y,z\in\mathbb{Z}^d}\sum_{y',z'\in\mathbb{Z}^d}|\mathcal{W}(y,z;y',z')|\mathrm{e}^{\delta(|y'-y|+|z'-z|)}\right). \tag{5.23}$$

Starting from the explicit definition of $\mathcal{J}_\kappa\, \mathcal{V}_t(\pi)\, \mathcal{J}_{-\kappa}$ (as in (3.2) and (5.9)) , one uses (5.23) and (5.19) with $\gamma' := \gamma + |\Im\kappa|$. This yields Statement 2). □

5.2.2. A combinatorial estimate. In the next step of our analysis of the Dyson series, we show that one can perform the integration over all pairings π and temporal coordinates $\underline{t}$ contributing to (5.11). The following lemma is purely combinatorial, i.e., it only employs notions introduced in Definition 5.1.

Lemma 5.2. *Consider a positive function h on $\mathbb{R}^+$ and a pairing $\pi \in \mathcal{P}$. We define*

$$\chi_t(\pi) := \int_{0=t_1\le\ldots\le t_{2n}=t} \Big(\prod_{i=2}^{2n-1}\mathrm{d}t_i\Big)\prod_{(r,s)\in\pi} h(t_s-t_r), \qquad \textit{with } n = |\pi|. \tag{5.24}$$

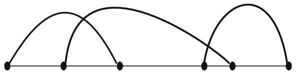

Fig. 5.4. This figure illustrates the change of variables from $(\pi, \underline{t})$, with $\pi \in \mathcal{P}_3$ and $t_1 < \ldots < t_6$, to $(u_i, v_i)_{i=1,2,3}$, with $u_i \leq v_i$ and $u_i \leq u_{i+1}$

Then

$$\sum_{\pi \text{ irr.}} \chi_t(\pi) \leq \left(\sum_{\pi \text{ min. irr.}} \chi_t(\pi) \right) \times \exp\left(t \int_{\mathbb{R}^+} \mathrm{d}w h(w) \right), \tag{5.25}$$

and, if π *is the minimally irreducible pairing in* $\mathcal{P}_n$ *and* $z \in \mathbb{R}$,

$$\int_{\mathbb{R}^+} \mathrm{d}t\, \mathrm{e}^{-tz} \chi_t(\pi) \leq \left(\int_{\mathbb{R}^+} \mathrm{d}w h(w) \mathrm{e}^{-wz} \right) \times \left(\int_{\mathbb{R}^+} \mathrm{d}y \int_{\mathbb{R}^+} \mathrm{d}w\, h(y+w) \mathrm{e}^{-wz} \right)^{n-1}. \tag{5.26}$$

Proof. Given $\pi \in \mathcal{P}_n$, we can relabel the times $t_1, \ldots, t_{2n}$ by setting

$$u_i = t_{r_i}, \qquad v_i = t_{s_i} \qquad \text{for} \quad i = 1, \ldots, n. \tag{5.27}$$

Using our conventions for the labels of the pairs (r_i, s_i), it follows that

$$0 \leq u_i \leq v_i \leq t, \qquad 0 \leq u_i \leq u_{i+1} \leq t, \qquad 0 = u_1, t = \max\{v_i\}. \tag{5.28}$$

Conversely, a set of n pairs of times (u_i, v_i), $i = 1, \ldots, n$, satisfying (5.28) uniquely determines a pairing $\pi \in \mathcal{P}_n$ and corresponding times $0 = t_1 \leq \ldots \leq t_{2n} = t$.

Consider an irreducible pairing $\pi' \in \mathcal{P}_{n'}$. It is easy to see that we can always find a subset $j_1, \ldots, j_n$ of $\{1, \ldots, n'\}$, for some $n \leq n'$, such that

1) the pairs (r_{j_i}, s_{j_i}), $i = 1, \ldots, n$ determine a minimally irreducible pairing $\pi \in \mathcal{P}_n$;
2) these pairs contain the boundary points, i.e. $r_{j_1} = 1$ and $\max_i\{s_{j_i}\} = 2n'$.

We write $\pi' \to \pi$ whenever π and π' are related in this way; (note, however, that π is not uniquely determined). It follows that

$$\sum_{\substack{|\pi'| = n' \\ \pi' \text{ irr.}}} \chi_t(\pi') \leq \sum_{\substack{|\pi| \leq n' \\ \pi \text{ min.irr.}}} \sum_{\substack{|\pi'| = n' \\ \pi' \to \pi}} \chi_t(\pi'). \tag{5.29}$$

For $n' \geq 2$, the inequality is strict, since π is not necessarily uniquely determined by π', and hence the same irreducible π' can appear more than once on the RHS of (5.29).

Using the change of variables (5.27), one can convince oneself that, for all $m := n' - n \geq 0$,

$$\sum_{\substack{|\pi'| = n' \\ \pi' \to \pi}} \chi_t(\pi') = \chi_t(\pi) \int_{\substack{0 \leq u_1 \leq \ldots \leq u_m \leq t \\ 0 \leq u_i \leq v_i \leq t}} \mathrm{d}\underline{u}\mathrm{d}\underline{v} \prod_{i=1}^m h(v_i - u_i), \tag{5.30}$$

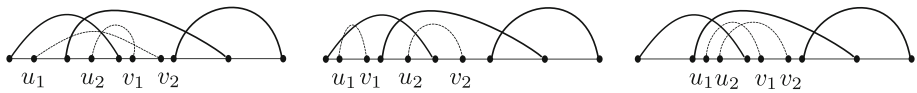

Fig. 5.5. Illustration of (5.30). Three pairings in $\mathcal{P}_5$ contributing to the LHS of (5.30). We have chosen π to be the minimally irreducible pairing (1, 3), (2, 5), (4, 6) in $\mathcal{P}_3$, as in Fig. 5.4. For each of these 3 pairings in $\mathcal{P}_5$, the five pairs $(u_i, v_i)_{i=1,...,5}$ contain a subset of three pairs identified with π. We have only shown the two other pairs, relabeling them as $(u_i, v_i)_{i=1,2}$. The same strategy is used to prove (5.30) in general

where π is the minimally irreducible pairing in $\mathcal{P}_n$, and where we have abbreviated $\mathrm{d}\underline{u} := \mathrm{d}u_1 \dots \mathrm{d}u_n$ and $\mathrm{d}\underline{v} := \mathrm{d}v_1 \dots \mathrm{d}v_n$. The relation (5.30) expresses the fact that one can add any set of pairs, corresponding to times $\underline{u}$, $\underline{v}$ satisfying the first two conditions of (5.28), to a minimally irreducible π, thus obtaining a new irreducible pairing (see also Fig. 5.5).

By explicit computation,

$$\sum_{m\in\mathbb{Z}^+} \int\limits_{\substack{0 \le u_1 \le \dots \le u_m \le t \\ 0 \le u_i \le v_i \le t}} \mathrm{d}\underline{u}\mathrm{d}\underline{v} \prod_{i=1}^{m} h(v_i - u_i) \le \sum_{m\in\mathbb{Z}^+} \int\limits_{0\le u_1 \le \dots \le u_m \le t} \mathrm{d}\underline{u} \left(\int\limits_{\mathbb{R}^+} \mathrm{d}w h(w) \right)^m$$
$$\le \exp\left(t \int\limits_{\mathbb{R}^+} \mathrm{d}w h(w) \right), \tag{5.31}$$

which proves the bound (5.25) starting from (5.29) and (5.30).

When we perform the change of variables (5.27) for a minimally irreducible pairing π, the variables $\underline{u}$, $\underline{v}$ satisfy the constraint $u_{i+1} \le v_i \le u_{i+2}$ in addition to the constraints $0 \le u_i \le u_{i+1} \le t$ and $0 \le u_i \le v_i \le t$. Let π be the minimally irreducible pairing in $\mathcal{P}_n$. Then ($u_1 = 0$ is a dummy variable)

$$\int\limits_{\mathbb{R}^+} \mathrm{d}t \mathrm{e}^{-tz} \chi_t(\pi) = \int\limits_0^\infty \mathrm{d}v_1 h(v_1 - u_1) \mathrm{e}^{-z(v_1-u_1)} \int\limits_0^{v_1} \mathrm{d}u_2 \int\limits_{v_1}^\infty \mathrm{d}v_2 \dots$$
$$\dots \int\limits_{v_{n-5}}^{v_{n-4}} \mathrm{d}u_{n-2} \int\limits_{v_{n-3}}^\infty \mathrm{d}v_{n-2} \dots \int\limits_{v_{n-3}}^{v_{n-2}} \mathrm{d}u_{n-1} \int\limits_{v_{n-2}}^\infty \mathrm{d}v_{n-1} \mathrm{e}^{-z(v_{n-1}-v_{n-2})} h(v_{n-1} - u_{n-1})$$
$$\int\limits_{v_{n-2}}^{v_{n-1}} \mathrm{d}u_n \int\limits_{v_{n-1}}^\infty \mathrm{d}v_n \mathrm{e}^{-z(v_n - v_{n-1})} h(v_n - u_n). \tag{5.32}$$

Performing the change of variables $w_i = v_i - v_{i-1}$ and $y_i = v_{i-1} - u_i$ (for $i > 1$) and extending the range of integration of y_i to $\mathbb{R}$, the above expression factorizes and one obtains the bound (5.26). □

5.3. Proof of Theorem 4.4. In this section, we prove Theorem 4.4. Statement 2) is proven separately for $\mathcal{L}(z)$ and $\mathcal{R}_\lambda^{\mathrm{ex}}(z)$ in Sects. 5.3.1 and 5.3.2, respectively. Statement 3) is proven in Sect. 5.3.1 and Statement 1) in Sect. 5.3.3.

It is mainly in Sect. 5.3.2 that we use the preparatory work summarized in Lemma 5.1 and Lemma 5.2, in order to obtain a bound on $\mathcal{R}^{\mathrm{ex}}_{\lambda}(z)$.

5.3.1. Properties of $\mathcal{L}(z)$. We compute $\mathcal{L}(z)$ starting from (5.9) and (5.12):

$$\mathcal{L}(z) = \int_{\mathbb{R}^+} \mathrm{d}t\, \mathrm{e}^{-tz} \sum_{x\in\mathbb{Z}^d} \sum_{l,l'\in\{L,R\}} \mathcal{I}_{l',x}\mathcal{U}_t\mathcal{I}_{l,x} \begin{cases} \hat{\psi}(t) & l = L \\ \hat{\psi}(-t) & l = R \end{cases}. \tag{5.33}$$

To display the result, we introduce the functions ψ_+, ψ_- as

$$\psi_+(z) = \int_{\mathbb{R}^+} \mathrm{d}t \hat{\psi}(t)\mathrm{e}^{\mathrm{i}tz}, \qquad \psi_-(z) = \int_{\mathbb{R}^-} \mathrm{d}t \hat{\psi}(t)\mathrm{e}^{\mathrm{i}tz}, \qquad z \in \mathbb{C}, \tag{5.34}$$

with $\hat{\psi}$ as defined in Sect. 2.3.2; (we recall that $\hat{\psi}(u)$ decays exponentially). Since $\hat{\psi}(-u) = \overline{\hat{\psi}(u)}$ (as follows from (2.18)), one has that

$$\psi_+(z) = \overline{\psi_-(\bar{z})}, \qquad \psi(z) = \psi_+(z) + \psi_-(z), \qquad \text{with } |\Im z| < g_{\mathrm{R}}. \tag{5.35}$$

Using (5.33), we calculate $\mathcal{L}(z)S$, for $S \in L^2(\mathbb{T}^d \times \mathbb{T}^d)$,

$$\begin{aligned} (\mathcal{L}(z)S)(k+\frac{p}{2}, k-\frac{p}{2}) \\ = \int_{\mathbb{T}^d} \mathrm{d}k' \, \Big(\psi_+\Big[\varepsilon\Big(k'-\frac{p}{2}\Big) - \varepsilon\Big(k+\frac{p}{2}\Big) + \mathrm{i}z\Big] + \psi_-\Big[\varepsilon\Big(k'+\frac{p}{2}\Big) - \varepsilon\Big(k-\frac{p}{2}\Big) - \mathrm{i}z\Big]\Big) \\ \times S\Big(k'+\frac{p}{2}, k'-\frac{p}{2}\Big) \\ - \int_{\mathbb{T}^d} \mathrm{d}k' \, \Big(\psi_+\Big[\varepsilon\Big(k-\frac{p}{2}\Big) - \varepsilon\Big(k'+\frac{p}{2}\Big) + \mathrm{i}z)\Big] + \psi_-\Big[\varepsilon\Big(k+\frac{p}{2}\Big) - \varepsilon(k'-\frac{p}{2}) - \mathrm{i}z\Big]\Big) \\ \times S\Big(k+\frac{p}{2}, k-\frac{p}{2}\Big). \end{aligned} \tag{5.36}$$

The claim about $\mathcal{L}(z)$ in Statement 2) of Theorem 4.4 follows by noticing that the above expression can be analytically continued in z and p. This follows from the analyticity of ε (Assumption 2.1) and ψ_+, ψ_- (consequences of Assumption 2.2).

To prove Statement 3), we first check that $(\mathcal{L}(0))_0 = M^0$ by setting $p = 0$ and $z = 0$ in (5.36), and using (5.35). It remains to verify that

$$\lambda^2(M^\kappa - M^0) = \mathrm{i}\lambda^2(\kappa, \nabla\varepsilon) = (\mathrm{ad}(\mathrm{i}H_{\mathrm{S}}))_{\lambda^2\kappa} + O((\lambda^2\kappa)^2) \tag{5.37}$$

as operators on $L^2(\mathbb{T}^d)$, where $(\kappa, \nabla\varepsilon)$ is the multiplication operator given by the function $k \mapsto (\kappa, \nabla\varepsilon)(k)$. Equation (5.37) follows by writing explicitly

$$((\mathrm{ad}(\mathrm{i}H_{\mathrm{S}}))_p\theta)(k) = \mathrm{i}\left(\varepsilon(k+\frac{p}{2}) - \varepsilon(k-\frac{p}{2})\right)\theta(k), \qquad \theta \in L^2(\mathbb{T}^d, \mathrm{d}k), \tag{5.38}$$

expanding in powers of p and putting $p = \lambda^2\kappa$.

5.3.2. Properties of $\mathcal{R}_\lambda^{\mathrm{ex}}(z)$. Choose positive constants $\gamma_1 > \gamma > 0$, as in Lemma 5.1, and define the quantity $\chi_t(\pi)$ as in Lemma 5.2, with h given by

$$h(t) := 2^2 b_d (\gamma_1 - \gamma - |\Im\kappa|)^2 \lambda^2 |\hat{\psi}(t)|. \tag{5.39}$$

It follows from Statement 2) of Lemma 5.1 and Eqs. (5.9), (5.11) that

$$\|\mathcal{J}_\kappa \mathcal{R}_\lambda^{\mathrm{ex}}(z) \mathcal{J}_{-\kappa}\| \leq b_d(2\gamma) \int_{\mathbb{R}^+} \mathrm{d}t\, \mathrm{e}^{2c_\varepsilon(\gamma_1)t} \mathrm{e}^{-\Re z t} \left(\sum_{\substack{|\pi|>1 \\ \pi \text{ irr.}}} \chi_t(\pi) \right), \tag{5.40}$$

and hence, using Lemma 5.2, that

$$\begin{aligned}
\|\mathcal{J}_\kappa \mathcal{R}_\lambda^{\mathrm{ex}}(z) \mathcal{J}_{-\kappa}\| &\leq b_d(2\gamma) \int_{\mathbb{R}^+} \mathrm{d}t \mathrm{e}^{-(\Re z - a)t} \sum_{\pi \text{ min. irr.}} \chi_t(\pi), \qquad \text{with} \quad a := 2c_\varepsilon(\gamma_1) \\
&\quad + \int_{\mathbb{R}^+} \mathrm{d}w\, h(w) \\
&\leq b_d(2\gamma) \left(\int_{\mathbb{R}^+} \mathrm{d}w\, h(w) \mathrm{e}^{-w(\Re z - a)} \right) \\
&\quad \times F\left(\int_{\mathbb{R}^+} \mathrm{d}y \int_{\mathbb{R}^+} \mathrm{d}w\, h(y+w) \mathrm{e}^{-w(\Re z - a)} \right),
\end{aligned}$$

where $F(x) := \frac{x}{1-x}$, provided that $|x| < 1$. To prove the first inequality above, we use (5.40) and (5.25), and, for the second inequality, we use (5.26) and sum the geometric series.

Statement 2) of Theorem 4.4 now follows by fixing the constants and using the exponential decay of $\hat{\psi}$. For example, choose γ_1, γ such that

$$2c_\varepsilon(\gamma_1) \leq \frac{1}{4} g_{\mathrm{R}}, \qquad \gamma := \frac{1}{2}\gamma_1, \tag{5.41}$$

and δ_2' small enough such that for $|\lambda| \leq \delta_2'$,

$$\int_{\mathbb{R}^+} \mathrm{d}w\, h(w) \leq \frac{1}{4} g_{\mathrm{R}}, \qquad \int_{\mathbb{R}^+} \mathrm{d}y \int_{\mathbb{R}^+} \mathrm{d}w\, h(y+w) \mathrm{e}^{-w(-\frac{1}{4}g_{\mathrm{R}} - a)} \leq 1. \tag{5.42}$$

Then (4.47) is satisfied with $\delta_1' := \frac{1}{4}\gamma_1$, $g' := \frac{1}{4} g_{\mathrm{R}}$ and δ_2' as determined above.

5.3.3. Proof of Equation (4.44) *in Statement 1) of Theorem 4.4*. To simplify the following calculations, we abbreviate

$$\mathcal{R}_\lambda^{\mathrm{irr}}(z) := \mathcal{R}_\lambda^{\mathrm{ex}}(z) + \lambda^2 \mathcal{L}(z), \qquad \mathcal{R}_{\mathrm{S}}(z) := (z - \mathrm{ad}(\mathrm{i}H_{\mathrm{S}}))^{-1}. \tag{5.43}$$

By the self-adjointness of $\mathrm{ad}(H_{\mathrm{S}})$, one has that $\|\mathcal{R}_{\mathrm{S}}(z)\| < |\Re z|^{-1}$. We choose λ and z such that $\Re z > 0$ and $\|\mathcal{R}_\lambda^{\mathrm{irr}}(z)\mathcal{R}_{\mathrm{S}}(z)\| \leq |\Re z|^{-1} \|\mathcal{R}_\lambda^{\mathrm{irr}}(z)\| < 1$. Then

$$\begin{aligned} \mathcal{R}_\lambda(z) &:= \int_{\mathbb{R}^+} \mathrm{d}t\, \mathrm{e}^{-tz} \mathcal{Z}_t^\lambda \\ &= \sum_{n \in \mathbb{Z}^+} \mathcal{R}_{\mathrm{S}}(z) \left(\mathcal{R}_\lambda^{\mathrm{irr}}(z)\mathcal{R}_{\mathrm{S}}(z)\right)^n \\ &= \mathcal{R}_{\mathrm{S}}(z) \left(1 - \mathcal{R}_\lambda^{\mathrm{irr}}(z)\mathcal{R}_{\mathrm{S}}(z)\right)^{-1} \\ &= \left(z - \mathrm{ad}(\mathrm{i}H_{\mathrm{S}}) - \mathcal{R}_\lambda^{\mathrm{irr}}(z)\right)^{-1} \\ &= \left(z - \mathrm{ad}(\mathrm{i}H_{\mathrm{S}}) - \lambda^2\mathcal{L}(z) - \mathcal{R}_\lambda^{\mathrm{ex}}(z)\right)^{-1}, \end{aligned} \tag{5.44}$$

where the second equality follows by Laplace transforming (5.10), and the third equality represents the sum of a geometric series. Hence, Statement 1) of Theorem 4.4 is proven.

6. Proof of Theorem 4.5

In this section we prove Theorem 4.5. Our reasoning is based on a standard application of analytic perturbation theory and the inverse Laplace transform.

We abbreviate

$$A(z, \lambda, \kappa) := \left(\mathrm{ad}(\mathrm{i}H_{\mathrm{S}}) + \lambda^2\mathcal{L}(z) + \mathcal{R}^{\mathrm{ex}}(z)\right)_{\lambda^2\kappa} - \lambda^2 M^\kappa \tag{6.1}$$

and we define

$$\mathbf{G} := \left\{ (z, \lambda, \kappa) \in \mathbb{C} \times \mathbb{R} \times \mathbb{C}^d \,\middle|\, \Re z > -g', |\kappa| < \delta_{\mathrm{kin}}, |\lambda| < \min\left(\delta_2', \sqrt{\frac{\delta_1'}{\delta_{\mathrm{kin}}}}\right) \right\}, \tag{6.2}$$

where g', δ_1', δ_2' are as described in Theorem 4.4 and δ_{kin} is as described in Theorem 4.3. Theorem 4.4 implies that, on the domain $\mathbf{G}$, the function $\lambda^2 M^\kappa + A(z, \lambda, \kappa)$ is analytic in the variables (z, κ) and, for $\Re z$ large enough,

$$(\mathcal{R}_\lambda(z))_{\lambda^2\kappa} = (z - \lambda^2 M^\kappa - A(z, \lambda, \kappa))^{-1}. \tag{6.3}$$

We may extend the (operator-valued) function $z \mapsto (\mathcal{R}_\lambda(z))_{\lambda^2\kappa}$ into the region $\Re z > -g'$. This will be useful, because, at the end of this section, we calculate the reduced evolution $(\mathcal{Z}_t^\lambda)_{\lambda^2\kappa}$ from the inverse Laplace transform of $(\mathcal{R}_\lambda(z))_{\lambda^2\kappa}$. From (6.3) we see that any singular point of the function $z \mapsto (\mathcal{R}_\lambda(z))_{\lambda^2\kappa}$ must satisfy

$$z \in \mathrm{sp}(\lambda^2 M^\kappa + A(z, \lambda, \kappa)). \tag{6.4}$$

Recall that by Theorem 4.3, M^{κ} has a simple isolated eigenvalue $f_{\text{kin}}(\kappa)$, and let $\Omega \subset \mathbb{C}$ be as defined in (4.30), i.e.,

$$\Omega := \bigcup_{|\kappa|<\delta_{\text{kin}}} \left(\text{sp} M^{\kappa} \setminus \{f_{\text{kin}}(\kappa)\}\right). \tag{6.5}$$

The following two lemmas describe the singularities of $(\mathcal{Z}_t^{\lambda})_{\lambda^2\kappa}$.

Lemma 6.1. *There is a constant c_1 and a function $c(\lambda)$ with $c(\lambda) \searrow 0$, as $\lambda \searrow 0$, such that, for any z satisfying (6.4), one of the following two statements holds:*

$$\text{dist}(z, \lambda^2\Omega) \leq \lambda^2 c(\lambda), \qquad \text{or} \qquad \text{dist}(z, \lambda^2 f_{\text{kin}}(\kappa)) \leq c_1\lambda^4. \tag{6.6}$$

Proof. From Theorem 4.4, we infer that

$$\|A(z,\lambda,\kappa)\| = \lambda^2 \|(\mathcal{L}(z)-\mathcal{L}(0))_{\lambda^2\kappa}\| + O(\lambda^4) + O((\lambda^2\kappa)^2) \qquad \text{as } \lambda \searrow 0, \lambda^2\kappa \searrow 0, \tag{6.7}$$

with $(\mathcal{L}(z)-\mathcal{L}(0))_{\lambda^2\kappa}$ bounded and analytic in (z,κ) on $\mathbf{G}$. Since M^{κ} is bounded, there is a constant $r(m) > 0$, for all $m > 0$, such that

$$\sup_{z\in\mathbb{C},\, \text{dist}(z,\text{sp}M^{\kappa})\geq r(m)} \|(z - M^{\kappa})^{-1}\| \leq m. \tag{6.8}$$

Choose $m^{-1} := \sup_{(z,\lambda,\kappa)\in\mathbf{G}} \lambda^{-2}\|A(z,\lambda,\kappa)\|$ (by (6.7), $m^{-1} = O(\lambda^0)$). Using the Neumann series for $(z-\lambda^2 M^{\kappa} - A(z,\lambda,\kappa))^{-1}$, it follows that, if $\text{dist}(z, \lambda^2\text{sp}M^{\kappa}) \geq \lambda^2 r(m)$, then z cannot satisfy (6.4).

If, however, $\text{dist}(z, \lambda^2\text{sp}M^{\kappa}) \leq \lambda^2 r(m)$, then $\|A(z,\lambda,\kappa)\| = O(\lambda^4)$, as $\lambda \searrow 0$; (this follows from (6.7) and the analyticity of $\mathcal{L}(z)$). The claim now follows from analytic perturbation theory, using that $\lambda^2 f_{\text{kin}}(\kappa)$ is an isolated simple eigenvalue. □

Lemma 6.2. *For sufficiently small $|\lambda|$, there is a unique $z =: \tilde{z}$ at a distance $O(\lambda^4)$ from $\lambda^2 f_{\text{kin}}(\kappa)$ satisfying (6.4). Let $P^{\lambda,\kappa}$ be the residue of $(z - \lambda^2 M^{\kappa} - A(z,\lambda,\kappa))^{-1}$ at $z = \tilde{z}$. It follows that $P^{\lambda,\kappa}$ is a rank one-operator and*

$$\|P^{\lambda,\kappa} - P_{\text{kin}}^{\kappa}\| = O(\lambda^2) \tag{6.9}$$

with P_{kin}^{κ} the one-dimensional spectral projection of M^{κ} corresponding to the isolated simple eigenvalue $f_{\text{kin}}(\kappa)$, as in Theorem 4.3.

Proof. By analytic perturbation theory, the operator $\lambda^2 M^{\kappa} + A(z,\lambda,\kappa)$ has at most one eigenvalue at a distance $O(\lambda^4)$ of $f_{\text{kin}}(\kappa)$. This means that (6.4) has at most one solution at a distance $O(\lambda^4)$ of $f_{\text{kin}}(\kappa)$. We now prove that there is at least one solution. Indeed, if no such solution existed, we could choose a contour

$$\mathbf{C}_{\kappa,a} = \{z \in \mathbb{C} \,|\, |z - f_{\text{kin}}(\kappa)| = a\}, \qquad a > 0, \tag{6.10}$$

with a small enough such that $\mathbf{C}_{\kappa,a}$ stays away from Ω. We then calculate

$$\begin{aligned} 2\pi\mathrm{i}(P_{\text{kin}}^{\kappa} - 0) &= \int_{\lambda^2\mathbf{C}_{\kappa,a}} \mathrm{d}z(z-\lambda^2 M^{\kappa})^{-1} - \int_{\lambda^2\mathbf{C}_{\kappa,a}} \mathrm{d}z(z - \lambda^2 M^{\kappa} - A(z,\lambda,\kappa))^{-1} \\ &= \int_{\lambda^2\mathbf{C}_{\kappa,a}} \mathrm{d}z(z-\lambda^2 M^{\kappa})^{-1} \left(1 - (1 - A(z,\lambda,\kappa)(z-\lambda^2 M^{\kappa})^{-1})^{-1}\right) \\ &\leq (2\pi a)\, b(a,\kappa) \left(1 - \frac{1}{1 - b(a,\kappa) O(\lambda^2)}\right), \end{aligned} \tag{6.11}$$

where

$$b(a,\kappa) := \sup_{z\in \mathbf{C}_{\kappa,a}} \|(z-M^{\kappa})^{-1}\|,$$

and, here and in what follows, the contour integrals are meant to be oriented clockwise. Since the last line of (6.11) is of order λ^2, we arrive at a contradiction to the fact that $P^{\kappa}_{\text{kin}} \neq 0$.

The claim about the residue is most easily seen in an abstract setting: Let $F(z)$ be a Banach-space valued analytic function in some open domain containing 0, and such that $0 \in \text{sp}F(0)$ is an isolated eigenvalue. We have hence the Taylor expansion

$$F(z) = \sum_{n\geq 0} \frac{z^n}{n!} F_n, \qquad F_n := F^{(n)}(0), \qquad 0 \in \text{sp}F_0. \tag{6.12}$$

If $\|F_1 - 1\|$ is small enough, then also $F_1^{-1}F_0$ has 0 as an isolated eigenvalue. We denote the corresponding spectral projection by $1_0(F_1^{-1}F_0)$ and we calculate

$$\text{Res}(F(z)^{-1}) = \text{Res}(F_0 + zF_1)^{-1} = \left(\text{Res}(F_1^{-1}F_0 + z)^{-1}\right) F_1^{-1} = 1_0(F_1^{-1}F_0)F_1^{-1}. \tag{6.13}$$

The last expression is clearly a rank-one operator. In the case at hand, $F_1^{-1} = 1 + O(\lambda^2)$, as $\lambda \searrow 0$, which yields (6.9). □

We set $f(\lambda,\kappa) := \tilde{z}$ and we define $P^{\lambda,\kappa}$ as the residue of $(z - \lambda^2 M^{\kappa} - A(z,\lambda,\kappa))^{-1}$ at $z = \tilde{z}$. It is clear that $f(\lambda,\kappa)$ and $P^{\lambda,\kappa}$ enjoy the analyticity properties claimed in Theorem 4.5.

We define the horizontal contours

$$\Gamma := \{z \in \mathbb{C} \,|\, z = l + \mathrm{i}\mathbb{R}\}, \qquad \Gamma' := \{z \in \mathbb{C} \,|\, z = -(g' - \epsilon) + \mathrm{i}\mathbb{R}\}, \tag{6.14}$$

with l large enough such that all singular points of $z \mapsto (\mathcal{R}_{\lambda}(z))_{\lambda^2\kappa}$ lie below Γ, and $\epsilon > 0$ small enough such that all singular points with $\Re z > -g'$ lie above Γ' (the notions 'below' and 'above' are meant as in Fig. 6.1). These contours are oriented from left to right. By Theorem 4.3, we can construct a contour $\mathbf{C}'$ which encircles Ω and such that $f_{\text{kin}}(\kappa)$ is separated by a gap g from this contour:

$$g := \inf_{|\kappa|\leq \delta_{\text{kin}}} \Re f_{\text{kin}}(\kappa) - \sup \Re \mathbf{C}' > 0. \tag{6.15}$$

By performing an inverse Laplace transform we find that

$$(\mathcal{Z}^{\lambda}_t)_{\lambda^2\kappa} = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma} \mathrm{d}z\, \mathrm{e}^{tz} (z - \lambda^2 M^{\kappa} - A(z,\lambda,\kappa))^{-1}. \tag{6.16}$$

For λ small enough, Lemma 6.1 ensures that one can deform contours and obtain

$$\int_{\Gamma} = \int_{\lambda^2 \mathbf{C}_{a,\kappa}} + \int_{\lambda^2 \mathbf{C}'} + \int_{\Gamma'}. \tag{6.17}$$

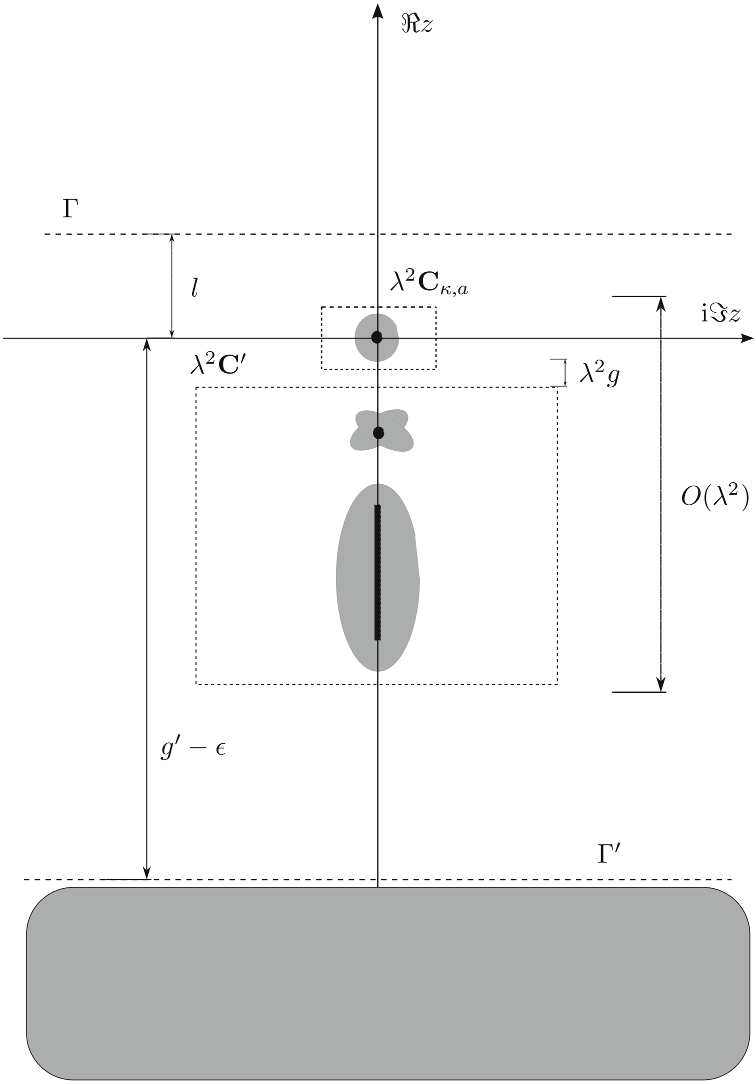

Fig. 6.1. The (rotated) complex plane. The black dots and thick black line indicate the spectrum of $\lambda^2 M^0$: The upper dot is the eigenvalue 0 and the thick vertical line is the continuous spectrum. In the picture, we have drawn only one other eigenvalue, but, in general, there can be more than one (or none) further eigenvalues. The function $\lambda^2 M^\kappa + A(z,\lambda,\kappa)$ is analytic above the lowest gray (rectangular) region. The other gray regions contain the singularities of the function $(\mathcal{R}_\lambda(z))_{\lambda^2\kappa}$ for $(z,\lambda,\kappa) \in \mathbf{G}$. The integration contours Γ, Γ' and $\lambda^2\mathbf{C}_{\kappa,a}$, $\lambda^2\mathbf{C}'$ are drawn in dashed lines. In this picture, the contour $\lambda^2\mathbf{C}_{\kappa,a}$ encircles $\lambda^2 f(\lambda,\kappa)$, for all (λ,κ), (i.e., such that $(z,\lambda,\kappa)\in\mathbf{G}$), which can be achieved by choosing a large enough

The first term on the RHS of (6.17) equals $\mathrm{e}^{t\lambda^2 f(\kappa,\lambda)} P^{\lambda,\kappa}$; this follows from Lemma 6.2. The second term is dominated by

$$\mathrm{e}^{\lambda^2 t(\sup(\Re\mathbf{C}'))} \int_{\lambda^2\mathbf{C}'} \frac{\mathrm{d}|z|}{2\pi} \,\|(z-\lambda^2 M^\kappa)^{-1}\|\,\|\left(1-(1-A(z,\lambda,\kappa)(z-\lambda^2 M^\kappa)^{-1}\right)^{-1}\|. \tag{6.18}$$

By the choice of $\mathbf{C}'_\lambda$ and the bound (6.7), the integral on the RHS is bounded by a constant, for λ small enough.

The third term of the RHS of (6.17) is split as

$$\int_{\Gamma'} dz\, e^{tz}(z-\lambda^2 M^\kappa - A(z,\lambda,\kappa))^{-1} = \int_{\Gamma'} dz\, e^{tz}(z-\lambda^2 M^\kappa)^{-1} + \int_{\Gamma'} dz\, e^{tz}(z-\lambda^2 M^\kappa)^{-1} A(z,\lambda,\kappa) \times (z-\lambda^2 M^\kappa - A(z,\lambda,\kappa))^{-1}. \tag{6.19}$$

The first integral can be closed in the lower half-plane and equals 0, the second integral has an integrand of order z^{-2} for large z, and hence its contribution is bounded by a constant times $e^{-t(g'-\epsilon)}$.

It follows that the crucial estimate (4.49) holds with $\delta_1 := \delta_{\mathrm{kin}}$ and g as in (6.15).

APPENDIX A

Here we consider the *effective* structure factor, which, in Sect. 2.3, has been introduced as the Fourier transform of the reservoir correlation function.

We use the spectral theorem to represent the positive operator ω as multiplication by $\xi \in \mathbb{R}^+$. There are Hilbert spaces $\mathfrak{h}_\xi$ for $\xi \in \mathbb{R}^+$ such that $\mathfrak{h} = \int_{\oplus \mathbb{R}^+} d\xi\, \mathfrak{h}_\xi$, and for all $\varphi \in \mathfrak{h}$, there are $\varphi_\xi \in \mathfrak{h}_\xi$ such that

$$\varphi = \int_{\oplus \mathbb{R}^+} d\xi\, \varphi_\xi, \qquad \omega\varphi = \int_{\oplus \mathbb{R}^+} d\xi\, \xi\, \varphi_\xi. \tag{A-1}$$

The structure factor $\phi \in \mathfrak{h}$ has been introduced in Sect. 2.3. We construct an effective form factor ϕ^β as an element of $\mathfrak{h} \oplus \mathfrak{h}$. We choose $\mathfrak{h}_{-\xi}$ to be isomorphic to $\mathfrak{h}_\xi$, and we define $\phi^\beta = \int_{\oplus \mathbb{R}} \phi^\beta_\xi$ as an element of $\mathfrak{h} \oplus \mathfrak{h} \sim \int_{\oplus \mathbb{R}} \mathfrak{h}_\xi$ by setting

$$\phi^\beta_\xi := \begin{cases} \frac{1}{\sqrt{e^{\beta\xi}-1}}\, \phi_\xi, & \xi > 0, \\ \frac{1}{\sqrt{1-e^{\beta\xi}}}\, \phi_{-\xi}, & \xi < 0. \end{cases} \tag{A-2}$$

The function ϕ^β plays the role of the form factor if one constructs the positive-temperature dynamical system. We just note that

$$\psi(\xi) = \|\phi^\beta_\xi\|^2_{\mathfrak{h}_\xi}. \tag{A-3}$$

Assume that the on-site one-particle space is given by $\mathfrak{h} = L^2(\mathbb{R}^d)$, and the one-particle Hamiltonian acts by multiplication with a function $\xi(r)$, where $r := |q|$, for $q \in \mathbb{R}^d$. We also assume that $r \mapsto \xi(r)$ is differentiable and monotonically increasing. Hence we can define the inverse function $\xi \mapsto r(\xi)$. The form factor $\phi \in L^2(\mathbb{R}^d)$ is taken to be spherically symmetric, $\phi(q) \equiv \phi(r)$. Then the Hilbert spaces $\mathfrak{h}_\xi$ are naturally identified with $L^2(\mathbb{S}^{d-1})$, and

$$\phi^\beta_\xi = r(|\xi|)^{\frac{d-1}{2}} \left(\frac{\partial r(|\xi|)}{\partial |\xi|}\right)^{-1/2} 1_{\mathbb{S}^{d-1}} \begin{cases} (e^{\beta\xi}-1)^{-1/2}\, \phi(r(\xi)), & \xi > 0, \\ (1-e^{\beta\xi})^{-1/2}\, \overline{\phi(r(-\xi))}, & \xi < 0, \end{cases} \tag{A-4}$$

where $1_{\mathbb{S}^{d-1}} \in L^2(\mathbb{S}^{d-1})$ is the constant function on $\mathbb{S}^{d-1}$ with $\|1_{\mathbb{S}^{d-1}}\| = 1$.

Next, we return to Assumption 2.2. By properties of the Fourier transform, e.g. Th. IX.14 of [19], this assumption is equivalent to the assumption that ψ extends to an analytic function in the strip $|\Im\xi| < g_{\mathrm{R}}$, and

$$\sup_{-g_{\mathrm{R}}<y<g_{\mathrm{R}}} \int_{\mathbb{R}} \mathrm{d}x\, |\psi(x+\mathrm{i}y)| < \infty. \tag{A-5}$$

Starting from expression (A-4), one can check condition (A-5) in concrete examples. E.g., for a relativistic dispersion law, $\xi(r) = r$, (A-5) is satisfied whenever

$$\sup_{-g_{\mathrm{R}}<y<g_{\mathrm{R}}} \int_{\mathbb{R}} \mathrm{d}x\, |x+\mathrm{i}y|^{d-2} |\phi(x+\mathrm{i}y)|^2 < \infty. \tag{A-6}$$

Acknowledgements. W.D.R. thanks J. Bricmont for helpful discussions on an early version of this model.

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Communicated by H.-T. Yau