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On second-order periodic elliptic operators in divergence form

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Abstract

We consider second-order, strongly elliptic, operators with complex coefficients in divergence form on \mathbf{R}^d . We assume that the coefficients are all periodic with a common period. If the coefficients are continuous we derive Gaussian bounds with the correct small and large time asymptotic behaviour on the heat kernel and all its Hölder derivatives. Secondly if the coefficients are Hölder continuous we prove that the first-order derivatives of the kernel satisfy good Gaussian bounds and the first-order Riesz transforms are bounded on the L_p -spaces with $p \in \langle 1, \infty \rangle$. Then we establish that the second-order derivatives exist and satisfy good bounds if, and only if, the coefficients are divergence-free or if, and only if, the second-order Riesz transforms are bounded. Finally if the third-order derivatives exist with good bounds then the coefficients must be constant.

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1 Introduction

We analyze the asymptotic behaviour of complex second-order strongly elliptic operators with periodic coefficients in divergence form acting on $L_2(\mathbf{R}^d)$. We establish that if the coefficients of the operators are continuous then the corresponding semigroups have bounded kernels which, together with their Hölder derivatives, satisfy good large time Gaussian bounds. Subsequently we establish a detailed hierarchy of asymptotic properties for periodic operators with Hölder continuous coefficients.

Auscher, McIntosh and Tchamitchian [AMT] proved the existence of Gaussian-type bounds for the kernels of complex operators with Hölder continuous coefficients but these bounds contain an extra factor with polynomial growth in time. Subsequently Auscher [Aus] extended these results to operators with uniformly continuous coefficients. We demonstrate that periodicity of the coefficients is sufficient to remove the growth factor and to give Gaussian bounds for the kernel and its Hölder derivatives for both small and large times. Moreover, the kernels of periodic operators with Hölder continuous coefficients have a remarkable $1, 2, \infty$ -structure. The kernels are automatically once-differentiable with the derivatives satisfying good Gaussian bounds, they are twice-differentiable with the second derivatives satisfying good asymptotic bounds if, and only if, the coefficients are divergence-free and existence of the third derivatives with the canonical behaviour implies the coefficients must be constant and hence the kernel is infinitely often differentiable. This hierarchy can also be characterized by the boundedness of the Riesz transforms; the first-order transforms are always bounded, boundedness of the second-order transforms is equivalent to the coefficients being divergence-free and boundedness of the third, or higher, order transforms implies the coefficients are constant.

The theory of complex second-order elliptic operators in divergence form differs substantially from the theory of their real counterparts. The complex theory shares the difficulties encountered with systems of real operators in divergence form or with single real operators in non-divergence form. In 1968 De Giorgi [Gio] gave an example of a system of real operators in divergence form which did not have the advantageous regularity features of the Nash–De Giorgi theory of single real operators with measurable coefficients. Several other authors subsequently gave refined examples of this nature (see, for example, [Gia], Section II.3). Then in 1981 Fabes and Kenig [FaK] constructed a class of real second-order elliptic operators in non-divergence form on \mathbf{R}^d such that the associated ‘parabolic measures’ were singular with respect to Lebesgue measure. The corresponding semigroups are contractive on $L_\infty(\mathbf{R}^d)$ but do not have bounded kernels. These examples are surprising since the operators have uniformly continuous coefficients and it is known that Hölder continuity of the coefficients is sufficient to ensure that the kernel exists and is at least twice differentiable (see [Fri], Chapter 9). The construction of the Fabes–Kenig examples was based on ideas of Modica, Mortola [MoM] which in turn used a suggestion of De Giorgi (see also [MMS] [Bau]). The theory of complex divergence form operators presents different structural difficulties. There are no problems in one or two dimensions; the principal regularity results of the Nash–De Giorgi theory are still valid [AMT]. But in 1985 Maz’ya, Nazarov and Plamenevskii [MNP] gave counterexamples for the complex theory in higher dimensions. Their ideas have been extended subsequently by various authors [ACT] [Dav] and result in examples of complex divergence form operators which generate continuous semigroups

on $L_p(\mathbf{R}^d)$ if, and only if, $|1/p - 1/2|$ is small. In particular the semigroups do not have bounded kernels. These examples require $d \geq 5$ and the status of the complex theory for $d = 3$ and $d = 4$ is not clear. Nevertheless the *reductio ad absurdum* argument given in [AMT], Remark 4.24, indicates that smoothness of the coefficients alone is not sufficient to obtain a satisfactory description in terms of bounded kernels. This conclusion is confirmed by our analysis of periodic operators.

Our approach to Gaussian bounds is through the homogenization theory of periodic systems [BLP] [ZKO]. The pointwise Gaussian-type bounds of Auscher, McIntosh and Tchamitchian [AMT], or Auscher [Aus], act as important *a priori* estimates. We use a Bloch–Zak decomposition and, following Zhikov [Zhi], we exploit L_2 -spectral estimates to prove that the kernel of the homogenized system provides a good asymptotic approximation to the semigroup kernel. Careful handling of the approximation, and interpolation with Auscher’s estimates, yields Gaussian bounds, for operators with continuous coefficients, both on the kernel and on its Hölder derivatives. A similar tactic works to provide detailed regularity properties for operators with Hölder continuous coefficients.

In the sequel H denotes the maximal accretive operator on the complex Hilbert space $L_2(\mathbf{R}^d)$ associated with the sectorial form (see, for example, [Kat] [ReS])

$$h(\varphi) = \sum_{k,l=1}^d (\partial_k \varphi, c_{kl} \partial_l \varphi) \quad (1)$$

where the $\partial_k = \partial/\partial x_k$ denote the usual partial derivatives and the domain of h is $D(h) = L_{2;1}(\mathbf{R}^d) = \bigcap_{k=1}^d D(\partial_k)$. The matrix $C = (c_{kl})$ of complex-valued coefficients $c_{kl} \in L_\infty(\mathbf{R}^d)$, which is not necessarily symmetric, is assumed to satisfy the ellipticity condition

$$\Re C = 2^{-1}(C + C^*) \geq \mu I > 0 \quad , \quad (2)$$

in the sense of $d \times d$ -matrices over \mathbf{C}^d , uniformly over \mathbf{R}^d , where $C^* = (c_{kl}^*)$ with $c_{kl}^* = \overline{c_{lk}}$. The ellipticity condition ensures that the form h is sectorial with vertex at the origin. The least upper bound μ_C of the μ satisfying this condition is called the ellipticity constant.

The operator H generates a continuous holomorphic semigroup S on $L_2(\mathbf{R}^d)$. The action of S is determined by a distribution kernel K . Our derivation of boundedness and smoothness properties of K is based on continuity and periodicity of the coefficients c_{kl} .

Theorem 1.1 *Assume the coefficients c_{kl} of H are continuous and periodic with a common period. Then the kernel K of the semigroup generated by H has the following bounds.*

I. *There exist $b, c > 0$ such that*

$$|K_t(x; y)| \leq c G_{b,t}(x - y)$$

for all $x, y \in \mathbf{R}^d$ and $t > 0$ where $G_{b,t}(x) = t^{-d/2} e^{-b|x|^2 t^{-1}}$.

II. *For all $\nu, \tau \in \langle 0, 1 \rangle$ and $\kappa > 0$ there exist $b, c > 0$ such that*

$$|K_t(x - h; y - k) - K_t(x; y)| \leq c \left(\frac{|h| + |k|}{|x - y| + t^{1/2}} \right)^\nu G_{b,t}(x - y)$$

for all $x, y, h, k \in \mathbf{R}^d$ and all $t > 0$ with $|h| + |k| \leq \tau|x - y| + \kappa t^{1/2}$.

Although we have stated these bounds for real positive t they can be extended to all complex t in an open subsector of the sector of holomorphy. A similar remark is true for all subsequent bounds of a similar nature. The passage from real t to complex $z = te^{i\alpha}$ corresponds to replacing H by $e^{i\alpha}H$ and for small α the latter operator is of the same type as H .

The situation with Hölder continuous coefficients is more detailed and introduces a new feature, boundedness of the Riesz transforms. For $p \in [1, \infty]$ define $L_{p;1}(\mathbf{R}^d) = \bigcap_{k=1}^d D(\partial_k)$, where ∂_k is the partial derivative in $L_p(\mathbf{R}^d)$.

Theorem 1.2 *Assume the coefficients c_{kl} of H are Hölder continuous and periodic with a common period. Then K is once-differentiable and there exist $b, c > 0$ such that*

$$|(\partial_{x_k} K_t)(x; y)| + |(\partial_{y_k} K_t)(x; y)| \leq c t^{-1/2} G_{b,t}(x - y)$$

for all $k \in \{1, \dots, d\}$, $x, y \in \mathbf{R}^d$ and all $t > 0$.

Moreover, if $p \in \langle 1, \infty \rangle$ then $D(H^{1/2}) = L_{p;1}(\mathbf{R}^d)$ and there exist $c_p, c'_p > 0$ such that

$$c_p \max_{1 \leq k \leq d} \|\partial_k \varphi\|_p \leq \|H^{1/2} \varphi\|_p \leq c'_p \max_{1 \leq k \leq d} \|\partial_k \varphi\|_p$$

for all $\varphi \in L_{p;1}(\mathbf{R}^d)$.

The uniform regularity properties given by this theorem are optimal as the next result shows. Increased regularity of the kernel for all t is characterized by a divergence-free property of the coefficients. In the fourth condition of the theorem U denotes the action of translations on the spaces $L_p(\mathbf{R}^d)$.

Theorem 1.3 *Assume the coefficients c_{kl} of H are Hölder continuous and periodic with a common period. The following conditions are equivalent.*

I. $\sum_{k=1}^d \partial_k c_{kl} = 0$, in the sense of distributions, for each $l \in \{1, \dots, d\}$.

II. There exist $c, \nu > 0$ such that

$$|(\partial_{x_k} K_t)(x - h; y) - (\partial_{x_k} K_t)(x; y)| \leq c t^{-1/2} (|h|t^{-1/2})^\nu t^{-d/2}$$

uniformly for all $k \in \{1, \dots, d\}$, $x, y, h \in \mathbf{R}^d$ with $|h| \leq 1$ and all $t \geq 1$.

III. K is twice-differentiable in the first variable and there exist $b, c > 0$ such that

$$|(\partial_{x_k} \partial_{x_l} K_t)(x; y)| \leq c t^{-1} G_{b,t}(x - y)$$

for all $k, l \in \{1, \dots, d\}$, $x, y \in \mathbf{R}^d$ and $t > 0$.

IV. There are $p \in [1, \infty]$ and $c_p, \nu > 0$ such that

$$\|(I - U(h))\partial_k S_t\|_{p \rightarrow p} \leq c_p t^{-1/2} (|h|t^{-1/2})^\nu \quad (3)$$

uniformly for all $k \in \{1, \dots, d\}$, all $|h| \leq 1$ and all $t \geq 1$.

V. If $p \in \langle 1, \infty \rangle$ then $D(H) = L_{p;2}(\mathbf{R}^d)$ and there exist $c_p, c'_p > 0$ such that

$$c_p \max_{1 \leq k, l \leq d} \|\partial_k \partial_l \varphi\|_p \leq \|H \varphi\|_p \leq c'_p \max_{1 \leq k, l \leq d} \|\partial_k \partial_l \varphi\|_p$$

for all $\varphi \in L_{p;2}(\mathbf{R}^d)$.

Further regularity only occurs for all t in the simple case that the coefficients are constant. Then of course the kernel is Gaussian and the Riesz transforms of all orders are bounded.

Theorem 1.4 *Assume the coefficients c_{kl} of H are Hölder continuous and periodic with a common period. The following conditions are equivalent.*

- I. *The coefficients c_{kl} are constant.*
- II. *K is twice-differentiable in the first variable and there exist $c, \nu > 0$ such that*

$$|(\partial_{x_k} \partial_{x_l} K_t)(x - h; y) - (\partial_{x_k} \partial_{x_l} K_t)(x; y)| \leq c t^{-1} (|h| t^{-1/2})^\nu t^{-d/2}$$

uniformly for all $k, l \in \{1, \dots, d\}$, $x, y, h \in \mathbf{R}^d$ with $|h| \leq 1$ and all $t \geq 1$.

- III. *There are $p \in [1, \infty]$ and $c_p, \nu > 0$ such that*

$$\|(I - U(h)) \partial_k \partial_l S_t\|_{p \rightarrow p} \leq c_p t^{-1} (|h| t^{-1/2})^\nu$$

uniformly for all $k, l \in \{1, \dots, d\}$, all $|h| \leq 1$ and all $t \geq 1$.

Although the regularity properties in these theorems are stated in terms of the first variable of the kernel one can readily draw similar conclusions for the second variable by symmetry. Interchange of the variables corresponds, by duality, to replacement of C by its transpose C^t , i.e., the matrix with coefficients $c_{kl}^t = c_{lk}$. For example, under the conditions of Theorem 1.2 the derivative with respect to the second variable is Hölder continuous with the canonical behaviour if, and only if, $\sum_{k=1}^d \partial_k c_{kl}^t = \sum_{k=1}^d \partial_k c_{lk} = 0$ as distributions for each $l \in \{1, \dots, d\}$. In fact one can deduce joint regularity properties from separate regularity properties by using the semigroup property

$$K_{s+t}(x; y) = \int_{\mathbf{R}^d} dz K_s(x; z) K_t(z; y) \quad .$$

For example, it follows in Theorem 1.2 that K is once-differentiable jointly with respect to both variables.

In Section 2 we summarize some basic elements of decomposition theory and homogenization theory for operators on $L_2(\mathbf{R}^d)$ with periodic coefficients and derive the essential spectral estimates. In Section 3 we prove Theorem 1.1. This follows by establishing that the kernel of the homogenized operator gives the best asymptotic approximation to K . We also deduce some results on first-order corrections to the asymptotic series for the kernel. In Section 4 we prove Theorems 1.2, 1.3 and 1.4. The conditions of Theorem 1.3 correspond to the first-order corrector, in the sense of homogenization theory, vanishing. The conditions of Theorem 1.4 correspond to the first and second order correctors vanishing.

2 Periodic systems

The proof of Theorem 1.1 relies on the *a priori* estimates of Auscher in combination with various Hilbert space properties of periodic systems which we develop in this section. Throughout the section we suppose that H is the maximal accretive operator associated

with the sectorial form (1) with the complex measurable coefficients satisfying the ellipticity assumption (2). We further assume that the coefficients are all periodic with a common period. Then, for simplicity, we choose units such that

$$c_{kl}(x+n) = c_{kl}(x) \quad , \quad (4)$$

for all $k, l \in \{1, \dots, d\}$, $x \in \mathbf{R}^d$ and $n \in \mathbf{Z}^d$. No continuity of the coefficients is required in this section.

2.1 Decomposition theory

Decomposition theory for operators with periodic coefficients has a long history dating back to Bloch [Blo]. We follow the description in [BJR] which is based on the Zak formalism commonly used in wavelet theory (see, for example [Dau]) although we then pass to the unitarily equivalent Bloch prescription.

If U denotes the unitary action of \mathbf{R}^d by left translations on $L_2(\mathbf{R}^d)$, i.e.,

$$(U(y)\varphi)(x) = \varphi(x-y)$$

for all $\varphi \in L_2(\mathbf{R}^d)$ and $y \in \mathbf{R}^d$, then $U(x)D(h) = D(h)$ for all $x \in \mathbf{R}^d$ and the periodicity (4) of the coefficients gives the invariance property $h(U(n)\varphi) = h(\varphi)$ for all $\varphi \in D(h)$ and all $n \in \mathbf{Z}^d$. Hence $U(n)D(H) = D(H)$ and $U(n)H = HU(n)$. Moreover,

$$U(n)S_t = S_tU(n)$$

on $L_2(\mathbf{R}^d)$ for all $n \in \mathbf{Z}^d$ and all $t > 0$. Next we introduce versions of H and S on $L_2(\mathbf{I}^d)$ where $\mathbf{I} = [0, 1]$.

Let ∂_k , for $k \in \{1, \dots, d\}$, denote the partial derivatives on $L_2(\mathbf{I}^d)$ corresponding to periodic boundary conditions, $\varphi(u_1, \dots, 0, \dots, u_d) = \varphi(u_1, \dots, 1, \dots, u_d)$ for almost every $u \in \mathbf{I}^d$, where the 0 and 1 are in the k -th position. Secondly, for all $\theta \in [-\pi, \pi]^d$ define H_θ as the maximal accretive operator on $L_2(\mathbf{I}^d)$ associated with the sectorial form

$$h_\theta(\varphi) = \sum_{k,l=1}^d ((\partial_k + i\theta_k)\varphi, c_{kl}(\partial_l + i\theta_l)\varphi) \quad (5)$$

where $D(h_\theta) = \bigcap_{k=1}^d D(\partial_k) = L_{2;1}(\mathbf{I}^d)$.

The H_θ are unitarily equivalent to versions \widetilde{H}_θ of H with θ -periodic boundary conditions, i.e., $\varphi(u_1, \dots, 0, \dots, u_d) = e^{i\theta_k}\varphi(u_1, \dots, 1, \dots, u_d)$ for all $k \in \{1, \dots, d\}$ and almost every $u \in \mathbf{I}^d$, where the 0 and 1 are in the k -th position. The unitarily equivalent description was used in [BJR], Section 2, and is related to the present description as follows. Let $V(\theta)$ be the unitary operator on $L_2(\mathbf{I}^d)$ defined by $(V(\theta)\varphi)(u) = e^{iu \cdot \theta}\varphi(u)$ for $u \in \mathbf{I}^d$. If $\varphi \in L_{2;1}(\mathbf{I}^d)$ then $V(\theta)\varphi$ satisfies the θ -periodic boundary conditions. Moreover,

$$h_\theta(\varphi) = \sum_{k,l=1}^d (\partial_k V(\theta)\varphi, c_{kl}\partial_l V(\theta)\varphi) \quad .$$

Hence $H_\theta = V(\theta)^*\widetilde{H}_\theta V(\theta)$ where the \widetilde{H}_θ are the operators used in [BJR].

One has a decomposition of $L_2(\mathbf{R}^d)$,

$$L_2(\mathbf{R}^d) \cong (2\pi)^{-d} \int_{[-\pi, \pi]^d}^{\oplus} d\theta L_2(\mathbf{I}^d)_\theta \quad ,$$

as a direct integral of copies of $L_2(\mathbf{I}^d)$ indexed by $\theta \in [-\pi, \pi]^d$ (for a description of the formalism of integral decompositions see, for example, [Dix], Chapter II, or [BrR], Chapter IV). The isomorphism is given as follows. Define $\Phi: L_2(\mathbf{R}^d) \rightarrow (2\pi)^{-d} \int_{[-\pi, \pi]^d}^{\oplus} d\theta L_2(\mathbf{I}^d)_\theta$ by $(\Phi(\varphi))(\theta) = \varphi_\theta$, where

$$\varphi_\theta(u) = \sum_{n \in \mathbf{Z}^d} e^{i(n-u) \cdot \theta} \varphi(u-n)$$

for all $\varphi \in L_2(\mathbf{R}^d)$, almost every $\theta \in [-\pi, \pi]^d$ and almost every $u \in \mathbf{I}^d$. By Fubini's and Parseval's theorems one verifies that Φ is a unitary operator. The inverse of Φ is given by

$$\left(\Phi^{-1} \left((\varphi_\theta)_{\theta \in [-\pi, \pi]^d} \right) \right) (u-n) = (2\pi)^{-d} \int_{[-\pi, \pi]^d} d\theta e^{-i(n-u) \cdot \theta} \varphi_\theta(u)$$

for all $(\varphi_\theta)_{\theta \in [-\pi, \pi]^d} \in (2\pi)^{-d} \int_{[-\pi, \pi]^d}^{\oplus} d\theta L_2(\mathbf{I}^d)_\theta$, $n \in \mathbf{Z}^d$ and almost every $u \in \mathbf{I}^d$.

It follows from [BJR] that the sectorial form h , the operator H and the semigroup S decompose in the same manner. Explicitly, if $\Phi(\varphi) = (\varphi_\theta)_{\theta \in [-\pi, \pi]^d}$ then

$$h(\varphi) = (2\pi)^{-d} \int_{[-\pi, \pi]^d} d\theta h_\theta(\varphi_\theta)$$

and

$$\Phi H \Phi^{-1} = (2\pi)^{-d} \int_{[-\pi, \pi]^d}^{\oplus} d\theta H_\theta$$

in the sense of direct integral decompositions of closed sectorial forms. Similarly

$$\Phi S_t \Phi^{-1} = (2\pi)^{-d} \int_{[-\pi, \pi]^d}^{\oplus} d\theta S_t^\theta \tag{6}$$

where S^θ denotes the semigroup generated by H_θ on $L_2(\mathbf{I}^d)$ (see [BJR], Theorem 2.3). If S has a bounded integrable kernel then the semigroup decomposition gives a similar kernel decomposition. We will use this fact extensively in Section 3.

Moreover, we need the following estimate on crossnorms. Note that the first crossnorm is on \mathbf{R}^d , whilst the second one is on \mathbf{I}^d . Moreover, both can be infinite.

Lemma 2.1 *Let T be a bounded operator on $L_2(\mathbf{R}^d)$ with a decomposition $\Phi^{-1} T \Phi = (2\pi)^{-d} \int_{[-\pi, \pi]^d}^{\oplus} d\theta T_\theta$ on the direct integral space $(2\pi)^{-d} \int_{[-\pi, \pi]^d}^{\oplus} d\theta L_2(\mathbf{I}^d)_\theta$. Then*

$$\|T\|_{1 \rightarrow \infty} \leq (2\pi)^{-d} \int_{[-\pi, \pi]^d} d\theta \|T_\theta\|_{1 \rightarrow \infty} \quad .$$

Proof If $\varphi \in C_c(\mathbf{R}^d)$ then $\|\varphi_\theta\|_1 \leq \|\varphi\|_1$ for all $\theta \in [-\pi, \pi]^d$. Therefore $|(\psi, T\varphi)| = |(2\pi)^{-d} \int_{[-\pi, \pi]^d} d\theta (\psi_\theta, T_\theta \varphi_\theta)| \leq (2\pi)^{-d} \int_{[-\pi, \pi]^d} d\theta \|\psi_\theta\|_1 \|T_\theta\|_{1 \rightarrow \infty} \|\varphi_\theta\|_1 \leq \|\psi\|_1 \|\varphi\|_1 (2\pi)^{-d} \int_{[-\pi, \pi]^d} d\theta \|T_\theta\|_{1 \rightarrow \infty}$, where $\varphi_\theta = (\Phi(\varphi))(\theta)$ and $\psi_\theta = (\Phi(\psi))(\theta)$, from which the lemma follows. \square

2.2 Spectral estimates

In this subsection we derive some basic spectral properties of the operators H_θ associated with the sectorial forms (5). It then follows that for large t the semigroup is determined by the small θ components S^θ in the periodic decomposition. Moreover, for small $|\theta|$ the large t behaviour of the S^θ is determined by the lowest eigenvalue and its eigenprojector.

It follows immediately from the definition (5) that the family h_θ of sectorial forms extends to a (multi-variable) holomorphic family of type (a), with $\theta \in \mathbf{C}^d$ (see [Kat], VII-§4.2). We denote the extension by h_θ and the associated m -sectorial operator by H_θ . Then the family H_θ , $\theta \in \mathbf{C}^d$, is a (multi-variable) holomorphic family of operators of type (B) by [Kat], Theorem VII-4.2. (Although we have a d -parameter extension of the formalism of Kato this does not affect any of the results we adopt from the standard theory.)

Each H_θ has a compact resolvent. This follows because H_0 has compact resolvent by [BJR], Lemma 2.1, and the family H_θ are a holomorphic family of type (B). Then every H_θ has compact resolvent for all $\theta \in \mathbf{C}^d$ (see [Kat], Theorem 4.3).

For all $\delta \in [0, \pi]$ set

$$B_\delta = \{\theta \in [-\pi, \pi]^d : \max_{k \in \{1, \dots, d\}} |\theta_k| \leq \delta\} \quad .$$

Then B_δ is closed in $[-\pi, \pi]^d$.

Lemma 2.2 *If $\delta \in [0, 1]$ then*

$$\operatorname{Re} h_\theta(\varphi) \geq \mu_C (1 - \delta) \|\nabla \varphi\|_2^2 + \mu_C |\theta|^2 \|\varphi\|_2^2$$

for all $\varphi \in L_{2,1}(\mathbf{I}^d)$ and $\theta \in B_\delta$.

Proof Let $(c_n)_{n \in \mathbf{Z}^d} \in C_c(\mathbf{Z}^d)$ and consider the trigonometric polynomial φ given by $\varphi(u) = \sum_{n \in \mathbf{Z}^d} c_n e^{2\pi i n \cdot u}$. Then

$$\begin{aligned} \operatorname{Re} h_\theta(\varphi) &= \operatorname{Re} \int_{\mathbf{I}^d} du \sum_{k,l=1}^d \overline{((\partial_k + i \theta_k) \varphi)(u)} c_{kl}(u) ((\partial_l + i \theta_l) \varphi)(u) \\ &\geq \mu_C \int_{\mathbf{I}^d} du \sum_{k=1}^d |((\partial_k + i \theta_k) \varphi)(u)|^2 = \mu_C \sum_{k=1}^d \sum_{n \in \mathbf{Z}^d} |c_n|^2 (2\pi n_k + \theta_k)^2 \quad . \end{aligned}$$

But if $m \in \mathbf{Z}$ and $\nu \in \mathbf{R}$ with $|\nu| \leq \delta \pi$ then $(2\pi m + \nu)^2 \geq 4\pi^2 m^2 (1 - \delta) + \nu^2$. Hence

$$\operatorname{Re} h_\theta(\varphi) \geq \mu_C \sum_{k=1}^d \sum_{n \in \mathbf{Z}^d} |c_n|^2 (4\pi^2 n_k^2 (1 - \delta) + |\theta_k|^2) = \mu_C (1 - \delta) \sum_{k=1}^d \|\partial_k \varphi\|_2^2 + \mu_C |\theta|^2 \|\varphi\|_2^2 \quad .$$

Since the trigonometric polynomials are dense in $L_{2,1}(\mathbf{I}^d)$ the lemma follows by a limiting argument. \square

The lemma has four immediate corollaries.

Corollary 2.3 *If $\theta \in [-\pi, \pi]^d$ then $\|S_t^\theta\|_{2 \rightarrow 2} \leq e^{-\mu_C |\theta|^2 t}$ for all $t > 0$.*

Corollary 2.4 *If $\theta \in [-\pi, \pi]^d$ and λ is an eigenvalue of H_θ then $\operatorname{Re} \lambda \geq \mu_C |\theta|^2$.*

These statements follow immediately since $\operatorname{Re} h_\theta(\varphi) \geq \mu_C |\theta|^2 \|\varphi\|_2^2$ for all $\varphi \in L_{2;1}(\mathbf{I}^d)$ and $\theta \in [-\pi, \pi]^d$.

Corollary 2.5 *There exists a $c > 0$ such that*

$$\operatorname{Re} h_\theta(\varphi) \geq c \operatorname{Re} h_0(\varphi)$$

for all $\varphi \in L_{2;1}(\mathbf{I}^d)$ and $\theta \in [-\pi, \pi]^d$.

Proof Let $\|C\| = \sup_{u \in \mathbf{I}^d} \|(c_{ki}(u))\|_{2 \rightarrow 2}$. Then it follows from the definition of h_θ that

$$\begin{aligned} |h_0(\varphi) - h_\theta(\varphi)| &\leq 2\|C\| \|\nabla\varphi\|_2 |\theta| \|\varphi\|_2 + \|C\| |\theta|^2 \|\varphi\|_2^2 \\ &\leq \varepsilon \mu_C \|\nabla\varphi\|_2^2 + \varepsilon^{-1} \mu_C^{-1} \|C\|^2 |\theta|^2 \|\varphi\|_2^2 + \|C\| |\theta|^2 \|\varphi\|_2^2 \\ &\leq \varepsilon \operatorname{Re} h_0(\varphi) + \mu_C^{-1} (\varepsilon^{-1} \mu_C^{-1} \|C\|^2 + \|C\|) \operatorname{Re} h_\theta(\varphi) \end{aligned}$$

for all $\varepsilon > 0$ and $\varphi \in L_{2;1}(\mathbf{I}^d)$, where, in the last step, we have used Lemma 2.2. The corollary follows by taking $\varepsilon = 1/2$. \square

Clearly the operator H_0 and its adjoint H_0^* have eigenvalue 0 with eigenfunction $\mathbf{1}$, the identity function. But it follows from the lemma that this eigenvalue is simple, i.e., it has multiplicity one.

Corollary 2.6 *If $\lambda \neq 0$ is an eigenvalue of H_0 then $\operatorname{Re} \lambda > 0$. Moreover, 0 is a simple eigenvalue of H_0 .*

Proof If ψ is a non-constant eigenfunction of the operator H_0 with eigenvalue λ then $\operatorname{Re} \lambda \|\psi\|_2^2 = \operatorname{Re} h_0(\psi) \geq \mu_C \|\nabla\psi\|_2^2 > 0$. This implies both statements. \square

For all $\delta > 0$ set

$$B_\delta^{\mathbf{C}} = \{\theta \in \mathbf{C}^d : \max_{k \in \{1, \dots, d\}} |\theta_k| < \delta\} .$$

Then $B_\delta^{\mathbf{C}}$ is open in \mathbf{C}^d .

Proposition 2.7 *There exist $\varepsilon_0, \theta_0 > 0$ and a holomorphic function $\lambda_0: B_{\theta_0}^{\mathbf{C}} \rightarrow \mathbf{C}$ such that $\lambda_0(0) = 0$ and $\lambda_0(\theta)$ is a simple eigenvalue of H_θ for all $\theta \in B_{\theta_0}^{\mathbf{C}}$. Moreover, $\lambda_0(\theta)$ is the unique eigenvalue λ of H_θ with $|\lambda| \leq \varepsilon_0$ for all $\theta \in B_{\theta_0}^{\mathbf{C}}$.*

Proof The first part follows by Corollary 2.6 and the proof of Theorem VII-1.7 in [Kat].

By Corollary 2.6 there exists an $\varepsilon_0 > 0$ such that 0 is the unique eigenvalue λ of H_0 with $|\lambda| \leq \varepsilon_0$. Moreover, the dimension of the eigenspace equals one. But these properties are stable under perturbation. It then follows from the proof of [Kat], Theorem VII-1.7, that for all sufficiently small $|\theta|$ the eigenvalue $\lambda_0(\theta)$ is the unique eigenvalue λ of H_θ with $|\lambda| < \varepsilon_0$. \square

Let ε_0, θ_0 and λ_0 be as in Proposition 2.7. For $\theta \in B_{\theta_0}^{\mathbf{C}}$ define the projection

$$P_0(\theta) = (2\pi i)^{-1} \int_{\Gamma_{\varepsilon_0}} d\lambda (\lambda I - H_\theta)^{-1}$$

where $\Gamma_{\varepsilon_0} = \{z \in \mathbf{C} : |z| = \varepsilon_0\}$. Then the map $\theta \mapsto P_0(\theta)$ is holomorphic near $\theta = 0$. This again follows by the proof of [Kat], Theorem VII-1.7. Therefore we may assume that $\theta_0 \leq \pi$, the map $\theta \mapsto P_0(\theta)$ is holomorphic on $B_{\theta_0}^{\mathbf{C}}$ and that

$$\|P_0(\theta) - P_0(0)\|_{2 \rightarrow 2} \leq 1/2$$

for all $\theta \in B_{\theta_0}^{\mathbf{C}}$. Note that $P_0(0)$ is the orthogonal projection onto the constant functions.

For all $\theta \in B_{\theta_0}^{\mathbf{C}}$ define $\varphi_\theta = P_0(\theta)\mathbf{1}$. Then $\|\varphi_\theta - \mathbf{1}\|_2 = \|(P_0(\theta) - P_0(0))\mathbf{1}\|_2 \leq 1/2$, so $\varphi_\theta \neq 0$. Since $P_0(\theta)$ projects onto the one-dimensional eigenspace corresponding to the eigenvalue $\lambda_0(\theta)$ it follows that φ_θ is an eigenfunction of H_θ with eigenvalue $\lambda_0(\theta)$. Obviously the map $\theta \mapsto \varphi_\theta$ is holomorphic from $B_{\theta_0}^{\mathbf{C}}$ into $L_2(\mathbf{I}^d)$. But $\varphi_\theta \in D(H_\theta) \subseteq D(h_\theta) = L_{2,1}(\mathbf{I}^d)$ for each $\theta \in B_{\theta_0}^{\mathbf{C}}$. We next show that the map $\theta \mapsto \varphi_\theta$ is also holomorphic from $B_{\theta_0}^{\mathbf{C}}$ into $L_{2,1}(\mathbf{I}^d)$.

Lemma 2.8 *For all $k \in \{1, \dots, d\}$ the map $\theta \mapsto \partial_k \varphi_\theta$ is holomorphic from $B_{\theta_0}^{\mathbf{C}}$ into $L_2(\mathbf{I}^d)$.*

Proof Obviously the map $\theta \mapsto (\psi, \partial_k \varphi_\theta) = -(\partial_k \psi, \varphi_\theta)$ is holomorphic on $B_{\theta_0}^{\mathbf{C}}$ for all $\psi \in L_{2,1}(\mathbf{I}^d)$ and since $L_{2,1}(\mathbf{I}^d)$ is dense in $L_2(\mathbf{I}^d)$ it suffices to show that the map $\theta \mapsto \partial_k \varphi_\theta$ from $B_{\theta_0}^{\mathbf{C}}$ into $L_2(\mathbf{I}^d)$ is locally bounded (see [Kat], Remark III-1.38). But

$$\|\partial_k \varphi_\theta\|_2 = \|e^{\lambda_0(\theta)} \partial_k S_1^\theta \varphi_\theta\|_2 \leq e^{\operatorname{Re} \lambda_0(\theta)} \|\partial_k S_1^\theta\|_{2 \rightarrow 2} \|\varphi_\theta\|_2$$

so it reduces the problem to showing that $\theta \mapsto \|\partial_k S_1^\theta\|_{2 \rightarrow 2}$ is locally bounded. Since

$$\operatorname{Re}(\varphi, H_\theta \varphi) \geq 2^{-1} \mu_C \|\nabla \varphi\|_2^2 - \|C\| |\theta|^2 (1 + 2\mu_C^{-1} \|C\|) \|\varphi\|_2^2$$

for all $\varphi \in D(H_\theta)$ and $\theta \in \mathbf{C}^d$ it follows by a straightforward argument that the map $\theta \mapsto \|\partial_k S_1^\theta\|_{2 \rightarrow 2}$ is locally bounded on \mathbf{C}^d (cf. the proof of [Rob], Lemma III.4.4). \square

Proposition 2.9 *There exists a $\mu > 0$ such that*

$$\operatorname{Re}(\varphi, H_\theta \varphi) \geq \mu \|\varphi\|_2^2$$

for all $\theta \in B_{2^{-1}\theta_0}$ and $\varphi \in (I - P_0(\theta))(D(H_\theta))$.

Proof Let $\theta \in B_{2^{-1}\theta_0}$ and $\varphi \in (I - P_0(\theta))(D(H_\theta))$. Then $\varphi \in D(H_\theta) \subseteq D(h_\theta) = L_{2,1}(\mathbf{I}^d)$ and

$$\operatorname{Re}(\varphi, H_\theta \varphi) \geq c \operatorname{Re} h_0(\varphi) = c \operatorname{Re} h_0((I - P_0(0))\varphi)$$

where c is the constant of Corollary 2.5 and we have used $H_0 P_0(0) = H_0^* P_0(0) = 0$. But the self-adjoint operator $\operatorname{Re} H_0$ associated with the quadratic form $\operatorname{Re} h_0$ has a discrete spectrum with simple lowest eigenvalue 0 and eigenfunction $\mathbf{1}$ (see Corollary 2.6). So if $\lambda_1 = \min(\sigma(\operatorname{Re} H_0) \setminus \{0\})$ then

$$\operatorname{Re}(\varphi, H_\theta \varphi) \geq c \lambda_1 \|(I - P_0(0))\varphi\|_2^2 = c \lambda_1 (\|\varphi\|_2^2 - (\varphi, P_0(0)\varphi)) \quad .$$

Since $\|P_0(\theta) - P_0(0)\|_{2 \rightarrow 2} \leq 2^{-1}$ for all $\theta \in B_{\theta_0}^{\mathbf{C}}$ one has

$$\operatorname{Re}(\varphi, H_\theta \varphi) \geq c \lambda_1 (2^{-1} \|\varphi\|_2^2 - \operatorname{Re}(\varphi, P_0(\theta)\varphi)) = 2^{-1} c \lambda_1 \|\varphi\|_2^2$$

for all $\theta \in B_{2^{-1}\theta_0}$ and $\varphi \in (I - P_0(\theta))(D(H_\theta))$. \square

Proposition 2.10 *There exists a $\mu > 0$ such that*

$$\|S_t^\theta(I - P_0(\theta))\varphi\|_2 \leq e^{-\mu t} \|(I - P_0(\theta))\varphi\|_2$$

uniformly for all $t > 0$, $\varphi \in L_2(\mathbf{I}^d)$ and $\theta \in B_{2^{-1}\theta_0}$.

Proof Let $\mu > 0$ be as in Proposition 2.9 and $\theta \in B_{2^{-1}\theta_0}$. The subspace $\mathcal{H} = (I - P_0(\theta))(L_2(\mathbf{I}^d))$ is the orthogonal complement of the one-dimensional subspace $P_0(\theta)^*L_2(\mathbf{I}^d)$. Since the latter subspace is invariant under the adjoint of S^θ it follows that \mathcal{H} is invariant under S^θ . Moreover, the restriction T of S^θ to \mathcal{H} is a continuous, holomorphic, semigroup with generator $H_\theta|_{\mathcal{H} \cap D(H_\theta)}$. But then it follows from Proposition 2.9 that $\operatorname{Re}(\varphi, H_\theta\varphi) \geq \mu \|\varphi\|_2^2$ for all $\varphi \in \mathcal{H} \cap D(H_\theta)$. So $\|T_t\|_{\mathcal{H} \rightarrow \mathcal{H}} \leq e^{-\mu t}$ for all $t > 0$, as required. \square

2.3 Homogenization

The asymptotic behaviour of periodic operators and the associated semigroups is often determined by the related, homogenized system (see [BLP] or [ZKO]). Next we define the homogenized operator corresponding to H and its decomposition. To this end we need a boundedness result for the Riesz transforms associated with H_0 .

First the self-adjoint operator $\operatorname{Re}H_0$ associated with the quadratic form $\operatorname{Re}h_0$ has a discrete spectrum with simple lowest eigenvalue 0 and eigenfunction $\mathbb{1}$. Hence by [Kat], Theorem III-6.17, the operator $\operatorname{Re}H_0$ leaves the orthogonal complement $L_2^\perp(\mathbf{I}^d) = (I - P_0(0))(L_2(\mathbf{I}^d))$ of the constant functions in $L_2(\mathbf{I}^d)$ invariant and the restriction of $\operatorname{Re}H_0$ to the space $L_2^\perp(\mathbf{I}^d)$ is invertible. With a slight abuse of notation we denote this inverse by $(\operatorname{Re}H_0)^{-1}$. In this section we shall use similar notation. Then the operator $(\operatorname{Re}H_0)^{-1/2} = ((\operatorname{Re}H_0)^{-1})^{1/2}$ is also bounded on $L_2^\perp(\mathbf{I}^d)$. But since

$$\operatorname{Re}h_0(\varphi) \geq \mu_C \|\nabla\varphi\|_2^2$$

it follows that $\partial_k(\operatorname{Re}H_0)^{-1/2}$ is bounded (has bounded closure) and $(\operatorname{Re}H_0)^{-1/2}\partial_l$ extends to a bounded operator, on $L_2^\perp(\mathbf{I}^d)$. Hence $\partial_k(\operatorname{Re}H_0)^{-1}\partial_l$ extends to a bounded operator, on $L_2^\perp(\mathbf{I}^d)$, for all $k, l \in \{1, \dots, d\}$. This last result has an analogue with $\operatorname{Re}H_0$ replaced by H_0 . Note that this does not require any continuity of the coefficients.

Lemma 2.11 *The inverse H_0^{-1} is bounded on $L_2^\perp(\mathbf{I}^d)$ and for all $k, l \in \{1, \dots, d\}$ the forms*

$$\begin{aligned} x_l(\varphi) &= (\varphi, H_0^{-1}\partial_l\varphi) \\ x_{kl}(\varphi) &= (\partial_k\varphi, H_0^{-1}\partial_l\varphi) \end{aligned}$$

with $D(x_l) = D(x_{kl}) = L_{2;1}(\mathbf{I}^d)$ have bounded extensions to $L_2(\mathbf{I}^d)$.

If X_l and X_{kl} denote the bounded operators associated with the bounded forms x_l and x_{kl} on $L_2(\mathbf{I}^d)$ then X_l and X_{kl} map $L_2(\mathbf{I}^d)$ into $L_2^\perp(\mathbf{I}^d)$. Moreover, $X_l L_2(\mathbf{I}^d) \subseteq L_{2;1}(\mathbf{I}^d)$ and $X_{kl} = -\partial_k X_l$.

Proof It follows from Corollary 2.6 that H_0^{-1} is bounded on $L_2^\perp(\mathbf{I}^d)$. But if $\varphi \in L_{2;1}(\mathbf{I}^d)$ then $\partial_k\varphi \in L_2^\perp(\mathbf{I}^d)$ for each $k \in \{1, \dots, d\}$. Hence the x_l and x_{kl} are well-defined. Then,

however, it follows from [Kat], Theorem VI-3.2, that there is a bounded symmetric operator B on $L_2^\perp(\mathbf{I}^d)$ such that

$$H_0^{-1} = (\operatorname{Re} H_0)^{-1/2} (I + iB)^{-1} (\operatorname{Re} H_0)^{-1/2} \quad . \quad (7)$$

Therefore

$$x_l(\varphi) = (\varphi, (\operatorname{Re} H_0)^{-1/2} (I + iB)^{-1} (\operatorname{Re} H_0)^{-1/2} \partial_l \varphi)$$

and

$$x_{kl}(\varphi) = ((\operatorname{Re} H_0)^{-1/2} \partial_k \varphi, (I + iB)^{-1} (\operatorname{Re} H_0)^{-1/2} \partial_l \varphi) \quad .$$

Since $\|(I + iB)^{-1}\|_{2 \rightarrow 2} \leq 1$ it follows that

$$|x_l(\varphi)| \leq \|(\operatorname{Re} H_0)^{-1/2}\|_{2 \rightarrow 2} \|\partial_l (\operatorname{Re} H_0)^{-1/2}\|_{2 \rightarrow 2} \|\varphi\|_2^2$$

and

$$|x_{kl}(\varphi)| \leq \|\partial_k (\operatorname{Re} H_0)^{-1/2}\|_{2 \rightarrow 2} \|\partial_l (\operatorname{Re} H_0)^{-1/2}\|_{2 \rightarrow 2} \|\varphi\|_2^2$$

where the operator norms are taken on $L_2^\perp(\mathbf{I}^d)$. Hence the x_l and x_{kl} extend to bounded forms on $L_2(\mathbf{I}^d)$. The associated bounded operators map $L_{2;1}(\mathbf{I}^d)$ into $L_2^\perp(\mathbf{I}^d)$ and since $L_2^\perp(\mathbf{I}^d)$ is closed in $L_2(\mathbf{I}^d)$ it implies that the operators map $L_2(\mathbf{I}^d)$ into $L_2^\perp(\mathbf{I}^d)$. \square

In the sequel we also use the notation $X_l = X_l(C)$ and $X_{kl} = X_{kl}(C)$ for the operators associated with the forms x_l and x_{kl} since it is sometimes necessary to track the dependence on the matrix C of coefficients. Hence $X_l(C^*)$ and $X_{kl}(C^*)$ will denote the operators corresponding to the adjoint operator.

The homogenization \widehat{H} of H is defined to be the elliptic operator on $L_2(\mathbf{R}^d)$ with constant coefficients \widehat{c}_{ij} associated with the form

$$\widehat{h}(\varphi) = \sum_{k,l=1}^d (\partial_k \varphi, \widehat{c}_{kl} \partial_l \varphi)$$

where the coefficients are defined by

$$\widehat{c}_{kl} = \int_{\mathbf{I}^d} du c_{kl}(u) - \sum_{m,n=1}^d (\overline{c_{km}}, X_{mn} c_{nl}) \quad .$$

This definition of \widehat{H} coincides with that of [BLP], pages 16 and 184, or that of [BBJR]. Note that the homogenized matrix $\widehat{C} = (\widehat{c}_{ij})$ satisfies the ellipticity condition (2) with $\mu = \mu_C$ (see, for example, [BLP] Chapter 1, Theorem 3.2). Let \widehat{K} be the kernel of the semigroup \widehat{S} generated by the operator \widehat{H} .

Since the coefficients of \widehat{H} are constant it can be decomposed in a similar manner to H . Then the components \widehat{H}_θ , $\theta \in [-\pi, \pi]^d$, in the decomposition are the maximal accretive operators on $L_2(\mathbf{I}^d)$ associated with the sectorial forms

$$\widehat{h}_\theta(\varphi) = \sum_{k,l=1}^d ((\partial_k + i\theta_k)\varphi, \widehat{c}_{kl} (\partial_l + i\theta_l)\varphi)$$

with $D(\widehat{h}_\theta) = L_{2;1}(\mathbf{I}^d)$.

Subsequently, we need the following lemma.

Lemma 2.12 *Let $\varphi \in L_{2;1}(\mathbf{I}^d)$ and $\tau_1, \dots, \tau_d \in L_2(\mathbf{I}^d)$. Suppose that*

$$h_0(\psi, \varphi) = \sum_{k=1}^d (\partial_k \psi, \tau_k)$$

for all $\psi \in L_{2;1}(\mathbf{I}^d)$. Then there is an $a \in \mathbf{C}$ such that $\varphi = a \mathbf{1} - \sum_{k=1}^d X_k \tau_k$.

Proof Since $h_0(\psi, \mathbf{1}) = 0$ we may assume that $\varphi \in L_2^\perp(\mathbf{I}^d) \cap L_{2;1}(\mathbf{I}^d)$. If $\chi \in L_2^\perp(\mathbf{I}^d)$ then $\psi = H_0^{*-1} \chi \in L_{2;1}(\mathbf{I}^d)$ by (7). So

$$(\chi, \varphi) = h_0(\psi, \varphi) = \sum_{k=1}^d (\partial_k \psi, \tau_k) = - \sum_{k=1}^d (X_k^* \chi, \tau_k) = - \sum_{k=1}^d (\chi, X_k \tau_k)$$

for all $\chi \in L_{2;1}(\mathbf{I}^d)$ from which the statement of the lemma follows. \square

3 Uniformly continuous coefficients

In this section we prove Theorem 1.1. Our reasoning is a variation of the argument of Zhikov [Zhi] who considered the asymptotic behaviour of real symmetric operators with periodic measurable coefficients. (Zhikov's argument is described in Section 2.6 of [ZKO].) In the real symmetric case one has good Gaussian bounds on the kernel and Zhikov used spectral estimates to obtain an asymptotic approximation of the kernel. Throughout this section we assume that the coefficients are continuous. Then the coefficients are uniformly continuous and one has the Gaussian-type bounds of [Aus], Theorem 4.3,

$$|K_t(x; y)| \leq c(1+t)^N G_{b,t}(x-y) \quad (8)$$

for some $N \in \mathbf{N}$ and $b, c > 0$ uniformly for all $x, y \in \mathbf{R}^d$ and $t > 0$. We will combine these with a variation of Zhikov's spectral estimates to obtain improved bounds.

3.1 Gaussian bounds

In this subsection we prove the first statement of Theorem 1.1. First note that by the decomposition theory of Section 2 the semigroups S^θ are given by bounded integral kernels K^θ which are related to K by

$$K_t^\theta(u; v) = \sum_{n \in \mathbf{Z}^d} e^{i(n-u+v)\cdot\theta} K_t(u; v+n) = \sum_{n \in \mathbf{Z}^d} e^{i(n-u+v)\cdot\theta} K_t(u-n; v) \quad (9)$$

for all $u, v \in \mathbf{I}^d$ and $\theta \in [-\pi, \pi]^d$. (This formula differs from the similar one given in [BJR], Theorem 2.4, by the presence of the factor $e^{-i(u-v)\cdot\theta}$ which arises because of the current unitarily equivalent description.) The sums in (9) are convergent for all $\theta \in \mathbf{C}^d$ and $u, v \in \mathbf{I}^d$, so one can use (9) to define a function K_t^θ for all $\theta \in \mathbf{C}^d$. Then we know that K_t^θ is the kernel of S_t^θ if $\theta \in [-\pi, \pi]^d$ and we next argue that this extends to all $\theta \in \mathbf{C}^d$.

It immediately follows from (8), (9) and the Jacobi identity, [ScD] Satz I.10.4, that the K^θ satisfy bounds similar to those of K : there exist $c, \omega > 0$ such that

$$|K_t^\theta(u; v)| \leq c(1+t)^N (1 \wedge t)^{-d/2} e^{-b\|u-v\|^2 t^{-1}} e^{\omega(\operatorname{Im} \theta)^2 t}$$

for all $\theta \in \mathbf{C}^d$, $u, v \in \mathbf{I}^d$ and $t > 0$, where

$$\|x\| = \min\{|x - n| : n \in \mathbf{Z}^d\}$$

for all $x \in \mathbf{R}^d$. For all $\theta \in \mathbf{C}^d$ and $t > 0$ let T_t^θ denote the operator on $L_2(\mathbf{I}^d)$ which has kernel K_t^θ . If $\varphi, \psi \in C_c(\mathbf{I}^d)$ and $t > 0$ then it follows again from the Gaussian estimates (8) that $\theta \mapsto (\psi, T_t^\theta \varphi)$ is a holomorphic function from \mathbf{C}^d into \mathbf{C} . But it equals the entire function $\theta \mapsto (\psi, S_t^\theta \varphi)$ for all $\theta \in [-\pi, \pi]^d$. Hence $(\psi, T_t^\theta \varphi) = (\psi, S_t^\theta \varphi)$ for all $\theta \in \mathbf{C}$. This implies that $T_t^\theta = S_t^\theta$ and therefore K^θ is the kernel of S^θ for all $\theta \in \mathbf{C}$.

It now follows from the well known estimates for the norm of the operator of convolution with a Gaussian that there exist $c, \omega > 0$ such that

$$\|S_t^\theta\|_{p \rightarrow q} \leq c(1+t)^N(1 \wedge t)^{-d(1/p-1/q)/2} e^{\omega(\operatorname{Im} \theta)^2 t} \quad (10)$$

uniformly for all $1 \leq p \leq q \leq \infty$, $t > 0$ and $\theta \in \mathbf{C}^d$, where N is as in (8).

Recall that $\theta \mapsto P_0(\theta)$ is a holomorphic function from $B_{\theta_0}^{\mathbf{C}}$ into $\mathcal{L}(L_2(\mathbf{I}^d))$ since the H_θ form a holomorphic family of operators on $L_2(\mathbf{I}^d)$. But the semigroup estimates give the following stronger conclusion.

Lemma 3.1 *The map $\theta \mapsto P_0(\theta)$ is holomorphic from $B_{\theta_0}^{\mathbf{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), L_\infty(\mathbf{I}^d))$.*

Proof First note that $P_0(\theta) = e^{2\lambda_0(\theta)} S_1^\theta P_0(\theta) S_1^\theta$. Hence

$$\|P_0(\theta)\|_{1 \rightarrow \infty} \leq e^{2\operatorname{Re} \lambda_0(\theta)} \|S_1^\theta\|_{1 \rightarrow 2} \|P_0(\theta)\|_{2 \rightarrow 2} \|S_1^\theta\|_{2 \rightarrow \infty}.$$

Therefore $\theta \mapsto \|P_0(\theta)\|_{1 \rightarrow \infty}$ is locally uniformly bounded.

Secondly, let $\psi, \varphi \in L_1(\mathbf{I}^d) \cap L_2(\mathbf{I}^d)$ and set $\varphi(\theta) = P_0(\theta)\varphi$. Then $\theta \mapsto \varphi(\theta)$ is a holomorphic function from $B_{\theta_0}^{\mathbf{C}}$ into $L_2(\mathbf{I}^d)$ and with derivative $\partial\varphi(\theta)/\partial\theta_j \in L_2(\mathbf{I}^d)$ for all j . Moreover, for all $\theta \in B_{\theta_0}^{\mathbf{C}}$ one has

$$\begin{aligned} (\psi, \varphi(\theta + \eta) - \varphi(\theta) - \sum_{j=1}^d \eta_j \frac{\partial}{\partial \theta_j} \varphi(\theta)) &= (2\pi i)^{-d} \int_{\Gamma^d} d\xi_1 \dots d\xi_d (\psi, \varphi(\xi)) \cdot \\ &\cdot \left(\prod_{j=1}^d (\xi_j - \theta_j - \eta_j)^{-1} - \prod_{j=1}^d (\xi_j - \theta_j)^{-1} - \sum_{k=1}^d \frac{\eta_k}{(\xi_k - \theta_k)} \prod_{j=1}^d (\xi_j - \theta_j)^{-1} \right) \end{aligned}$$

for all $\eta \in \mathbf{C}^d$ with $|\eta|$ small enough, where Γ is a positively-oriented circle around the origin with radius $2^{-1}(\theta_0 + \max_{k \in \{1, \dots, d\}} |\theta_j|)$. One readily deduces that there is an $M > 0$ such that

$$\begin{aligned} |(\psi, \varphi(\theta + \eta) - \varphi(\theta) - \sum_{j=1}^d \eta_j \frac{\partial}{\partial \theta_j} \varphi(\theta))| &\leq M |\eta|^2 \|\psi\|_1 \sup_{\xi \in \Gamma^d} \|\varphi(\xi)\|_\infty \\ &\leq M |\eta|^2 \sup_{\xi \in \Gamma^d} \|P_0(\xi)\|_{1 \rightarrow \infty} \|\psi\|_1 \|\varphi\|_1 \end{aligned}$$

uniformly for all $\psi, \varphi \in L_1(\mathbf{I}^d) \cap L_2(\mathbf{I}^d)$ and all small $|\eta|$. Then $\partial\varphi(\theta)/\partial\theta_j \in L_\infty(\mathbf{I}^d)$ for all j and

$$\|\varphi(\theta + \eta) - \varphi(\theta) - \sum_{j=1}^d \eta_j \frac{\partial}{\partial \theta_j} \varphi(\theta)\|_\infty \leq M |\eta|^2 \sup_{\xi \in \Gamma^d} \|P_0(\xi)\|_{1 \rightarrow \infty} \|\varphi\|_1$$

uniformly for all $\varphi \in L_1(\mathbf{I}^d) \cap L_2(\mathbf{I}^d)$ and all small $|\eta|$. So $\theta \mapsto \varphi(\theta)$ is holomorphic from $B_{\theta_0}^{\mathbf{C}}$ into $L_\infty(\mathbf{I}^d)$ and the desired conclusion follows immediately since $L_1(\mathbf{I}^d) \cap L_2(\mathbf{I}^d)$ is dense in $L_1(\mathbf{I}^d)$. \square

After these preliminaries we come to the first important step in the derivation of the Gaussian bounds. We prove that for large t the essential contribution to the kernel comes from the small θ components in the periodic decomposition and these contributions are dominated by the lowest eigenstate. For $\delta \in \langle 0, \theta_0 \rangle$ define

$$P_0(B_\delta) = \Phi^{-1} \left((2\pi)^{-d} \int_{B_\delta}^{\oplus} d\theta P_0(\theta) \right) \Phi \quad .$$

Then $P_0(B_\delta)$ is a projection on $L_2(\mathbf{R}^d)$.

Lemma 3.2 *There exist $\mu > 0$ and for all $\delta \in \langle 0, \theta_0 \rangle$ a $c > 0$ such that*

$$\|S_t(I - P_0(B_\delta))\|_{1 \rightarrow \infty} \leq c e^{-\mu t}$$

uniformly for all $t \geq 1$.

Proof Let $\mu > 0$ be as in Proposition 2.10 and $\delta \in \langle 0, \theta_0 \rangle$. Then it follows from (6) and Lemma 2.1 that

$$\|S_t(I - P_0(B_\delta))\|_{1 \rightarrow \infty} \leq (2\pi)^{-d} \int_{[-\pi, \pi]^d \setminus B_\delta} d\theta \|S_t^\theta\|_{1 \rightarrow \infty} + (2\pi)^{-d} \int_{B_\delta} d\theta \|S_t^\theta(I - P_0(\theta))\|_{1 \rightarrow \infty}$$

for all $t > 0$. We estimate the two terms separately.

It follows from Corollary 2.3, the estimates (10) and the semigroup property that there exists a $c > 0$ such that $\|S_t^\theta\|_{1 \rightarrow \infty} \leq c e^{-2^{-1}\mu_C \delta^2 t}$ uniformly for all $t \geq 1$ and $\theta \in [-\pi, \pi]^d \setminus B_\delta$. So

$$(2\pi)^{-d} \int_{[-\pi, \pi]^d \setminus B_\delta} d\theta \|S_t^\theta\|_{1 \rightarrow \infty} \leq c e^{-2^{-1}\mu_C \delta^2 t}$$

for all $t \geq 1$.

Alternatively, for the integral over B_δ we use the semigroup property. Then

$$\|S_t^\theta(I - P_0(\theta))\|_{1 \rightarrow \infty} \leq \|S_{t/3}^\theta\|_{1 \rightarrow 2} \|S_{t/3}^\theta(I - P_0(\theta))\|_{2 \rightarrow 2} \|S_{t/3}^\theta\|_{2 \rightarrow \infty}$$

for all $\theta \in [-\pi, \pi]^d$ and $t > 0$. But $\|P_0(\theta) - P_0(0)\|_{2 \rightarrow 2} \leq 1$ for all $\theta \in B_{\theta_0}^{\mathbf{C}}$. Hence $\|S_{t/3}^\theta(I - P_0(\theta))\|_{2 \rightarrow 2} \leq 2e^{-3^{-1}\mu t}$ uniformly for all $t > 0$ and $\theta \in B_\delta$, by Proposition 2.10. Again using the estimates (10) it follows that there is a $c' > 0$ such that

$$\|S_t^\theta(I - P_0(\theta))\|_{1 \rightarrow \infty} \leq c' e^{-4^{-1}\mu t}$$

uniformly for all $t \geq 1$ and $\theta \in B_\delta$. Combination of these estimates completes the proof. \square

The second important step in the proof of Gaussian bounds is the comparison of the kernel K with the corresponding kernel \widehat{K} of the homogenized system. Now the semigroup \widehat{S} generated by the homogenized operator \widehat{H} can be approximated as in Lemma 3.2 but with the eigenvalue $\hat{\lambda}_0(\theta)$ and eigenprojector $\widehat{P}_0(\theta)$ corresponding to \widehat{H}_θ . Hence to compare K and \widehat{K} one must compare the eigenvalues λ_0 , $\hat{\lambda}_0$ and the eigenprojectors P_0 , \widehat{P}_0 . The next proposition gives the key eigenvalue comparison.

Let $\hat{\varepsilon}_0$, $\hat{\theta}_0$ and $\hat{\lambda}_0$ be the parameters of Proposition 2.7 corresponding to the operator \widehat{H} .

Proposition 3.3 *There exists a $c > 0$ such that $|\lambda_0(\theta) - \hat{\lambda}_0(\theta)| \leq c|\theta|^3$ uniformly for $\theta \in B_{2^{-1}(\theta_0 \wedge \hat{\theta}_0)}^{\mathbf{C}}$.*

Proof Since \widehat{H}_θ is an operator with constant coefficients one has $\widehat{H}_\theta \mathbf{1} = (\theta, \widehat{C}\theta) \mathbf{1}$. So $\hat{\lambda}_0(\theta) = (\theta, \widehat{C}\theta)$ for all $\theta \in B_{\hat{\theta}_0}^{\mathbf{C}}$ by the last statement of Proposition 2.7.

The maps λ_0 and $\theta \mapsto \varphi_\theta$ are holomorphic on $B_{\theta_0}^{\mathbf{C}}$, so by Lemma 2.8 for all $\alpha \in J(d) = \bigcup_{n=0}^{\infty} \{1, \dots, d\}^n$ there are $\lambda_\alpha \in \mathbf{C}$ and $\varphi_\alpha \in L_{2;1}(\mathbf{I}^d)$ such that

$$\lambda_0(\theta) = \sum_{\alpha \in J(d)} \lambda_\alpha \theta^\alpha \quad \text{and} \quad \varphi_\theta = \sum_{\alpha \in J(d)} \theta^\alpha \varphi_\alpha$$

for all $\theta \in B_{\theta_0}^{\mathbf{C}}$. The second series converges both in $L_2(\mathbf{I}^d)$ and in $L_{2;1}(\mathbf{I}^d)$. Then $\lambda_\alpha = 0$ and $\varphi_\alpha = \mathbf{1}$ if $|\alpha| = 0$, since $\lambda_0(0) = 0$ and $\varphi_0 = \mathbf{1}$, where $|\alpha| = n$ if $\alpha = (i_1, \dots, i_n) \in J(d)$. But for all $\psi \in L_{2;1}(\mathbf{R}^d)$ one has

$$\begin{aligned} \sum_{\beta \in J(d)} \lambda_\beta \theta^\beta \sum_{\gamma \in J(d)} (\psi, \theta^\gamma \varphi_\gamma) &= \lambda_0(\theta) (\psi, \varphi_\theta) = (\psi, H_\theta \varphi_\theta) \\ &= \sum_{k,l=1}^d \sum_{\alpha \in J(d)} ((\partial_k + i\bar{\theta}_k)\psi, c_{ki}(\partial_l + i\theta_l)\theta^\alpha \varphi_\alpha) \end{aligned} \quad (11)$$

for all $\theta \in B_{\theta_0}^{\mathbf{C}}$.

Let $m \in \{1, \dots, d\}$. Then comparing coefficients of θ_m gives

$$\lambda_{(m)}(\psi, \mathbf{1}) = h_0(\psi, \varphi_{(m)}) + \sum_{k=1}^d i(\partial_k \psi, c_{km} \mathbf{1}) \quad .$$

Taking $\psi = \mathbf{1}$ gives $\lambda_{(m)} = 0$. Moreover,

$$h_0(\psi, \varphi_{(m)}) = -i \sum_{k=1}^d (\partial_k \psi, c_{km} \mathbf{1}) \quad (12)$$

for all $\psi \in L_{2;1}(\mathbf{I}^d)$ and hence

$$\partial_l \varphi_{(m)} = -i \sum_{k=1}^d X_{lk} c_{km} \quad (13)$$

for all $l \in \{1, \dots, d\}$, by Lemmas 2.11 and 2.12.

Next let $m, n \in \{1, \dots, d\}$ with $m \neq n$. Then comparing coefficients of $\theta_m \theta_n$ in (11) gives

$$\begin{aligned} \lambda_{(m,n)}(\psi, \mathbf{1}) + \lambda_{(n,m)}(\psi, \mathbf{1}) &= h_0(\psi, \varphi_{(m,n)}) + h_0(\psi, \varphi_{(n,m)}) \\ &\quad + \sum_{l=1}^d (i\psi, c_{ml} \partial_l \varphi_{(n)}) + \sum_{k=1}^d (\partial_k \psi, c_{km} i \varphi_{(n)}) \\ &\quad + \sum_{l=1}^d (i\psi, c_{nl} \partial_l \varphi_{(m)}) + \sum_{k=1}^d (\partial_k \psi, c_{kn} i \varphi_{(m)}) \\ &\quad + (\psi, c_{mn} \mathbf{1}) + (\psi, c_{nm} \mathbf{1}) \end{aligned}$$

for all $\psi \in L_{2;1}(\mathbf{I}^d)$. Substituting $\psi = \mathbf{1}$ one finds

$$\begin{aligned} \lambda_{(m,n)} + \lambda_{(n,m)} &= -i \sum_{l=1}^d (\mathbf{1}, c_{ml} \partial_l \varphi_{(n)}) - i \sum_{l=1}^d (\mathbf{1}, c_{nl} \partial_l \varphi_{(m)}) + \int_{\mathbf{I}^d} c_{mn} + \int_{\mathbf{I}^d} c_{nm} \\ &= - \sum_{k,l=1}^d (\mathbf{1}, c_{ml} X_{lk} c_{kn}) - \sum_{k,l=1}^d (\mathbf{1}, c_{nl} X_{lk} c_{km}) + \int_{\mathbf{I}^d} c_{mn} + \int_{\mathbf{I}^d} c_{nm} \\ &= \hat{c}_{mn} + \hat{c}_{nm} \end{aligned}$$

by (13). Similarly,

$$\lambda_{(n,n)} = - \sum_{k,l=1}^d (\mathbf{1}, c_{nl} X_{lk} c_{kn}) + \int_{\mathbf{I}^d} c_{nn} = \hat{c}_{nn}$$

for all $n \in \{1, \dots, d\}$. So

$$\lambda_0(\theta) = \hat{\lambda}_0(\theta) + \sum_{|\alpha| \geq 3} \lambda_\alpha \theta^\alpha$$

for all $\theta \in B_{\theta_0 \wedge \hat{\theta}_0}^{\mathbf{C}}$ and the proposition follows. \square

The above calculation also gives the first-order term in the Taylor expansion of the holomorphic function $\theta \mapsto P_0(\theta)$. For $m \in \{1, \dots, d\}$ define

$$\chi_m = \sum_{k=1}^d X_k(C) c_{km} \in L_2(\mathbf{I}^d) \quad \text{and} \quad \chi_m^t = \sum_{k=1}^d X_k(C^t) c_{km}^t \in L_2(\mathbf{I}^d) \quad ,$$

where $C^t = (c_{km}^t)$ with $c_{km}^t = c_{mk}$ denotes the transpose matrix. These functions are the first-order correctors of homogenization theory ([BLP], [ZKO]). For $\theta \in B_{\theta_0}^{\mathbf{C}}$ and $m \in \{1, \dots, d\}$ let $P_0^{(m)}(\theta) = \partial P_0(\theta) / \partial \theta_m$.

Corollary 3.4 *If $m \in \{1, \dots, d\}$ then $\chi_m, \chi_m^t \in L_\infty(\mathbf{I}^d)$. Moreover,*

$$P_0^{(m)}(0) \varphi = i \chi_m P_0(0) \varphi - i P_0(0) (\chi_m^t \varphi)$$

for all $\varphi \in L_2(\mathbf{I}^d)$.

Proof If $\varphi_\theta = P_0(\theta) \mathbf{1}$ and $\varphi_\theta^\dagger = P_0(\theta)^* \mathbf{1}$ then

$$(\psi, P_0(\theta) \varphi) = \frac{(\psi, \varphi_\theta)(\varphi_\theta^\dagger, \varphi)}{(\varphi_\theta^\dagger, \varphi_\theta)} \quad .$$

Hence we must calculate the coefficient of θ_m on the right hand side and identify it with the expression for $(\psi, P_0^{(m)}(0) \varphi)$. But it follows from (12) and Lemma 2.12 that

$$\varphi_\theta = \mathbf{1} + i \sum_{m=1}^d \theta_m \left(\sum_{k=1}^d X_k(C) c_{km} + a_m \mathbf{1} \right) + O(|\theta|^2) = \mathbf{1} + i \sum_{m=1}^d \theta_m \mathbf{1} (\chi_m + a_m \mathbf{1}) + O(|\theta|^2)$$

for some $a \in \mathbf{C}^d$. Similarly

$$\varphi_\theta^\dagger = \mathbf{1} + i \sum_{m=1}^d \overline{\theta_m} \left(\sum_{k=1}^d \overline{X_k(C^t)} \overline{c_{km}^t} + a_m^\dagger \mathbf{1} \right) + O(|\theta|^2) = \mathbf{1} + i \sum_{m=1}^d \overline{\theta_m} (\overline{\chi_m^t} + a_m^\dagger \mathbf{1}) + O(|\theta|^2)$$

for some $a^\dagger \in \mathbf{C}^d$. Hence

$$(\varphi_\theta^\dagger, \varphi_\theta) = 1 + i \sum_{m=1}^d (a_m - \overline{a_m^\dagger}) \theta_m + O(|\theta|^2)$$

because $(\mathbf{1}, X_k(C)c_{km}) = 0 = (X_k(C^t)c_{km}^t, \mathbf{1})$. Therefore

$$(\psi, P_0^{(m)}(\mathbf{0})\varphi) = (\psi, i\chi_m)(\mathbf{1}, \varphi) + (\psi, \mathbf{1})(i\overline{\chi_m^t}, \varphi) \quad (14)$$

for all $\varphi, \psi \in L_2(\mathbf{I}^d)$, by a simple calculation. The a_m, a_m^\dagger give no contribution to the first order terms.

Next, the map $\theta \mapsto P_0(\theta)$ is holomorphic from $B_{\hat{\theta}_0}^{\mathbf{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), L_\infty(\mathbf{I}^d))$, by Lemma 3.1. So $P_0^{(m)}(\theta) \in \mathcal{L}(L_1(\mathbf{I}^d), L_\infty(\mathbf{I}^d))$ for all $\theta \in B_{\hat{\theta}_0}^{\mathbf{C}}$. Therefore $\chi_m = -iP_0^{(m)}(\mathbf{0})\mathbf{1} \in L_\infty(\mathbf{I}^d)$ since χ_m^t has mean value zero. Replacing C by C^t gives the same for χ_m^t . Note that this implies that

$$\varphi_\theta = \mathbf{1} + i \sum_{m=1}^d \theta_m \chi_m + O(|\theta|^2) \quad (15)$$

both in the L_2 -, and the L_∞ -sense. The last statement rephrases (14). \square

The most important step in the proof of Gaussian bounds is to show that the homogenized kernel \widehat{K} gives a first-order asymptotic approximation to K .

Theorem 3.5 *There exists a $c > 0$ such that*

$$\|K_t - \widehat{K}_t\|_\infty \leq c t^{-1/2} t^{-d/2}$$

uniformly for all $t \geq 1$.

Proof Since $\widehat{H}_\theta \mathbf{1} = (\theta, \widehat{C}\theta)\mathbf{1}$ it follows that $\widehat{P}_0(\theta)$ is a (possibly non-orthogonal) projection onto the constant functions. But similarly $(\widehat{H}_\theta)^* \mathbf{1} = (\theta, \widehat{C}\theta)^* \mathbf{1}$ and hence $\widehat{P}_0(\theta)^*$ is also a projection onto the constant functions. Therefore $\widehat{P}_0(\theta) = P_0(\mathbf{0})$ is the orthogonal projection onto the constant functions for all $\theta \in B_{\hat{\theta}_0}^{\mathbf{C}}$.

Next, by Lemma 3.2 there exist $c, \mu > 0$ such that

$$\|S_t(I - P_0(B_\delta))\|_{1 \rightarrow \infty} \leq c e^{-\mu t} \quad \text{and} \quad \|\widehat{S}_t(I - \widehat{P}_0(B_\delta))\|_{1 \rightarrow \infty} \leq c e^{-\mu t}$$

uniformly for all $t \geq 1$, where $\delta = 2^{-1}(\theta_0 \wedge \hat{\theta}_0)$. Then

$$\|S_t - \widehat{S}_t\|_{1 \rightarrow \infty} \leq 2c e^{-\mu t} + \|S_t P_0(B_\delta) - \widehat{S}_t \widehat{P}_0(B_\delta)\|_{1 \rightarrow \infty}$$

for all $t \geq 1$. Hence it follows from Lemma 2.1 that one needs to estimate $\|e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\hat{\lambda}_0(\theta)t} P_0(\mathbf{0})\|_{1 \rightarrow \infty}$ for all $\theta \in B_\delta$. Obviously one has the decomposition

$$\begin{aligned} \|e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\hat{\lambda}_0(\theta)t} P_0(\mathbf{0})\|_{1 \rightarrow \infty} &\leq |e^{-\lambda_0(\theta)t} - e^{-\hat{\lambda}_0(\theta)t}| \|P_0(\mathbf{0})\|_{1 \rightarrow \infty} \\ &\quad + |e^{-\lambda_0(\theta)t}| \|P_0(\theta) - P_0(\mathbf{0})\|_{1 \rightarrow \infty} \end{aligned} \quad (16)$$

and we estimate the two terms separately.

The first term is easily handled with the eigenvalue estimates of Proposition 3.3. It follows from this proposition, Corollary 2.4 and a Duhamel estimate that

$$\begin{aligned} |e^{-\lambda_0(\theta)t} - e^{-\hat{\lambda}_0(\theta)t}| &= \left| t \int_0^1 ds e^{-t(s\lambda_0(\theta) + (1-s)\hat{\lambda}_0(\theta))} (\hat{\lambda}_0(\theta) - \lambda_0(\theta)) \right| \\ &\leq ct \int_0^1 ds e^{-t\mu c|\theta|^2} |\theta|^3 = ct |\theta|^3 e^{-t\mu c|\theta|^2} \end{aligned}$$

for a suitable $c > 0$ uniformly for all $t > 0$ and $\theta \in B_\delta$.

Next we consider the second term in (16). It follows from Lemma 3.1 that there is a $c > 0$ such that

$$\|P_0(\theta) - P_0(0)\|_{1 \rightarrow \infty} \leq c |\theta|$$

for all $\theta \in B_\delta$. Hence one deduces from Corollary 2.4 that there is a $c' > 0$ such that

$$\|e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\hat{\lambda}_0(\theta)t} P_0(0)\|_{1 \rightarrow \infty} \leq c' (|\theta| + t |\theta|^3) e^{-\mu c |\theta|^2 t} \quad (17)$$

uniformly for all $t > 0$ and $\theta \in B_\delta$. Then

$$\begin{aligned} \|S_t P_0(B_\delta) - \hat{S}_t \hat{P}_0(B_\delta)\|_{1 \rightarrow \infty} &\leq c' \int_{B_\delta} d\theta (|\theta| + t |\theta|^3) e^{-\mu c |\theta|^2 t} \\ &\leq c' \int_{\mathbf{R}^d} d\theta (|\theta| + t |\theta|^3) e^{-\mu c |\theta|^2 t} = c'' t^{-1/2} t^{-d/2} \quad , \end{aligned}$$

where $c'' = c' \int_{\mathbf{R}^d} d\theta e^{-\mu c |\theta|^2} (|\theta| + |\theta|^3)$.

It now follows by combination of these estimates that

$$\|S_t - \hat{S}_t\|_{1 \rightarrow \infty} \leq 2c e^{-\mu t} + c'' t^{-1/2} t^{-d/2} \quad (18)$$

uniformly for all $t \geq 1$. Thus one can now choose a $c' > 0$ such that

$$\|K_t - \widehat{K}_t\|_\infty = \|S_t - \hat{S}_t\|_{1 \rightarrow \infty} \leq c' t^{-1/2} t^{-d/2}$$

uniformly for all $t \geq 1$. □

By interpolation one deduces Gaussian bounds for the difference of K and \widehat{K} , together with a multiplicative factor which is almost $t^{-1/2}$.

Corollary 3.6 *For all $\varepsilon > 0$ there exist $b, c > 0$ such that*

$$|K_t(x; y) - \widehat{K}_t(x - y)| \leq ct^{-(1-\varepsilon)/2} G_{b,t}(x - y)$$

uniformly for all $t \geq 1$ and $x, y \in \mathbf{R}^d$.

Proof By Theorem 3.5 there exists a $c > 0$ such that

$$|K_t(x; y) - \widehat{K}_t(x - y)| \leq ct^{-1/2} t^{-d/2}$$

uniformly for all $t \geq 1$ and $x, y \in \mathbf{R}^d$. Next K satisfies the bounds (8) and because \widehat{H} is a strongly elliptic operator with constant coefficients \widehat{K} satisfies Gaussian bounds

$$|\widehat{K}_t(x - y)| \leq c' G_{b,t}(x - y) \quad .$$

Therefore there exist $b, c' > 0$ and $N \in \mathbf{N}$ such that

$$|K_t(x; y) - \widehat{K}_t(x - y)| \leq c' t^N t^{-d/2} e^{-b|x-y|^2 t^{-1}}$$

uniformly for all $t \geq 1$ and $x, y \in \mathbf{R}^d$. Then

$$\begin{aligned} |K_t(x; y) - \widehat{K}_t(x - y)| &= |K_t(x; y) - \widehat{K}_t(x - y)|^\varepsilon |K_t(x; y) - \widehat{K}_t(x - y)|^{1-\varepsilon} \\ &\leq (c')^\varepsilon c^{1-\varepsilon} t^{-(1-\varepsilon(1+2N))/2} t^{-d/2} e^{-b\varepsilon|x-y|^2 t^{-1}} \end{aligned}$$

for all $\varepsilon \in \langle 0, 1 \rangle$, $t \geq 1$ and $x, y \in \mathbf{R}^d$. The proof of the corollary is complete. \square

Finally the Gaussian bounds of Theorem 1.1.I are an immediate consequence. Since \widehat{K} satisfies Gaussian bounds uniformly for $t > 0$ the bounds follow for large t from Corollary 3.6. But for small t the bounds are well known.

3.2 Hölder estimates

In this subsection we prove the second statement of Theorem 1.1, the Gaussian bounds on the Hölder derivatives of the kernel K . The proof is similar in outline to the proof of Gaussian bounds in Subsection 3.1. We begin with the bounds of Auscher, [Aus] Theorem 4.3, which establish that for all $\nu \in \langle 0, 1 \rangle$ there exist $b, c > 0$ and $N \in \mathbf{N}$ such that

$$|K_t(x - h; y) - K_t(x; y)| \leq c (|h|t^{-1/2})^\nu (1 + t)^N G_{b,t}(x - y) \quad (19)$$

for all $h, x, y \in \mathbf{R}^d$ and $t > 0$ with $|h| \leq t^{1/2}$. These bounds rely on the uniform continuity of the coefficients. We use the spectral estimates to improve these bounds by removing the growth factor. The tactic is to estimate the difference between the Hölder derivative of K and the Hölder derivative of \widehat{K} .

Theorem 3.7 *There exists a $c > 0$ such that*

$$|(K_t - \widehat{K}_t)(x - h; y) - (K_t - \widehat{K}_t)(x; y)| \leq c t^{-(1-\nu)/2} (|h|t^{-1/2})^\nu t^{-d/2}$$

uniformly for all $t \geq 1$ and $x, y, h, \in \mathbf{R}^d$.

Proof The basic idea of the proof is to prove first uniform bounds

$$\|(I - U(h))(S_t - \widehat{S}_t)\|_{1 \rightarrow \infty} \leq c |h|^\nu t^{-1/2} t^{-d/2} \quad (20)$$

uniformly for all $h \in \mathbf{R}^d$ and $t \geq 1$ with $|h| \leq 1$ and then remove the restriction on $|h|$.

Again we use decomposition theory to isolate the principal contribution which comes from the lowest eigenstate. This is an elaboration of the arguments of Subsection 3.1 but the decomposition of translations introduces an additional term.

Fix $\nu \in \langle 0, 1 \rangle$. If $\delta = 2^{-1}(\theta_0 \wedge \widehat{\theta}_0)$, as before, then by Lemma 3.2 there exist $c, \mu > 0$ such that $\|S_t(I - P_0(B_\delta))\|_{1 \rightarrow \infty} \leq c e^{-\mu t}$ uniformly for all $t \geq 1$. Then there is a $c' > 0$ such that

$$\|(I - U(h))S_t(I - P_0(B_\delta))\|_{1 \rightarrow \infty} \leq \|(I - U(h))S_1\|_{\infty \rightarrow \infty} \|S_{t-1}(I - P_0(B_\delta))\|_{1 \rightarrow \infty} \leq c' |h|^\nu e^{-\mu t}$$

uniformly for all $h \in \mathbf{R}^d$ with $|h| \leq 1$ and $t \geq 2$. Since similar estimates are valid for \widehat{S} we will have proved (20) once we can show that there is a $c > 0$ such that

$$\|(I - U(h))(S_t P_0(B_\delta) - \widehat{S}_t \widehat{P}_0(B_\delta))\|_{1 \rightarrow \infty} \leq c |h|^\nu t^{-1/2} t^{-d/2}$$

uniformly for all $h \in \mathbf{R}^d$ and $t \geq 1$ with $|h| \leq 1$.

If $\varphi \in L_2(\mathbf{I}^d)$ and $h \in \mathbf{R}^d$ define $L(h)\varphi \in L_2(\mathbf{I}^d)$ by $(L(h)\varphi)(u) = \tau(e^{2\pi i(u-h)})$ where $\tau \in L_2(\mathbf{T}^d)$ is given by $\tau(e^{2\pi i u}) = \varphi(u)$. Then $L(h)$ is a unitary operator and it follows that the operator U of translations on \mathbf{R}^d has the decomposition

$$\Phi U(h) \Phi^{-1} = (2\pi)^{-d} \int_{[-\pi, \pi]^d}^\oplus d\theta e^{-i\theta \cdot h} L(h) \quad (21)$$

for all $h \in \mathbf{R}^d$. Therefore

$$\begin{aligned} & \Phi(I - U(h))(S_t P_0(B_\delta) - \widehat{S}_t \widehat{P}_0(B_\delta))\Phi^{-1} \\ &= (2\pi)^{-d} \int_{B_\delta} d\theta (1 - e^{-i\theta \cdot h})(e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\widehat{\lambda}_0(\theta)t} P_0(0)) \\ & \quad + (2\pi)^{-d} \int_{B_\delta} d\theta e^{-i\theta \cdot h} (I - L(h))(e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\widehat{\lambda}_0(\theta)t} P_0(0)) \end{aligned}$$

for all $h \in \mathbf{R}^d$ and $t > 0$. Then by Lemma 2.1

$$\begin{aligned} & \|(I - U(h))(S_t P_0(B_\delta) - \widehat{S}_t \widehat{P}_0(B_\delta))\|_{1 \rightarrow \infty} \\ & \leq (2\pi)^{-d} \int_{B_\delta} d\theta |1 - e^{-i\theta \cdot h}| \|e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\widehat{\lambda}_0(\theta)t} P_0(0)\|_{1 \rightarrow \infty} \\ & \quad + (2\pi)^{-d} \int_{B_\delta} d\theta \|(I - L(h))(e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\widehat{\lambda}_0(\theta)t} P_0(0))\|_{1 \rightarrow \infty} \quad . \quad (22) \end{aligned}$$

The first term on the right hand side is the additional contribution from the decomposition of the translation. If c' is as in (17) then

$$\begin{aligned} & (2\pi)^{-d} \int_{B_\delta} d\theta |1 - e^{-i\theta \cdot h}| \|e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\widehat{\lambda}_0(\theta)t} P_0(0)\|_{1 \rightarrow \infty} \\ & \leq (2\pi)^{-d} c' \int_{B_\delta} d\theta |h| |\theta| (|\theta| + t |\theta|^3) e^{-\mu c |\theta|^2 t} \\ & \leq c' |h| \int_{\mathbf{R}^d} d\theta |\theta| (|\theta| + t |\theta|^3) e^{-\mu c |\theta|^2 t} \\ & = c'' |h| t^{-(d+2)/2} \leq c'' t^{-1/2} (|h| t^{-1/2})^\nu t^{-d/2} \end{aligned}$$

for all $h \in \mathbf{R}^d$ and $t > 0$ with $|h| \leq t^{1/2}$ and $c'' = c' \int_{\mathbf{R}^d} d\theta e^{-\mu c |\theta|^2} |\theta| (|\theta| + |\theta|^3)$.

The second term on the right hand side of (22) can be estimated by the reasoning of Subsection 3.1. First we need some preliminary estimates comparable to (10).

If one extends the function $u \mapsto K_t^\theta(u; v)$ to a periodic function on \mathbf{R}^d for all $v \in \mathbf{I}^d$ then

$$K_t^\theta(x; v) = \sum_{n \in \mathbf{Z}^d} e^{i(n-x+v) \cdot \theta} K_t(x - n; v)$$

for all $\theta \in \mathbf{C}^d$, $t > 0$, $x \in \mathbf{R}^d$ and $v \in \mathbf{I}^d$. Using the bounds (19) and the Gaussian bounds of Theorem 1.1.I it follows that there are $b, c, \omega > 0$ and $N \in \mathbf{N}$ such that

$$\begin{aligned} |K_t^\theta(u-h;v) - K_t^\theta(u;v)| &\leq \sum_{n \in \mathbf{Z}^d} |e^{i(n-u+h+v)\cdot\theta} - e^{i(n-u+v)\cdot\theta}| |K_t(u-n;v)| \\ &\quad + \sum_{n \in \mathbf{Z}^d} |e^{i(n-u+h+v)\cdot\theta}| |K_t(u-h-n;v) - K_t(u-n;v)| \\ &\leq c|h|t^{1/2}(1 \wedge t)^{-d/2}e^{-b\|u-v\|^2t^{-1}}e^{\omega(\operatorname{Im}\theta)^2t} \\ &\quad + c(|h|t^{-1/2})^\nu(1+t)^N(1 \wedge t)^{-d/2}e^{-b\|u-h-v\|^2t^{-1}}e^{\omega(\operatorname{Im}\theta)^2t} \end{aligned}$$

uniformly for all $\theta \in \mathbf{C}^d$, $t > 0$, $h \in \mathbf{R}^d$ and $u, v \in \mathbf{I}^d$ with $|h| \leq t^{1/2} \wedge 1$. Since $(u, v) \mapsto K^\theta(u-h;v)$ is the kernel of the operator $L(h)S_t^\theta$ it follows that there are $c, \omega > 0$ such that

$$\|(I-L(h))S_t^\theta\|_{p \rightarrow q} \leq c(|h|t^{-1/2})^\nu(1+t)^N(1 \wedge t)^{-d(1/p-1/q)/2}e^{\omega(\operatorname{Im}\theta)^2t} \quad (23)$$

uniformly for all $1 \leq p \leq q \leq \infty$, $\theta \in \mathbf{C}^d$, $t > 0$ and $h \in \mathbf{R}^d$ with $|h| \leq t^{1/2} \wedge 1$.

Next define the Banach space

$$\mathcal{C}^\nu = \{\varphi \in C(\mathbf{I}^d) : \sup_{0 < |h| \leq 1} |h|^{-\nu} \|(I-L(h))\varphi\|_\infty < \infty\}$$

with norm $\|\varphi\|_{\mathcal{C}^\nu} = \|\varphi\|_\infty + \sup_{0 < |h| \leq 1} |h|^{-\nu} \|(I-L(h))\varphi\|_\infty$. Note that $\varphi(u_1, \dots, 0, \dots, u_d) = \varphi(u_1, \dots, 1, \dots, u_d)$ for all $\varphi \in \mathcal{C}^\nu$, $u \in \mathbf{I}^d$ and $k \in \{1, \dots, d\}$, where the 0 and 1 are in the k -th position. Then (23) together with (10) implies that S_t^θ is a bounded operator from $L_1(\mathbf{I}^d)$ into \mathcal{C}^ν and

$$\|S_t^\theta\|_{L_1(\mathbf{I}^d) \rightarrow \mathcal{C}^\nu} \leq c(1+t)^N(1 \wedge t)^{-d(1/p-1/q)/2}e^{\omega(\operatorname{Im}\theta)^2t}$$

uniformly for all $1 \leq p \leq q \leq \infty$, $\theta \in \mathbf{C}^d$ and $t > 0$. In particular, the family of operators is bounded locally uniform in θ . Arguing as in the proof of Lemma 3.1 it follows that the spectral projections $\theta \mapsto P_0(\theta)$ form a holomorphic family of operators from $B_{\theta_0}^{\mathbf{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), \mathcal{C}^\nu)$. Hence there is a $c > 0$ such that $\|P_0(\theta) - P_0(0)\|_{L_1(\mathbf{I}^d) \rightarrow \mathcal{C}^\nu} \leq c|\theta|$ uniformly for all $\theta \in B_\delta$. In particular

$$\|(I-L(h))(P_0(\theta) - P_0(0))\|_{1 \rightarrow \infty} \leq c|\theta||h|^\nu$$

for all $\theta \in B_\delta$ and $h \in \mathbf{R}^d$ with $|h| \leq 1$. This gives estimates, as in the proof of Theorem 3.5,

$$(2\pi)^{-d} \int_{B_\delta} d\theta \|(I-L(h))(e^{-\lambda_0(\theta)t}P_0(\theta) - e^{-\hat{\lambda}_0(\theta)t}P_0(0))\|_{1 \rightarrow \infty} \leq c't^{-1/2}|h|^\nu t^{-d/2}$$

uniformly for all $h \in \mathbf{R}^d$ and $t \geq 1$ with $|h| \leq 1$ which bound the second term in (22).

Adding the contributions it follows that there exists a $c > 0$ such that

$$\|(I-U(h))(S_t - \hat{S}_t)\|_{1 \rightarrow \infty} \leq c t^{-1/2} |h|^\nu t^{-d/2} \quad (24)$$

uniformly for all $h \in \mathbf{R}^d$ and $t \geq 2$ with $|h| \leq 1$. But then it follows from (18) that (24) is also valid for all $h \in \mathbf{R}^d$ with $|h| \geq 1$ and by (19) also for $t \in [1, 2]$, with a possibly larger

value of c . So the estimates (24) are valid uniformly for all $h \in \mathbf{R}^d$ and $t \geq 1$ and the theorem follows. \square

With several applications of interpolation one can deduce rather sharp Gaussian bounds for the Hölder derivatives of the difference.

Theorem 3.8 *For all $\varepsilon, \nu, \tau \in \langle 0, 1 \rangle$ and $\kappa > 0$ there exist $b, c > 0$ such that*

$$|(K_t - \widehat{K}_t)(x - h; y - k) - (K_t - \widehat{K}_t)(x; y)| \leq c t^{-(1-\varepsilon)(1-\nu)/2} \left(\frac{|h| + |k|}{|x - y| + t^{1/2}} \right)^\nu G_{b,t}(x - y) \quad (25)$$

uniformly for all $t \geq 1$ and $x, y, h, k \in \mathbf{R}^d$ with $|h| + |k| \leq \tau|x - y| + \kappa t^{1/2}$.

Proof Interpolation of the bounds of Theorem 3.7 with the bounds (19) of Auscher, which are of course also valid for \widehat{K} , implies that for all $\varepsilon \in \langle 0, 1 \rangle$ there exist $b, c > 0$ such that

$$|(K_t - \widehat{K}_t)(x - h; y) - (K_t - \widehat{K}_t)(x; y)| \leq c (|h|t^{-1/2})^\nu t^{-(1-\varepsilon)(1-\nu)/2} G_{b,t}(x - y)$$

uniformly for all $t \geq 1$ and $h, x, y \in \mathbf{R}^d$ with $|h| \leq t^{1/2}$.

These bounds are a special case of (25). To obtain the general bounds we use two additional arguments.

First it follows from the last bounds that for all $\varepsilon \in \langle 0, 1 \rangle$ there exists a $c > 0$ such that

$$\|(I - U(h))(S_t - \widehat{S}_t)\|_{2 \rightarrow \infty} \leq c (|h|t^{-1/2})^\nu t^{-(1-\varepsilon)(1-\nu)/2} t^{-d/4} \quad (26)$$

uniformly for all $h \in \mathbf{R}^d$ and $t \geq 1$ with $|h| \leq t^{1/2}$. But by Theorem 3.5 and increasing the value of c it follows that the bounds (26) are valid uniformly for all $h \in \mathbf{R}^d$ and $t \geq 1$. The semigroup \widehat{S} satisfies similar bounds: there exists a $c > 0$ such that

$$\|(I - U(h))\widehat{S}_t\|_{2 \rightarrow \infty} \leq c (|h|t^{-1/2})^\nu t^{-d/4}$$

for all $h \in \mathbf{R}^d$ and $t > 0$. So there is a $c > 0$ such that

$$\|(I - U(h))S_t\|_{2 \rightarrow \infty} \leq c (|h|t^{-1/2})^\nu t^{-d/4}$$

for all $h \in \mathbf{R}^d$ and $t \geq 1$. Then by the previous estimates and duality one deduces that for all $\varepsilon \in \langle 0, 1 \rangle$ there exists a $c > 0$ such that

$$\begin{aligned} \|(I - U(h))(S_t - \widehat{S}_t)(I - U(k))\|_{1 \rightarrow \infty} &\leq \|(I - U(h))S_{t/2}\|_{2 \rightarrow \infty} \|(S_{t/2} - \widehat{S}_{t/2})(I - U(k))\|_{1 \rightarrow 2} \\ &\quad + \|(I - U(h))(S_{t/2} - \widehat{S}_{t/2})\|_{2 \rightarrow \infty} \|\widehat{S}_{t/2}(I - U(k))\|_{1 \rightarrow \infty} \\ &\leq c (|h| |k| t^{-1})^\nu t^{-(1-\varepsilon)(1-\nu)/2} t^{-d/2} \end{aligned}$$

for all $h, k \in \mathbf{R}^d$ and $t \geq 2$. Together with the estimates of Theorem 3.7 and duality one establishes that for all $\varepsilon \in \langle 0, 1 \rangle$ there exists a $c > 0$ such that

$$\begin{aligned} |(K_t - \widehat{K}_t)(x - h; y - k) - (K_t - \widehat{K}_t)(x; y)| \\ \leq c \left((|h| |k| t^{-1})^\nu + (|h|t^{-1/2})^\nu + (|k|t^{-1/2})^\nu \right) t^{-(1-\varepsilon)(1-\nu)/2} t^{-d/2} \end{aligned}$$

uniformly for all $h, k, x, y \in \mathbf{R}^d$ and $t \geq 1$.

Finally we can apply Lemma 4.2 of [ELR2]. This lemma allows one to interpolate between the last bounds and the bounds of Corollary 3.6 to obtain the bounds (25) for any slightly smaller ν . \square

Obviously Theorem 1.1.II is an immediate consequence of Theorem 3.8.

3.3 Asymptotic estimates

In the foregoing derivation of kernel bounds the estimate of Theorem 3.5 played a key role. The proof of this estimate can, in principle, be extended to obtain a complete asymptotic expansion of K in terms of \widehat{K} , the derivatives of \widehat{K} and the correctors of homogenization theory. In this subsection we discuss the first-order term in this expansion.

The zero-order term in the expansion was derived by first making a spectral decomposition, secondly approximating the components in terms of an integral over small $|\theta|$ of the contribution coming from the eigenprojector $P_0(\theta)$ and the eigenvalue $\lambda_0(\theta)$ and thirdly approximating the eigenprojector and eigenvalue by the lowest order terms in their holomorphic expansions. The first-order term in the expansion is derived by the same process but arises from the next terms in the holomorphic expansions. In the case of the eigenprojector this is the linear term in θ and for the eigenvalue the term of order θ^3 . The expansion for the eigenvalue has the form

$$\lambda_0(\theta) = \hat{\lambda}_0(\theta) + \sum_{\alpha \in J(d); |\alpha| \geq 3} \lambda_\alpha \theta^\alpha$$

for $\theta \in B_{\theta_0 \wedge \hat{\theta}_0}^{\mathbf{C}}$ as a consequence of Proposition 3.3.

Lemma 3.9 *For all $m \in \{1, \dots, d\}$ the correctors χ_m and χ_m^t extend to continuous periodic functions on \mathbf{R}^d .*

Proof It follows from (15) that $P_0(\theta)\mathbb{1} = \varphi_\theta = \mathbb{1} + i \sum_{m=1}^d \theta_m \chi_m + O(|\theta|^2)$ in the L_∞ -sense. But the map $\theta \mapsto P_0(\theta)$ is holomorphic from $B_{\theta_0}^{\mathbf{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), \mathcal{C}^\nu)$, by the proof of Theorem 3.7. Hence $\chi_m \in \mathcal{C}^\nu$ for all $m \in \{1, \dots, d\}$ and it extends to a continuous periodic function on \mathbf{R}^d . \square

Proposition 3.10 *There exists a $c > 0$ such that*

$$\begin{aligned} |K_t(x; y) - \widehat{K}_t(x - y) - \sum_{m=1}^d (\chi_m(x) - \chi_m^t(y)) (\partial_m \widehat{K}_t)(x - y) \\ - it \sum_{\alpha \in J(d); |\alpha|=3} \lambda_\alpha (\partial^\alpha \widehat{K}_t)(x - y)| \leq c t^{-1} t^{-d/2} \end{aligned}$$

uniformly for all $t \geq 1$ and $x, y \in \mathbf{R}^d$.

Remark Each term occurring in the difference estimated in the proposition satisfies a Gaussian bound. Therefore one can interpolate between the uniform bound of the proposition and the Gaussian bounds to obtain a Gaussian bound for the difference. Then, for each $\varepsilon > 0$, one obtains a bound $c t^{-(1-\varepsilon)} G_{b,t}(x - y)$ for $t \in [1, \infty)$.

Proof of Proposition 3.10 The proof is based on the same reasoning used to prove Theorem 3.5 and we only sketch the main ideas. First it follows from the previous proof that one has bounds

$$\|S_t - \widehat{S}_t - S_t P_0(B_\delta) + \widehat{S}_t \widehat{P}_0(B_\delta)\|_{1 \rightarrow \infty} \leq c e^{-\mu t} \quad (27)$$

for all $t \geq 1$. To estimate $S_t P_0(B_\delta) - \widehat{S}_t \widehat{P}_0(B_\delta)$ we now use the identity

$$\begin{aligned} e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\widehat{\lambda}_0(\theta)t} P_0(0) &= e^{-\widehat{\lambda}_0(\theta)t} \left((P_0(\theta) - P_0(0)) + t(\widehat{\lambda}_0(\theta) - \lambda_0(\theta)) P_0(0) \right) \\ &\quad + t e^{-\widehat{\lambda}_0(\theta)t} (\widehat{\lambda}_0(\theta) - \lambda_0(\theta)) (P_0(\theta) - P_0(0)) \\ &\quad + t^2 (\widehat{\lambda}_0(\theta) - \lambda_0(\theta))^2 \int_0^1 ds (1-s) e^{-\widehat{\lambda}_0(\theta)t(1-s) - \lambda_0(\theta)ts} P_0(\theta) \end{aligned}$$

which is readily verified with two applications of the Duhamel identity.

The most significant contribution to the operator crossnorm comes from the term

$$L_t(\theta) = e^{-\widehat{\lambda}_0(\theta)t} \left(\sum_{m=1}^d \theta_m P_0^{(m)}(0) - t \sum_{\alpha; |\alpha|=3} \lambda_\alpha \theta^\alpha P_0(0) \right)$$

arising from the expansion of the the bracketed factor in the first term, where $P^{(m)}$ is as in Corollary 3.4 and the λ_α as in the proof of Proposition 3.3. All other contributions are bounded by a multiple of $t^{-1} t^{-d/2}$. But it follows from Corollary 3.4 and the observation that $P_0(0) = \widehat{P}_0(\theta)$ for $|\theta| < \delta$, that

$$L_t(\theta) = \sum_{m=1}^d i \theta_m e^{-\widehat{\lambda}_0(\theta)t} \left(\chi_m \widehat{P}_0(\theta) - \widehat{P}_0(\theta) M_{\chi_m^t} \right) - i t \sum_{\alpha; |\alpha|=3} \lambda_\alpha (i\theta)^\alpha e^{-\widehat{\lambda}_0(\theta)t} \widehat{P}_0(\theta)$$

where $M_{\chi_m^t}$ denotes the multiplication operator with the function χ_m^t on the space $L_2(\mathbf{I}^d)$.

If one differentiates (21) then

$$\Phi \partial_m \widehat{S}_t \Phi^{-1} = (2\pi)^{-d} \int_{[-\pi, \pi]^d}^\oplus d\theta (i\theta_m \widehat{S}_t^\theta + \partial_m \widehat{S}_t^\theta)$$

and

$$\Phi \partial_m \widehat{S}_t \widehat{P}_0(B_\delta) \Phi^{-1} = (2\pi)^{-d} \int_{B_\delta}^\oplus d\theta i e^{-\widehat{\lambda}_0(\theta)t} \theta_m P_0(0)$$

since $\partial_m \widehat{P}_0(\theta) = \partial_m P_0(0) = 0$. We next determine a decomposition for $\chi_m \partial_m \widehat{S}_t \widehat{P}_0(B_\delta)$ for all $m \in \{1, \dots, d\}$.

If $\varphi \in C_c(\mathbf{R}^d)$ with $\Phi(\varphi) = (\varphi_\theta)_{\theta \in [-\pi, \pi]^d}$ then $(\Phi(\varphi \chi_m))(\theta) = \chi_m \varphi_\theta$ for all $\theta \in [-\pi, \pi]^d$. So

$$\Phi \chi_m \partial_m \widehat{S}_t \widehat{P}_0(B_\delta) \Phi^{-1} = (2\pi)^{-d} \int_{B_\delta}^\oplus d\theta e^{-\widehat{\lambda}_0(\theta)t} i \theta_m \chi_m P_0(0) \quad (28)$$

for all $t > 0$. Similarly the terms with χ_m^t and third order terms in θ can be handled. Therefore (27) gives an estimate

$$\|S_t - \widehat{S}_t - \sum_{m=1}^d (\chi_m \partial_m \widehat{S}_t - \partial_m \widehat{S}_t M_{\chi_m^t}) \widehat{P}_0(B_\delta) - i t \sum_{\alpha; |\alpha|=3} \lambda_\alpha \partial^\alpha \widehat{S}_t \widehat{P}_0(B_\delta)\|_{1 \rightarrow \infty} \leq c t^{-1} t^{-d/2}$$

uniformly for $t \geq 1$. But then $\widehat{P}_0(B_\delta)$ can be replaced by the identity because this only introduces exponential corrections. The resulting bounds translate directly into the uniform bounds on the kernels given in the proposition. \square

Under some quite general circumstances the first-order correction in the asymptotic expansion of K are zero. Define $\operatorname{div} C = 0$ to mean that $\sum_{k=1}^d \partial_k c_{km} = 0$, in the sense of distributions, for each $m \in \{1, \dots, d\}$.

Lemma 3.11

- I. The correctors $\chi_m = 0$ for all $m \in \{1, \dots, d\}$ if, and only if, $\operatorname{div} C = 0$.
- II. The correctors $\chi_m^t = 0$ for all $m \in \{1, \dots, d\}$ if, and only if, $\operatorname{div} C^t = 0$.
- III. If $\operatorname{div} C = \operatorname{div} C^t = 0$ then $\lambda_\alpha = 0$ for all $\alpha \in J(d)$ with $|\alpha| = 3$.

Proof First

$$(H_0^* \chi, \chi_m) = - \sum_{k=1}^d (\partial_k \chi, c_{km})$$

for all $\chi \in D(H_0^*) \cap L_2^\perp(\mathbf{I}^d)$ and hence for all $\chi \in D(H_0^*)$ and $m \in \{1, \dots, d\}$. But $D(H_0^*)$ is dense in $L_{2;1}(\mathbf{I}^d)$. Hence if $\chi_m = 0$ for all $m \in \{1, \dots, d\}$ then $\operatorname{div} C = 0$. Conversely, if $\operatorname{div} C = 0$ then $(H_0^* \chi, \chi_m) = 0$ for all $\chi \in D(H_0^*)$ since $C_c^\infty(\mathbf{I}^d)$ is dense in $L_{2;1}(\mathbf{I}^d)$ and $L_{2;1}(\mathbf{I}^d) \subseteq D(H_0^*)$. As $H_0^*(L_2^\perp(\mathbf{I}^d) \cap D(H_0^*)) = L_2^\perp(\mathbf{I}^d)$ and $\chi_m \in L_2^\perp(\mathbf{I}^d)$ by Lemma 2.11 it follows that $\chi_m = 0$.

The second statement follows from the first by replacing C with C^t .

Next for $\theta \in B_{\theta_0}$ set $R(\theta) = \lambda_0(\theta) - (\theta, \widehat{C}\theta)$. If $\operatorname{div} C^t = 0$ then

$$\lambda_0(\theta)(\mathbf{1}, P_0(\theta)\mathbf{1}) = (\mathbf{1}, H_\theta P_0(\theta)\mathbf{1}) = (\mathbf{1}, (\theta, C\theta) P_0(\theta)\mathbf{1})$$

and hence

$$R(\theta) = (\mathbf{1}, ((\theta, C\theta) - (\theta, \widehat{C}\theta)) P_0(\theta)\mathbf{1}) / (\mathbf{1}, P_0(\theta)\mathbf{1}) .$$

Moreover, $\operatorname{div} C^t = 0$ implies that \widehat{C} is the mean of C over \mathbf{I}^d and hence $(\mathbf{1}, ((\theta, C\theta) - (\theta, \widehat{C}\theta)) P_0(0)\mathbf{1}) = 0$. Therefore

$$R(\theta) = (\mathbf{1}, ((\theta, C\theta) - (\theta, \widehat{C}\theta)) (P_0(\theta) - P_0(0))\mathbf{1}) / (\mathbf{1}, P_0(\theta)\mathbf{1}) .$$

But if, in addition, $\operatorname{div} C = 0$ then $\|P_0(\theta) - P_0(0)\|_{2 \rightarrow 2} = O(|\theta|^2)$ by Corollary 3.4. Hence $|R(\theta)| = O(|\theta|^4)$. \square

Note that if $\operatorname{div} C^t = 0$ then the coefficients $\lambda_{(k,l,m)}$ of the third-order terms in $R(\theta)$ are given by

$$\lambda_{(k,l,m)} = i \sum_{n=1}^d (\mathbf{1}, (c_{kl} - (\mathbf{1}, c_{kl}\mathbf{1})) X_n c_{nm}). \quad (29)$$

where we have use the explicit form of the correctors given in Subsection 2.3 and Corollary 3.4.

The last two results allow one to conclude that the asymptotic estimate (18) is usually optimal.

Proposition 3.12 *The following conditions are equivalent.*

- I. There is a $c > 0$ such that $\|S_t - \widehat{S}_t\|_{1 \rightarrow \infty} \leq ct^{-1} t^{-d/2}$ uniformly for $t \geq 1$.
- II. There are $c, \varepsilon > 0$ such that $\|S_t - \widehat{S}_t\|_{1 \rightarrow \infty} \leq ct^{-(1+\varepsilon)/2} t^{-d/2}$ uniformly for $t \geq 1$.
- III. $\operatorname{div} C = \operatorname{div} C^t = 0$.

Proof It follows from Lemma 3.11 and Proposition 3.10 that III \Rightarrow I. But it is evident that I \Rightarrow II.

If I is valid then it follows from Proposition 3.10 that there is a $c' > 0$ such that

$$\left| \sum_{m=1}^d \left(\chi_m(x) - \chi_m^t(y) \right) (\partial_m \widehat{K}_t)(x-y) + it \sum_{\alpha \in J(d); |\alpha|=3} \lambda_\alpha(\partial^\alpha \widehat{K}_t)(x-y) \right| \leq c' t^{-\varepsilon/2} t^{-(d+1)/2}$$

for all $t \geq 1$ and $x, y \in \mathbf{R}^d$. Then

$$\begin{aligned} & \left| \sum_{m=1}^d \left(\chi_m(x) - \chi_m^t(x - t^{1/2}y) \right) (\partial_m \widehat{K}_1)(y) + i \sum_{\alpha \in J(d); |\alpha|=3} \lambda_\alpha(\partial^\alpha \widehat{K}_1)(y) \right| \\ &= t^{(d+1)/2} \left| \sum_{m=1}^d \left(\chi_m(x) - \chi_m^t(x - t^{1/2}y) \right) (\partial_m \widehat{K}_t)(t^{1/2}y) + it \sum_{\alpha \in J(d); |\alpha|=3} \lambda_\alpha(\partial^\alpha \widehat{K}_t)(t^{1/2}y) \right| \\ &\leq c' t^{-\varepsilon/2} \end{aligned}$$

for all $x, y \in \mathbf{R}^d$ and $t \geq 1$. Since the χ_m and χ_m^t are periodic functions with mean value zero, integration with respect to x over \mathbf{I}^d gives

$$\left| \sum_{\alpha \in J(d); |\alpha|=3} \lambda_\alpha(\partial^\alpha \widehat{K}_1)(y) \right| \leq c' t^{-\varepsilon/2}$$

for all $y \in \mathbf{R}^d$ and $t \geq 1$. Then $\sum_{\alpha \in J(d); |\alpha|=3} \lambda_\alpha(\partial^\alpha \widehat{K}_1)(y) = 0$ by taking the limit $t \rightarrow \infty$. So

$$\left| \sum_{m=1}^d \left(\chi_m(x) - \chi_m^t(x - t^{1/2}y) \right) (\partial_m \widehat{K}_1)(y) \right| \leq c' t^{-\varepsilon/2}$$

for all $x, y \in \mathbf{R}^d$ and $t \geq 1$. Now let $x, y_0 \in \mathbf{R}^d$. Since χ_m^t has again mean value zero it follows by integration with respect to y over the set $y_0 + t^{-1/2}\mathbf{I}^d$ that

$$\begin{aligned} & \left| \sum_{m=1}^d \chi_m(x) t^{d/2} \int_{y_0 + t^{-1/2}\mathbf{I}^d} dy (\partial_m \widehat{K}_1)(y) \right. \\ & \quad \left. - \sum_{m=1}^d t^{d/2} \int_{y_0 + t^{-1/2}\mathbf{I}^d} dy \chi_m^t(x - t^{1/2}y) \left((\partial_m \widehat{K}_1)(y) - (\partial_m \widehat{K}_1)(y_0) \right) \right| \\ & \leq c' t^{-\varepsilon/2} \end{aligned}$$

for all $t > 0$. But $\lim_{t \rightarrow \infty} t^{d/2} \int_{y_0 + t^{-1/2}\mathbf{I}^d} dy (\partial_m \widehat{K}_1)(y) = (\partial_m \widehat{K}_1)(y_0)$ and $|(\partial_m \widehat{K}_1)(y) - (\partial_m \widehat{K}_1)(y_0)| \leq \|\nabla \partial_m \widehat{K}_1\|_\infty |y - y_0| = d^{1/2} \|\nabla \partial_m \widehat{K}_1\|_\infty t^{-1/2}$ for all $y \in y_0 + t^{-1/2}\mathbf{I}^d$. So taking the limit $t \rightarrow \infty$ one deduces that

$$\sum_{m=1}^d \chi_m(x) (\partial_m \widehat{K}_1)(y_0) = 0$$

for all $x, y_0 \in \mathbf{R}^d$. Scaling then gives $\sum_{m=1}^d \chi_m(x) (\partial_m \widehat{K}_t)(y) = 0$ for all $x, y \in \mathbf{R}^d$ and $t > 0$. Then for all $\eta, x \in \mathbf{R}^d$ one has

$$\begin{aligned} \sum_{m=1}^d \chi_m(x) \eta_m &= \lim_{t \downarrow 0} \int_{\mathbf{R}^d} dy \sum_{m=1}^d \chi_m(x) \widehat{K}_t(y) \frac{\partial}{\partial y_m} e^{\eta \cdot y} \\ &= - \lim_{t \downarrow 0} \int_{\mathbf{R}^d} dy e^{\eta \cdot y} \sum_{m=1}^d \chi_m(x) (\partial_m \widehat{K}_t)(y) = 0 \end{aligned}$$

and $\chi_m = 0$ for all $m \in \{1, \dots, d\}$.

Similarly $\chi_m^t = 0$ for all $m \in \{1, \dots, d\}$. Then Statement I is a consequence of Lemma 3.11. \square

Finally we note that the third order terms in the holomorphic expansion of $\theta \mapsto \lambda_0(\theta)$ vanish in the case of symmetric coefficients. We temporarily adopt the notation $H_\theta(C) = H_\theta, \lambda_0(\theta; C)$, etc. to denote the dependence of the various element on the matrix of coefficients.

Lemma 3.13 *There is a $\delta > 0$ such that*

$$\lambda_0(\theta; C) = \lambda_0(-\theta; C^t)$$

for all $\theta \in B_\delta^C$. Hence if C is symmetric, i.e., if $C = C^t$, then $\theta \mapsto \lambda_0(\theta; C)$ is an even function for small $|\theta|$.

Proof Since $\lambda_0(\theta; C)$ is an eigenvalue of $H_\theta(C)$ it follows that $\overline{\lambda_0(\theta; C)}$ is an eigenvalue of $H_\theta(C)^*$. Let $\varphi_\theta^*(C)$ be a corresponding eigenfunction. Then

$$\overline{H_\theta(C)^* \varphi_\theta^*(C)} = \lambda_0(\theta; C) \overline{\varphi_\theta^*(C)} \quad .$$

Since $\overline{H_\theta(C)^*} = H_{-\theta}(C^t)$ one deduces that

$$H_\theta(C) \overline{\varphi_{-\theta}^*(C^t)} = \lambda_0(-\theta; C^t) \overline{\varphi_{-\theta}^*(C^t)} \quad .$$

Thus $\lambda_0(-\theta; C^t)$ is an eigenvalue of $H_\theta(C)$ such that $\lambda_0(-\theta; C^t) \rightarrow 0$ as $|\theta| \rightarrow 0$. Hence, by simplicity of the eigenvalue, $\lambda_0(-\theta; C^t) = \lambda_0(\theta; C)$ for all small $|\theta|$ (see Proposition 2.7). \square

Despite this last result there are non-symmetric examples for which the third-order terms are non-zero. If $C = I + \varepsilon B$ then H is a perturbation of the Laplacian for small ε . Now for $d = 2$ set

$$B(x) = \begin{pmatrix} e^{2\pi i x_2} & 0 \\ e^{-2\pi i x_2} & 0 \end{pmatrix} \quad .$$

Then $\operatorname{div} B^t = 0$, $(\mathbf{1}, B\mathbf{1}) = 0$ and $\operatorname{div} B(x) = (-2\pi i e^{-2\pi i x_2}, 0)$. Since $H_0\tau = 4\pi^2 \tau$ if $\tau(x) = e^{-2\pi i x_2}$ it follows from (29) that the coefficient $\lambda_{(1,1,1)} = (2\pi)^{-1} \varepsilon^2 \neq 0$.

4 Hölder continuous coefficients

If the coefficients are Hölder continuous of order $\nu \in \langle 0, 1 \rangle$ then it follows from [AMT] or [ElR1] that the kernel is once-differentiable in both variables and the derivatives are Hölder continuous of order ν . Moreover, these derivatives satisfy Gaussian bounds but with an extra factor which grows polynomially with the t variable. In this section we establish the hierarchy of regularity estimates for periodic systems described in Theorems 1.2, 1.3 and 1.4 which are uniform in time.

4.1 Derivatives on the kernel

In this subsection we prove Theorem 1.2.

Suppose $\nu \in \langle 0, 1 \rangle$ is such that $c_{kl} \in \mathcal{C}^\nu$ for all $k, l \in \{1, \dots, d\}$. We begin with the derivatives. Since the statements concerning the derivative of the kernel with respect to the second variable follow by duality from similar statements with respect to the first variable, we only need to consider the first variable. We set $\partial_k = \partial/\partial x_k$, the derivative with respect to the first variable in the k -th direction.

The proofs then follow by a variation of the methods of Section 3.

Lemma 4.1 *For all $\theta \in \mathbf{C}^d$ with $|\theta| < \theta_0$ the projection $P_0(\theta)$ is bounded from $L_1(\mathbf{I}^d)$ into $L_{\infty;1}(\mathbf{I}^d)$ and $\partial_k P_0(\theta) \in \mathcal{L}(\mathbf{I}^d, \mathcal{C}^\nu)$ for all $k \in \{1, \dots, d\}$. Moreover, the map $\theta \mapsto \partial_k P_0(\theta)$ is holomorphic from $B_{\theta_0}^{\mathcal{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), L_\infty(\mathbf{I}^d))$ and from $B_{\theta_0}^{\mathcal{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), \mathcal{C}^\nu)$ for all $k \in \{1, \dots, d\}$.*

Proof It follows from [AMT], Theorem 4.15, that there exist $b, c > 0$ and $N \in \mathbf{N}$ such that

$$|(\partial_k K_t)(x; y)| \leq ct^{-1/2} (1+t)^N G_{b,t}(x-y)$$

for all $k \in \{1, \dots, d\}$, $x, y \in \mathbf{R}^d$ and $t > 0$. Using the identity (9) one sees that K^θ is differentiable, the derivative of S_t^θ maps $L_1(\mathbf{I}^d)$ into $L_\infty(\mathbf{I}^d)$ and $\theta \mapsto \|\partial_k S_t^\theta\|_{1 \rightarrow \infty}$ is locally uniformly bounded. Then the proof is a variation of the arguments given in the proof of Lemma 3.1.

Finally, the Hölder estimates follow by a small change of the argument starting from the kernel bounds

$$|(\partial_k K_t)(x; y) - (\partial_k K_t)(x-h; y)| \leq ct^{-1/2} (|h|t^{-1/2})^\nu (1+t)^N G_{b,t}(x-y)$$

of Theorem 4.15 in [AMT]. □

Obviously $\partial_k P_0(0) = 0$ for all k . For $k, l \in \{1, \dots, d\}$ let $P_{kl} \in \mathcal{L}(L_1(\mathbf{I}^d), L_\infty(\mathbf{I}^d))$ be the partial derivatives of $\theta \mapsto \partial_k P_0(\theta)$. So

$$M = \sup_{k \in \{1, \dots, d\}} \sup_{\substack{\theta \in \mathbf{C}^d \\ 0 < |\theta| \leq 2^{-1} \theta_0}} |\theta|^{-2} \|\partial_k P_0(\theta) - \sum_{l=1}^d \theta_l P_{kl}\|_{1 \rightarrow \infty} < \infty \quad .$$

Comparison with Corollary 3.4 identifies the operators P_{kl} in terms of the correctors χ_l .

Lemma 4.2 *If $k, l \in \{1, \dots, d\}$ then $\chi_l \in L_{\infty;1}(\mathbf{I}^d)$, $\partial_k \chi_l \in \mathcal{C}^\nu$ and $P_{kl} = i(\partial_k \chi_l) P_0(0)$.*

Proof It follows from (15) that

$$P_0(\theta)\mathbf{1} = \varphi_\theta = \mathbf{1} + i \sum_{l=1}^d \theta_l \chi_l + O(|\theta|^2)$$

in the L_2 -sense. But the map $\theta \mapsto \partial_k P_0(\theta)$ from $B_{\theta_0}^{\mathcal{C}}$ into $\mathcal{L}(L_2(\mathbf{I}^d), L_2(\mathbf{I}^d))$ is also holomorphic for all $k \in \{1, \dots, d\}$ and, moreover, $\chi_l \in L_{2;1}(\mathbf{I}^d)$ for all $l \in \{1, \dots, d\}$, by Lemma 2.11. Hence

$$\partial_k P_0(\theta)\mathbf{1} = i \sum_{l=1}^d \theta_l \partial_k \chi_l + O(|\theta|^2)$$

in the L_2 -sense. On the other hand the map $\theta \mapsto \partial_k P_0(\theta)$ from $B_{\theta_0}^{\mathcal{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), L_\infty(\mathbf{I}^d))$ is also holomorphic. Therefore $\partial_k \chi_l \in L_\infty(\mathbf{I}^d)$ for all $l \in \{1, \dots, d\}$ and hence $\chi_k \in L_{\infty;1}(\mathbf{I}^d)$. Similarly, $\partial_k \chi_l \in \mathcal{C}^\nu$.

It follows from Corollary 3.4 that $(\psi, P_{kl}\varphi) = (\psi, i \partial_k \chi_l)(\mathbf{1}, \varphi)$ for all $\varphi, \psi \in L_1(\mathbf{I}^d)$, which implies the last statement. \square

We are now able to formulate an analogue of Theorems 3.5, 3.7 and 3.8 and Corollary 3.6 for the asymptotic behaviour of $\partial_k K_t$ for large t . Then the Gaussian bounds for $\partial_k K_t$ follow as before.

Theorem 4.3 *Assume the coefficients are Hölder continuous and periodic with a common period. Then there exists a $c > 0$ such that*

$$|(\partial_k K_t)(x; y) - (\partial_k \widehat{K}_t)(x - y) - \sum_{l=1}^d (\partial_k \chi_l)(x) (\partial_l \widehat{K}_t)(x - y)| \leq c t^{-1} t^{-d/2}$$

uniformly for all $k \in \{1, \dots, d\}$, $t \geq 1$ and $x, y \in \mathbf{R}^d$.

Moreover, for all $\varepsilon \in (0, 1)$ there exist $b, c > 0$ such that

$$|(\partial_k K_t)(x; y) - (\partial_k \widehat{K}_t)(x - y) - \sum_{l=1}^d (\partial_k \chi_l)(x) (\partial_l \widehat{K}_t)(x - y)| \leq c t^{-(1-\varepsilon)/2} t^{-1/2} G_{b,t}(x - y)$$

uniformly for all $k \in \{1, \dots, d\}$, $t \geq 1$ and $x, y \in \mathbf{R}^d$.

Proof Fix $k \in \{1, \dots, d\}$. Since

$$(x, y) \mapsto (\partial_k K_t)(x; y) - (\partial_k \widehat{K}_t)(x - y) - \sum_{l=1}^d (\partial_k \chi_l)(x) (\partial_l \widehat{K}_t)(x - y)$$

is the kernel of the operator $\partial_k S_t - \partial_k \widehat{S}_t - \sum_{l=1}^d (\partial_k \chi_l) \partial_l \widehat{S}_t$ it suffices, by Lemma 3.2, to prove that there is a $c > 0$ such that

$$\|\partial_k S_t P_0(B_\delta) - \partial_k \widehat{S}_t \widehat{P}_0(B_\delta) - \sum_{l=1}^d (\partial_k \chi_l) \partial_l \widehat{S}_t \widehat{P}_0(B_\delta)\|_{1 \rightarrow \infty} \leq c t^{-1} t^{-d/2} \quad (30)$$

for all $t \geq 1$, where $\delta = 2^{-1}(\theta_0 \wedge \widehat{\theta}_0)$. If one differentiates (21) then

$$\Phi \partial_k S_t \Phi^{-1} = (2\pi)^{-d} \int_{[-\pi, \pi]^d}^{\oplus} d\theta (i\theta_k S_t^\theta + \partial_k S_t^\theta)$$

and arguing as in (28) gives

$$\Phi (\partial_k \chi_l) \partial_l \widehat{S}_t \widehat{P}_0(B_\delta) \Phi^{-1} = (2\pi)^{-d} \int_{B_\delta}^{\oplus} d\theta e^{-\widehat{\lambda}_0(\theta)t} i\theta_l (\partial_k \chi_l) P_0(0) = (2\pi)^{-d} \int_{B_\delta}^{\oplus} d\theta e^{-\widehat{\lambda}_0(\theta)t} \theta_l P_{kl}$$

for all $t > 0$, where we used Lemma 4.2 in the last step. Hence

$$\begin{aligned} & \Phi \left(\partial_k S_t P_0(B_\delta) - \partial_k \widehat{S}_t \widehat{P}_0(B_\delta) - \sum_{l=1}^d (\partial_k \chi_l) \partial_l \widehat{S}_t \widehat{P}_0(B_\delta) \right) \Phi^{-1} \\ &= (2\pi)^{-d} \int_{B_\delta} d\theta \left(i\theta_k (e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\widehat{\lambda}_0(\theta)t} P_0(0)) + e^{-\lambda_0(\theta)t} \left(\partial_k P_0(\theta) - \sum_{l=1}^d \theta_l P_{kl} \right) \right. \\ & \quad \left. + (e^{-\lambda_0(\theta)t} - e^{-\widehat{\lambda}_0(\theta)t}) \sum_{l=1}^d \theta_l P_{kl} \right). \end{aligned}$$

Arguing as before (30) is valid and the proof of Theorem 4.3 is complete. \square

The estimates of Theorem 1.2 on the derivatives $(\partial_{x_k} K_t)(x; y)$ now follow from Theorem 4.3 and similar estimates on the derivatives of the Gaussian kernel \widehat{K}_t .

Next we examine the second statement of Theorem 1.2 on the first-order Riesz transforms. The proof of this result is simplified by noting that if one has the inclusion $D(H^{1/2}) \subseteq L_{p,1}(\mathbf{R}^d)$ and the lower bounds

$$c_p \max_{1 \leq k \leq d} \|\partial_k \varphi\|_p \leq \|H^{1/2} \varphi\|_p \quad (31)$$

for all $\varphi \in D(H^{1/2})$ then it follows that $L_{q,1}(\mathbf{R}^d) \subseteq D((H^*)^{1/2})$ and the upper bounds

$$\|(H^*)^{1/2} \psi\|_q \leq c'_p \max_{1 \leq k \leq d} \|\partial_k \psi\|_q$$

are valid for all $\psi \in L_{q,1}(\mathbf{R}^d)$ with q dual to p . This follows starting from the identity

$$((H^*)^{1/2} \psi, \varphi) = (H^* \psi, H^{-1/2} \varphi) = \sum_{k,l=1}^d (\partial_l \psi, c_{kl} \partial_k H^{-1/2} \varphi)$$

for all $\varphi \in D(H^{-1/2}) \subset L_p(\mathbf{R}^d)$ and $\psi \in D(H^*) \subset L_q(\mathbf{R}^d)$. Hence we need only establish the lower bounds (31) for H .

Fix $p \in \langle 1, \infty \rangle$. As the coefficients are Hölder continuous, it is known (see [EIR1], Theorem 4.6) that $D(H^{1/2}) = L_{p,1}(\mathbf{R}^d)$. Therefore the operators $R_{k,\varepsilon} = \partial_k (\varepsilon I + H)^{-1/2}$ are bounded on $L_p(\mathbf{R}^d)$ for all $\varepsilon > 0$. The essence of the proof of (31) is to establish a uniform bound

$$\max_{1 \leq k \leq d} \sup_{\varepsilon > 0} \|R_{k,\varepsilon}\|_{p \rightarrow p} < \infty \quad .$$

This bound is obtained by first observing that

$$R_{k,\varepsilon} = \Gamma(1/2)^{-1} \partial_k \int_0^\infty dt e^{-\varepsilon t} t^{-1/2} S_t = R_{k,\varepsilon}^{(1)} + R_{k,\varepsilon}^{(2)}$$

with

$$R_{k,\varepsilon}^{(1)} = \Gamma(1/2)^{-1} \partial_k \int_0^\infty dt e^{-(1+\varepsilon)t} t^{-1/2} S_t = \partial_k ((1+\varepsilon)I + H)^{-1}$$

and

$$R_{k,\varepsilon}^{(2)} = \Gamma(1/2)^{-1} \int_0^\infty dt e^{-\varepsilon t} (1 - e^{-t}) t^{-1/2} \partial_k S_t \quad .$$

But one has bounds

$$\|R_{k,\varepsilon}^{(1)}\|_{p \rightarrow p} \leq \|\partial_k (I + H)^{-1/2}\|_{p \rightarrow p} \|(I + H)^{1/2} ((1+\varepsilon)I + H)^{-1/2}\|_{p \rightarrow p} \leq c_1 \|\partial_k (I + H)^{-1/2}\|_{p \rightarrow p}$$

with c_1 independent of ε because H has a bounded H_∞ -holomorphic functional calculus. This is true for $p = 2$ since H is injective and maximal accretive [ADM], Theorem G, and it then follows for $p \in \langle 1, \infty \rangle$ by [DuR], Theorem 3.4. Fix $\delta \in \langle 0, 1 \rangle$. Next we use the estimates

$$\|\partial_k S_t - \partial_k \widehat{S}_t - \sum_{l=1}^d (\partial_k \chi_l) \partial_l \widehat{S}_t\|_{p \rightarrow p} \leq c' t^{-1/2} (1+t)^{-\delta/2} \quad .$$

These follow for $t \leq 1$ from the bounds on $\partial_k S_t$ and $\partial_k \widehat{S}_t$ and they follow for $t \geq 1$ as an immediate corollary of Theorem 4.3. One deduces that

$$\begin{aligned} \|R_{k,\varepsilon}^{(2)}\|_{p \rightarrow p} &\leq c' \Gamma(1/2)^{-1} \int_0^\infty dt e^{-\varepsilon t} (1 - e^{-t}) t^{-1} (1+t)^{-\delta/2} \\ &\quad + \Gamma(1/2)^{-1} \left\| \int_0^\infty dt e^{-\varepsilon t} (1 - e^{-t}) t^{-1/2} \left(\partial_k \widehat{S}_t + \sum_{l=1}^d (\partial_k \chi_l) \partial_l \widehat{S}_t \right) \right\|_{p \rightarrow p} . \end{aligned}$$

But the first term on the right hand side has a finite bound, uniform for all $\varepsilon > 0$, since $\delta \in (0, 1)$. Moreover, the second term on the right is the L_p -norm of the operator

$$\partial_k \left((\varepsilon I + \widehat{H})^{-1/2} - ((1 + \varepsilon)I + \widehat{H})^{-1/2} \right) + \sum_{l=1}^d (\partial_k \chi_l) \left(\partial_l (\varepsilon I + \widehat{H})^{-1/2} - \partial_l ((1 + \varepsilon)I + \widehat{H})^{-1/2} \right)$$

which is bounded, uniformly for $\varepsilon > 0$, since the Riesz transforms of \widehat{H} are bounded. Thus $R_{k,\varepsilon}^{(1)}$, $R_{k,\varepsilon}^{(2)}$ and $R_{k,\varepsilon}$ are all norm bounded uniformly in ε .

It follows from the foregoing that

$$\max_{1 \leq k \leq d} \|\partial_k \varphi\|_p \leq C \|(\varepsilon I + H)^{1/2} \varphi\|_p$$

for all $\varepsilon > 0$ and $\varphi \in L_{p,1}(\mathbf{R}^d)$ with C independent of ε . Then (31) follows by taking the limit $\varepsilon \rightarrow 0$.

4.2 Higher order derivatives of the kernel

The hierarchy of smoothness of the kernel together with optimal Gaussian bounds does not usually extend beyond one derivative. The situation is comparable with the scale of genuine Gaussian bounds for derivatives of the kernel of the Laplacian on groups with polynomial growth (see [ERS]).

In this subsection we prove the equivalence of the conditions in Theorem 1.3 by proving the implications III \Rightarrow II \Rightarrow IV \Rightarrow I \Rightarrow III and then I \Rightarrow V \Rightarrow IV. Finally we prove Theorem 1.4.

Obviously the implication Theorem 1.3.III \Rightarrow II is trivial.

Proof of Theorem 1.3.II \Rightarrow IV By (15) in Lemma 4.2 of [ElR2] and Theorem 1.2 it follows that there are $b, c > 0$ such that

$$|(\partial_k K_t)(x - h; y) - (\partial_k K_t)(x; y)| \leq c t^{-1/2} G_{b,t}(x - y) \quad (32)$$

uniformly for all $x, y, h \in \mathbf{R}^d$, $t > 0$ and $k \in \{1, \dots, d\}$ with $|h| \leq t^{1/2}$. Interpolation with the bounds of Condition II establishes that for all $\varepsilon \in (0, \nu)$ there are $b', c' > 0$ such that

$$|(\partial_k K_t)(x - h; y) - (\partial_k K_t)(x; y)| \leq c' t^{-1/2} (|h| t^{-1/2})^{\nu - \varepsilon} G_{b',t}(x - y)$$

uniformly for all $x, y, h \in \mathbf{R}^d$, $t \geq 1$ and $k \in \{1, \dots, d\}$ with $|h| \leq 1$. Then the bounds of Condition IV follow by integration of the kernel.

We next show that the implication IV \Rightarrow I is a consequence of Theorem 4.3.

Proof of Theorem 1.3.IV \Rightarrow I Suppose Condition IV is valid and that $\nu \in (0, 1)$, $c_p > 0$ and $p \in [1, \infty]$ are such that (3) is satisfied. Fix $k \in \{1, \dots, d\}$. Then

$$\|(I - L(h))\partial_k S_t\|_{p \rightarrow p} \leq c_p t^{-(1+\nu)/2} \quad (33)$$

for all $t \geq 1$ and $h \in \mathbf{R}^d$ with $|h| \leq 1$. We first show that these bounds are also valid with p replaced by 2. The Gaussian bounds of Theorem 1.2 imply that there is a $c > 0$ such that

$$\|\partial_k S_t\|_{q \rightarrow q} \leq c t^{-1/2} \quad (34)$$

uniformly for all $q \in [1, \infty]$ and $t > 0$. Interpolating between (33) and (34) by taking $q = 1$ if $p > 2$ and $q = \infty$ if $p < 2$ establishes that there are (probably different) $c > 0$ and $\nu \in \langle 0, 1 \rangle$ such that

$$\|(I - U(h))\partial_k S_t\|_{2 \rightarrow 2} \leq c t^{-(1+\nu)/2}$$

uniformly for all $t \geq 1$ and $h \in \mathbf{R}^d$ with $|h| \leq 1$.

It follows from Theorem 4.3 that there is a $c' > 0$ such that

$$\|\partial_k S_t - \partial_k \widehat{S}_t - \sum_{l=1}^d (\partial_k \chi_l) \partial_l \widehat{S}_t\|_{2 \rightarrow 2} \leq c' t^{-(1+\nu)/2}$$

uniformly for all $t \geq 1$. So

$$\|(I - U(h))\partial_k S_t - (I - U(h))\partial_k \widehat{S}_t - (I - U(h)) \sum_{l=1}^d (\partial_k \chi_l) \partial_l \widehat{S}_t\|_{2 \rightarrow 2} \leq 2c' t^{-(1+\nu)/2}$$

uniformly for all $t \geq 1$. Since \widehat{S}_t satisfies bounds

$$\|(I - U(h))\partial_l \widehat{S}_t\|_{2 \rightarrow 2} \leq c'' t^{-1/2} (|h| t^{-1/2})^\nu \quad (35)$$

uniformly for all $t > 0$ and $h \in \mathbf{R}^d$ it follows that

$$\|(I - U(h)) \sum_{l=1}^d (\partial_k \chi_l) \partial_l \widehat{S}_t\|_{2 \rightarrow 2} \leq (c + 2c' + c'' |h|^\nu) t^{-(1+\nu)/2} \leq (c + 2c' + c'') t^{-(1+\nu)/2}$$

for all $t \geq 1$ and $h \in \mathbf{R}^d$ with $|h| \leq 1$. Using the bounds (35) once again, the boundedness of the $\partial_k \chi_l$ and the identity $((U(h) - I)(\varphi\psi)) = (U(h)\varphi)((U(h) - I)\psi) + ((U(h) - I)\varphi)\psi$ one establishes that there is a $c''' > 0$ such that

$$\left\| \sum_{l=1}^d \left((I - U(h))(\partial_k \chi_l) \right) \partial_l \widehat{S}_t \right\|_{2 \rightarrow 2} \leq c''' t^{-(1+\nu)/2} \quad (36)$$

uniformly for all $t \geq 1$ and $h \in \mathbf{R}^d$ with $|h| \leq 1$.

Fix $h \in \mathbf{R}^d$ with $|h| \leq 1$ and set

$$\psi_l = (I - U(h))(\partial_k \chi_l)$$

for all $l \in \{1, \dots, d\}$. We show that the periodic function ψ_l vanishes for all l . (The following elegant argument is due to Nick Dungey.) It follows from (36) and the semigroup property that

$$\left\| \sum_{l=1}^d \psi_l \partial_l \widehat{K}_{2t} \right\|_2 = \left\| \sum_{l=1}^d \psi_l \partial_l \widehat{S}_t \widehat{K}_t \right\|_2 \leq c''' t^{-(1+\nu)/2} \|\widehat{K}_t\|_2 \leq c t^{-(1+\nu)/2} t^{-d/4}$$

uniformly for all $t \geq 1$ and for a suitable $c > 0$. Then by scaling

$$\left\| \sum_{l=1}^d \psi_l^{(t)} \partial_l \widehat{K}_2 \right\|_2 \leq c t^{-\nu/2}$$

for all $t \geq 1$, where $\psi_l^{(t)}(x) = \psi_l(t^{1/2}x)$. In particular, $\lim_{t \rightarrow \infty} \left\| \sum_{l=1}^d \psi_l^{(t)} \partial_l \widehat{K}_2 \right\|_2 = 0$. But

$$\begin{aligned} \lim_{t \rightarrow \infty} \left\| \sum_{l=1}^d \psi_l^{(t)} \partial_l \widehat{K}_2 \right\|_2^2 &= \lim_{t \rightarrow \infty} \sum_{l,m=1}^d \int_{\mathbf{R}^d} dx \overline{\psi_m(t^{1/2}x)} \psi_l(t^{1/2}x) \overline{(\partial_m \widehat{K}_2)(x)} (\partial_l \widehat{K}_2)(x) \\ &= \sum_{l,m=1}^d \int_{\mathbf{I}^d} du \overline{\psi_m(u)} \psi_l(u) \cdot \int_{\mathbf{R}^d} dx \overline{(\partial_m \widehat{K}_2)(x)} (\partial_l \widehat{K}_2)(x) \\ &= \int_{\mathbf{I}^d \times \mathbf{R}^d} du dx \left| \sum_{l=1}^d \psi_l(u) (\partial_l \widehat{K}_2)(x) \right|^2 \end{aligned}$$

because $\overline{\psi_m^{(t)}} \psi_l^{(t)}$ converges in the weak* topology on $L_\infty(\mathbf{R}^d)$ to its average value over \mathbf{I}^d (see [ZKO] page 5). So $\sum_{l=1}^d \psi_l(u) (\partial_l \widehat{K}_2)(x) = 0$ for almost every $(u, x) \in \mathbf{I}^d \times \mathbf{R}^d$. Since ψ_l and \widehat{K}_2 are continuous by Lemma 4.2 this implies that $\sum_{l=1}^d \psi_l(u) (\partial_l \widehat{K}_2)(x) = 0$ for all $(u, x) \in \mathbf{I}^d \times \mathbf{R}^d$. Arguing as at the end of the proof of Proposition 3.12 gives $(I - U(h))(\partial_k \chi_l) = \psi_l = 0$ for all $l \in \{1, \dots, d\}$. This is valid for all $k \in \{1, \dots, d\}$ and $h \in \mathbf{R}^d$ with $|h| \leq 1$. But then $\partial_k \chi_l$ is constant. On the other hand, $\partial_k \chi_l \in L_2^\perp(\mathbf{I}^d)$, so $\partial_k \chi_l = 0$. But then χ_l is constant and since $\chi_l \in L_2^\perp(\mathbf{I}^d)$ one has $\chi_l = 0$ for all $l \in \{1, \dots, d\}$. Then Condition I follows from Lemma 3.11.I.

Before we can prove the remaining implications of Theorem 1.3 we need some preparation.

Lemma 4.4 *If $\operatorname{div} C = 0$ then $L_{2;2}(\mathbf{R}^d) \subseteq D(H)$ and*

$$H\varphi = - \sum_{k,l=1}^d c_{kl} \partial_k \partial_l \varphi$$

for all $\varphi \in L_{2;2}(\mathbf{R}^d)$.

Proof If $\psi \in L_{2;1}(\mathbf{R}^d)$ and $\varphi \in L_{2;2}(\mathbf{R}^d)$ then

$$h(\psi, \varphi) = \sum_{k,l=1}^d (\partial_k \psi, c_{kl} \partial_l \varphi) = - \sum_{k,l=1}^d (\psi, c_{kl} \partial_k \partial_l \varphi) + \sum_{l=1}^d r(\psi, \partial_l \varphi)$$

with

$$r(\psi, \chi) = \sum_{k=1}^d \left((\partial_k \psi, c_{kl} \chi) + (\psi, c_{kl} \partial_k \chi) \right)$$

for all $\psi, \chi \in L_{2;1}(\mathbf{R}^d)$. But then

$$r(\psi, \chi) = \sum_{k=1}^d \int_{\mathbf{R}^d} dx \left(\partial_k (\overline{\psi} \chi) \right)(x) c_{kl}(x)$$

and since $\operatorname{div} C = 0$ one has $r(\psi, \chi) = 0$. □

Since H can be expressed in non-divergent form, and since the coefficients are Hölder continuous, it follows that the kernel K is at least twice-differentiable in the first variable and the derivatives satisfy Gaussian bounds with an exponential growth in time (see the remark on page 255 in [Fri]). Explicitly, there are $b, c > 0$ and $\omega \geq 0$ such that

$$|(\partial_k \partial_l K_t)(x; y)| \leq ct^{-1} e^{\omega t} G_{b,t}(x - y) \quad (37)$$

and

$$|(\partial_k \partial_l K_t)(x - h; y) - (\partial_k \partial_l K_t)(x; y)| \leq ct^{-1} (|h|t^{-1/2})^{\nu/2} e^{\omega t} G_{b,t}(x - y) \quad (38)$$

for all $h, x, y \in \mathbf{R}^d$, $k, l \in \{1, \dots, d\}$ and $t > 0$ with $|h| \leq t^{1/2}$. This allows us to extend the conclusions of Lemmas 3.1 and 4.1.

Lemma 4.5 *For all $\theta \in B_{\theta_0}^{\mathbf{C}}$ the projection $P_0(\theta)$ is bounded from $L_1(\mathbf{I}^d)$ into $L_{\infty;2}(\mathbf{I}^d)$ and $\partial_k \partial_l P_0(\theta)$ is bounded from $L_1(\mathbf{I}^d)$ into $\mathcal{C}^{\nu/2}$ for all $k, l \in \{1, \dots, d\}$. Moreover, the map $\theta \mapsto \partial_k \partial_l P_0(\theta)$ is holomorphic from $B_{\theta_0}^{\mathbf{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), L_{\infty}(\mathbf{I}^d))$ and from $B_{\theta_0}^{\mathbf{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), \mathcal{C}^{\nu/2})$ for all $k, l \in \{1, \dots, d\}$.*

Proof Using (9) and (37) one sees that K^θ is twice-differentiable and there are $b, c, \omega > 0$ such that

$$|(\partial_k \partial_l K_t^\theta)(u; v)| \leq c (|\theta|^2 + t^{-1})(1 \wedge t)^{-d/2} e^{-b\|u-v\|^2 t^{-1}} e^{\omega(1+(\operatorname{Im}\theta)^2)t}$$

for all $\theta \in \mathbf{C}^d$, $t > 0$ and $u, v \in \mathbf{I}^d$. Arguing as in the proof of Lemma 3.1 the $L_{\infty;2}$ -statements of the lemma follow.

The Hölder bounds follow from (38). \square

Next we examine the second-order terms in the holomorphic expansion of $\theta \mapsto P_0(\theta)$. In general this is complicated but simplifications occur because we are assuming $\operatorname{div} C = 0$. Hence the correctors $\chi_m = 0$ by Lemma 3.11. As $\operatorname{div} C = 0$ it also follows that \hat{c}_{mn} is the average of c_{mn} over \mathbf{I}^d and one can define

$$\chi_{mn} = 2^{-1} H_0^{-1} \left((c_{mn} + c_{nm}) - (\hat{c}_{mn} + \hat{c}_{nm}) \mathbf{1} \right)$$

for all $m, n \in \{1, \dots, d\}$, where $H_0^{-1}: L_2^\perp(\mathbf{I}^d) \rightarrow L_2^\perp(\mathbf{I}^d)$ is as in Subsection 2.3. Then it follows from the proof of Proposition 3.3 that one can identify the second-order term in the expansion of the eigenvector φ_θ as $\varphi_{(m,n)} = -\chi_{mn} + a_{mn}$ for some $a_{mn} \in \mathbf{C}$. The second-order term $\varphi_{(m,n)}^\dagger$ in the expansion of φ_θ^\dagger has a more complicated form which we will not require. But one verifies that $(\varphi_\theta^\dagger - (\varphi_\theta^\dagger, \mathbf{1}) \mathbf{1}, \varphi_\theta) - 1 = O(|\theta|^3)$ and

$$(\psi, P_0^{(mn)}(0)\varphi) = -(\psi, \chi_{mn})(\mathbf{1}, \varphi) + (\psi, \mathbf{1})(\varphi_{(m,n)}^\dagger - (\varphi_\theta^\dagger, \mathbf{1}) \mathbf{1}, \varphi)$$

for all $\psi, \varphi \in L_2(\mathbf{I}^d)$, where $P_0^{(mn)}(\theta) = \partial^2 P_0(\theta) / (\partial \theta_m \partial \theta_n)$. As in Corollary 3.4 the constant a_{mn} gives no contribution. Then it follows that

$$(\partial_k \partial_l \psi, P_0^{(mn)}(0)\varphi) = -(\partial_k \partial_l \psi, \chi_{mn})(\mathbf{1}, \varphi)$$

for $\psi \in L_{2;2}(\mathbf{I}^d) \cap L_{1;2}(\mathbf{I}^d)$ and $\varphi \in L_2$ and $\varphi_{(m,n)}^\dagger$ also plays no role. Since $\theta \mapsto \partial_k \partial_l P_0(\theta)$ is holomorphic from $B_{\theta_0}^{\mathbf{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), L_{\infty}(\mathbf{I}^d))$ and from $B_{\theta_0}^{\mathbf{C}}$ into $\mathcal{L}(L_1(\mathbf{I}^d), \mathcal{C}^{\nu/2})$ it follows that $\chi_{mn} \in L_{\infty;2}$ and $\partial_k \partial_l \chi_{mn} \in \mathcal{C}^{\nu/2}$. Moreover,

$$\partial_k \partial_l P_0^{(mn)}(0) = -(\partial_k \partial_l \chi_{mn}) P_0(0)$$

for all $k, l, m, n \in \{1, \dots, d\}$.

We extend the χ_{mn} to periodic functions on $C(\mathbf{R}^d)$.

Proposition 4.6 *If $\operatorname{div} C = 0$ then there is a $c > 0$ such that*

$$|(\partial_k \partial_l K_t)(x; y) - (\partial_k \partial_l \widehat{K}_t)(x - y) + \sum_{m, n=1}^d (\partial_k \partial_l \chi_{mn})(x) (\partial_m \partial_n \widehat{K}_t)(x - y)| \leq c t^{-3/2} t^{-d/2}$$

uniformly for all $k, l \in \{1, \dots, d\}$, $x, y \in \mathbf{R}^d$ and $t \geq 1$.

Proof Fix $k, l \in \{1, \dots, d\}$. Then with $\delta = 2^{-1}(\theta_0 \wedge \hat{\theta}_0)$ one has

$$\begin{aligned} & \Phi \left(\partial_k \partial_l S_t P_0(B_\delta) - \partial_k \partial_l \widehat{S}_t \widehat{P}_0(B_\delta) \right) \Phi^{-1} \\ &= (2\pi)^{-d} \int_{B_\delta} d\theta \left((i\theta_k + \partial_k)(i\theta_l + \partial_l) S_t^\theta P_0(\theta) + \theta_k \theta_l \widehat{S}_t^\theta P_0(0) \right) \end{aligned}$$

for all $t > 0$. If $\theta \in B_\delta$ then

$$\begin{aligned} & (i\theta_k + \partial_k)(i\theta_l + \partial_l) S_t^\theta P_0(\theta) + \theta_k \theta_l \widehat{S}_t^\theta P_0(0) \\ &= e^{-\lambda_0(\theta)t} \left(-\theta_k \theta_l P_0(\theta) + i\theta_k \partial_l P_0(\theta) + i\theta_l \partial_k P_0(\theta) + \partial_k \partial_l P_0(\theta) \right) + e^{-\hat{\lambda}_0(\theta)t} \theta_k \theta_l P_0(0) \\ &= \sum_{m, n=1}^d e^{-\hat{\lambda}_0(\theta)t} \theta_m \theta_n \partial_k \partial_l P_0^{(mn)}(0) - \theta_k \theta_l (e^{-\lambda_0(\theta)t} P_0(\theta) - e^{-\hat{\lambda}_0(\theta)t} P_0(0)) \\ & \quad + i e^{-\lambda_0(\theta)t} \theta_k \partial_l P_0(\theta) + i e^{-\lambda_0(\theta)t} \theta_l \partial_k P_0(\theta) + (e^{-\lambda_0(\theta)t} - e^{-\hat{\lambda}_0(\theta)t}) \partial_k \partial_l P_0(\theta) \\ & \quad + e^{-\hat{\lambda}_0(\theta)t} \left(\partial_k \partial_l P_0(\theta) - \sum_{m, n=1}^d \theta_m \theta_n \partial_k \partial_l P_0^{(mn)}(0) \right) \end{aligned}$$

for all $t > 0$. But $\partial_k P_0^{(m)}(0) = 0$ for all $k, m \in \{1, \dots, d\}$ by Lemmas 3.11.I and 4.2 since $\operatorname{div} C = 0$. So $\|\partial_k P_0(\theta)\|_{1 \rightarrow \infty} = O(|\theta|^2)$. Then also $\partial_k \partial_l P_0^{(m)}(0) = 0$ for all $k, l, m \in \{1, \dots, d\}$ and therefore $\|\partial_k \partial_l P_0(\theta)\|_{1 \rightarrow \infty} = O(|\theta|^2)$. Moreover,

$$\|\partial_k \partial_l P_0(\theta) - \sum_{m, n=1}^d \theta_m \theta_n \partial_k \partial_l P_0^{(mn)}(0)\|_{1 \rightarrow \infty} = O(|\theta|^3) \quad .$$

So only the first term gives a big contribution. Since $\partial_k \partial_l P_0^{(mn)}(0) = -(\partial_k \partial_l \chi_{mn}) P_0(0)$ this contribution comes from the kernel of the operator $-(\partial_k \partial_l \chi_{mn}) \partial_m \partial_n \widehat{S}_t$ and the proposition follows by the earlier arguments. \square

Now we can complete the proof of the equivalence of the first four conditions of Theorem 1.3.

Proof of Theorem 1.3.I \Rightarrow III We first show that one can replace the exponential factor $e^{\omega t}$ in the bounds (37) by a factor $(1 + t)$.

It follows from the semigroup property, the estimates (37) and the Gaussian bounds on the kernel that

$$|(\partial_k \partial_l K_t)(x; y)| \leq c \int_{\mathbf{R}^k} dz G_{b,1}(x - z) G_{b,t-1}(z - y) \quad .$$

Hence

$$|(\partial_k \partial_l K_t)(x; y)| \leq c' G_{b',t}(x - y)$$

uniformly for all $t \geq 1$ and $x, y \in \mathbf{R}^d$.

Since similar bounds are also valid for the kernel \widehat{K} there exist $b, c > 0$ such that

$$|(\partial_k \partial_l K_t)(x; y) - (\partial_k \partial_l \widehat{K}_t)(x - y) + \sum_{m,n=1}^d (\partial_k \partial_l \chi_{mn})(x) (\partial_m \partial_n \widehat{K}_t)(x - y)| \leq c(1+t)t^{-1} G_{b,t}(x - y)$$

uniformly for all $t > 0$ and $x, y \in \mathbf{R}^d$. Then by interpolation with the bounds of Proposition 4.6 one deduces that for all $\varepsilon \in (0, 1)$ there exist $b, c > 0$ such that

$$\begin{aligned} |(\partial_k \partial_l K_t)(x; y) - (\partial_k \partial_l \widehat{K}_t)(x - y) + \sum_{m,n=1}^d (\partial_k \partial_l \chi_{mn})(x) (\partial_m \partial_n \widehat{K}_t)(x - y)| \\ \leq c t^{-\varepsilon/2} t^{-1} G_{b,t}(x - y) \end{aligned} \quad (39)$$

uniformly for all $t \geq 1$ and $x, y \in \mathbf{R}^d$. This immediately implies Condition III.

Proof of Theorem 1.3.I \Rightarrow V The proof is similar to the proof of the boundedness of the first-order Riesz transforms in Theorem 1.2. Fix $p \in \langle 1, \infty \rangle$. It follows from Lemma 4.4 that H can be expressed in non-divergence form. But then $D(H) = L_{p;2}(\mathbf{R}^d)$ and one has estimates

$$\max_{1 \leq k, l \leq d} \|\partial_k \partial_l \varphi\|_p \leq c(\|H\varphi\|_p + \|\varphi\|_p)$$

for all $\varphi \in L_{p;2}(\mathbf{R}^d)$. (These estimates follow from similar estimates for operators with constant coefficients, the uniform continuity of the coefficients and a partition of the identity, by standard arguments.) Therefore the operators $R_{k,l,\varepsilon} = \partial_k \partial_l (\varepsilon I + H)^{-1}$ are bounded on $L_p(\mathbf{R}^d)$ for each $\varepsilon > 0$ and again it is necessary to obtain a norm bound uniform for small ε . But

$$R_{k,l,\varepsilon} = \partial_k \partial_l \int_0^\infty dt e^{-\varepsilon t} S_t = R_{k,l,\varepsilon}^{(1)} + R_{k,l,\varepsilon}^{(2)}$$

with

$$R_{k,l,\varepsilon}^{(1)} = \partial_k \partial_l \int_0^\infty dt e^{-\varepsilon t} (2e^{-t} - e^{-2t}) S_t = 2\partial_k \partial_l ((1 + \varepsilon)I + H)^{-1} - \partial_k \partial_l ((2 + \varepsilon)I + H)^{-1}$$

and

$$R_{k,l,\varepsilon}^{(2)} = \int_0^\infty dt e^{-\varepsilon t} (1 - e^{-t})^2 \partial_k \partial_l S_t \quad .$$

Then $\|R_{k,l,\varepsilon}^{(1)}\|_{p \rightarrow p}$ is bounded uniformly in ε because H has a bounded H_∞ -holomorphic functional calculus. Moreover, (39) together with the bounds of III, which are a consequence of I, give bounds

$$\|\partial_k \partial_l S_t - \partial_k \partial_l \widehat{S}_t + \sum_{m,n=1}^d (\partial_k \partial_l \chi_{mn}) \partial_m \partial_n \widehat{S}_t\|_{p \rightarrow p} \leq c t^{-1} (1 + t)^{-\nu/2}$$

for some $\nu \in \langle 0, 1 \rangle$ and all $t > 0$. Therefore one estimates easily that $\|R_{k,l,\varepsilon}^{(2)}\|_{p \rightarrow p}$ is also bounded uniformly in ε .

It follows from these estimates that

$$\max_{1 \leq k, l \leq d} \|\partial_k \partial_l \varphi\|_p \leq c \|(\varepsilon I + H)\varphi\|_p$$

for all $\varphi \in D(H)$ with c independent of ε . Hence taking the limit $\varepsilon \rightarrow 0$ one obtains

$$\max_{1 \leq k, l \leq d} \|\partial_k \partial_l \varphi\|_p \leq c \|H\varphi\|_p$$

for all $\varphi \in D(H)$. But the complementary bounds

$$c' \|H\varphi\|_p \leq \max_{1 \leq k, l \leq d} \|\partial_k \partial_l \varphi\|_p$$

are elementary since H is in non-divergence form.

Proof of Theorem 1.3. V \Rightarrow IV Suppose Condition V is valid and $p \in \langle 1, \infty \rangle$. Then there is a $c > 0$ such that $\|\partial_k \partial_l \varphi\|_p \leq c \|H\varphi\|_p$ for all $k, l \in \{1, \dots, d\}$ and $\varphi \in L_{p;2}(\mathbf{R}^d)$. But the operator H has a bounded H_∞ -functional calculus on $L_p(\mathbf{R}^d)$. Hence there is a $c' > 0$ such that $\|HS_t\|_{p \rightarrow p} \leq c' t^{-1}$ for all $t > 0$. Then $\|\partial_k \partial_l S_t \varphi\|_p \leq c c' t^{-1} \|\varphi\|_p$ and Condition IV follows.

For derivatives higher than second-order on the kernel, or the semigroup, the canonical small time behaviour cannot be expected to extend to large times except in the case that all coefficients are constant and derivatives of all orders are well-behaved.

Proof of Theorem 1.4 The proof of the implication I \Rightarrow II is well known.

“II \Rightarrow III”. The proof is the similar to the proof of Theorem 1.3. II \Rightarrow IV although one more interpolation argument is necessary. It is a consequence of the Duhamel formula that

$$(\partial_k \varphi)(x) = -s^{-1} (\varphi(x - se_k) - \varphi(x)) - s^{-1} \int_0^s du \left((\partial_k \varphi)(x - ue_k) - (\partial_k \varphi)(x) \right)$$

for any continuously differentiable function φ , all $x \in \mathbf{R}^d$, $s > 0$ and $k \in \{1, \dots, d\}$, where e_k is the unit vector in the k -th direction. Setting $\varphi(x) = (\partial_l K_t)(x; y)$ it follows from the bounds (32) and the bounds of Condition II that there are $b, c > 0$ such that

$$\begin{aligned} |(\partial_k \partial_l K_t)(x; y)| &\leq c s^{-1} t^{-1/2} G_{b,t}(x - y) + c s^{-1} \int_0^s du t^{-1} (ut^{-1/2})^\nu t^{-d/2} \\ &= c t^{-(d+1)/2} \left(s^{-1} e^{-b|x-y|^2 t^{-1}} + (1 + \nu)^{-1} s^\nu t^{-(1+\nu)/2} \right) \\ &\leq 2c t^{-(d+1)/2} e^{-2^{-1}\nu b|x-y|^2 t^{-1}} \end{aligned}$$

uniformly for all $t \geq 1$ and $x, y \in \mathbf{R}^d$, if one chooses $s = e^{-2^{-1}b|x-y|^2 t^{-1}} \leq 1$. Hence there are $b', c' > 0$ such that

$$|(\partial_k \partial_l K_t)(x - h; y) - (\partial_k \partial_l K_t)(x; y)| \leq c' (|h|t^{-1/2})^\nu G_{b',t}(x - y)$$

uniformly for all $t \geq 1$ and $h, x, y \in \mathbf{R}^d$ with $|h| \leq 1$. Interpolation with the bounds of Condition II gives bounds

$$\begin{aligned} |(\partial_k \partial_l K_t)(x - h; y) - (\partial_k \partial_l K_t)(x; y)| &\leq c'' t^{-(1-\varepsilon)} (|h|t^{-1/2})^\nu G_{\varepsilon b',t}(x - y) \\ &\leq c'' t^{-1} (|h|t^{-1/2})^{\nu-2\varepsilon} G_{\varepsilon b',t}(x - y) \end{aligned}$$

uniformly for all $\varepsilon \in \langle 0, \nu/2 \rangle$, $t \geq 1$ and $h, x, y \in \mathbf{R}^d$ with $|h| \leq 1$. Hence III is valid.

“III \Rightarrow I”. If Condition III is valid then $\|(I-U(h))(I-U(g))\partial_t S_t\|_{p \rightarrow p} \leq c_p t^{-(2+\nu)/2} |h|^\nu |g|$ for all $g, h \in \mathbf{R}^d$, $t \geq 1$ and $l \in \{1, \dots, d\}$ with $|h| \leq 1$. Arguing as in the proof of Theorem 1.3.IV \Rightarrow I it follows that $(I-U(h))(I-U(g))\partial_k \chi_l = 0$ for all $k, l \in \{1, \dots, d\}$ and $g, h \in \mathbf{R}^d$ with $|h| \leq 1$. Hence $\chi_l = 0$ for all l and $\operatorname{div} C = 0$. Then one can apply Proposition 4.6 and argue as in the proof of the implication in Theorem 1.3.IV \Rightarrow I. One deduces that Condition I is valid.

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