LONG TIME BEHAVIOUR OF HEAT FLOW: GLOBAL ESTIMATES AND EXACT ASYMPTOTICS

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Abstract. We obtain global upper and lower bounds on the heat kernel of an elliptic second order differential operator, which become sharp in certain long-time and large-space asymptotics. We prove a generalization of Aronson's Gaussian bounds which identifies correctly an effective drift for heat flow. In the case of periodic coefficients we give variational characterizations of the effective conductivity, which is then made to appear in heat kernel bounds. These results are for heat kernels with measurable coefficients. For differentiable coefficients we prove tighter estimates, in which the rate of homogenization is known to be optimal.

1 Introduction

The flow of heat over long intervals of time, in an inhomogeneous medium, can sometimes be approximated by that in a uniform medium. There is an extensive literature on the asymptotic approach to this approximation, see for example the books of Bensoussan, Lions and Papanicolaou [BLP] and Jikov, Kozlov and Olienik [JKO]. The results obtained there identify effective constants which characterize explicitly certain asymptotics of the heat flow. Our object in this paper is to obtain, in the case of periodic structure, *global* estimates on the heat kernel in terms of these effective constants. These estimates, from above and below, become sharp in an explicit way in certain long-time and large-space asymptotics, which involve a combination of homogenization and large deviations. We do not recover the classical homogenization results, but our results, as well as giving explicit control of the heat kernel prior to any asymptotics, give a more detailed picture of the tail of the heat kernel, and reveal the importance of the *speed* with which heat is expected to pass from one point to another.

Global estimates on the heat kernel have previously been developed by Aronson [A], Davies [D], Fabes and Stroock [FS] and many others. Some recent references are the papers of Benjamini, Chavel and Feldman [BCF] and Grigor'yan [G]. Although some of these estimates identify exact constants in the regime of small time asymptotics, the identification of exact constants for long-time behaviour has

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proved relatively difficult. One possible complication is that the global structure may become important, but this is not a problem in the periodic case. Another difficulty is that the first and zeroth order parts of the heat operator, which had hitherto been dealt with as perturbations of the second order part, now become dominant.

In this paper we obtain sharp long-time estimates by combining the methods for short-time estimates, found in [FS] and [NS] with ideas from the homogenization theory for the heat equation as found for example in [BLP] and [JKO]. We extend our work on the simplest self-adjoint case [N] to a general second order elliptic operator, including in particular the case of convection enhanced diffusion studied by Fannjiang and Papanicolaou [FP]. We obtain upper and lower bounds on the heat kernel corresponding to different classes of test-function or test-field. When these bounds are optimized, the effective conductivity appears naturally by means of its variational characterizations. The main results are Theorems 1.1, 1.2, 1.3 and 1.4.

Consider a second order differential operator L on $L^2(\mathbb{R}^n)$ given by the Dirichlet form

$$\int_{\mathbb{R}^n} fLg\,dm = -\int_{\mathbb{R}^n} \langle df, (a+\beta)dg\rangle dm + \int_{\mathbb{R}^n} \langle f\bar{b}, dg\rangle dx,$$

with domain $W^{1,2}(\mathbb{R}^n)$ where m is a Borel measure on $\mathbb{R}^n$, where

$$a : \mathbb{R}^n \to \mathbb{R}^n \otimes \mathbb{R}^n, \quad \beta : \mathbb{R}^n \to \mathbb{R}^n \otimes \mathbb{R}^n$$

are measurable, respectively symmetric and anti-symmetric, and where $\bar{b} \in \mathbb{R}^n$ is a constant vector. We shall assume throughout that m is uniformly equivalent to Lebesgue measure, with density μ, that a is uniformly equivalent to the standard metric on $\mathbb{R}^n$, and that β is uniformly bounded. Let $\lambda \in (0,\infty)$ be a constant, chosen so that

$$\lambda^{-1}|v^*|^2 \le \langle a(x)v^*, v^*\rangle \le \lambda|v^*|^2, \quad \lambda^{-1} \le \mu(x) \le \lambda, \tag{1.1}$$

and

$$|\beta(x)| \le \lambda \tag{1.2}$$

for all $x \in \mathbb{R}^n$ and $v^* \in (\mathbb{R}^n)^*$. In the case $\bar{b} \neq 0$, we shall also assume that for some bounded measurable vector field ξ on $\mathbb{R}^n$ we have

$$\int_{\mathbb{R}^n} f\,dm - \int_{\mathbb{R}^n} f\,dx = \int_{\mathbb{R}^n} \langle \xi, df\rangle dm \tag{1.3a}$$

for all test-functions f. We choose λ so that

$$|\bar{b}||\xi(x)| \le \lambda \tag{1.3b}$$

for all $x \in \mathbb{R}^n$. Formally we may write

$$Lg = \operatorname{div}\big((a+\beta)dg\big) + \langle \bar{b}/\mu, dg\rangle \tag{1.4}$$

and

$$\operatorname{div}\xi = (1/\mu) - 1,$$

where div denotes the divergence associated to m:

$$\int_{\mathbb{R}^n} \langle \xi, df\rangle dm = -\int_{\mathbb{R}^n} f \operatorname{div}\xi dm.$$

Thus

$$\operatorname{div}\xi = \overline{\operatorname{div}}\,(\mu\xi)/\mu$$

where $\overline{\operatorname{div}}$ denotes the standard divergence on $\mathbb{R}^n$, and when μ is differentiable

$$\operatorname{div}\xi = \overline{\operatorname{div}}\,\xi + \langle \xi, d\log\mu\rangle.$$

Note that the adjoint operator for L with respect to m is obtained by changing the signs of β and $\bar{b}$.

Conditions (1.1) and (1.2) are known to ensure that there is a unique strongly continuous semigroup $(P_t)_{t\geq 0}$ on $L^2(\mathbb{R}^n)$ such that for $g \in L^2(\mathbb{R}^n)$

$$(s, x) \mapsto (P_s g)(x) \in L^2([0,t], W^{1,2}(\mathbb{R}^n))$$

and

$$\int_{\mathbb{R}^n} f P_t g dm = \int_{\mathbb{R}^n} f g dm + \int_0^t \int_{\mathbb{R}^n} f L P_s g dm ds \tag{1.5}$$

for all $f \in W^{1,2}(\mathbb{R}^n)$. Moreover, each P_t extends to a contraction on L^p for all $1 \leq p \leq \infty$ and, for $t > 0$, P_t is given by a non-negative density function:

$$P_t f(x) = \int_{\mathbb{R}^n} p(t, x, y) f(y) m(dy).$$

See for example Sturm [Stu]. The case where $\mu \equiv 1$, or indeed where μ has a bounded derivative, is covered in many standard texts on parabolic theory. Our object is *a priori* estimation of the *heat kernel* $p(t, x, y)$ by means of equation (1.5).

The fundamental Gaussian estimates for heat kernels of uniformly elliptic operators were proved by Aronson [A]; Fabes and Stroock [FS],[S] later gave a more direct approach. Given bounded measurable functions $b : \mathbb{R}^n \to \mathbb{R}^n$ and $c : \mathbb{R}^n \to \mathbb{R}^n$, suppose we choose λ so that for all $x \in \mathbb{R}^n$

$$|b(x)| \leq \lambda, \quad |c(x)| \leq \lambda. \tag{1.6}$$

Then the heat kernel of the operator

$$L^c f = \overline{\operatorname{div}}\,(a df) + \langle b, df\rangle + cf \tag{1.7}$$

satisfies for all $x, y \in \mathbb{R}^n$ and $t \leq 1$,

$$C^{-1} t^{-n/2} \exp\{-C|y-x|^2/t\} \leq p^c(t, x, y) \leq C t^{-n/2} \exp\{-|y-x|^2/Ct\}. \tag{1.8}$$

Here and throughout we denote by C some finite constant depending only on λ and n. Estimates for $t > 1$ then follow from the semigroup property

$$p^c(s+t,x,y) = \int_{\mathbb{R}^n} p^c(s,x,z)p^c(t,z,y)dz.$$

But these estimates involve spurious factors $e^{\pm Ct}$ and are never sharp. The problem lies with the assumption (1.6), which is not invariant under diffusion scaling. On the other hand, for an operator in the form (1.4)

$$Lf = \operatorname{div}\big((a+\beta)df\big) + \langle \bar{b}/\mu, df\rangle,$$

we may instead make assumptions (1.2),(1.3) which are invariant under diffusion scaling. Formally the operators (1.4) and (1.7) coincide when $c = 0$ and $b = \operatorname{div}\beta + d\log\mu + \bar{b}/\mu$. In §2 we shall prove:

Theorem 1.1. *Suppose that L is given by (1.4) and that (1.1),(1.2),(1.3) hold. There is a constant $C < \infty$, depending only on λ and n, such that for all $x, y \in \mathbb{R}^n$ and $t > 0$ we have*

$$C^{-1}t^{-n/2}\exp\{-C|y-x|^2/t\} \le p(t,x,y+\bar{b}t) \le Ct^{-n/2}\exp\{-|y-x|^2/Ct\}.$$

These estimates correctly identify the *effective drift* $\bar{b}$, as one can read off directly the large deviations asymptotics

$$\bar{b}^i = \lim_{\delta\to 0}\lim_{t\to\infty}(\delta t)^{-1}\log\int_{\mathbb{R}^n} e^{\delta(y^i - x^i)}p(t,x,y)m(dy).$$

Besides being appropriate mathematically, the canonical form (1.4) is also natural physically. In a solid medium one would normally take $\beta = 0$ and $\bar{b} = 0$. Then a represents the thermal conductivity, and would reduce to a multiple of the identity were the medium isotropic. The density μ represents the heat capacity of the medium. For diffusion of some quantity in an incompressible fluid, a and μ are naturally constants and the volume-preserving drift field is given by $\operatorname{div}\beta + \bar{b}/\mu$. We shall refer to β as a *vector potential* for the vector field $\operatorname{div}\beta$.

From §3 on we restrict attention to the case where a, β and μ are periodic, of period $T = [0,1]^n$. We shall always assume in this case that

$$m(T) = 1, \quad |\bar{b}| \le \lambda. \tag{1.9}$$

Then $(1/\mu) - 1$ is periodic of mean zero, so there is a periodic vector field ξ such that

$$\operatorname{div}\xi = (1/\mu) - 1, \quad \int_T \xi dm = 0$$

and such that for all $x \in \mathbb{R}^n$

$$|\xi(x)| \le C.$$

In particular (1.9) effectively implies (1.3).

The effective conductivity is found by solving the following elliptic problem in the unit cell T, with periodic boundary conditions

$$\operatorname{div}\big((a+\beta)(v^* - d\psi)\big) + \langle \bar{b}/\mu, v^* - d\psi\rangle = \langle \bar{b}, v^*\rangle. \tag{1.10}$$

For each $v^* \in (\mathbb{R}^n)^*$ there is a unique solution $\psi \in W^{1,2}(T)$ up to an additive constant, which is called the *corrector* for v^*. Note that $d\psi$ depends linearly on v^*. The *effective conductivity* $\bar{a}$ is then the symmetric matrix determined by

$$|v^*|_{\bar{a}}^2 = \int_T |v^* - d\psi|_a^2 dm$$

where $|v^*|_{\bar{a}}^2 = \langle \bar{a}v^*, v^*\rangle$ and $|v^* - d\psi|_a^2$ is defined similarly. We make frequent use of such notation below.

The following standard result in homogenization explains why $\bar{a}$ is called the effective conductivity: in the case where $\bar{b} = 0$, uniformly on compacts in $(0,\infty)\times\mathbb{R}^n\times\mathbb{R}^n$, as $\sigma\to\infty$ we have

$$\sigma^{n/2}p(\sigma^2 t, \sigma x, \sigma y) \to \bar{p}(t,x,y)$$

where $\bar{p}$ is the constant coefficient heat kernel

$$\bar{p}(t,x,y) = (4\pi t)^{-n/2}(\det \bar{a})^{-1/2}\exp\{-|y-x|_{\bar{a}^{-1}}^2/4t\}.$$

See for example [JKO]. We shall not use this result. Indeed our results are rather different although they reflect the same phenomenon. We make *global* estimates of p in terms of $\bar{p}$, and these estimates become sharp when $|y-x|^2/t$ is *large* rather than small.

In §3 we show how to characterize $\bar{a}$ by variational principles, from both above and below. These are the key to obtaining estimates on $\bar{a}$. A different procedure for obtaining essentially the same variational principles, in the case $\bar{b} = 0$ and $\mu = 1$, is described in Milton [M], incorporating ideas of Cherkaev and Gibiansky. We also sketch two examples, considered in detail by Fannjiang and Papanicolaou [FP], where the effect of drift in long time is to make $\bar{a}$ very much greater than a.

In §4 and §5 we prove the following refinement of Theorem 1.1.

Theorem 1.2. *Suppose that L is given by (1.4) with periodic coefficients and that (1.1),(1.2),(1.9) hold. There are constants $\alpha\in(0,1)$ and $C<\infty$, depending only on λ and n, such that for all $x, y\in\mathbb{R}^n$ and $t>0$ we have*

$$\begin{aligned}
t^{-n/2}&\exp\{-Ct^{-\alpha}e^{C|y-x|^2/t} - C(1+|y-x|^2/t)^{1/2} - |y-x|_{\bar{a}^{-1}}^2/4t\}\\
&\le p(t,x,y+\bar{b}t)\\
&\le Ct^{-n/2}(1+|y-x|^2/t)^{n/2}\exp\{Ct^{-\alpha}e^{C|y-x|^2/t} - |y-x|_{\bar{a}^{-1}}^2/4t\}.
\end{aligned}$$

We had previously obtained upper and lower bounds in terms of $\bar{a}$ for the case $\beta = 0$, $\mu = 1$ and $\bar{b} = 0$. See [N], Theorems 4 and 5. Our new estimates improve the upper bound, but the new lower bound is weaker, though of course more general.

The method used for the lower bound in [N] does not readily transfer to the general case.

In the asymptotic regime $|y-x|^2/(t\log t) \to 0$ the error terms $Ct^{-\alpha}e^{C|y-x|^2/t}$ become negligible. In fact as $|y-x|^2/(t\log t) \to 0$ with $|y-x|^2/t \to \infty$ we have the exact large deviations asymptotics

$$(n/2)\log t + \log p(t,x,y+\bar{b}t) \sim -|y-x|^2_{\bar{a}^{-1}}/4t. \tag{1.11}$$

We write $\sim$ to mean that the ratio of the left and right sides tends to 1. Thus our estimates identify correctly the effective conductivity $\bar{a}$. The asymptotic regime $|y-x|^2/(t\log t) \to 0$ includes the diffusion scaling limit, which is the usual context for homogenization in the heat equation.

For coefficients with bounded derivatives we can strengthen the conclusion of Theorem 1.2, and also give a simpler proof. We make the condition that a, β and μ are weakly differentiable and for all $i,j=1,\dots,n$ and $x\in\mathbb{R}^n$

$$|da^{ij}(x)| \le \lambda, \quad |d\mu(x)| \le \lambda \tag{1.12}$$

and

$$|d\beta^{ij}(x)| \le \lambda. \tag{1.13}$$

Theorem 1.3. *Suppose that L is given by (1.4) with periodic coefficients and that (1.1),(1.2),(1.9),(1.12),(1.13) hold. There is a constant $C<\infty$, depending only on λ and n, such that for all $x,y\in\mathbb{R}^n$ and all $t>0$ we have*

$$\begin{aligned} t^{-n/2}e^{-C(VE+E^{1/2})}&\exp\{-|y-x|^2_{\bar{a}^{-1}}/4t\} \\ &\le p(t,x,y+\bar{b}t) \le Ct^{-n/2}E^{n/2}e^{CVE}\exp\{-|y-x|^2_{\bar{a}^{-1}}/4t\}, \end{aligned}$$

where $V=|y-x|/t$ and $E=1+|y-x|^2/t$.

The proof is given in §6. We note that in the proof the hypotheses (1.12),(1.13) are used only to ensure that the correctors for L and for its adjoint have bounded derivatives. So this property may be used as an alternative hypothesis. Now the error term CVE becomes negligible as $|y-x|/t\to 0$. The large deviations asymptotics (1.11) hold as $|y-x|/t \to 0$ and $|y-x|^2/t\to\infty$. We have already shown in [N] and in a special case that as $|y-x|/t\to\infty$ and $|y-x|^2/t\to\infty$ one has

$$\log p(t,x,y) \sim -d(x,y)^2/4t,$$

where $d(x,y)$ is the Riemannian distance function associated to the inner product a^{-1}. Thus as $|y-x|/t \to \infty$ the large deviations localize around the shortest path, whereas as $|y-x|/t\to 0$ the local structure is lost by homogenization. The fact that the slow-path ($|y-x|/t\to 0$) and fast-path asymptotics are different shows that Theorem 1.3 would fail without the error terms $e^{\pm CVE}$. We discuss the consequences of this dichotomy further in the context of some examples in §3.

Independently, and by probabilistic methods, Mark Freidlin and Richard Sowers have recently obtained similar large deviations estimates [FSo]. Discussions with

Richard Sowers on the asymptotic regime necessary for (1.11) helped to motivate Theorem 1.3.

We shall refer to the representation (1.4) as the *canonical form* for a second order elliptic differential operator on $\mathbb{R}^n$. To justify this let us consider an operator of the form

$$L^c f = \operatorname{div}(adf) + \langle b, df\rangle + cf \tag{1.14}$$

where a, b, c and the density μ determining the divergence are periodic and satisfy (1.1),(1.6),(1.9). In addition suppose that a and μ have weak derivatives and b has a weak divergence satisfying (1.12) and for all $x \in \mathbb{R}^n$

$$|\operatorname{div} b(x)| \leq \lambda. \tag{1.15}$$

The case $\mu = 1$, where div is the standard divergence, is of course included. We shall transform L^c to the canonical form and thus deduce estimates on the heat kernel $p^c(t,x,y)$ for L^c.

We can write

$$L^c f = \overline{\operatorname{div}}(adf) + \langle b + ad\log\mu, df\rangle + cf.$$

Since $|ad\log\mu(x)| \leq C$, the heat kernel estimate (1.8) applies. So the heat semigroup on the torus associated to L^c has a density function $\pi(t,x,y)$, with respect to Lebesgue measure, such that

$$C^{-1} \leq \pi(1,x,y) \leq C.$$

By a standard result of ergodic theory it follows that L^c has a unique positive periodic eigenfunction γ, normalized by

$$\int_T \gamma dm = 1,$$

and for all $x \in \mathbb{R}^n$

$$C^{-1} \leq \gamma(x) \leq C. \tag{1.16}$$

See for example Harris ([H], Chapter III, §10). We denote the eigenvalue of γ by $\bar{c}$. The condition (1.12)

$$|da^{ij}(x)| \leq \lambda$$

gives us uniform control of the derivative of γ. For we may choose some smooth cut-off function ϕ of compact support and consider

$$(L^c - \bar{c})(\phi\gamma) - 2\langle d\phi, ad(\phi\gamma)\rangle = \big(\operatorname{div}(ad\phi) + \langle b, d\phi\rangle - 2\langle d\log\phi, ad\phi\rangle\big)\gamma$$

as an equation for $\phi\gamma$ in some bounded domain containing the support of ϕ. Then by a standard result of elliptic partial differential equations, γ is differentiable and satisfies for all $x \in \mathbb{R}^n$

$$|d\gamma(x)| \leq C. \tag{1.17}$$

See for example Ladyženskaja and Ural'ceva ([LU], Chapter III, §15). Now set

$$Lf = \gamma^{-1}(L^c - \bar{c})(\gamma f).$$

Then

$$Lf = \operatorname{div}(adf) + \langle \tilde{b}, df \rangle$$

where $\tilde{b} = b + 2ad \log \gamma$. The explicit relation

$$p^c(t,x,y) = e^{\bar{c}t}\gamma(x)p(t,x,y)\gamma(y)^{-1},$$

together with (1.16), reduces the problem of estimating p^c to that of estimating p. Next, the operator L has a unique periodic invariant density ν, satisfying

$$\operatorname{div}(ad\nu - \tilde{b}\nu) = 0$$

and

$$\int_T \nu dm = 1$$

and then for all $x \in \mathbb{R}^n$

$$C^{-1} \leq \nu(x) \leq C.$$

See again [H]. The condition (1.12), together with (1.15), gives us uniform control of the derivative of ν. For we have the following equation for ν/γ,

$$\operatorname{div}\big(ad(\nu/\gamma)\big) - \langle b, d(\nu/\gamma)\rangle + (c - \bar{c} - \operatorname{div} b)(\nu/\gamma) = 0$$

and an argument similar to that used for (1.16) shows that ν is differentiable and satisfies for all $x \in \mathbb{R}^n$

$$|d\nu(x)| \leq C.$$

Hence $\eta = -\mu(ad\nu - \tilde{b}\nu)$ is a bounded periodic vector field with $\overline{\operatorname{div}}\,\eta = 0$. Hence we can find $\bar{b} \in \mathbb{R}^n$ and $\beta : \mathbb{R}^n \to \mathbb{R}^n \otimes \mathbb{R}^n$, periodic, differentiable and anti-symmetric such that for all $i, j = 1, \dots, n$ and $x \in \mathbb{R}^n$

$$|\bar{b}| \leq C, \quad |\beta(x)| \leq C, \quad |d\beta^{ij}(x)| \leq C$$

and

$$\eta = \bar{b} + \overline{\operatorname{div}}\,(\mu\nu\beta).$$

Denote by $\widetilde{\operatorname{div}}$ the divergence associated with density $\mu\nu$. Then we may rewrite the last equation in the form

$$\tilde{b} = ad \log \nu + (\bar{b}/\mu\nu) + \widetilde{\operatorname{div}}\,\beta$$

and

$$Lf = \widetilde{\operatorname{div}}\big((a+\beta)df\big) + \langle \bar{b}/\mu\nu, df\rangle.$$

This is the canonical form, and moreover a, β and $\mu\nu$ satisfy all the conditions required for Theorem 1.3. Hence we obtain:

Theorem 1.4. *Suppose L^c is given by (1.14) and that a, b, c and μ are periodic and satisfy (1.1),(1.6),(1.9),(1.12) and (1.15). Then L^c determines effective constants $\bar{a} \in \mathbb{R}^n \otimes \mathbb{R}^n$, $\bar{b} \in \mathbb{R}^n$ and $\bar{c} \in \mathbb{R}$ and there is a constant $C < \infty$, depending only on λ and n, such that for all $x, y \in \mathbb{R}^n$ and $t > 0$ we have*

$$e^{-C(VE+E^{1/2})}\bar{p}(t,x,y) \leq p^c(t,x,y) \leq CE^{n/2}e^{CVE}\bar{p}(t,x,y)$$

where

$$V = 1 \wedge (|y - x - \bar{b}t|/t), \quad E = (1 + |y - x - \bar{b}t|^2/t)$$

and where $\bar{p}$ is the heat kernel of the associated uniform medium

$$\bar{p}(t,x,y) = (4\pi t)^{-n/2}(\det \bar{a})^{-1/2} \exp\{\bar{c}t - |y - x - \bar{b}t|^2_{\bar{a}^{-1}}/4t\}.$$

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2 Extension of Aronson's estimates

We consider an elliptic second order differential operator in the canonical form (1.4)

$$Lf = \operatorname{div}\big((a+\beta)df\big) + \langle \bar{b}/\mu, df\rangle$$

and satisfying conditions (1.1),(1.2),(1.3). We shall prove the following estimate, which extends the case $\mu = 1$ and $\bar{b} = 0$ due to Aronson [A]:

$$C^{-1}t^{-n/2}\exp\{-C|y-x|^2/t\} \leq p(t,x,y+\bar{b}t) \leq Ct^{-n/2}\exp\{-|y-x|^2/Ct\}.$$

The method we shall use for the general case is based on the rederivation by Fabes and Stroock [FS] of the case $\beta = 0$ of Aronson's estimate. We begin with a technical lemma, which at a formal level is a simple consequence of the heat equation.

Lemma 2.1. *Let $u_0 \in L^2 \cap L^\infty(\mathbb{R}^n)$ and set $u_t = P_t u_0$. Assume that $\phi : [0,\infty) \times \mathbb{R}^n \to \mathbb{R}$ is weakly differentiable and satisfies for all $t \geq 0$*

$$\phi \in L^1 \cap L^\infty([0,t] \times \mathbb{R}^n),$$

and

$$\int_0^t \int_{\mathbb{R}^n} \left(\left| \frac{\partial \phi}{\partial s} \right| + |d\phi_s|^2 \right) dmds < \infty.$$

Then, for all $f \in C^2(\mathbb{R}^n)$,

$$\begin{aligned}
&\int_{\mathbb{R}^n} \phi_t f(u_t)dm - \int_{\mathbb{R}^n} \phi_0 f(u_0)dm \\
&\quad = \int_0^t \int_{\mathbb{R}^n} \frac{\partial \phi}{\partial s} f(u_s)dmds - \int_0^t \int_{\mathbb{R}^n} \phi_s f''(u_s)|du_s|^2 dmds \\
&\quad\quad - \int_0^t \int_{\mathbb{R}^n} \phi_s f'(u_s)\langle d\phi_s, du_s\rangle dmds.
\end{aligned}$$

Proof. Consider
$$u_t^{(n)} = n^{-1}\int_t^{t+n^{-1}} u_s ds.$$
Then $u_t^{(n)} \to u_t$ in $L^2(\mathbb{R}^n)$ and $u^{(n)} \to u$ in $L^2([0,t], W^{1,2}(\mathbb{R}^n))$ for all t, as $n \to \infty$. So it suffices to prove the identity for $u^{(n)}$. In addition to being a solution, $u^{(n)}$ has the property that $t \mapsto u_t^{(n)} : [0,\infty) \to W^{1,2}(\mathbb{R}^n)$ is continuous. Let us assume then that u has this property.

We deal first with the case where ϕ is independent of t. Denote by $\mathcal{A}$ the set of those $f \in C^2(\mathbb{R})$ for which the identity holds. We shall show that $\mathcal{A} = C^2(\mathbb{R})$. Obviously $\mathcal{A}$ is a vector space, which contains the constants. By dominated convergence, $\mathcal{A}$ is closed in $C^2(\mathbb{R})$. The fact that u is a solution says that $f(u) = u$ belongs to $\mathcal{A}$. So by the density of polynomials in $C^2(\mathbb{R})$, it suffices to show that $\mathcal{A}$ is an algebra.

Let $f, g \in \mathcal{A}$ and let $\phi \in L^1 \cap W^{1,2} \cap L^\infty(\mathbb{R}^n)$. Then, for all fixed t, we have $\phi f(u_t), \phi g(u_t) \in L^1 \cap W^{1,2} \cap L^\infty(\mathbb{R}^n)$. Fix n and set $\underline{s} = n^{-1}\lfloor ns/t\rfloor, \bar{s} = n^{-1}\lceil ns/t\rceil$. Then by splitting the interval $[0,t]$ into n subintervals, we deduce from the identities for f and g that
$$\begin{aligned}
&\int_{\mathbb{R}^n} \phi f(u_t)g(u_t)dm - \int_{\mathbb{R}^n} \phi f(u_0)g(u_0)dm \\
&= -\int_0^t \int_{\mathbb{R}^n} \phi\{f(u_{\bar{s}})g''(u_s) + f''(u_s)g(u_{\underline{s}})\}|du_s|^2 dmds \\
&\quad - \int_0^t \int_{\mathbb{R}^n} \phi f'(u_{\bar{s}})g'(u_s)\langle du_{\bar{s}}, du_s\rangle dmds \\
&\quad - \int_0^t \int_{\mathbb{R}^n} \phi f'(u_s)g'(u_{\underline{s}})\langle du_{\underline{s}}, du_s\rangle dmds \\
&\quad - \int_0^t \int_{\mathbb{R}^n} \{f(u_{\bar{s}})g'(u_s) + f'(u_s)g(u_{\underline{s}})\}\langle d\phi, du_s\rangle dmds.
\end{aligned}$$
This yields the desired identity for the product fg on letting $n \to \infty$.

We extend to the case where ϕ depends on t by a similar argument, first reducing to the case where $t \mapsto \phi_t : [0,\infty) \to W^{1,2}(\mathbb{R}^n)$ is continuous, and then letting $n \to \infty$ in the identity
$$\begin{aligned}
&\int_{\mathbb{R}^n} \phi_t f(u_t)dm - \int_{\mathbb{R}^n} \phi_0 f(u_0)dm \\
&= \int_0^t \int_{\mathbb{R}^n} \frac{\partial\phi}{\partial s} f(u_{\bar{s}})dmds - \int_0^t \int_{\mathbb{R}^n} \phi_{\underline{s}} f''(u_s)|du_s|^2 dmds \\
&\quad - \int_0^t \int_{\mathbb{R}^n} \phi_{\underline{s}} f'(u_s)\langle d\phi_{\underline{s}}, du_s\rangle dmds.
\end{aligned}$$
□

Proof of the upper bound. Let $v^* \in (\mathbb{R}^n)^*$ and let $\phi_0 \in L^2 \cap L^\infty(\mathbb{R}^n)$ with $\phi \geq 0$. Let $\theta \in W^{1,2} \cap W^{1,\infty}(\mathbb{R}^n)$, with $|d\theta| \leq |v^*|$. Set $\theta_t(x) = \langle v^*, \bar{b}t\rangle + \theta(x)$ and $\rho_t = e^{\theta_t}$. Set
$$\phi_t(x) = \int_{\mathbb{R}^n} p(t,x,z)\phi_0(z)m(dz).$$

Consider for $q = 2, 4, 8, \ldots,$

$$G_q(t) = \left(\int_{\mathbb{R}^n} (\phi_t \rho_t)^q dm \right)^{1/q}.$$

Then, by Lemma 2.1, for almost all t,

$$G_q'(t) = -G_q(t)^{1-q} \int_{\mathbb{R}^n} \left\{ \langle d\phi_t, (a-\beta) d(\phi_t^{q-1} \rho_t^q) \rangle + \langle v^*, \bar{b} \rangle \phi_t^q \rho_t^q (1/\mu - 1) \right\} dm.$$

Set $\psi_t = (\phi_t \rho_t)^{q/2}$, then

$$\langle d\phi_t, (a-\beta) d(\phi_t^{q-1} \rho_t) \rangle = (4/q^2)(q-1) |d\psi_t|_a^2 - \langle d\psi_t, \psi_t \big((2-4/q) a + 2\beta \big) \, d\theta \rangle - \psi_t^2 \, |d\theta|_a^2$$

and

$$\int_{\mathbb{R}^n} \phi_t^q \rho_t^q (1/\mu - 1) dm = \int_{\mathbb{R}^n} \psi_t^2 \operatorname{div} \xi \, dm = -2 \int_{\mathbb{R}^n} \langle d\psi_t, \psi_t \xi \rangle dm.$$

Hence by a quadratic inequality

$$G_q'(t) \le G_q(t)^{1-q} \left\{ -\frac{1}{Cq} \int_{\mathbb{R}^n} |d\psi_t|^2 dm + Cq|v^*|^2 \int_{\mathbb{R}^n} \psi_t^2 dm \right\}.$$

We now use the fundamental inequality of Nash

$$\int_{\mathbb{R}^n} |d\psi|^2 dz \ge \left(\int_{\mathbb{R}^n} \psi^2 dz \right)^{1+2/n} \Big/ \left(C \int_{\mathbb{R}^n} \psi dz \right)^{4/n}$$

to deduce the following system of differential inequalities:

$$G_q'(t) \le -\frac{1}{Cq} \frac{G_q(t)^{1+2q/n}}{G_{q/2}(t)^{2q/n}} + C|v^*|^2 q G_q(t).$$

Let us assume that ϕ_0 satisfies

$$G_2(0) = \left(\int_{\mathbb{R}^n} (\phi_0 \rho_0)^2 dm \right)^{1/2} = 1, \tag{2.1}$$

then we may deduce as in [FS], [S] or [NS] that

$$G_q(t) \le C t^{-n/4} e^{C|v^*|^2 t}. \tag{2.2}$$

Now

$$p(t, x, y) = \int_{\mathbb{R}^n} p(t/2, x, z) p(t/2, z, y) m(dz) \le I_1 I_2$$

where

$$I_1 = \left(\int_{\mathbb{R}^n} p(t/2, x, z)^2 / \rho_0(z)^2 m(dz) \right)^{1/2},$$

$$I_2 = \left(\int_{\mathbb{R}^n} p(t/2, z, y)^2 \rho_0(z)^2 m(dz) \right)^{1/2}.$$

We optimize (2.2) subject to (2.1) to obtain

$$\begin{aligned}\rho_{t/2}(x)I_1 &= \sup_{\phi_0}\int_{\mathbb{R}^n}\rho_{t/2}(x)p(t/2,x,z)\phi_0(z)m(dz)\\ &\leq \sup_{\phi_0}\limsup_{q\to\infty}G_q(t/2)\leq Ct^{-n/4}e^{C|v^*|^2t}\end{aligned}$$

so

$$I_1\leq Ct^{-n/4}e^{-\theta(x)-\langle v^*,\bar{b}t/2\rangle+C|v^*|^2t}$$

and by duality

$$I_2\leq Ct^{-n/4}e^{\theta(y)-\langle v^*,\bar{b}t/2\rangle+C|v^*|^2t}.$$

We can choose $\theta(z)$ so that $\theta(y)-\theta(x)=\langle v^*,y-x\rangle$ and so obtain

$$p(t,x,y)\leq Ct^{-n/2}e^{\langle v^*,y-x-\bar{b}t\rangle+C|v^*|^2t}.$$

The upper bound follows on optimizing over v^*. □

Proof of the lower bound. We shall first show for $|y-x-\bar{b}t|\leq 3\sqrt{t}$ that

$$p(t,x,y)\geq C^{-1}t^{-n/2}. \tag{2.3}$$

By a scaling argument this reduces to showing for $|x|\leq 2$ and $|y|\leq 2$ that

$$p(2,x-b,y+b)\geq C^{-1}.$$

Set $\gamma_s=(s-1)\bar{b}$. Fix $\sigma\in(0,\infty)$ and consider

$$\rho_s(z)=\begin{cases}\big(4\pi\sigma(2-s)\big)^{-n/2}e^{-|z-\gamma_s|^2/4\sigma(2-s)}, & \text{for } 0\leq s\leq 1,\\ (4\pi\sigma s)^{-n/2}e^{-|z-\gamma_s|^2/4\sigma s}, & \text{for } 1\leq s\leq 2.\end{cases}$$

Then

$$\rho_1(z)=(4\pi\sigma)^{-n/2}e^{-|z|^2/4\sigma}$$

and

$$\partial\rho/\partial s=\begin{cases}-\sigma^2\Delta\rho_s+\langle\bar{b},d\rho_s\rangle, & \text{for } 0\leq s\leq 1,\\ \sigma^2\Delta\rho_s+\langle\bar{b},d\rho_s\rangle, & \text{for } 1\leq s\leq 2.\end{cases}$$

By Jensen's inequality

$$\begin{aligned}\log p(2,x-\bar{b},y+\bar{b}) &= \log\int_{\mathbb{R}^n}p(1,x-\bar{b},z)p(1,z,y+\bar{b})m(dz)\\ &\geq \log\int_{\mathbb{R}^n}p(1,x-\bar{b},z)p(1,z,y+\bar{b})(4\pi\sigma)^{n/2}\rho_1(z)m(dz)\\ &\geq C\log\sigma+G(1)+\hat{G}(1)\end{aligned}$$

where

$$\begin{aligned}G(s) &= \int_{\mathbb{R}^n}\rho_s(z)\big(\log p(s,x-\bar{b},z)-C\big)m(dz), \quad \text{for } 0\leq s\leq 1,\\ \hat{G}(s) &= \int_{\mathbb{R}^n}\rho_s(z)\big(\log p(s,z,y-\bar{b})-C\big)m(dz), \quad \text{for } 1\leq s\leq 2.\end{aligned}$$

It is convenient to assume, as we may by the upper bound, that the constant C here is chosen so that the integrands are negative for $1/2 \leq s \leq 3/2$. We shall show that $G(1) \geq -C$ for a choice of σ depending only on λ and n. By duality also $\hat{G}(1) \geq -C$, thus establishing (2.3).

Set $p_s(z) = p(s, x - \bar{b}, z)$. Observe that for $R, K > 0$ we have

$$1 = \int_{\mathbb{R}^n} p_s dm \leq \int_{|z-\gamma_s| \geq R} p_s dm + e^{-K} m(|z - \gamma_s| \leq R) \\ + \|p_s\|_\infty m\big(|z - \gamma_s| \leq R, \quad p_s(z) \geq e^{-K}\big).$$

Then by the upper bound for p_s, for $1/2 \leq s \leq 1$, by choosing $R(\lambda, n) < \infty$ sufficiently large, then $K(\lambda, n) < \infty$ sufficiently large, we obtain

$$m\big(|z - \gamma_s| \leq R, \quad p_s(z) \geq e^{-K}\big) \geq C^{-1}.$$

We note that for $0 \leq s \leq 1$

$$|\langle \xi, d\langle d\rho_s, \bar{b}\rangle\rangle| \leq C\left(\frac{|z - \gamma_s|^2}{\sigma^2(2-s)} + \frac{1}{\sigma(2-s)}\right)\rho_s \leq \sigma^2 \Delta\rho_s + C\rho_s$$

for sufficiently large $\sigma(\lambda, n) < \infty$.

By the spectral gap inequality for the classical Laplacian, for $0 \leq s \leq 1$,

$$\int_{\mathbb{R}^n} \left(\psi - \int_{\mathbb{R}^n} \psi\rho_s dz\right)^2 \rho_s dz \leq 2\sigma(2-s) \int_{\mathbb{R}^n} |d\psi|^2 \rho_s dz.$$

We are now ready for the main calculation. In order to apply Lemma 2.1, we fix $\kappa \in (0, 1]$ and set $p_s^\kappa = p_s + \kappa$ and

$$G_\kappa(s) = \int_{\mathbb{R}^n} \rho_s(\log p_s^\kappa - C) dm.$$

Then p_s^κ is uniformly positive, so by truncating log away from the range of p_s^κ we can apply Lemma 2.1 to deduce, for almost all $s \in [1/2, 1]$

$$\begin{aligned}
G'_\kappa(s) &= -\int_{\mathbb{R}^n} (\sigma^2\Delta\rho_s - \langle\bar{b}, d\rho_s\rangle)(\log p_s^\kappa - C) dm \\
&\quad - \int_{\mathbb{R}^n} \langle d\log p_s^\kappa, (a + \beta) d\log(\rho_s/p_s^\kappa) + \bar{b}/\mu\rangle \rho_s dm \\
&= \int_{\mathbb{R}^n} \langle d\log p_s^\kappa, a d\log p_s^\kappa\rangle dm - \int_{\mathbb{R}^n} \langle d\log p_s^\kappa, (a+\beta) d\log\rho_s\rangle \rho_s dm \\
&\quad - \int_{\mathbb{R}^n} \langle d\log p_s^\kappa, \xi\rangle\langle d\log\rho_s, \bar{b}\rangle \rho_s dm \\
&\quad - \int_{\mathbb{R}^n} (\sigma^2\Delta\rho_s - \langle\xi, d\langle d\rho_s, \bar{b}\rangle\rangle)(\log p_s^\kappa - C) dm \\
&\geq \frac{1}{C}\int_{\mathbb{R}^n} |d\log p_s^\kappa|^2 \rho_s dz + CG_\kappa(s) - C \\
&\geq \frac{1}{C}\int_{\mathbb{R}^n} \big(G_\kappa(s) - \log p_s^\kappa\big)^2 \rho_s dz + CG_\kappa(s) - C \\
&\geq C^{-1} e^{-R^2/4\sigma} \big(G_\kappa(s) + K\big)^2 m\big(|z - \gamma_s| \leq R, p_s^\kappa(z) \geq e^{-K}\big) + CG_\kappa(s) - C \\
&\geq C^{-1} G_\kappa(s)^2 + CG_\kappa(s) - C \geq C^{-1} G_\kappa(s)^2 - C
\end{aligned}$$

and this differential inequality forces $G_\kappa(1) \ge -C$ with C independent of κ. Hence $G(1) \ge -C$ as required.

Finally we deduce the lower bound from (2.3) by a standard chaining argument. It suffices to show that

$$p(t,x,y) \ge t^{-n/2}e^{-Ck}$$

whenever $|y - x - \bar{b}t| \le (kt)^{1/2}$ and $k = 1, 2, \dots$. We choose points $x = x_0, x_1, \dots, x_{k-1}, x_k = y$ such that

$$|x_{j+1} - x_j - \bar{b}t/k| \le (t/k)^{1/2}$$

for all j, and note that when $|z_j - x_j| \le (t/k)^{1/2}$ this forces

$$|z_{j+1} - z_j - \bar{b}t/k| \le 3(t/k)^{1/2}$$

so by (2.3)

$$p(t/k, z_j, z_{j+1}) \ge C^{-1}t^{-n/2}.$$

Then

$$\begin{aligned} p(t,x,y) &\ge \underset{|z_j - x_j| \le (t/k)^{1/2}}{\int \dots \int} \prod_{j=0}^{k-1} p(t/k, z_j, z_{j+1}) m(dz_1) \dots m(dz_{k-1}) \\ &\ge (\Omega_n/3^n C)^{k-1}(t/k)^{n(k-1)/2} C^{-k}(t/k)^{-nk/2} \ge t^{-n/2}e^{-Ck} \end{aligned}$$

where Ω_n is the volume of the unit ball. □

The arguments we have used apply with no essential change to the case where a, β and $\bar{b}$ are time-dependent, as in [FS] and [NS]. We shall need one simple case below, where β_t and $\bar{b}_t$ take one value for $t < 0$ say and another for $t \ge 0$. Then for $s < 0 < t$, with an obvious notation

$$p(s,x;t,y) = \int_{\mathbb{R}^n} p_1(-s,x,z)p_2(t,z,y)m(dz)$$

so the relevant Gaussian bounds follow from those for p_1 and p_2.

In general, given a time-dependent elliptic second-order differential operator $\tilde{L}_t$, whose heat kernel $\tilde{p}$ with respect to Lebesgue measure satisfies for $s < t$

$$\begin{aligned} &C^{-1}(t-s)^{-n/2}\exp\{-C|y-x|^2/(t-s)\} \\ &\qquad \le \tilde{p}(s,x;t,y) \le C(t-s)^{-n/2}\exp\{-|y-x|^2/C(t-s)\}, \end{aligned}$$

Fabes and Stroock [FS] have shown that Nash's Hölder estimate applies. We can apply this to

$$\tilde{p}(s,x;t,y) = p(s, x+\gamma_s; t, y+\gamma_t)\mu(y+\gamma_t)$$

to deduce

$$\sup_{|x|,|x'| \le 1} |p(s,x;t,y) - p(s,x';t,y)| \le C(t-s)^{-(n+\alpha)/2} \tag{2.4}$$

for some constant $\alpha \in (0,1)$ depending only on λ and n. This is crucial to the averaging estimates in §4 and §5.

3 Variational characterizations of the effective conductivity

Suppose we are given an operator in the canonical form (1.4)

$$Lf = \operatorname{div}\big((a+\beta)df\big) + \langle \bar{b}/\mu, df\rangle$$

where a, β and μ are periodic, of period $T = [0,1]^n$, and that conditions (1.1),(1.2), (1.9) apply.

We described in §1 how one may identify, for a general elliptic second order differential operator with periodic coefficients, first an effective *potential* $\bar{c}$, and then an *effective drift* $\bar{b}$. At this point the operator is naturally written in the form (1.4). Next the *effective conductivity* $\bar{a}$ is identified by solving the cell problem (1.10). For our heat kernel estimates, indeed for any problem which involves estimating the effective conductivity, a variational characterization of $\bar{a}$ is more useful than a defining differential equation. We shall prove a single variational principle in Lemma 3.1, which allows us to deduce variational characterizations for $\bar{a}$ from both above and below. Immediate consequences are that diffusion in an incompressible fluid is always enhanced by motion of the fluid, whereas heat conduction in a solid is retarded by variability in the heat capacity.

Consider the relation

$$(v/\mu) - \operatorname{div}\chi = (a+\beta)(v^* - d\theta) + \langle \bar{b}, v^*\rangle\xi - \bar{b}\theta/\mu \tag{3.1}$$

where $v \in \mathbb{R}^n$, $v^* \in (\mathbb{R}^n)^*$, where θ is a periodic weakly differentiable potential with

$$\int_T \theta\, dm = 0,$$

and where χ is a periodic weakly differentiable vector potential. Recall that div is the divergence associated to m; in particular $\operatorname{div}\chi$ is the vector field characterized by

$$\int_T \langle \operatorname{div}\chi, \omega\rangle dm = -\int_T \langle \chi, d\omega\rangle dm$$

for all one-forms ω. For each v^* this relation serves to define uniquely v, θ and $\operatorname{div}\chi$, which then depend linearly on v^*. The same is true of the adjoint relation

$$(w/\mu) - \operatorname{div}\eta = (a-\beta)(w^* - d\psi) - \langle \bar{b}, w^*\rangle\xi + \bar{b}\psi/\mu.$$

One way to see this is to take the divergence in (3.1), so obtaining an elliptic equation for θ. Alternatively the variational arguments used in Lemma 3.1 below lead to the same conclusion. We may then write

$$v = (\bar{a}+\bar{\beta})v^*, \quad w = (\bar{a}-\bar{\beta})w^*$$

for constant matrices $\bar{a}$ and $\bar{\beta}$.

Observe that

$$\begin{aligned}&\int_T \langle v^* - d\theta, \langle \bar{b}, v^*\rangle \xi - \bar{b}\theta/\mu\rangle dm \\ &\quad = \int_T \langle d\theta, \theta\bar{b}/\mu\rangle dm - \langle v^*, \bar{b}\rangle \int_T \big(\theta(1/\mu - 1) + \langle \xi, d\theta\rangle\big) dm = 0 \qquad (3.2)\end{aligned}$$

where we have used the facts

$$\int_T \theta dm = 0, \quad \int_T \xi dm = 0, \quad (1/\mu) - 1 = \operatorname{div} \xi.$$

The following calculation confirms the suggestion of the notation that $\bar{a}$ is symmetric and $\bar{\beta}$ is anti-symmetric:

$$\begin{aligned}&\langle (\bar{a} - \bar{\beta})w^*, v^*\rangle = \langle w, v^*\rangle \\ &\quad = \int_T \langle (w/\mu) - \operatorname{div} \eta, v^* - d\theta\rangle dm \\ &\quad = \int_T \langle (a - \beta)(w^* - d\psi) - \langle \bar{b}, w^*\rangle \xi + \bar{b}\psi/\mu, v^* - d\theta\rangle dm \\ &\quad = \int_T \langle w^* - d\psi, (a + \beta)(v^* - d\theta) + \langle \bar{b}, v^*\rangle \xi - \bar{b}\theta/\mu\rangle dm \\ &\quad = \int_T \langle w^* - d\psi, (v/\mu) - \operatorname{div} \chi\rangle dm \\ &\quad = \langle w^*, v\rangle = \langle w^*, (\bar{a} + \bar{\beta})v^*\rangle.\end{aligned}$$

We used a polarization of (3.2) for the central equality. Moreover on taking $w^* = v^*$ we find

$$\langle \bar{a}v^*, v^*\rangle = \int_T |v^* - d\theta|_a^2 dm \geq 0$$

with equality only if $v^* = 0$, so $\bar{a}$ is positive-definite. On taking the divergence in (3.1) we obtain the cell problem, so θ is the corrector for v^* and our definition of $\bar{a}$ is compatible with §1.

Lemma 3.1. *For all $v \in \mathbb{R}^n$ and $v^* \in (\mathbb{R}^n)^*$ we have*

$$\begin{aligned}&|v - (\bar{a} + \bar{\beta})v^*|_{\bar{a}^{-1}}^2 \\ &\quad = \inf_{\theta,\chi} \int_T |(v/\mu) - \operatorname{div} \chi - (a + \beta)(v^* - d\theta) - \langle \bar{b}, v^*\rangle \xi + \bar{b}\theta/\mu|_{a^{-1}}^2 dm.\end{aligned}$$

Proof. Fix v and v^*. By a standard weak compactness argument in L^2 the infimum is attained, at θ and χ say, and by considering variations about the minimum we must have

$$\begin{aligned}(v/\mu) - \operatorname{div} \chi - (a + \beta)(v^* - d\theta) - \langle \bar{b}, v^*\rangle \xi + \bar{b}\theta/\mu &= 2a(w^* - d\psi), \\ (a - \beta)(w^* - d\psi) - \langle \bar{b}, w^*\rangle \xi + \bar{b}\psi/\mu &= -(w/\mu - \operatorname{div} \eta)\end{aligned}$$

for some $w \in \mathbb{R}^n, w^* \in (\mathbb{R}^n)^*$, some periodic weakly differentiable potential ψ of mean zero, and some period weakly differentiable vector potential η. On adding these equations we obtain

$$(v+w)/\mu - \operatorname{div}(\chi+\eta) = (a+\beta)\big((v^*+w^*) - d(\theta+\psi)\big) + \langle \bar{b}, v^*+w^*\rangle\xi - \bar{b}(\theta+\psi)/\mu.$$

Hence

$$v+w = (\bar{a}+\bar{\beta})(v^*+w^*), \quad w = -(\bar{a}-\bar{\beta})w^*$$

and hence

$$2\bar{a}w^* = v - (\bar{a}+\bar{\beta})v^*.$$

Therefore

$$\begin{aligned}\int_T &|(v/\mu) - \operatorname{div}\chi - (a+\beta)(v^*-d\theta) - \langle \bar{b}, v^*\rangle\xi + \bar{b}\theta/\mu|^2_{a^{-1}}\, dm \\ &= 4\int_T |w^* - d\psi|^2_a dm = 4|w^*|^2_{\bar{a}} = |v - (\bar{a}+\bar{\beta})v^*|^2_{\bar{a}^{-1}}. \qquad \square\end{aligned}$$

The lemma contains variational characterizations of the *effective conductivity* $\bar{a}$ both from below and from above. These will be applied in our lower and upper bounds respectively. From below we have

$$|v|^2_{\bar{a}^{-1}} = \inf_{\theta,\chi}\int_T |(v/\mu) - \operatorname{div}\chi + (a+\beta)d\theta + \bar{b}\theta/\mu|^2_{a^{-1}}\, dm. \tag{3.3}$$

Note that

$$|v - (\bar{a}+\bar{\beta})v^*|^2_{\bar{a}^{-1}} = |v - \bar{\beta}v^*|^2_{\bar{a}^{-1}} - 2\langle v, v^*\rangle + |v^*|^2_{\bar{a}},$$

so from above we have

$$|v^*|^2_{\bar{a}} = \inf_{v,\theta,\chi}\int_T |(v/\mu) - \operatorname{div}\chi - (a+\beta)(v^*-d\theta) - \langle \bar{b}, v^*\rangle\xi + \bar{b}\theta/\mu|^2_{a^{-1}}\, dm \tag{3.4}$$

where the infimum is taken over vectors v such that $\langle v^*, v\rangle = 0$.

We shall need to know that the minimizing potentials θ in (3.3) and (3.4) satisfy uniform bounds of the form

$$|\theta(x)| \le C|v| \quad (\text{respectively } C|v^*|). \tag{3.5}$$

By the proof of Lemma 3.1, these potentials are linear combinations of correctors, so it suffices to establish such bounds when θ satisfies

$$\operatorname{div}\big((a+\beta)(v^*-d\theta)\big) + \langle \bar{b}/\mu, v^*-d\theta\rangle = \langle \bar{b}, v^*\rangle,$$

and

$$\int_T \theta\, dm = 0.$$

Then obviously
$$\int_T |d\theta|^2 dm \leq C|v^*|^2$$
so also
$$\int_T |\theta|^2 dm \leq C|v^*|^2.$$
We have
$$\frac{\partial}{\partial t}\int_{\mathbb{R}^n} p(t,x,y)\big(\langle v^*, y\rangle - \theta(y)\big)m(dy) = \langle \bar{b}, v^*\rangle$$
so
$$\langle v^*, x\rangle - \theta(x - \bar{b}t) = \int_{\mathbb{R}^n} p(t, x - \bar{b}t, y)\big(\langle v^*, y\rangle - \theta(y)\big)m(dy).$$
Hence the desired estimate follows from Theorem 1.1.

We end this section by discussing for certain special cases some implications of the the variational characterizations (3.3) and (3.4) and the heat kernel estimates of §1. These special cases make it clear that the problem we consider can in no way be treated as small perturbation of the case $\mu = 1$ and $\beta = 0$.

The case where $a = \varepsilon I$ and $\mu = 1$ may be interpreted as diffusion at rate ε in an incompressible fluid undergong convection with velocity field $\bar{b} + \operatorname{div}\beta$. By taking $\theta = 0$ and $\chi = 0$ in (3.3) we see that here the effective conductivity $\bar{a} \geq a$. Thus the fluid motion always enhances the diffusion. Fannjiang and Papanicolaou [FP] have investigated the asymptotics of $\bar{a}$ as $\varepsilon \downarrow 0$ for various given motions of the fluid. The case
$$\operatorname{div}\beta = \begin{pmatrix} -\sin x \cos y \\ \cos x \sin y \end{pmatrix}, \quad \bar{b} = 0$$
in two dimensions gives a cellular flow: no fluid crosses the boundaries of the period cells. Nevertheless for small $\varepsilon > 0$ the effect of the fluid motion dramatically enhances the diffusion, so that
$$\bar{a} \sim c^* \sqrt{\varepsilon} I$$
where $c^* > 0$ is a known constant. The case where
$$\operatorname{div}\beta = \begin{pmatrix} \sin y \\ 0 \end{pmatrix}, \quad \bar{b} = 0$$
gives a shear layer flow. As $\varepsilon \downarrow 0$ one gets
$$\bar{a} \sim \begin{pmatrix} c^*\varepsilon^{-1} & 0 \\ 0 & \varepsilon \end{pmatrix}$$
where $c^* > 0$ is another known constant. Thus in one direction the effective diffusivity actually increases as the microscopic diffusivity decreases.

The case where $a = I$ and $\beta = 0$ may be interpreted as heat flow in a medium of variable heat capacity μ. By taking $v = 0$, $\theta = 0$ and $\chi = 0$ in (3.4) we see that here always $\bar{a} \leq a$. Thus the variability of μ serves to retard the conduction of heat.

It is instructive to consider the asymptotic results on the heat kernel that we obtain in the light of these examples. Consider first the cellular flow example with $\varepsilon \ll 1$. By our slow-path asymptotics for $t \gg 1$ and $\sqrt{t} \ll |x-y| \ll t$, $p(t,x,y)$ is approximated by the heat kernel with constant conductivity $c^*\sqrt{\varepsilon}$. But the fast-path asymptotics show for $t \gg 1$ and $t \ll |x-y|$ we should approximate by the heat kernel for conductivity ε: in this regime the fluid motion is no longer fast enough to boost conduction. Secondly, consider a solid medium of unit conductivity where the heat capacity varies periodically, with bounded derivative. The effective conductivity is then less than unity, and this is relevant in the asymptotic regime where $t \gg 1$ and $\sqrt{t} \ll |x-y| \ll t$. But in the extreme tail of the heat kernel where $t \gg 1$ and $t \ll |x-y|$ the retarding effect of the periodic structure is no longer felt.

4 The upper bound for measurable coefficients

Assume that L takes the canonical form (1.4)

$$Lf = \operatorname{div}\big((a+\beta)df\big) + \langle \bar{b}/\mu, df\rangle$$

where a, β and μ are periodic, of period $T = [0,1]^n$, and that conditions (1.1),(1.2), (1.9) apply. We shall show there are constants $\alpha \in (0,1)$ and $C < \infty$, depending only on λ and n such that, for all $x, y \in \mathbb{R}^n$ and $t > 0$

$$p(t,x,y+\bar{b}t) \le Ct^{-n/2}(1+|y-x|^2/t)^{1/2}\exp\{Ct^{-\alpha}e^{C|y-x|^2/t} - |y-x|^2_{\bar{a}^{-1}}/4t\}.$$

This is the upper bound of Theorem 1.2.

Fix x, y and t, and set $\varepsilon = (|y-x-\bar{b}t|^2/t)^{-1}$ and $v^* = \bar{a}^{-1}(y-x-\bar{b}t)/2t$. We may assume that $t > 1$ and

$$C \le |y-x-\bar{b}t|^2/t \le \log t/C$$

or the claimed bound follows from Theorem 1.1. Then

$$|v^*| \le C|y-x-\bar{b}t|/t \le (\log t/t)^{1/2} \le 1.$$

Denote by v, θ and χ the minimizing vector, potential and vector potential in the variational characterization (3.4) of $|v^*|^2_{\bar{a}}$. Set $\rho(z) = e^{\langle v^*, z\rangle - \theta(z)}$ and consider the operator

$$\begin{aligned}\tilde{L}f &= \rho^{-1}(L(\rho f)\\ &= Lf + 2\langle a(v^*-d\theta), df\rangle\\ &\qquad + \Big(\operatorname{div}\big((a+\beta)(v^*-d\theta)\big) + \langle \bar{b}/\mu, v^*-d\theta\rangle + |v^*-d\theta|^2_a\Big)f.\end{aligned}$$

Set

$$\phi_s(z) = \tilde{p}(s,z,y) = \rho(z)^{-1}p(s,z,y)\rho(y) = e^{\langle v^*, y-z\rangle - (\theta(y)-\theta(z))}p(s,z,y)$$

and consider

$$G(s) = \Big(\int_{\mathbb{R}^n} \phi_s^2 dm \Big)^{1/2}.$$

By the upper bound of Theorem 1.1 and the uniform bound (3.5) for θ we have

$$\phi_s(z) \le Cs^{-n} e^{\langle v^*, y-z\rangle} e^{-|y-z-\bar{b}s|^2/Cs},$$

so

$$G(s) \le Cs^{-n/4} e^{\langle v^*, \bar{b}s\rangle + C|v^*|^2 s},$$

and so

$$G(\varepsilon t/2) \le Ct^{-n/4}(|y-x-\bar{b}t|^2/t)^{n/4} e^{\langle v^*, \bar{b}\rangle \varepsilon t/2}.$$

We shall show below that there is a constant $\alpha \in (0,1)$, depending only on λ and n, such that, for any periodic measurable function g, for $\varepsilon t/2 \le s \le t/2$,

$$\Big| \int_{\mathbb{R}^n} g\phi_s^2 dm - \int_T g dm \int_{\mathbb{R}^n} \phi_s^2 dm \Big| \le Ct^{-\alpha} \int_T |g| dm \int_{\mathbb{R}^n} \phi_s^2 dm. \tag{4.1}$$

The constant α is in fact derived in a simple way from the Hölder exponent of Nash discussed at the end of §2. By a straightforward extension of Lemma 2.1, exploiting the Gaussian bounds we now have for $p(t,x,y)$, for almost all $s \in [\varepsilon t/2, t/2]$, we have

$$\begin{aligned}
\frac{1}{2}\frac{d}{ds} \int_{\mathbb{R}^n} \phi_s^2 dm &= \int_{\mathbb{R}^n} \phi_s \tilde{L} \phi_s dm \\
&= -\int_{\mathbb{R}^n} \langle d\phi_s, a d\phi_s\rangle dm + 2\int_{\mathbb{R}^n} \langle d\phi_s, \phi_s\big((v/\mu) - \operatorname{div}\chi - \beta(v^* - d\theta)\big)\rangle dm \\
&\quad + \int_{\mathbb{R}^n} (\langle \bar{b}/\mu, v^* - d\theta\rangle + |v^* - d\theta|_a^2)\phi_s^2 dm.
\end{aligned}$$

We have

$$\begin{aligned}
&\int_{\mathbb{R}^n} \langle \bar{b}/\mu, v^* - d\theta\rangle \phi_s^2 dm \\
&\qquad = \langle \bar{b}, v^*\rangle \int_{\mathbb{R}^n} \phi_s^2 dm - \int_{\mathbb{R}^n} (\langle \bar{b}/\mu, d\theta\rangle + (1 - 1/\mu)\langle \bar{b}, v^*\rangle)\phi_s^2 dm \\
&\qquad = \langle \bar{b}, v^*\rangle \int_{\mathbb{R}^n} \phi_s^2 dm + 2\int_{\mathbb{R}^n} \langle d\phi_s, \phi_s\big((\theta\bar{b}/\mu) - \xi\langle \bar{b}, v^*\rangle\big)\rangle dm.
\end{aligned}$$

By a quadratic inequality,

$$\begin{aligned}
\frac{1}{2}\frac{d}{ds} \int_{\mathbb{R}^n} \phi_s^2 dm &\le \int_{\mathbb{R}^n} |v^* - d\theta|_a^2 \phi_s^2 dm + \langle \bar{b}, v^*\rangle \int_{\mathbb{R}^n} \phi_s^2 dm \\
&\qquad + \int_{\mathbb{R}^n} |(v/\mu) - \operatorname{div}\chi - \beta(v^* - d\theta) + (\theta\bar{b}/\mu) - \xi\langle \bar{b}, v^*\rangle|_{a^{-1}}^2 \phi_s^2 dm \\
&\le \big(Ct^{-\alpha}|v^*|^2 + \langle \bar{b}, v^*\rangle + |v^*|_{\bar{a}}^2\big) \int_{\mathbb{R}^n} \phi_s^2 dm.
\end{aligned}$$

For the final inequality we used the averaging estimate (4.1), twice, and then the orthogonality relation (3.2), which shows

$$|v^*|^2_{\bar a} = \int_T |v^* - d\theta|^2_a dm + \int_T |(v/\mu) - \operatorname{div}\chi - \beta(v^* - d\theta) + (\theta\bar b/\mu) - \xi\langle \bar b, v^*\rangle|^2_{a^{-1}} dm.$$

Hence we obtain for $\varepsilon t/2 \le s \le t/2$,

$$G'(s) \le \big(Ct^{-\alpha}|v^*|^2 + \langle \bar b, v^*\rangle + |v^*|^2_{\bar a}\big)G(s).$$

Note that $|v^*|^2 t \le C\log t$. Then

$$\begin{aligned} G(t/2) &\le \exp\{Ct^{-\alpha}|v^*|^2 t + \langle \bar b, v^*\rangle(1-\varepsilon)t/2 + |v^*|^2_{\bar a}t/2\}G(\varepsilon t/2) \\ &\le Ct^{-n/4}(|y-x-\bar b t|^2/t)^{n/4}\exp\{Ct^{-\alpha} + \langle \bar b, v^*\rangle t/2 + |v^*|^2_{\bar a}t/2\}. \end{aligned}$$

We have

$$\begin{aligned} p(t,x,y) &= \rho(x)\int_{\mathbb{R}^n} \tilde p(t/2,x,z)\tilde p(t/2,z,y)m(dz)\rho(y)^{-1} \\ &\le Ce^{-\langle v^*, y-x\rangle}\hat G(t/2)G(t/2) \end{aligned}$$

where

$$\hat G(t/2) = \left(\int_{\mathbb{R}^n} \tilde p(t/2,x,z)^2 m(dz)\right)^{1/2}.$$

By symmetry $\hat G(t/2)$ satisfies the bound obtained for $G(t/2)$. Hence

$$p(t,x,y) \le Ct^{-n/2}(|y-x-\bar b t|^2/t)^{n/2}\exp\{Ct^{-\alpha} - \langle v^*, y-x-\bar b t\rangle + |v^*|^2_{\bar a}t\}$$

which gives the desired bound on setting $v^* = \bar a^{-1}(y-x-\bar b t)/2t$. □

Proof of (4.1). We have to show that *there are constants $\alpha \in (0,1)$ and $C < \infty$, depending only on λ and n, such that, for any measurable function g, for $\varepsilon t/2 \le s \le t/2$*

$$\left|\int_{\mathbb{R}^n} g\phi_s^2 dm - \int_T g\,dm\int_{\mathbb{R}^n}\phi_s^2 dm\right| \le Ct^{-\alpha}\int_T |g|dm\int_{\mathbb{R}^n}\phi_s^2 dm.$$

Let ψ be a bounded function, integrable over $\mathbb{R}^n$, and let g be a periodic function, integrable over T. Then

$$\left|\int_{\mathbb{R}^n} g\psi dm - \int_T g\,dm\int_{\mathbb{R}^n}\psi dm\right| \le \sum_N \delta_N(\psi)\int_T |g|dm \tag{4.2}$$

where N ranges over $\mathbb{Z}^n$ and

$$\delta_N(\psi) = \sup_{w,z\in T}|\psi(w+N) - \psi(z+N)|.$$

In estimating $\sum_N \delta_N(\psi)$ for certain functions ψ we shall use

$$\delta_N(\psi\phi) \leq \delta_N(\psi)|\phi|_N + |\psi|_N \delta_N(\phi)$$

where

$$|\psi|_N = \sup_{z\in T} |\psi(z+N)|.$$

We also note that a Gaussian bound such as

$$|\psi(z)| \leq Ct^{-n/2}e^{-|z|^2/Ct}$$

for some $t \geq 1$, allows the following estimate for all $R \geq 0$:

$$\sum_{|N|\geq Rt^{1/2}} \delta_N(\psi) \leq 2 \sum_{|N|\geq Rt^{1/2}} |\psi|_N \leq Ce^{-R^2/C}.$$

We turn to the case

$$\psi(z) = \left(e^{\langle v^*, y-z-\bar{b}s\rangle - (\theta(y)-\theta(z))} p(s,z,y)\right)^2$$

which is relevant to (4.1). It suffices to consider the case $y = \bar{b}s$, when we have

$$C^{-1}s^{-n/2}e^{-C|z|^2/s} \leq p(s,z,y) \leq Cs^{-n/2}e^{-|z|^2/Cs}$$

and by (2.4)

$$\delta_N\big(p(s,\cdot,y)\big) \leq Cs^{-(n+\alpha)/2}.$$

By (3.5) we have $|\theta(z)| \leq C|v^*| \leq C$, so

$$\int_{\mathbb{R}^n} \psi dm \geq C^{-1}s^{-n/2},$$

$$\psi(z) \leq Cs^{-n/2}e^{Cs|v^*|^2}\big(s^{-n/2}e^{-|z|^2/Cs}\big)$$

and

$$\delta_N(\psi) \leq Cs^{-n}e^{Cs|v^*|^2}(|v^*| + s^{-\alpha/2}).$$

Recall that $|v^*| \leq (\log t/t)^{1/2} \leq 1$ and $\varepsilon t/2 \geq t/\log t \geq 1$. Then, for $\varepsilon t/2 \leq s \leq t/2$ and $R = (C\log s)^{1/2}$,

$$\begin{aligned}
\sum_N \delta_N(\psi) &= \Bigg(\sum_{|N|<Rs^{1/2}} + \sum_{|N|\geq Rs^{1/2}}\Bigg)\delta_N(\psi) \\
&\leq Cs^{-n/2}e^{Cs|v^*|^2}\big((|v^*| + s^{-\alpha/2})R^n + e^{-R^2/C}\big) \\
&\leq Cs^{-n/2}t^{-\alpha/2} \leq Ct^{-\alpha/2}\int_{\mathbb{R}^n} \psi dm.
\end{aligned}$$

On substituting this estimate into (4.2) we obtain (4.1). □

5 The lower bound for measurable coefficients

Under the same conditions as §4 we shall show there are constants $\alpha \in (0,1)$ and $C < \infty$, depending only on λ and n, such that for all $x, y \in \mathbb{R}^n$ and $t > 0$

$$p(t,x,y+\bar{b}t) \geq t^{-n/2} \exp\{-Ct^{-\alpha} e^{C|y-x|^2/t} - C(1+|y-x|^2/t)^{1/2} - |y-x|^2_{\bar{a}^{-1}}/4t\}.$$

This is the lower bound in Theorem 1.2.

Fix x, y and t, and set $\varepsilon = (|y-x-\bar{b}t|^2/t)^{-1/2}$ and $v = (y-x-\bar{b}t)/(1-\varepsilon)t$. We may assume that $t > 1$ and

$$C \leq |y-x-\bar{b}t|^2/t \leq \log t/C$$

or the claimed bound follows from Theorem 1.1. Then

$$|v| \leq C|y-x-\bar{b}t|/t \leq (\log t/t)^{1/2} \leq 1.$$

Denote by θ and χ the minimizing potential and vector potential in the variational characterization (3.4) of $|v|^2_{\bar{a}^{-1}}$. Set $\tilde{\mu} = e^{-\theta}\mu$, $d\tilde{m}/dz = \tilde{\mu}$, $\tilde{\beta} = \beta - \chi$ and $\tilde{b} = \bar{b} + v$. We denote by $\widetilde{\operatorname{div}}$ the divergence associated to $\tilde{m}$.

Set

$$\tilde{p}_{t/2}(z) = \tilde{q}\big(t/2, z, (x+y)/2\big)$$

where $\tilde{q}$ is the heat kernel of $\widetilde{\operatorname{div}}(adf)$ with respect to $\tilde{m}$, which is symmetric. We note that

$$\int_{\mathbb{R}^n} \tilde{p}_{t/2} d\tilde{m} = 1$$

and by Theorem 1.1

$$\tilde{p}_{t/2}(z) \leq Ct^{-n/2} e^{-|z-(x+y)/2|^2/Ct}.$$

For $0 \leq s \leq t/2$, define $\tilde{p}_s(z)$ by the backward heat equation

$$\partial\tilde{p}/\partial s + \widetilde{\operatorname{div}}\big((a+\tilde{\beta})d\tilde{p}_s\big) + \langle \tilde{b}/\tilde{\mu}, d\tilde{p}_s\rangle = 0$$

with final value $\tilde{p}_{t/2}$. By Theorem 1.1 we have

$$\tilde{p}_{\varepsilon t/2}(z) \leq Ct^{-n/2} e^{-|z-x-\varepsilon\bar{b}t/2|^2/Ct}.$$

We shall prove below the following averaging estimate: there is a constant $\alpha \in (0,1)$, depending only on λ and n, such that for $0 \leq s \leq t/2$, for any non-negative measurable periodic function g,

$$\int_{\mathbb{R}^n} g\tilde{p}_s d\tilde{m} \leq (1+Ct^{-\alpha}) \int_T g dm. \tag{5.1}$$

Set $p_s(z) = p(s, x, z)$ and, for $\kappa \in [0, 1]$, set $p_s^\kappa = p_s + \kappa$ and

$$G_\kappa(s) = \int_{\mathbb{R}^n} \tilde{p}_s \log p_s^\kappa d\tilde{m}.$$

By Theorem 1.1 we know that

$$\log p_s(z) \geq -C - (n/2) \log s - |z - x - \bar{b}s|^2/s.$$

Hence

$$G_0(\varepsilon t/2) \geq -C - (n/2)\log(\varepsilon t/2) - C/\varepsilon \geq -(n/2)\log t - C/\varepsilon.$$

We would now like to appeal to Lemma 2.1 to compute the derivative $G'_\kappa(s)$. But in general we may not have

$$\int_0^t \int_{\mathbb{R}^n} \left| \frac{\partial \tilde{p}}{\partial s} \right| d\tilde{m} ds < \infty.$$

Indeed $\partial \tilde{p}/\partial s$ may not be a function. However we can still arrive at the conclusion of Lemma 2.1, by exploiting the fact that $\tilde{p}$ solves the heat equation. The only point in question, coming at the end of the proof of Lemma 2.1, is to pass to limit as $n \to \infty$ in

$$\int_0^t \int_{\mathbb{R}^n} \frac{\partial \tilde{p}}{\partial s} f(p_{\bar{s}}) d\tilde{m} ds$$

where $\bar{s} = n^{-1}\lceil ns/t \rceil$. But by the heat equation, the limit exists and is given by

$$\int_{\mathbb{R}^n} \langle f'(p_s) dp_s, (a + \tilde{\beta}) d\tilde{p}_s + \tilde{b}\tilde{p}_s/\tilde{\mu} \rangle d\tilde{m} ds.$$

So for $\kappa > 0$, for almost all $s \in [\varepsilon t/2, t/2]$ we have

$$\begin{aligned}
G'_\kappa(s) &= \int_{\mathbb{R}^n} \langle d \log p_s^\kappa, (a + \tilde{\beta}) d \log \tilde{p}_s \rangle \tilde{p}_s d\tilde{m} + \int_{\mathbb{R}^n} \langle d \log p_s^\kappa, \tilde{b}/\tilde{\mu} \rangle \tilde{p}_s d\tilde{m} \\
&\quad - \int_{\mathbb{R}^n} \langle (a + \beta) d(e^{-\theta} \tilde{p}_s / p_s^\kappa), dp_s^\kappa \rangle dm - \int_{\mathbb{R}^n} \langle d \log p_s^\kappa, \bar{b}/\mu \rangle \tilde{p}_s d\tilde{m} \\
&= \int_{\mathbb{R}^n} \langle d \log p_s^\kappa, a d \log p_s^\kappa \rangle \tilde{p}_s d\tilde{m} \\
&\quad + \int_{\mathbb{R}^n} \langle d \log p_s^\kappa, (v/\mu) - \operatorname{div} \chi + (a + \beta) d\theta + \bar{b}\theta/\mu \rangle \tilde{p}_s d\tilde{m} \\
&\quad + \int_{\mathbb{R}^n} \langle d \log p_s^\kappa, (e^\theta - 1 - \theta)\bar{b}/\mu - \chi d\theta - (e^\theta - 1) v/\mu \rangle \tilde{p}_s d\tilde{m} \\
&\geq -\frac{1}{4(1-\delta)} \int_{\mathbb{R}^n} |(v/\mu) - \operatorname{div} \chi + (a + \beta) d\theta + \bar{b}\theta/\mu|_{a^{-1}}^2 \tilde{p}_s d\tilde{m} \\
&\quad - \frac{1}{4\delta} \int_{\mathbb{R}^n} |(e^\theta - 1 - \theta)(\bar{b}/\mu) - \chi d\theta - (e^\theta - 1) v/\mu|_{a^{-1}}^2 \tilde{p}_s d\tilde{m} \\
&\geq -Ct^{-\alpha}|v|^2 - C|v|^4/\delta - |v|_{\bar{a}^{-1}}^2 / 4(1-\delta)
\end{aligned}$$

where we have used the averaging estimate (5.1). We take $\delta = |v|/2$ to obtain

$$G'_\kappa(s) \geq -Ct^{-\alpha}|v|^2 - C|v|^3 - |v|^2_{\bar{a}^{-1}}/4.$$

Hence

$$\begin{aligned} G_\kappa(t/2) &= G_\kappa(\varepsilon t/2) + \int_{\varepsilon t/2}^{t/2} G'_\kappa(s)ds \\ &\geq -(n/2)\log t - (C/\varepsilon) - Ct^{-\alpha} - (1-\varepsilon)|v|^2_{\bar{a}^{-1}} t/8 \\ &\geq -(n/2)\log t - Ct^{-\alpha} - C(|y-x-\bar{b}t|^2/t)^{1/2} - |y-x-\bar{b}t|^2_{\bar{a}^{-1}}/8t. \end{aligned}$$

This estimate is independent of $\kappa > 0$, so extends to $\kappa = 0$. Now

$$\begin{aligned} p(t,x,y) &= \int_{\mathbb{R}^n} p(t/2,x,z)p(t/2,z,y)m(dz) \\ &\geq Ct^{n/2}\int_{\mathbb{R}^n} p(t/2,x,z)p(t/2,z,y)\tilde{p}_{t/2}(z)\tilde{m}(dz), \end{aligned}$$

so by Jensen's inequality

$$\log p(t,x,y) \geq (n/2)\log t + G_0(t/2) + \hat{G}_0(t/2),$$

where

$$\hat{G}_0(t/2) = \int_{\mathbb{R}^n} \tilde{p}_{t/2}(z)\log p(t/2,z,y)\tilde{m}(dz).$$

By symmetry, $\hat{G}_0(t/2)$ satisfies the same lower bound as $G_0(t/2)$. So

$$\log p(t,x,y) \geq -(n/2)\log t - Ct^{-\alpha} - C(|y-x-\bar{b}t|^2/t)^{1/2} - |y-x-\bar{b}t|^2_{\bar{a}^{-1}}/4t$$

which is the desired lower bound. □

Proof of (5.1). We have to show *there are constants $\alpha \in (0,1)$ and $C < \infty$, depending only on λ and n, such that for $0 \leq s \leq t/2$, for any non-negative measurable periodic function g we have*

$$\int_{\mathbb{R}^n} g\tilde{p}_s d\tilde{m} \leq (1 + Ct^{-\alpha})\int_T g dm.$$

We refer to the notation used in the proof of (4.1). For $0 \leq s \leq t/2$ we have the following estimates from §2:

$$\begin{aligned} &\tilde{p}_s(z) \leq Ct^{-n/2}e^{-|z-\gamma_s|^2/Ct}, \\ &\delta_N(\tilde{p}_s) \leq Ct^{-(n+\alpha)/2} \end{aligned}$$

where $\gamma_s = (x+y)/2 + (s-t/2)\tilde{b}$. Hence for $R = (C\log t)^{1/2}$

$$\begin{aligned} \sum_N \delta_N(\tilde{p}_s) &= \Bigg(\sum_{|N-\gamma_s|\leq Rt^{1/2}} + \sum_{|N-\gamma_s|>Rt^{1/2}}\Bigg)\delta_N(\tilde{p}_s) \\ &\leq CR^n t^{-\alpha/2} + Ce^{-R^2/C} = C\big(t^{-\alpha/2}(\log t)^{n/2} + t^{-1}\big). \end{aligned}$$

Then for $g \geq 0$ measurable and periodic

$$\left| \int_{\mathbb{R}^n} g\tilde{p}_s d\tilde{m} - \int_T g d\tilde{m} \right| \leq Ct^{-\alpha/2} \int_T g d\tilde{m}$$

so

$$\int_{\mathbb{R}^n} g\tilde{p}_s d\tilde{m} \leq (1 + Ct^{-\alpha/2}) \int_T g d\tilde{m}.$$

Finally

$$\left| \int_T g d\tilde{m} - \int_T g dm \right| = \left| \int_T g(e^{-\theta} - 1) dm \right| \leq C|v| \int_T g dm \leq Ct^{-\alpha/2} \int_T g dm. \quad \square$$

6 Estimates for coefficients with bounded derivatives

Assume that L takes the canonical form (1.4)

$$Lf = \operatorname{div}\big((a + \beta) df\big) + \langle \bar{b}/\mu, df \rangle$$

where a, β and μ are periodic, of period $T = [0, 1]^n$, and that conditions (1.1),(1.2), (1.9) apply. Assume in addition that a, β and μ have weak derivatives satisfying (1.12),(1.13):

$$|da^{ij}(x)| \leq \lambda, \quad |d\beta^{ij}(x)| \leq \lambda, \quad |d\mu(x)| \leq \lambda$$

for all $i, j = 1, \dots, n$ and $x \in T$. We know already that, for any bounded measurable periodic function g of mean zero, the equation $Lf = g$ has a unique periodic solution f in $W_2^1(T)$, up to an additive constant. Now conditions (1.12),(1.13) ensure that f is continuously differentiable and satisfies an estimate of the form

$$|df(x)| \leq C \sup_{x \in T} |g(x)|. \tag{6.1}$$

See for example ([LU], Chapter III, Theorem 15.1).

Consider the relation (3.1)

$$(v/\mu) - \operatorname{div} \chi = (a + \beta)(v^* - d\theta) + \langle \bar{b}, v^* \rangle \xi - \bar{b}\theta/\mu.$$

On taking the divergence we obtain

$$\operatorname{div}\big((a + \beta) d\theta\big) + \langle \bar{b}/\mu, d\theta \rangle = \operatorname{div}\big((a + \beta) v^*\big) + \langle \bar{b}(1/\mu - 1), v^* \rangle$$

and hence, by (6.1), the uniform bound

$$|d\theta(x)| \leq C|v^*|. \tag{6.2}$$

Then from (3.1) itself

$$|\operatorname{div} \chi(x)| \leq C|v^*|. \tag{6.3}$$

The same argument applies to the adjoint operator. Also, the minimizing potential and vector potential in Lemma 3.1 were seen to be linear combinations of such θ and χ and hence satisfy estimates of the forms (6.2) and (6.3) themselves.

We shall show there is a constant $C < \infty$, depending only on λ and n, such that for all $x, y \in \mathbb{R}^n$ and $t > 0$

$$\begin{aligned} t^{-n/2}e^{-C(VE+E^{1/2})}&\exp\{-|y-x|^2_{\bar{a}^{-1}}/4t\} \\ &\leq p(t,x,y+\bar{b}t) \leq Ct^{-n/2}E^{n/2}e^{CVE}\exp\{-|y-x|^2_{\bar{a}^{-1}}/4t\}, \end{aligned}$$

where $V = |y-x|/t$ and $E = 1 + |y-x|^2/t$. This will prove Theorem 1.3.

Proof of the upper bound. To emphasise the power of (6.2) we shall start from scratch, making no appeal to Theorem 1.1. Suppose we are given $v^* \in (\mathbb{R}^n)^*$ and a potential θ. Set $\gamma(x) = e^{\langle v^*, x\rangle - \theta(x)}$ and define a new operator by

$$\tilde{L}f = \gamma^{-1}L(\gamma f).$$

Explicitly

$$\tilde{L}f = Lf + 2\langle a(v^* - d\theta), df\rangle + \Big\{\operatorname{div}\big((a+\beta)(v^*-d\theta)\big) + \langle \bar{b}/\mu, v^* - d\theta\rangle + |v^* - d\theta|^2_a\Big\} f.$$

The heat kernel of $\tilde{L}$ is given by

$$\tilde{p}(t,x,y) = \gamma(x)^{-1}p(t,x,y)\gamma(y).$$

We follow the usual method, of finding upper bounds on $\tilde{p}(t,x,y)$ depending on γ, and then optimizing over γ. Fix $y \in \mathbb{R}^n$ and set $\phi_t(x) = \tilde{p}(t,x,y)$. Then, by a simple extension of Lemma 2.1, for almost all t we have

$$\begin{aligned} \frac{d}{dt}\int_{\mathbb{R}^n} \phi_t dm = &\int_{\mathbb{R}^n} |v^* - d\theta|^2_a \phi_t dm \\ &- \int_{\mathbb{R}^n} \Big\{\operatorname{div}\big((a-\beta)(v^*-d\theta)\big) - \langle \bar{b}/\mu, v^* - d\theta\rangle\Big\}\phi_t dm. \end{aligned} \tag{6.4}$$

The adjoint corrector ψ for v^* satisfies

$$\operatorname{div}\big((a-\beta)(v^*-d\psi)\big) - \langle \bar{b}/\mu, v^* - d\psi\rangle = -\langle \bar{b}, v^*\rangle$$

with periodic boundary conditions and satisfies the uniform bound (6.2)

$$|d\psi(x)| \leq C|v^*|.$$

On taking $\theta = \psi$ we obtain

$$\frac{d}{dt}\int_{\mathbb{R}^n} \phi_t dm \leq (\langle \bar{b}, v^*\rangle + C|v^*|^2)\int_{\mathbb{R}^n} \phi_t dm.$$

We deduce the estimate

$$\int_{\mathbb{R}^n} e^{\langle v^*, y-x\rangle} p(t,x,y) m(dx) \le e^{C|v^*|+C|v^*|^2 t+\langle v^*,\bar{b}\rangle t}. \tag{6.5}$$

We digress to derive a more refined estimate of the same type, of which no further use is made. We know that

$$|v^*|_{\bar{a}}^2 = \int_T |v^* - d\psi|_a^2 dm$$

so we can find a periodic function $\omega \in W_2^1(T)$ such that

$$\operatorname{div}\big((a-\beta)d\omega\big) - \langle \bar{b}/\mu, d\omega\rangle = |v^*|_{\bar{a}}^2 - |v^* - d\psi|_a^2.$$

Then by (6.1), ω is differentiable and satisfies

$$|d\omega(x)| \le C|v^*|^2.$$

On taking $\theta = \psi + \omega$ in (6.4) we obtain

$$\frac{d}{dt}\int_{\mathbb{R}^n} \phi_t dm \le \big(\langle \bar{b}, v^*\rangle + |v^*|_{\bar{a}}^2 + C|v^*|^3\big)\int_{\mathbb{R}^n} \phi_t dm.$$

We deduce for $|v^*| \le 1$ the estimate

$$\int_{\mathbb{R}^n} e^{\langle v^*, y-x\rangle} p(t,x,y) m(dx) \le e^{C|v^*|+C|v^*|^3 t} e^{\langle v^*,\bar{b}\rangle t + |v^*|_{\bar{a}}^2 t}$$

which is then valid for all v^* by (6.5).

We turn from L^1 to L^2. By a simple extension of Lemma 2.1, we have the counterpart of (6.4): for almost all t

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^n} \phi_t^2 dm = &-\int_{\mathbb{R}^n} \langle d\phi_t, a d\phi_t\rangle dm + \langle \bar{b}, v^*\rangle \int_{\mathbb{R}^n} \phi_t^2 dm + \int_{\mathbb{R}^n} |v^* - d\theta|_a^2 \phi_t^2 dm \\ &+ 2\int_{\mathbb{R}^n} \langle d\phi_t, \phi_t\{(v/\mu) - \operatorname{div}\chi - \beta(v^* - d\theta) + (\theta\bar{b}/\mu) - \xi\langle \bar{b}, v^*\rangle\}\rangle dm.\end{aligned} \tag{6.6}$$

It is advantageous to introduce $v \in \mathbb{R}^n$ and a vector potential χ here, which by an integration by parts contribute nothing to the formula. On taking $\theta = 0$, $v = 0$ and $\chi = 0$, we obtain by a quadratic inequality

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^n} \phi_t^2 dm \le -\frac{1}{C}\int_{\mathbb{R}^n} |d\phi_t|^2 dx + (\langle \bar{b}, v^*\rangle + C|v^*|^2)\int_{\mathbb{R}^n} \phi_t^2 dm.$$

Consider

$$G(t) = \Big(\int_{\mathbb{R}^n} \phi_t^2 dm\Big)^{1/2}.$$

By Nash's inequality

$$G'(t) \le -G(t)^{1+4/n} / \Big(C \int_{\mathbb{R}^n} \phi_t dm\Big)^{4/n} + (\langle \bar{b}, v^* \rangle + C|v^*|^2) G(t)$$

so by the L^1 estimate (6.5)

$$(\log G)'(t) \le -\big(G(t)/Ce^{C|v^*|+C|v^*|^2 t + \langle v^*, \bar{b}\rangle t}\big)^{4/n} + \langle v^*, \bar{b}\rangle + C|v^*|^2.$$

Hence

$$G(t) \le Ct^{-n/4} e^{C|v^*| + \langle v^*, \bar{b}\rangle t + C|v^*|^2 t}$$

and hence

$$\Big(\int_{\mathbb{R}^n} \big(e^{\langle v^*, y-x\rangle} p(t,x,y)\big)^2 m(dx)\Big)^{1/2} \le Ct^{-n/4} e^{C|v^*| + C|v^*|^2 t + \langle v^*, \bar{b}\rangle t}. \tag{6.7}$$

This is in fact equivalent to the estimate

$$p(t, x, y + \bar{b}t) \le Ct^{-n/2} \exp\{C|y-x|/t - |y-x|^2/Ct\}$$

which is the upper bound of Theorem 1.1 in the case $|y-x|/t \le 1$. The condition $|y-x|/t \le 1$ may be seen as allowing some homogenization to take place. Without it, instead of an $L^1 \to L^2$ estimate we have to take the longer route $L^2 \to L^4 \to \ldots \to L^\infty$ used in proving Theorem 1.1.

For a more refined estimate we choose v, θ and χ to be the minimizing vector, potential and vector potential in the variational characterization (3.4) of $|v^*|^2_{\bar{a}}$. By conditions (6.2),(6.3) we have uniformly

$$|d\theta(x)| \le C|v^*|, \quad |\operatorname{div} \chi(x)| \le C|v^*|.$$

Set

$$\rho = |v^* - d\theta|_a^2 + |(v/\mu) - \operatorname{div}\chi - \beta(v^* - d\theta) + (\theta\bar{b}/\mu) - \xi\langle \bar{b}, v^*\rangle|^2_{a^{-1}} - |v^*|^2_{\bar{a}}$$

then ρ is a bounded periodic function of mean zero, so there is a periodic vector field η such that

$$\operatorname{div} \eta = \rho$$

and uniformly

$$|\eta(x)| \le C|v^*|^2.$$

Assume for now that

$$|v^*| \le 1 \le |v^*|^2 t \tag{6.8}$$

and set $\varepsilon = (|v^*|^2 t)^{-1}$ and $\delta = |v^*|/2$. Consider

$$G(t) = \Big(\int_{\mathbb{R}^n} \phi_t^2 dm\Big)^{1/2}.$$

By the estimate (6.7) we know

$$G(\varepsilon t) \leq C(\varepsilon t)^{-n/4} e^{C|v^*|+C\varepsilon|v^*|^2 t+\langle v^*,\varepsilon \bar{b} t\rangle}.$$

By applying a quadratic inequality in (6.6) we obtain

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^n}\phi_t^2 dm \leq -\delta\int_{\mathbb{R}^n}\langle d\phi_t, a d\phi_t\rangle dm \\ + \left(\langle \bar{b}, v^*\rangle + \frac{|v^*|_{\bar{a}}^2}{1-\delta}\right)\int_{\mathbb{R}^n}\phi_t^2 dm + \frac{1}{1-\delta}\int_{\mathbb{R}^n}\rho\phi_t^2 dm\end{aligned}$$

and by another quadratic inequality

$$\begin{aligned}\frac{1}{1-\delta}\int_{\mathbb{R}^n}\rho\phi_t^2 dm &= -\frac{2}{1-\delta}\int_{\mathbb{R}^n}\langle d\phi_t, \phi_t\eta\rangle dm \\ &\leq \delta\int_{\mathbb{R}^n}\langle d\phi_t, a d\phi_t\rangle dm + \frac{C|v^*|^4}{\delta}\int_{\mathbb{R}^n}\phi_t^2 dm,\end{aligned}$$

so

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^n}\phi_t^2 dm \leq (C|v^*|^3 + \langle \bar{b}, v^*\rangle + |v^*|_{\bar{a}}^2)\int_{\mathbb{R}^n}\phi_t^2 dm.$$

Therefore

$$G'(t) \leq (C|v^*|^3 + \langle \bar{b}, v^*\rangle + |v^*|_{\bar{a}}^2) G(t)$$

and combining this with our estimate for $G(\varepsilon t)$ we obtain

$$G(t) \leq Ct^{-n/4}(|v^*|^2 t)^{n/4} e^{C|v^*|+C|v^*|^3 t+\langle v^*,\bar{b}\rangle t+|v^*|_{\bar{a}}^2 t}.$$

We deduce the estimate

$$\begin{aligned}\left(\int_{\mathbb{R}^n}\left(e^{\langle v^*,y-x\rangle}p(t,x,y)\right)^2 m(dx)\right)^{1/2} \\ \leq Ct^{-n/4}(1+|v^*|^2 t)^{n/4} e^{C|v^*|+C|v^*|^3 t} e^{\langle v^*,\bar{b}\rangle t+|v^*|_{\bar{a}}^2 t}\end{aligned}$$

which remains valid when (6.8) fails by (6.7). By symmetry also

$$\begin{aligned}\left(\int_{\mathbb{R}^n}\left(e^{\langle v^*,y-x\rangle}p(t,x,y)\right)^2 m(dy)\right)^{1/2} \\ \leq Ct^{-n/4}(1+|v^*|^2 t)^{n/4} e^{C|v^*|+C|v^*|^3 t} e^{\langle v^*,\bar{b}\rangle t+|v^*|_{\bar{a}}^2 t}.\end{aligned}$$

Hence by the Cauchy–Schwarz inequality, for all v^*,

$$\begin{aligned}p(t,x,y) &= \int_{\mathbb{R}^n} p(t/2,x,z)p(t/2,z,y)m(dz) \\ &= e^{-\langle v^*,y-x\rangle}\int_{\mathbb{R}^n}\left(e^{\langle v^*,z-x\rangle}p(t/2,x,z)\right)\left(e^{\langle v^*,y-z\rangle}p(t/2,z,y)\right)m(dz) \\ &\leq Ct^{-n/2}(1+|v^*|^2 t)^{n/2} e^{C|v^*|+C|v^*|^3 t} e^{-\langle v^*,y-x-\bar{b}t\rangle+|v^*|_{\bar{a}}^2 t}.\end{aligned}$$

We take $v^* = \bar{a}^{-1}(y - x - \bar{b}t)/2t$ to obtain the desired upper bound. $\square$

Proof of the lower bound. We modify the proof of the lower bound for measurable coefficients, taking advantage of the extra regularity assumptions (1.12),(1.13). Fix $x, y \in \mathbb{R}^n$ and $t > 0$ and set $\varepsilon = (1+|y-x-\bar{b}t|^2/t)^{-1/2}$ and $v = (y-x-\bar{b}t)/(1-\varepsilon)t$. Denote by θ and χ the minimizing potential and vector potential in the variational characterization (3.3) of $|v|^2_{\bar{a}^{-1}}$. Then we have uniformly

$$|d\theta(x)| \leq C|v|, \quad |\operatorname{div}\chi(x)| \leq C|v|$$

so there is a periodic vector field η such that

$$\operatorname{div}\eta = |(v/\mu) - \operatorname{div}\chi + (a+\beta)d\theta + \bar{b}\theta/\mu|^2_{a^{-1}} - |v|^2_{\bar{a}^{-1}}$$

and uniformly

$$|\eta(x)| \leq C|v|^2.$$

We define $\tilde{p}_s$ as in §5 and note that, as a special case of the functional used in §5, for almost all $s \in [0, t/2]$, we have

$$\frac{d}{ds}\int_{\mathbb{R}^n} \tilde{p}_s \log \tilde{p}_s d\tilde{m} = \int_{\mathbb{R}^n} \langle d\log\tilde{p}_s, ad\log\tilde{p}_s\rangle \tilde{p}_s d\tilde{m}.$$

Also, by Theorem 1.1,

$$-C - (n/2)\log(t-s) \leq \int_{\mathbb{R}^n} \tilde{p}_s \log\tilde{p}_s d\tilde{m} \leq C - (n/2)\log(t-s)$$

so

$$\int_{\mathbb{R}^n} \tilde{p}_{t/2}\log\tilde{p}_{t/2} d\tilde{m} - \int_{\mathbb{R}^n} \tilde{p}_{\varepsilon t/2}\log\tilde{p}_{\varepsilon t/2} d\tilde{m} \leq C.$$

As in §5 we set $p_s(z) = p(s,x,z)$ and consider

$$G(s) = \int_{\mathbb{R}^n} \tilde{p}_s \log p_s d\tilde{m},$$

for which we have

$$G(\varepsilon t/2) \geq -(n/2)\log t - C/\varepsilon,$$

and the estimate

$$\begin{aligned} G'(s) \geq \frac{1}{4(1-\delta)} &\int_{\mathbb{R}^n} |(v/\mu) - \operatorname{div}\chi + (a+\beta)d\theta + \bar{b}\theta/\mu|^2_{a^{-1}}\tilde{p}_s d\tilde{m} \\ &- \frac{1}{4\delta}\int_{\mathbb{R}^n} |(e^\theta - 1 - \theta)(\bar{b}/\mu) - \chi d\theta - (e^\theta - 1)v/\mu|^2_{a^{-1}}\tilde{p}_s d\tilde{m}. \end{aligned}$$

We may assume $|v| \leq 1$ or the result follows from Theorem 1.1. Set $\delta = |v|/2$ to obtain

$$G'(s) \geq -C|v|^3 - C\int_{\mathbb{R}^n} \tilde{p}_s \operatorname{div}\eta d\tilde{m} - |v|^2_{\bar{a}^{-1}}/4.$$

Now by a quadratic inequality

$$\int_{\mathbb{R}^n} \tilde{p}_s \operatorname{div} \eta d\tilde{m} = \int_{\mathbb{R}^n} \langle \eta, d\log \tilde{p}_s \rangle \tilde{p}_s d\tilde{m} + \int_{\mathbb{R}^n} \langle \eta, d\theta \rangle \tilde{p}_s d\tilde{m}$$
$$\leq C|v|^3 + |v| \int_{\mathbb{R}^n} \langle d\log \tilde{p}_s, a d\log \tilde{p}_s \rangle \tilde{p}_s d\tilde{m}.$$

Hence

$$G(t/2) = G(\varepsilon t/2) + \int_{2t/2}^{t/2} G'(s) ds$$
$$\geq -(n/2)\log t - (C/\varepsilon) - C|v|^3 t - C|v| - (1-\varepsilon)|v|^2_{\bar{a}^{-1}} t/8.$$

For the rest we follow §5. □

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