Homogenization of the Periodic Schrödinger-type Equations

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Mathematical and Theoretical Physics,
dedicated to Ludwig Faddeev
St. Petersburg,
28–31 May 2024

Statement of the problem

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Let $\varepsilon > 0$ be a parameter. We use the notation

$$f^\varepsilon(\mathbf{x}) := f\left(\frac{\mathbf{x}}{\varepsilon}\right).$$

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Main object

By A_ε *we denote the operator in* $L_2(\mathbb{R}^d;\mathbb{C}^n)$ *given by*

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Here $g(\mathbf{x})$ *is a* Γ*-periodic* $(m \times m)$*-matrix-valued function such that*

$$c' \mathbf{1}_m \leqslant g(\mathbf{x}) \leqslant c'' \mathbf{1}_m, \quad 0 < c' \leqslant c'' < \infty;$$

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$b(\mathbf{D}) = \sum_{j=1}^d b_j D_j$ *is a first order* $(m \times n)$*-matrix DO. We assume that* $m \geqslant n$ *and that the symbol* $b(\boldsymbol{\xi}) = \sum_{j=1}^d b_j \xi_j$ *has maximal rank:*

$$\mathrm{rank}\, b(\boldsymbol{\xi}) = n, \quad 0 \neq \boldsymbol{\xi} \in \mathbb{R}^d.$$

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The precise definition of A_ε is given in terms of the quadratic form

$$a_\varepsilon[\mathbf{u},\mathbf{u}] = \int_{\mathbb{R}^d} \langle g^\varepsilon(\mathbf{x}) b(\mathbf{D})\mathbf{u}, b(\mathbf{D})\mathbf{u}\rangle \, d\mathbf{x}, \quad \mathbf{u} \in H^1(\mathbb{R}^d;\mathbb{C}^n).$$

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We have

$$c_0 \int_{\mathbb{R}^d} |\mathbf{D}\mathbf{u}|^2 \, d\mathbf{x} \leqslant a_\varepsilon[\mathbf{u},\mathbf{u}] \leqslant c_1 \int_{\mathbb{R}^d} |\mathbf{D}\mathbf{u}|^2 \, d\mathbf{x}, \quad \mathbf{u} \in H^1(\mathbb{R}^d;\mathbb{C}^n).$$

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Example:

$$A_\varepsilon = -\operatorname{div} g^\varepsilon(\mathbf{x})\nabla = \mathbf{D}^* g^\varepsilon(\mathbf{x})\mathbf{D}.$$

In this case, we have $n = 1$ and $m = d$.

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$$\begin{aligned} i\partial_\tau \mathbf{u}_\varepsilon(\mathbf{x},\tau) &= (A_\varepsilon \mathbf{u}_\varepsilon)(\mathbf{x},\tau), \quad \mathbf{x} \in \mathbb{R}^d, \ \tau \in \mathbb{R}; \\ \mathbf{u}_\varepsilon(\mathbf{x},0) &= \phi(\mathbf{x}). \end{aligned}$$

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The solution can be represented as

$$\mathbf{u}_\varepsilon(\cdot,\tau) = e^{-i\tau A_\varepsilon}\phi.$$

The effective operator

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Definition of the effective matrix g^0:
Let $\Lambda(\mathbf{x})$ be the $(n \times m)$-matrix-valued Γ-periodic solution of the problem

$$b(\mathbf{D})^* g(\mathbf{x})(b(\mathbf{D})\Lambda(\mathbf{x}) + \mathbf{1}_m) = 0, \quad \int_\Omega \Lambda(\mathbf{x})\, d\mathbf{x} = 0.$$

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Then g^0 is an $(m \times m)$-matrix given by

$$g^0 = |\Omega|^{-1} \int_\Omega \widetilde{g}(\mathbf{x})\, d\mathbf{x}, \quad \widetilde{g}(\mathbf{x}) = g(\mathbf{x})(b(\mathbf{D})\Lambda(\mathbf{x}) + \mathbf{1}_m).$$

Survey

- In 2001, **Birman** and **Suslina** proved that
$$\left\|(A_\varepsilon + I)^{-1} - (A^0 + I)^{-1}\right\|_{L_2(\mathbb{R}^d)\to L_2(\mathbb{R}^d)} \leqslant C\varepsilon \qquad (1)$$
by the *operator-theoretic* (spectral) *approach*.

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$$\left\|(A_\varepsilon + I)^{-1} - (A^0 + I)^{-1} - \varepsilon K(\varepsilon)\right\|_{L_2(\mathbb{R}^d)\to L_2(\mathbb{R}^d)} \leqslant C\varepsilon^2. \qquad (2)$$

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Here a *corrector* $K_1(\varepsilon)$ is given by

$$K_1(\varepsilon) = \Lambda^\varepsilon \Pi_\varepsilon b(\mathbf{D})(A^0+I)^{-1}, \quad (\Pi_\varepsilon \mathbf{u})(\mathbf{x}) = (2\pi)^{-d/2}\int_{\widetilde{\Omega}/\varepsilon} e^{i\langle \mathbf{x},\boldsymbol{\xi}\rangle}\widehat{\mathbf{u}}(\boldsymbol{\xi})\, d\boldsymbol{\xi},$$

and $K(\varepsilon)$ has a more complicated structure:

$$K(\varepsilon) = K_1(\varepsilon) + K_1(\varepsilon)^* + K_3.$$

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- A different approach to operator error estimates (the *shift method*) was suggested by **Zhikov** and **Pastukhova** in 2005. See a survey by Zhikov and Pastukhova (Russian Math. Surveys, 2016).

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- Similar results were obtained for $\cos(\tau A_\varepsilon^{1/2})$ and $A_\varepsilon^{-1/2}\sin(\tau A_\varepsilon^{1/2})$ by **Birman** and **Suslina**, **Meshkova**, **Dorodnyi** and **Suslina**.

Main questions

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Is it possible to approximate the operator $e^{-i\tau A_\varepsilon}$ *in the* $(H^s \to L_2)$*-norm with error* $O(\varepsilon^2)$ *and in the* $(H^s \to H^1)$*-norm with error* $O(\varepsilon)$*?*

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The results with corrector can be applied to the Cauchy problem

$$\begin{aligned} & i\partial_\tau \mathbf{u}_\varepsilon(\mathbf{x},\tau) = (A_\varepsilon \mathbf{u}_\varepsilon)(\mathbf{x},\tau), \quad \mathbf{x} \in \mathbb{R}^d,\ \tau \in \mathbb{R}; \\ & \mathbf{u}_\varepsilon(\mathbf{x},0) = \psi_\varepsilon(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}, \end{aligned} \tag{9}$$

with initial data from a special class:

$$\psi_\varepsilon := \phi + \varepsilon \Lambda^\varepsilon b(\mathbf{D})\Pi_\varepsilon \phi, \quad \phi \in H^s(\mathbb{R}^d; \mathbb{C}^n) \text{ with a suitable } s. \tag{10}$$

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Note that

$$(I + \varepsilon\Lambda^\varepsilon b(\mathbf{D})\Pi_\varepsilon)^{-1} = I - \varepsilon\Lambda^\varepsilon b(\mathbf{D})\Pi_\varepsilon \ \Rightarrow \ \boldsymbol{\phi} = \boldsymbol{\psi}_\varepsilon - \varepsilon\Lambda^\varepsilon b(\mathbf{D})\Pi_\varepsilon\boldsymbol{\psi}_\varepsilon.$$

Reduction 1: Scaling transformation

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We apply the operator-theoretic method based on the scaling transformation, the Floquet–Bloch theory and analytic perturbation theory. By the scaling transformation, the study of $e^{-i\tau A_\varepsilon}$ is reduced to the study of the operator

$$e^{-i\tau\varepsilon^{-2}A},$$

where $A = b(\mathbf{D})^* g(\mathbf{x}) b(\mathbf{D})$.

Reduction 2: Direct integral expansion

Using the unitary Gelfand transform, we expand the operator A in the direct integral:

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We have to approximate the operator

$$e^{-i\tau\varepsilon^{-2} A(\mathbf{k})}$$

uniformly in $\mathbf{k} \in \widetilde{\Omega}$.

Analytic perturbation theory

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$$\mathfrak{N} := \operatorname{Ker} A(0) = \{\mathbf{u} \in L_2(\Omega; \mathbb{C}^n) : \mathbf{u}(\mathbf{x}) = \mathbf{c} \in \mathbb{C}^n\}.$$

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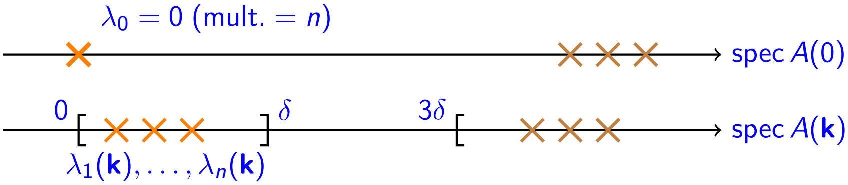
Let P be the orthogonal projection onto $\mathfrak{N}$: $P\mathbf{u} = |\Omega|^{-1} \int_\Omega \mathbf{u}(\mathbf{x})\, d\mathbf{x}$. So, $\lambda_0 = 0$ is an n-multiple isolated eigenvalue of $A(0)$. Then for $|\mathbf{k}| \leqslant t_0$ the perturbed operator $A(\mathbf{k})$ has exactly n eigenvalues $\lambda_1(\mathbf{k}), \dots, \lambda_n(\mathbf{k})$ on $[0, \delta]$, while the interval $(\delta, 3\delta)$ is free of the spectrum.



Analytic perturbation theory

We put $\mathbf{k} = t\boldsymbol{\theta}$, $t = |\mathbf{k}|$, $\boldsymbol{\theta} \in \mathbb{S}^{d-1}$, and study the operator family

$$A(\mathbf{k}) = A(t\boldsymbol{\theta}) =: A(t, \boldsymbol{\theta})$$

by means of the *analytic perturbation theory* with respect to t.

Analytic perturbation theory

We put $\mathbf{k} = t\boldsymbol{\theta}$, $t = |\mathbf{k}|$, $\boldsymbol{\theta} \in \mathbb{S}^{d-1}$, and study the operator family

$$A(\mathbf{k}) = A(t\boldsymbol{\theta}) =: A(t, \boldsymbol{\theta})$$

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By the Kato–Rellich theorem, for $t \leqslant t_0$ there exist real-analytic branches of the eigenvalues $\lambda_l(t, \boldsymbol{\theta})$ and the eigenvectors $\varphi_l(t, \boldsymbol{\theta})$ of $A(t, \boldsymbol{\theta})$:

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and the set $\{\varphi_l(t, \boldsymbol{\theta})\}$ forms an orthonormal basis in the eigenspace of $A(t, \boldsymbol{\theta})$ corresponding to $[0, \delta]$.

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$$\lambda_l(t, \boldsymbol{\theta}) = \gamma_l(\boldsymbol{\theta})t^2 + \mu_l(\boldsymbol{\theta})t^3 + \nu_l(\boldsymbol{\theta})t^4 + \dots, \tag{11}$$

$$\varphi_l(t, \boldsymbol{\theta}) = \omega_l(\boldsymbol{\theta}) + t\varphi_l^{(1)}(\boldsymbol{\theta}) + \dots, \tag{12}$$

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$l = 1, \dots, n$. Here $\gamma_l(\boldsymbol{\theta}) \geqslant c_* > 0$, and $\mu_l(\boldsymbol{\theta}), \nu_l(\boldsymbol{\theta}) \in \mathbb{R}$. The embryos $\omega_1(\boldsymbol{\theta}), \dots, \omega_n(\boldsymbol{\theta})$ form an orthonormal basis in $\mathfrak{N}$.

Analytic perturbation theory

Let $F(t,\boldsymbol{\theta})$ be the spectral projection of $A(t,\boldsymbol{\theta})$ for the interval $[0,\delta]$. We have the following *threshold approximations* for small t:

$$F(t,\boldsymbol{\theta}) = P + tF_1(\boldsymbol{\theta}) + O(t^2), \tag{13}$$

$$A(t,\boldsymbol{\theta})F(t,\boldsymbol{\theta}) = t^2 S(\boldsymbol{\theta})P + t^3 K(\boldsymbol{\theta}) + O(t^4). \tag{14}$$

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The operators $F_1(\boldsymbol{\theta})$, $S(\boldsymbol{\theta})$ and $K(\boldsymbol{\theta})$ can be described in the invariant terms, as well as in terms of the coefficients of power series expansions for $\lambda_l(t, \boldsymbol{\theta})$ and $\varphi_l(t, \boldsymbol{\theta})$.

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The operator $S(\boldsymbol{\theta}) = b(\boldsymbol{\theta})^* g^0 b(\boldsymbol{\theta})$ is called the *spectral germ* of the operator family $A(t,\boldsymbol{\theta})$ at $t=0$. The coefficients $\gamma_l(\boldsymbol{\theta})$ and the elements $\omega_l(\boldsymbol{\theta})$ are eigenvalues and eigenvectors of the spectral germ:

$$S(\boldsymbol{\theta})\omega_l(\boldsymbol{\theta}) = \gamma_l(\boldsymbol{\theta})\omega_l(\boldsymbol{\theta}), \quad l = 1, \dots, n.$$

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In terms of the coefficients,

$$N(\boldsymbol{\theta}) = N_0(\boldsymbol{\theta}) + N_*(\boldsymbol{\theta}),$$
$$N_0(\theta) = \sum_{l=1}^{n} \mu_l(\boldsymbol{\theta}) (\cdot, \omega_l(\boldsymbol{\theta})) \omega_l(\boldsymbol{\theta}),$$
$$N_*(\theta) = \sum_{l=1}^{n} \gamma_l(\boldsymbol{\theta}) \left((\cdot, P\varphi_l^{(1)}(\boldsymbol{\theta})) \omega_l(\boldsymbol{\theta}) + (\cdot, \omega_l(\boldsymbol{\theta})) P\varphi_l^{(1)}(\boldsymbol{\theta}) \right).$$

Results

Theorem 1 [Birman and Suslina, 2008]

For $\varepsilon > 0$ *and* $\tau \in \mathbb{R}$ *we have*

$$\left\| e^{-i\tau A_\varepsilon} - e^{-i\tau A^0} \right\|_{H^3(\mathbb{R}^d) \to L_2(\mathbb{R}^d)} \leqslant C(1 + |\tau|)\varepsilon.$$

Results with corrector

Theorem 2 [Suslina, 2023]

For $\varepsilon > 0$ *and* $\tau \in \mathbb{R}$ *we have*

$$\left\| e^{-i\tau A_\varepsilon}(I + \varepsilon \Lambda^\varepsilon b(\mathbf{D})\Pi_\varepsilon) - e^{-i\tau A^0} - \varepsilon K(\varepsilon,\tau) \right\|_{H^6(\mathbb{R}^d)\to L_2(\mathbb{R}^d)} \leqslant C(1+|\tau|)^2\varepsilon^2.$$

Here the corrector $K(\varepsilon,\tau)$ *is given by*

$$K(\varepsilon,\tau) := [\Lambda^\varepsilon] b(\mathbf{D})\Pi_\varepsilon e^{-i\tau A^0} - i\int_0^\tau e^{-i(\tau-\rho)A^0} b(\mathbf{D})^* L(\mathbf{D}) b(\mathbf{D}) e^{-i\rho A^0}\, d\rho.$$

Results with corrector

Theorem 3 [Suslina, 2023]

For $\varepsilon > 0$ and $\tau \in \mathbb{R}$ we have

$$\left\| e^{-i\tau A_\varepsilon} (I + \varepsilon \Lambda^\varepsilon b(\mathbf{D}) \Pi_\varepsilon) - e^{-i\tau A^0} - \varepsilon K_1(\varepsilon, \tau) \right\|_{H^4(\mathbb{R}^d) \to H^1(\mathbb{R}^d)} \leqslant C(1 + |\tau|)\varepsilon.$$

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Remark. 1) The correctors $K(\varepsilon, \tau)$ and $K_1(\varepsilon, \tau)$ are different. This agrees with the results for elliptic and parabolic equations.
2) We see that the "expected" first order approximation $e^{-i\tau A^0} + \varepsilon K_1(\varepsilon, \tau)$ is close not to the operator $e^{-i\tau A_\varepsilon}$, but to $e^{-i\tau A_\varepsilon} (I + \varepsilon \Lambda^\varepsilon b(\mathbf{D})\Pi_\varepsilon)$.

Discussion

It is impossible to approximate the operator $\varepsilon e^{-i\tau A_\varepsilon}[\Lambda^\varepsilon]b(\mathbf{D})\Pi_\varepsilon$ in terms of the spectral characteristics at the bottom of the spectrum.

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Improvement of the results under additional assumptions

The results can be improved under the following condition.

Condition 1

Suppose that at least one of the following assumptions is satisfied:
1°. $N(\boldsymbol{\theta}) = 0$ *for any* $\boldsymbol{\theta} \in \mathbb{S}^{d-1}$.
2°. $N_0(\boldsymbol{\theta}) = 0$ *for any* $\boldsymbol{\theta} \in \mathbb{S}^{d-1}$ *(i. e.,* $\mu_l(\boldsymbol{\theta}) \equiv 0$ *for* $l = 1, \dots, n$*) and the number of different eigenvalues of* $S(\boldsymbol{\theta})$ *does not depend on* $\boldsymbol{\theta}$.

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Theorem 4 [Dorodnyi, 2022]

Suppose that Condition 1 is satisfied. Then for $\varepsilon > 0$ *and* $\tau \in \mathbb{R}$

$$\| e^{-i\tau A_\varepsilon} - e^{-i\tau A^0} \|_{H^2(\mathbb{R}^d) \to L_2(\mathbb{R}^d)} \leqslant C(1 + |\tau|)^{1/2}\varepsilon. \qquad (15)$$

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Theorem 5 [Suslina, 2023]

Suppose that Condition 1 is satisfied. Then for $\varepsilon > 0$ *and* $\tau \in \mathbb{R}$

$$\left\| e^{-i\tau A_\varepsilon} (I + \varepsilon \Lambda^\varepsilon b(\mathbf{D}) \Pi_\varepsilon) - e^{-i\tau A^0} - \varepsilon K(\varepsilon, \tau) \right\|_{H^4(\mathbb{R}^d) \to L_2(\mathbb{R}^d)} \leqslant C(1 + |\tau|)\varepsilon^2.$$

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Sharpness of the results

In the general case, all the results are sharp with respect to the norm type and the dependence of estimates on τ.

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Theorem 7 [Suslina, 2017; Dorodnyi, 2022]

Suppose that $N_0(\boldsymbol{\theta}_0) \neq 0$ for some $\boldsymbol{\theta}_0 \in \mathbb{S}^{d-1}$, i. e., $\mu_l(\boldsymbol{\theta}_0) \neq 0$ for some l.
1) *Let $\tau \neq 0$ and $s < 3$. Then there does not exist a constant $C(\tau) > 0$ such that the estimate*

$$\left\| e^{-i\tau A_\varepsilon} - e^{-i\tau A^0} \right\|_{H^s(\mathbb{R}^d) \to L_2(\mathbb{R}^d)} \leqslant C(\tau)\varepsilon \tag{16}$$

holds for all sufficiently small ε.
2) *Let $s \geqslant 3$. There does not exist a positive function $C(\tau)$ such that $\lim_{|\tau|\to\infty} C(\tau)/|\tau| = 0$ and estimate (16) holds for $\tau \in \mathbb{R}$ and sufficiently small ε.*

Theorem 7 confirms that Theorem 1 is sharp.

Sharpness of the results

Theorem 8 [Suslina, 2023]

Suppose that $N_0(\boldsymbol{\theta}_0) \neq 0$ for some $\boldsymbol{\theta}_0 \in \mathbb{S}^{d-1}$, i. e., $\mu_l(\boldsymbol{\theta}_0) \neq 0$ for some l. Then the results of Theorem 2 and 3 are sharp both with respect to the norm type and with respect to the dependence of estimates on τ.

Sharpness of the results

Finally, we show that the improved results (that are valid under Condition 1) are also sharp.

Theorem 9 [Dorodnyi, 2022]

Suppose that $N_0(\boldsymbol{\theta}) = 0$ *for any* $\boldsymbol{\theta} \in \mathbb{S}^{d-1}$*, i. e.,* $\mu_l(\boldsymbol{\theta}) \equiv 0$ *for* $l = 1, \dots, n$*. Suppose that* $\nu_j(\boldsymbol{\theta}_0) \neq 0$ *for some* j *and* $\boldsymbol{\theta}_0 \in \mathbb{S}^{d-1}$*.*
1) *Let* $\tau \neq 0$ *and* $s < 2$*. Then there does not exist a constant* $C(\tau) > 0$ *such that the estimate*

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Theorem 9 shows that Theorem 4 is sharp.

Sharpness of the results

Theorem 10 [Suslina, 2023]

Suppose that $N_0(\boldsymbol{\theta}) = 0$ *for any* $\boldsymbol{\theta} \in \mathbb{S}^{d-1}$*, i. e.,* $\mu_l(\boldsymbol{\theta}) \equiv 0$ *for* $l = 1, \dots, n$*. Suppose that* $\nu_j(\boldsymbol{\theta}_0) \neq 0$ *for some* j *and* $\boldsymbol{\theta}_0 \in \mathbb{S}^{d-1}$*. Then the results of Theorems 5 and 6 are sharp both with respect to the norm type and with respect to the dependence of estimates on* τ*.*

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