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SEVERAL ESTIMATES OF MUSIELAK–ORLICZ–HARDY–SOBOLEV TYPE FOR SCHRÖDINGER TYPE OPERATORS

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Abstract. Let $L := -\mathrm{div}(A\nabla) + V$ be a Schrödinger type operator with the nonnegative potential V belonging to the reverse Hölder class $RH_q(\mathbb{R}^n)$ for some $q \in (n/2, \infty]$ and $n \geq 3$, where A satisfies the uniformly elliptic condition. Assume that $\varphi : \mathbb{R}^n \times [0, \infty) \to [0, \infty)$ is a function such that $\varphi(x, \cdot)$ is an Orlicz function and $\varphi(\cdot, t) \in \mathbb{A}_\infty(\mathbb{R}^n)$ (the class of uniformly Muckenhoupt weights). In this article, the author proves that the operators VL^{-1}, $V^{1/2}\nabla L^{-1}$ and $\nabla^2 L^{-1}$ are bounded from the Musielak–Orlicz–Hardy space associated with L, $H_{\varphi,L}(\mathbb{R}^n)$, to the Musielak-Orlicz space $L^\varphi(\mathbb{R}^n)$ or $H_{\varphi,L}(\mathbb{R}^n)$ under some further assumptions for φ and A, which further implies a maximal inequality for L in the scale of $H_{\varphi,L}(\mathbb{R}^n)$. All these results improve the known results by weakening the assumption for φ and L.

1. Introduction

Let $L := -\Delta + V$ be the Schrödinger operator on the Euclidean space $\mathbb{R}^n$ with $n \geq 3$. When V is a nonnegative polynomial on $\mathbb{R}^n$, the boundedness of $V^{1/2}\nabla L^{-1}$ and $\nabla^2 L^{-1}$ on $L^p(\mathbb{R}^n)$ with $p \in (1, \infty)$ was obtained by Zhong in [41]. Based on this, Shen [33] generalized these results via extending the nonnegative polynomial V to the case that $0 \leq V$ belongs to the reverse Hölder class $RH_q(\mathbb{R}^n)$ with some $q \in [n/2, \infty]$. Recall that a nonnegative function w on $\mathbb{R}^n$ is said to belong to the *reverse Hölder class* $RH_q(\mathbb{R}^n)$ with $q \in (1, \infty]$, denoted by $w \in RH_q(\mathbb{R}^n)$, if,

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when $q \in (1, \infty)$, $w \in L^q_{\mathrm{loc}}(\mathbb{R}^n)$ and

$$[w]_{RH_q(\mathbb{R}^n)} := \sup_{B\subset\mathbb{R}^n} \left\{\frac{1}{|B|}\int_B [w(x)]^q\,dx\right\}^{1/q} \left\{\frac{1}{|B|}\int_B w(x)\,dx\right\}^{-1} < \infty \tag{1.1}$$

or, when $q = \infty$, $w \in L^\infty_{\mathrm{loc}}(\mathbb{R}^n)$ and

$$[w]_{RH_\infty(\mathbb{R}^n)} := \sup_{B\subset\mathbb{R}^n} \left\{\operatorname*{ess\,sup}_{x\in B}\, w(x)\right\} \left\{\frac{1}{|B|}\int_B w(x)\,dx\right\}^{-1} < \infty, \tag{1.2}$$

where the suprema are taken over all balls $B \subset \mathbb{R}^n$. We remark that $RH_p(\mathbb{R}^n) \subset RH_q(\mathbb{R}^n)$ for any $1 < q < p \le \infty$ and, if V is a nonnegative polynomial, then $V \in RH_\infty(\mathbb{R}^n)$ (see, for example, [33]). It follows from [13] that $RH_q(\mathbb{R}^n)$ has the property of self-improvement. More precisely, if $V \in RH_q(\mathbb{R}^n)$ for some $q \in (1, \infty)$, then there exists $\epsilon \in (0, \infty)$, depending only on n and the constant C in (1.1), such that $V \in RH_{q+\epsilon}(\mathbb{R}^n)$. Thus, for any $V \in RH_q(\mathbb{R}^n)$ with $q \in (1, \infty]$, we introduce the *critical index* q_+ for V as follows:

$$q_+ := \sup\left\{q \in (1, \infty] :\ V \in RH_q(\mathbb{R}^n)\right\}. \tag{1.3}$$

It is easy to see that the boundedness of $\nabla^2 L^{-1}$ on $L^p(\mathbb{R}^n)$ implies immediately the Sobolev $W^{2,p}(\mathbb{R}^n)$ regularity for the solution u to the equation $-\Delta u + Vu = f$ when $f \in L^p(\mathbb{R}^n)$ with some $p \in (1, \infty)$. Furthermore, Shen [33] also established the boundedness of VL^{-1} on $L^p(\mathbb{R}^n)$, which, together with the boundedness of $\nabla^2 L^{-1}$ on $L^p(\mathbb{R}^n)$, further implies the following *maximal inequality* in $L^p(\mathbb{R}^n)$ (see also [1]):

$$\|-\Delta f\|_{L^p(\mathbb{R}^n)} + \|Vf\|_{L^p(\mathbb{R}^n)} \le C\,\|(-\Delta + V)f\|_{L^p(\mathbb{R}^n)},$$

where $f \in C_c^\infty(\mathbb{R}^n)$ and C is a positive constant independent of f. Moreover, the weighted $L^p(\mathbb{R}^n)$-boundedness of these operators was studied in [37]. Recently, Ly [27] proved that VL^{-1} and $\nabla^2 L^{-1}$ are bounded from the Hardy space $H^p_L(\mathbb{R}^n)$, associated with L, to $L^p(\mathbb{R}^n)$ when $p \in (0, 1]$, and $\nabla^2 L^{-1}$ is also bounded from $H^p_L(\mathbb{R}^n)$ to the classical Hardy space $H^p(\mathbb{R}^n)$ when $p \in (\frac{n}{n+1}, 1]$, via the boundedness of $\nabla^2 L^{-1}$ on $L^p(\mathbb{R}^n)$ with some $p \in (1, \infty)$ and some Sobolev type estimates for the heat kernel of L. Moreover, the boundedness of $\nabla^2 L^{-1}$ and VL^{-1} on the Musielak–Orlicz–Hardy space $H_{\varphi,L}(\mathbb{R}^n)$ was independently studied in [7] by different method. Very recently, the boundedness of VL^{-1}, $V^{1/2}(\nabla - i\vec{a})L^{-1}$ and $(\nabla - i\vec{a})^2 L^{-1}$ from the Musielak–Orlicz–Hardy space $H_{\varphi,L}(\mathbb{R}^n)$, associated with the magnetic Schrödinger operator L, to the Musielak–Orlicz space $L^\varphi(\mathbb{R}^n)$ was established in [8], where $L := -(\nabla - i\vec{a})\cdot(\nabla - i\vec{a}) + V$ with $\vec{a} := (a_1, a_2, \ldots, a_n)$ and $0 \le V \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$ satisfying some additional assumptions (see [8, Theorem 1.1] for the details).

Recall that the Musielak–Orlicz–Hardy space is a function space of Hardy-type which unify the classical Hardy space, the weighted Hardy space, the Orlicz-Hardy space and the weighted Orlicz-Hardy space, in which the spatial and the time variables may not be separable (see [12, 19, 35, 30, 32, 36, 38] for more details on the developments of Hardy-type spaces and Musielak-Orlicz spaces). We also remark that the Musielak–Orlicz–Hardy space appears naturally in many applications (see, for example, [5, 24, 25, 26]). This kind of Musielak–Orlicz–Hardy spaces associated with operators generalizes the (Orlicz-)Hardy space and the (weighted) (Orlicz-)Hardy space associated with operators, which has attracted great interests in recent years. Such function spaces associated with operators play important roles in the study for the boundedness of singular integrals associated with some differential operators, which may not fall within the scope of the classical Calderón-Zygmund theory (see, for example, [2, 6, 9, 11, 16, 17, 20, 21, 39]).

Let the matrix $A := \{a_{ij}\}_{1\le i,\,j\le n}$ satisfies the following assumptions.

(A$_1$) For any $i,\, j \in \{1,\, \dots,\, n\}$, a_{ij} is a measurable function on $\mathbb{R}^n$. Moreover, there exists a constant $\lambda \in (0,1]$ such that, for all $i,\, j \in \{1,\, \dots,\, n\}$ and $x,\, \xi \in \mathbb{R}^n$,

$$a_{ij}(x) = a_{ji}(x) \quad \text{and} \quad \lambda|\xi|^2 \le \sum_{i,\,j=1}^{n} a_{ij}(x)\xi_i\xi_j \le \lambda^{-1}|\xi|^2.$$

(A$_2$) There exist constants $\alpha \in (0,1]$ and $K \in (0,\infty)$ such that, for all $i,\, j \in \{1,\, \dots,\, n\}$,

$$\|a_{ij}\|_{C^\alpha(\mathbb{R}^n)} \le K,$$

where, for $f \in C^\alpha(\mathbb{R}^n)$, $\|f\|_{C^\alpha(\mathbb{R}^n)} := \sup_{x,\,y\in\mathbb{R}^n,\,x\neq y} \frac{|f(x)-f(y)|}{|x-y|^\alpha}$.

(A$_3$) For all $i,\, j \in \{1,\, \dots,\, n\}$, $x \in \mathbb{R}^n$ and $z \in \mathbb{Z}^n$,

$$a_{ij}(x+z) = a_{ij}(x) \text{ and } \sum_{k=1}^{n} \frac{\partial a_{kj}(x)}{\partial x_k} = 0.$$

Assume that $0 \le V$ belongs to the reserve Hölder class $RH_{q_0}(\mathbb{R}^n)$ for some $q_0 \in [n/2,\infty]$ and $n \ge 3$. Denote by $W^{1,\,2}(\mathbb{R}^n)$ the usual *Sobolev space on* $\mathbb{R}^n$ equipped with the norm $(\|f\|^2_{L^2(\mathbb{R}^n)} + \|\nabla f\|^2_{L^2(\mathbb{R}^n)})^{1/2}$, where ∇f denotes the *distributional gradient* of f. Let $V \in RH_{q_0}(\mathbb{R}^n)$ and

$$W^{1,\,2}_V(\mathbb{R}^n) := \left\{u \in W^{1,\,2}(\mathbb{R}^n) : \int_{\mathbb{R}^n} |u(x)|^2 V(x)\, dx < \infty\right\}.$$

Denote by L the *maximal-accretive operator* (see [31, p. 23, Definition 1.46] for the definition) on $L^2(\mathbb{R}^n)$ with largest domain $D(L) \subset W^{1,\,2}_V(\mathbb{R}^n)$ such that, for any $f \in D(L)$ and $g \in W^{1,\,2}_V(\mathbb{R}^n)$,

$$\langle Lf, g\rangle := \int_{\mathbb{R}^n} A(x)\nabla f(x) \cdot \overline{\nabla g(x)}\, dx + \int_{\mathbb{R}^n} f(x)\overline{g(x)}V(x)\, dx,$$

where $\langle\cdot,\cdot\rangle$ denotes the interior product in $L^2(\mathbb{R}^n)$ and A satisfies the assumption (A_1). In this sense, for all $f \in D(L)$, we write

$$Lf := -\mathrm{div}(A\nabla)f + Vf. \tag{1.4}$$

For the elliptic operator $L_0 := -\mathrm{div}(A\nabla)$ with A satisfying (A_1), (A_2) and (A_3), Avellaneda and Lin [4, Theorem B] proved that $\nabla^2 L_0$ is bounded on $L^p(\mathbb{R}^n)$ for any $p \in (1,\infty)$. It was also proved in [4, Theorem B] that the assumption (A_3) is necessary for the $L^p(\mathbb{R}^n)$-boundedness of $\nabla^2 L_0$. Moreover, for the operator L as in (1.4), Kurata and Sugano [23] studied the boundedness of VL^{-1}, $V^{1/2}\nabla L^{-1}$ and $\nabla^2 L^{-1}$ on weighted Lebesgue spaces and Morrey spaces under the assumptions that A satisfies (A_1), (A_2) and (A_3), $V \in RH_\infty(\mathbb{R}^n)$ and that, for all $i,\, j \in \{1,\, \ldots,\, n\}$, $a_{ij} \in C^{1+\alpha}(\mathbb{R}^n)$ with some $\alpha \in (0, 1]$.

Based on the work in [23], the boundedness of VL^{-1}, $V^{1/2}\nabla L^{-1}$ and $\nabla^2 L^{-1}$, from the Musielak–Orlicz–Hardy space $H_{\varphi,\,L}(\mathbb{R}^n)$ to $L^\varphi(\mathbb{R}^n)$ or $H_{\varphi,\,L}(\mathbb{R}^n)$, was studied in [40]. More precisely, assume that the Musielak-Orlicz function φ satisfies some assumptions (see [40, Theorems 1.4 and 1.6] or Remark 1.7 below for the details). It was proved in [40] that VL^{-1} and $V^{1/2}\nabla L^{-1}$ are bounded from $H_{\varphi,\,L}(\mathbb{R}^n)$ to $L^\varphi(\mathbb{R}^n)$ under the assumptions (A_1), (A_2) and $V \in RH_q(\mathbb{R}^n)$ with $q \in [n, \infty)$; $\nabla^2 L^{-1}$ is bounded from $H_{\varphi,\,L}(\mathbb{R}^n)$ to $L^\varphi(\mathbb{R}^n)$ or $H_\varphi(\mathbb{R}^n)$ under the assumptions (A_1), (A_2), (A_3), $V \in RH_q(\mathbb{R}^n)$ with $q \in [n, \infty)$ and that, for any $i,\, j \in \{1,\, \ldots,\, n\}$, $a_{ij} \in C^{1+\alpha}(\mathbb{R}^n)$ with some $\alpha \in (0, 1]$, and VL^{-1} is bounded on $H_{\varphi,\,L}(\mathbb{R}^n)$ under the same assumptions. Here, $H_\varphi(\mathbb{R}^n)$ denotes the Musielak–Orlicz–Hardy space introduced by Ky [24].

The main intention of this article is to improve the results obtained in [7, 40] by weakening the assumption for φ and L. More precisely, let L be as in (1.4) and $H_{\varphi,\,L}(\mathbb{R}^n)$ the Musielak–Orlicz–Hardy space associated with L. We establish the boundedness of the operators VL^{-1}, $V^{1/2}\nabla L^{-1}$ and $\nabla^2 L^{-1}$ from $H_{\varphi,\,L}(\mathbb{R}^n)$ to $L^\varphi(\mathbb{R}^n)$ or $H_{\varphi,\,L}(\mathbb{R}^n)$ under weaker assumptions than those in [7, 40].

In order to state the main results of this article, let us first recall some notation and definitions.

We first describe the growth function considered in this article. Recall that a function $\Phi : [0, \infty) \to [0, \infty)$ is called an *Orlicz function* if it is nondecreasing, $\Phi(0) = 0$, $\Phi(t) > 0$ for any $t \in (0, \infty)$ and $\lim_{t\to\infty} \Phi(t) = \infty$ (see, for example, [30, 32]). Moreover, Φ is said to be of *upper* (resp. *lower*) *type* p for some $p \in [0, \infty)$, if there exists a positive constant C such that, for all $s \in [1, \infty)$ (resp. $s \in [0, 1]$) and $t \in [0, \infty)$, $\Phi(st) \le Cs^p\Phi(t)$.

For a given function $\varphi : \mathbb{R}^n \times [0, \infty) \to [0, \infty)$ such that, for any $x \in \mathbb{R}^n$, $\varphi(x, \cdot)$ is an Orlicz function, φ is said to be of *uniformly upper* (resp. *lower*) *type* p for some $p \in (0, \infty)$ if there exists a positive constant C such that, for all $x \in \mathbb{R}^n$, $t \in [0, \infty)$ and $s \in [1, \infty)$ (resp. $s \in [0, 1]$), $\varphi(x, st) \le Cs^p\varphi(x, t)$. Let

$$I(\varphi) := \inf\{p \in (0, \infty) : \ \varphi \text{ is of uniformly upper type } p\} \tag{1.5}$$

and

$$i(\varphi) := \sup\{p \in (0, \infty) : \ \varphi \text{ is of uniformly lower type } p\}. \tag{1.6}$$

In what follows, $I(\varphi)$ and $i(\varphi)$ are, respectively, called the *uniformly critical upper type index* and the *uniformly critical lower type index* of φ. Observe that $I(\varphi)$ and $i(\varphi)$ may not be attainable, namely, φ may not be of uniformly upper type $I(\varphi)$ and uniformly lower type $i(\varphi)$ (see, for example, [6, 7, 39] for some examples). Moreover, it is easy to see that, if φ is of uniformly upper type $p_1 \in (0, \infty)$ and lower type $p_0 \in (0, \infty)$, then $p_1 \ge p_0$. Thus, $I(\varphi) \ge i(\varphi)$.

Definition 1.1. Let $\varphi : \mathbb{R}^n \times [0, \infty) \to [0, \infty)$ satisfy that $\varphi(\cdot, t)$ is measurable for all $t \in [0, \infty)$. The function φ is said to satisfy the *uniformly Muckenhoupt* *condition for some* $q \in [1, \infty)$, denoted by $\varphi \in \mathbb{A}_q(\mathbb{R}^n)$, if, when $q \in (1, \infty)$,

$$\mathbb{A}_q(\varphi) := \sup_{t\in(0,\infty)} \sup_{B\subset\mathbb{R}^n} \frac{1}{|B|^q} \int_B \varphi(x,t)\,dx \left\{ \int_B [\varphi(y,t)]^{1-q}\,dy \right\}^{q-1} < \infty$$

or, when $q = 1$,

$$\mathbb{A}_1(\varphi) := \sup_{t\in(0,\infty)} \sup_{B\subset\mathbb{R}^n} \frac{1}{|B|} \int_B \varphi(x,t)\,dx \left\{ \operatorname*{ess\,sup}_{y\in B} [\varphi(y,t)]^{-1} \right\} < \infty.$$

Here the first suprema are taken over all $t \in (0, \infty)$ and the second ones over all balls $B \subset \mathbb{R}^n$.

The function φ is said to satisfy the *uniformly reverse Hölder condition for some* $q \in (1, \infty]$, denoted by $\varphi \in \mathbb{RH}_q(\mathbb{R}^n)$, if $\sup_{t\in(0,\infty)}[\varphi(\cdot,t)]_{RH_q(\mathbb{R}^n)} < \infty$, where $[\varphi(\cdot,t)]_{RH_q(\mathbb{R}^n)}$ for any given $t \in (0, \infty)$ is defined as in (1.1) and (1.2) with w replaced by $\varphi(\cdot, t)$.

Recall that, in Definition 1.1, $\mathbb{A}_p(\mathbb{R}^n)$, with $p \in [1, \infty)$, and $\mathbb{RH}_q(\mathbb{R}^n)$, with $q \in (1, \infty]$, were respectively introduced in [24] and [39].

Let $\mathbb{A}_\infty(\mathbb{R}^n) := \cup_{q\in[1,\infty)}\mathbb{A}_q(\mathbb{R}^n)$. The *critical indices* for $\varphi \in \mathbb{A}_\infty(\mathbb{R}^n)$ is defined as follows:

$$q(\varphi) := \inf \{q \in [1, \infty) : \ \varphi \in \mathbb{A}_q(\mathbb{R}^n)\} \tag{1.7}$$

and

$$r(\varphi) := \sup \{q \in (1, \infty] : \ \varphi \in \mathbb{RH}_q(\mathbb{R}^n)\}. \tag{1.8}$$

Now we recall the notion of growth functions from Ky [24].

Definition 1.2. A function $\varphi : \mathbb{R}^n \times [0, \infty) \to [0, \infty)$ is called a *growth function* if the following hold:

(i) φ is a *Musielak-Orlicz function*, namely,
  (a) $\varphi(x, \cdot) : \ [0, \infty) \to [0, \infty)$ is an Orlicz function for all $x \in \mathbb{R}^n$;
  (b) $\varphi(\cdot, t)$ is a measurable function for all $t \in [0, \infty)$.

(ii) $\varphi \in \mathbb{A}_\infty(\mathbb{R}^n)$.

(iii) The function φ is of uniformly lower type p for some $p \in (0, 1]$ and of uniformly upper type 1.

Clearly, $\varphi(x, t) := \omega(x)\Phi(t)$ is a growth function if $\omega \in A_\infty(\mathbb{R}^n)$ and Φ is an Orlicz function of lower type p for some $p \in (0, 1]$ and upper type 1. Here, $A_q(\mathbb{R}^n)$ with $q \in [1, \infty]$ denotes the class of Muckenhoupt weights (see, for example, [15]). A typical example of such Orlicz function Φ is $\Phi(t) := t^p$, with $p \in (0, 1]$, for all $t \in [0, \infty)$ (see, for example, [38, 39] for more examples of such Φ). Another typical example of growth function is

$$\varphi(x, t) := \frac{t}{\ln(e + |x|) + \ln(e + t)} \tag{1.9}$$

for all $x \in \mathbb{R}^n$ and $t \in [0, \infty)$. It is worth to remark that for such φ as in (1.9), the corresponding Musielak–Orlicz–Hardy space $H_\varphi(\mathbb{R}^n)$ or $H_{\varphi,L}(\mathbb{R}^n)$, associated with the Schrödinger operator $L := -\Delta + V$ on $\mathbb{R}^n$, appears naturally when studying the products of functions in $H^1(\mathbb{R}^n)$ and $\mathrm{BMO}(\mathbb{R}^n)$, the endpoint estimates for the div-curl lemma and endpoint estimates for commutators of singular integrals related to the Schrödinger operator L (see [5, 25, 26] for the details).

Recall that, for a function φ as in Definition 1.2, a measurable function f on $\mathbb{R}^n$ is said to be in the *Musielak-Orlicz space* $L^\varphi(\mathbb{R}^n)$ if $\int_{\mathbb{R}^n}\varphi(x,|f(x)|)\,dx<\infty$. Moreover, for any $f\in L^\varphi(\mathbb{R}^n)$, define

$$\|f\|_{L^\varphi(\mathbb{R}^n)}:=\inf\left\{\lambda\in(0,\infty):\ \int_{\mathbb{R}^n}\varphi\left(x,\frac{|f(x)|}{\lambda}\right)\,dx\le 1\right\}.$$

Let L and φ be, respectively, as in (1.4) and Definition 1.2. We remark that, L is a nonnegative self-adjoint operator in $L^2(\mathbb{R}^n)$. Moreover, the Gaussian upper bound estimate for the kernels of the semigroup $\{e^{-tL}\}_{t>0}$ (see Lemma 4.5 below) further implies that the semigroup $\{e^{-tL}\}_{t>0}$ satisfies the reinforced $(1,\infty,1)$ off-diagonal estimates (see [6, Assumption (B)] for the details). Thus, L is a nonnegative self-adjoint operator on $L^2(\mathbb{R}^n)$ satisfying the reinforced $(1,\infty,1)$ off-diagonal estimates. Now we recall the Musielak–Orlicz–Hardy space $H_{\varphi,L}(\mathbb{R}^n)$, associated with L, introduced in [6].

For $f\in L^2(\mathbb{R}^n)$ and $x\in\mathbb{R}^n$, the *Lusin area function* $S_L(f)(x)$, associated with L, is defined by

$$S_L(f)(x):=\left\{\int_{\Gamma(x)}\left|t^2Le^{-t^2L}(f)(y)\right|^2\frac{dy\,dt}{t^{n+1}}\right\}^{1/2},$$

where $\Gamma(x):=\{(y,t)\in\mathbb{R}^n\times(0,\infty):\ |y-x|<t\}$. A function $f\in L^2(\mathbb{R}^n)$ is said to be in the set $\widetilde{H}_{\varphi,L}(\mathbb{R}^n)$ if $S_L(f)\in L^\varphi(\mathbb{R}^n)$; moreover, define $\|f\|_{H_{\varphi,L}(\mathbb{R}^n)}:=\|S_L(f)\|_{L^\varphi(\mathbb{R}^n)}$.

The *Musielak–Orlicz–Hardy space* $H_{\varphi,L}(\mathbb{R}^n)$ is defined to be the completion of $\widetilde{H}_{\varphi,L}(\mathbb{R}^n)$ respect with to the quasi-norm $\|\cdot\|_{H_{\varphi,L}(\mathbb{R}^n)}$.

Now we give out the first main result of this article.

Theorem 1.3. *Let L and φ be, respectively, as in (1.4) and Definition 1.2. Assume that $q_+>n/2$ and $q_+>I(\varphi)[r(\varphi)]'$, where q_+, $I(\varphi)$ and $r(\varphi)$ are, respectively, as (1.3), (1.5) and (1.8), and $[r(\varphi)]'$ denotes the conjugate exponent of $r(\varphi)$.*

(i) *If A in (1.4) satisfies the assumption (A_1), then VL^{-1} is bounded from $H_{\varphi,L}(\mathbb{R}^n)$ to $L^\varphi(\mathbb{R}^n)$.*

(ii) *If A in (1.4) satisfies the assumptions (A_1) and (A_2), then $V^{1/2}\nabla L^{-1}$ is bounded from $H_{\varphi,L}(\mathbb{R}^n)$ to $L^\varphi(\mathbb{R}^n)$.*

(iii) *If A satisfies the assumptions (A_1), (A_2) and (A_3), then ∇^2L^{-1} is bounded from $H_{\varphi,L}(\mathbb{R}^n)$ to $L^\varphi(\mathbb{R}^n)$.*

For any $t\in(0,\infty)$, denote by K_t the kernel of the semigroup operator e^{-tL}. To prove Theorem 1.3, we first establish some suitable estimates for VK_t, ∇K_t and ∇^2K_t (see Proposition 2.2 below). To end this, we borrow some ideas from [7, 27, 28]. Moreover, the functional calculus $L^{-1}=\int_0^\infty e^{-tL}\,dt$, the atomic characterization of $H_{\varphi,L}(\mathbb{R}^n)$ obtained in [6] (see also Lemma 3.2 below) and the boundedness of VL^{-1}, $V^{1/2}\nabla L^{-1}$ and ∇^2L^{-1} on $L^p(\mathbb{R}^n)$ with some $p\in(1,\infty)$ are used in the proof of Theorem 1.3.

To state the second main result of this article, we recall the definition of the Musielak–Orlicz–Hardy space $H_\varphi(\mathbb{R}^n)$ introduced in [24]. Denote by $\mathcal{S}(\mathbb{R}^n)$ the *space of all Schwartz functions* and by $\mathcal{S}'(\mathbb{R}^n)$ its *dual space* (namely, the *space of all tempered distributions*). For all $f \in \mathcal{S}'(\mathbb{R}^n)$, let $\mathcal{G}(f)$ denote its *non-tangential grand maximal function* (see [24] for the details).

Definition 1.4. Let φ be as in Definition 1.2. The *Musielak–Orlicz–Hardy space* $H_\varphi(\mathbb{R}^n)$ is defined to be the space of all $f \in \mathcal{S}'(\mathbb{R}^n)$ such that $\mathcal{G}(f) \in L^\varphi(\mathbb{R}^n)$ with the quasi-norm $\|f\|_{H_\varphi(\mathbb{R}^n)} := \|\mathcal{G}(f)\|_{L^\varphi(\mathbb{R}^n)}$.

Moreover, we have the following conclusion, which was stated in [3].

Lemma 1.5. *Let $L_0 := -\mathrm{div}(A\nabla)$ with A satisfying the assumption (A_1) and p_t be the kernel of the heat semigroup e^{-tL_0} generated by L_0. Then there exists $\alpha_0 \in (0, 1]$ such that, for any $\alpha \in (0, \alpha_0)$, there exist positive constants $C_{(\alpha)}$ and c_0 satisfying that, for all x, $x + h$, $y \in \mathbb{R}^n$ and $t \in (0,\infty)$ with $|h| \le \sqrt{t}$,*

$$|p_t(x+h, y) - p_t(x, y)| + |p_t(y, x+h) - p_t(y, x)| \le \frac{C_{(\alpha)}}{t^{n/2}} \left[\frac{|h|}{\sqrt{t}}\right]^\alpha e^{-\frac{c_0|x-y|^2}{t}}.$$

Let

$$\sigma_0 := \min\left\{\alpha_0,\, 2 - \frac{n}{q_+}\right\} \tag{1.10}$$

with α_0 and q_+, respectively, as in Lemma 1.5 and (1.3).

Now we give out the second main result of this article as follows.

Theorem 1.6. *Let L and φ be, respectively, as in (1.4) and Definition 1.2. Assume that $I(\varphi)$, $i(\varphi)$, $q(\varphi)$, $r(\varphi)$, q_+ and σ_0 are, respectively, as in (1.5), (1.6), (1.7), (1.8), (1.3) and (1.10), $q_+ > n/2$ and $q_+ > I(\varphi)[r(\varphi)]'$.*

(i) *If A in (1.4) satisfy the assumption (A_1) and $n + \sigma_0 > \frac{nq(\varphi)}{i(\varphi)}$, then VL^{-1} is bounded on $H_{\varphi,L}(\mathbb{R}^n)$.*

(ii) *If A in (1.4) satisfy the assumptions (A_1), (A_2) and (A_3), and $n + \frac{\sigma_0}{2} > \frac{nq(\varphi)}{i(\varphi)}$, then $V^{1/2}\nabla L^{-1}$ is bounded on $H_{\varphi,L}(\mathbb{R}^n)$.*

(iii) *If A in (1.4) satisfy the assumptions (A_1), (A_2) and (A_3), and $n + \sigma_0 > \frac{nq(\varphi)}{i(\varphi)}$, then $\nabla^2 L^{-1}$ is bounded on $H_{\varphi,L}(\mathbb{R}^n)$.*

(iv) *If A in (1.4) satisfy the assumptions (A_1), (A_2) and (A_3), $n + 1 > \frac{nq(\varphi)}{i(\varphi)}$ and $q(\varphi)[r(\varphi)]' < q_+$, then $\nabla^2 L^{-1}$ is bounded from $H_{\varphi,L}(\mathbb{R}^n)$ to $H_\varphi(\mathbb{R}^n)$.*

To prove Theorem 1.6, we introduce an atomic Musielak–Orlicz–Hardy space $H^{q,\varepsilon}_{\varphi,L}(\mathbb{R}^n)$ (see Definition 4.1 below) and then establish the inclusion relation $H^{q,\varepsilon}_{\varphi,L}(\mathbb{R}^n) \subset H_{\varphi,L}(\mathbb{R}^n)$ (see Lemma 4.3 below), which is motivated by [26]. Via this inclusion, $L^p(\mathbb{R}^n)$-boundedness of VL^{-1}, $V^{1/2}\nabla L^{-1}$ and $\nabla^2 L^{-1}$ for some $p \in (1,\infty)$, the atomic characterization of $H_{\varphi,L}(\mathbb{R}^n)$ obtained in [6, Theorem 5.4] (see also Lemma 3.2 below) and the molecular characterization of $H_\varphi(\mathbb{R}^n)$ obtained in [18, Theorem 4.13] (see also Lemma 4.8 below), we prove Theorem 1.6. It is worth pointing out that, the proof of Theorem 1.6 is different from that of [40, Theorem 1.6], and the new ingredient appeared in the proof of Theorem 1.6 is that we fully excavate some connotative information of the $(\varphi, q, M)_L$-atoms associated with L (see Definition 3.1 below).

Remark 1.7. Let $I(\varphi)$, $i(\varphi)$, $q(\varphi)$, $r(\varphi)$, q_+, α_0 and σ_0 are, respectively, as in (1.5), (1.6), (1.7), (1.8), (1.3), Lemma 1.5 and (1.10).

(a) Theorem 1.3 was obtained in [40, Theorem 1.4] under the assumptions that $V \in RH_{q_0}(\mathbb{R}^n)$ with $q_0 \in [n, \infty)$, $i(\varphi) \in (\frac{n}{n+\alpha_0}, 1]$ and

$$[r(\varphi)]' < \frac{n}{nq(\varphi)/i(\varphi) - \alpha_0}.$$

We also remark that, the additional assumption that, for any $i,\, j \in \{1, \ldots, n\}$, $a_{ij} \in C^{1+\alpha}(\mathbb{R}^n)$ with some $\alpha \in (0, 1]$, is necessary in [40, Theorem 1.4] when establishing the boundedness of $\nabla^2 L^{-1}$ from $H_{\varphi,\,L}(\mathbb{R}^n)$ to $L^{\varphi}(\mathbb{R}^n)$. Moreover, $I(\varphi)[r(\varphi)]' < q_+$ automatically holds true under these assumptions for φ. Thus, Theorem 1.3 improves the results in [40, Theorem 1.4] by weakening the assumptions for φ and A.

(b) When $A := I$ with I being the unit matrix, $L = -\Delta + V$ is just the Schrödinger operator on $\mathbb{R}^n$. Let $\varphi(x, t) := t^p$, for all $x \in \mathbb{R}^n$ and $t \in [0, \infty)$, with $p \in (0, 1]$. In this case the spaces $H_{\varphi,\,L}(\mathbb{R}^n)$ and $L^{\varphi}(\mathbb{R}^n)$ are, respectively, just the Hardy space $H^p_L(\mathbb{R}^n)$ studied in [11] and $L^p(\mathbb{R}^n)$. The boundedness of VL^{-1} and $\nabla^2 L^{-1}$, from $H^p_L(\mathbb{R}^n)$ to $L^p(\mathbb{R}^n)$, was obtained in [27, Theorem 1.2(a)]. Moreover, in this case, $r(\varphi) = \infty$, which implies that $I(\varphi)[r(\varphi)]' < q_+$ holds true. Thus, (i) and (iii) of Theorem 1.3 completely cover [27, Theorem 1.2(a)] by taking $A := I$ and $\varphi(x, t) := t^p$, for all $x \in \mathbb{R}^n$ and $t \in [0, \infty)$, with $p \in (0, 1]$.

(c) It follows from [40, Remark 2.4(iii)] that $H_{\varphi}(\mathbb{R}^n) \subset H_{\varphi,\,L}(\mathbb{R}^n)$ and there exists a positive constant C such that, for all $f \in H_{\varphi}(\mathbb{R}^n)$, $\|f\|_{H_{\varphi,\,L}(\mathbb{R}^n)} \le C\|f\|_{H_{\varphi}(\mathbb{R}^n)}$ under the assumption $n + \sigma_0 > \frac{nq(\varphi)}{i(\varphi)}$. Thus, as a corollary of (i), (ii) and (iii) of Theorem 1.6, we know that VL^{-1}, $V^{1/2}\nabla L^{-1}$ and $\nabla^2 L^{-1}$ are bounded from $H_{\varphi}(\mathbb{R}^n)$ to $H_{\varphi,\,L}(\mathbb{R}^n)$ under the assumptions of the terms (i), (ii) and (iii) of Theorem 1.6. Furthermore, as a corollary of Theorem 1.6(iv), we see that $\nabla^2 L^{-1}$ is bounded on $H_{\varphi}(\mathbb{R}^n)$ under the assumption of Theorem 1.6(iv) and that $n + \sigma_0 > \frac{nq(\varphi)}{i(\varphi)}$.

(d) (i), (iii) and (iv) of Theorem 1.6 were obtained in [40, Theorem 1.6 and Remark 1.8(i)] under the assumptions that A in (1.4) satisfies (A_1), (A_2), (A_3) and $a_{ij} \in C^{1+\alpha}(\mathbb{R}^n)$ with some $\alpha \in (0, 1]$ for any $i,\, j \in \{1, \ldots, n\}$, $V \in RH_{q_0}(\mathbb{R}^n)$ with $q_0 \in [n, \infty)$, $i(\varphi) \in (\frac{n}{n+\alpha_0}, 1]$ and

$$q(\varphi)[r(\varphi)]' < \frac{n}{nq(\varphi)/i(\varphi) - \alpha_0}.$$

It is easy to see that, $q(\varphi)[r(\varphi)]' < q_+$ and $n+\sigma_0 > \frac{nq(\varphi)}{i(\varphi)}$ automatically holds true under these assumptions for φ. Thus, (i), (iii) and (iv) of Theorem 1.6 improves [40, Theorem 1.6 and Remark 1.8(i)] by weakening the assumptions for φ and A.

(e) Theorem 1.6(ii) is new even when $A := I$ in (1.4) and $\varphi(x, t) := t^p$, for all $x \in \mathbb{R}^n$ and $t \in [0, \infty)$, with $p \in (\frac{n}{n+\sigma_0/2}, 1]$.

(f) From [40, Remarks 1.7 and 1.8], we deduce that the function φ as in (1.9) satisfies the assumptions in Theorems 1.3 and 1.6. Thus, the conclusion in Theorems 1.3 and 1.6 holds true for the space $H_{\varphi,\,L}(\mathbb{R}^n)$ and $H_{\varphi}(\mathbb{R}^n)$ associated with

φ as in (1.9) (see [40, Remarks 1.7 and 1.8] for more examples of φ satisfying the assumptions in Theorems 1.3 and 1.6).

As a corollary of Theorem 1.6, we have the following maximal inequality for L in the scale of the space $H_{\varphi,\,L}(\mathbb{R}^n)$.

Corollary 1.8. *Let φ, L and V be the same as in Theorem 1.6. Then there exists a positive constant C such that, for all $f \in C_c^\infty(\mathbb{R}^n)$,*

$$\|-\Delta f\|_{H_{\varphi,\,L}(\mathbb{R}^n)} + \|Vf\|_{H_{\varphi,\,L}(\mathbb{R}^n)} \le C\,\|Lf\|_{H_{\varphi,\,L}(\mathbb{R}^n)}\,.$$

The layout of this article is as follows. In Section 2, we establish several useful Sobolev type estimates for the heat kernel of L. Then, in Sections 3 and 4, we give the proofs of Theorems 1.3 and 1.6, respectively.

Finally we make some conventions on notation. Throughout the whole article, we denote by C a *positive constant* which is independent of the main parameters, but it may vary from line to line. We also use $C_{(\gamma,\beta,\dots)}$ to denote a *positive constant* depending on the indicated parameters γ, β, $\dots$. The *symbol* $A \lesssim B$ means that $A \le CB$. If $A \lesssim B$ and $B \lesssim A$, then we write $A \sim B$. For any given (quasi-)normed spaces $\mathcal{A}$ and $\mathcal{B}$ with the corresponding norms $\|\cdot\|_{\mathcal{A}}$ and $\|\cdot\|_{\mathcal{B}}$, the *symbol* $\mathcal{A} \subset \mathcal{B}$ means that, for all $f \in \mathcal{A}$, then $f \in \mathcal{B}$ and $\|f\|_{\mathcal{B}} \lesssim \|f\|_{\mathcal{A}}$. For any measurable subset E of $\mathbb{R}^n$, we denote by $E^{\complement}$ the *set* $\mathbb{R}^n \setminus E$ and by χ_E its *characteristic function*. We also set $\mathbb{N} := \{1, \dots\}$ and $\mathbb{Z}_+ := \{0\} \cup \mathbb{N}$. Moreover, for each ball $B \subset \mathbb{R}^n$, let $S_0(B) := 2B$ and $S_j(B) := 2^{j+1}B \setminus (2^jB)$ for $j \in \mathbb{N}$. Finally, for $q \in [1,\infty]$, we denote by q' the *conjugate exponent* of q, namely, $1/q + 1/q' = 1$.

2. Sobolev type estimates for heat kernel of L

In this section, we establish some useful Sobolev type estimates for the heat kernels of L. Assume that U is a nonnegative function on $\mathbb{R}^n$ and $U \in RH_q(\mathbb{R}^n)$ with $q \in [n/2, \infty]$. Then, for all $x \in \mathbb{R}^n$, the *auxiliary function* $m(x, U)$ associated with U is defined by

$$[m(x,U)]^{-1} := \sup\left\{r \in (0,\infty):\ \frac{r^2}{|B(x,r)|}\int_{B(x,r)} U(y)\,dy \le 1\right\}, \tag{2.1}$$

which was introduced by Shen [33]. To state the main results of this section, we first recall the following useful conclusion for the auxiliary function as in (2.1), which is just [33, Lemma 1.4].

Lemma 2.1. *Let the nonnegative function $U \in RH_q(\mathbb{R}^n)$ with $q \in [n/2, \infty]$ and $m(\cdot, U)$ be as in (2.1). Then there exist positive constants C_1, C_2 and k_0 such that, for all x, $y \in \mathbb{R}^n$,*

$$\frac{C_1 m(x,U)}{[1 + |x-y|m(x,U)]^{k_0/(k_0+1)}} \le m(y,U) \le C_2[1 + |x-y|m(x,U)]^{k_0} m(x,U).$$

Now we state the main results of this section, which play a key role in the proof of Theorem 1.3.

Proposition 2.2. *Let L be as in (1.4) and K_t the heat kernel of L. Assume that $q_+ \in (n/2, \infty)$ with q_+ as in (1.3).*

(i) *For all $p \in [1, 2q_+)$, $k \in \mathbb{Z}_+$, $x \in \mathbb{R}^n$ and $t,\ s \in (0,\infty)$, there exist positive constants $C_{(k,p)}$, $\xi_{(k,p)}$ and $c_{(k,p)}$, depending on k and p, such that*

$$\begin{aligned}&\left[\int_{\{y\in\mathbb{R}^n:\,|y-x|\geq\sqrt{s}\}}\left|\nabla\frac{\partial^k K_t(y,x)}{\partial t^k}\right|^p\,dy\right]^{1/p}\\&\quad\leq \frac{C_{(k,p)}}{t^{1/2+n/(2p')+k}}\exp\left\{-\xi_{(k,p)}\frac{s}{t}\right\}\exp\left\{-c_{(k,p)}(1+t[m(x,V)]^2)^\delta\right\}.\end{aligned}\tag{2.2}$$

(ii) *For all $p \in [1, q_+)$, $k \in \mathbb{Z}_+$, $x \in \mathbb{R}^n$ and $t,\ s \in (0,\infty)$, there exist positive constants $C_{(k,p)}$, $\xi_{(k,p)}$ and $c_{(k,p)}$, depending on k and p, such that*

$$\begin{aligned}&\left[\int_{\{y\in\mathbb{R}^n:\,|y-x|\geq\sqrt{s}\}}\left|\nabla^2\frac{\partial^k K_t(y,x)}{\partial t^k}\right|^p\,dy\right]^{1/p}\\&\quad\leq \frac{C_{(k,p)}}{t^{1+n/(2p')+k}}\exp\left\{-\xi_{(k,p)}\frac{s}{t}\right\}\exp\left\{-c_{(k,p)}(1+t[m(x,V)]^2)^\delta\right\}\end{aligned}$$

and

$$\begin{aligned}&\left[\int_{\{y\in\mathbb{R}^n:\,|y-x|\geq\sqrt{s}\}}\left|V(y)\frac{\partial^k K_t(y,x)}{\partial t^k}\right|^p\,dy\right]^{1/p}\\&\quad\leq \frac{C_{(k,p)}}{t^{1+n/(2p')+k}}\exp\left\{-\xi_{(k,p)}\frac{s}{t}\right\}\exp\left\{-c_{(k,p)}(1+t[m(x,V)]^2)^\delta\right\},\end{aligned}\tag{2.3}$$

here and hereafter, $m(\cdot, V)$ is as in (2.1) and $\delta := 1/[2(k_0+1)]$ with k_0 as in Lemma 2.1.

Obviously, the conclusion of Proposition 2.2 could be derived from the following Lemma 2.3. Thus, we only need to prove Lemma 2.3.

Lemma 2.3. *Let L, q_+ and K_t be as in Proposition 2.2.*

(i) *For all $p \in [1, 2q_+)$, $k \in \mathbb{Z}_+$, $x \in \mathbb{R}^n$ and $t \in (0,\infty)$,*

$$\begin{aligned}&\left\{\int_{\mathbb{R}^n}\left|\nabla\frac{\partial^k K_t(y,x)}{\partial t^k}\right|^p e^{p\xi_{(k,p)}\frac{|y-x|^2}{t}}\,dy\right\}^{1/p}\\&\quad\leq \frac{C_{(k,p)}}{t^{1/2+n/(2p')+k}}\exp\left\{-c_{(k,p)}(1+t[m(x,V)]^2)^\delta\right\}.\end{aligned}$$

(ii) *For all $p \in [1, q_+)$, $k \in \mathbb{Z}_+$, $x \in \mathbb{R}^n$ and $t \in (0,\infty)$,*

$$\begin{aligned}&\left\{\int_{\mathbb{R}^n}\left|\nabla^2\frac{\partial^k K_t(y,x)}{\partial t^k}\right|^p e^{p\xi_{(k,p)}\frac{|y-x|^2}{t}}\,dy\right\}^{1/p}\\&\quad\leq \frac{C_{(k,p)}}{t^{1+n/(2p')+k}}\exp\left\{-c_{(k,p)}(1+t[m(x,V)]^2)^\delta\right\}\end{aligned}\tag{2.4}$$

and

$$\begin{aligned}&\left\{\int_{\mathbb{R}^n}\left|V(y)\frac{\partial^k K_t(y,x)}{\partial t^k}\right|^p e^{p\xi_{(k,p)}\frac{|y-x|^2}{t}}\,dy\right\}^{1/p}\\&\quad\leq \frac{C_{(k,p)}}{t^{1+n/(2p')+k}}\exp\left\{-c_{(k,p)}(1+t[m(x,V)]^2)^\delta\right\},\end{aligned}$$

where the positive constants $\xi_{(k,p)}$, $C_{(k,p)}$, $c_{(k,p)}$ and δ are as in Proposition 2.2, and $m(\cdot,V)$ is as in (2.1).

To prove Lemma 2.3, we need the following auxiliary conclusions.

Lemma 2.4. *Let L, q_+ and K_t be as in Proposition 2.2. Then there exist positive constants C_3, C_4 and C_5 such that, for all x, $y\in\mathbb{R}^n$ and $t\in(0,\infty)$,*

$$0\le K_t(x,y)\le \frac{C_3}{t^{n/2}}\exp\left\{-C_4(1+t[m(x,V)]^2)^\delta\right\}\exp\left\{-C_5\frac{|x-y|^2}{t}\right\},$$

where $m(\cdot,V)$ and δ are, respectively, as in (2.1) and Proposition 2.2. Moreover, $t^k\frac{\partial^k K_t}{\partial t^k}$ with $k\in\mathbb{N}$ also satisfies the same estimate as K_t.

Lemma 2.4 is just [22, Theorem 1(b)].

Lemma 2.5. *Let L, q_+ and K_t be as in Proposition 2.2. Then, for all $p\in[1,2q_+)$, $x\in\mathbb{R}^n$ and $t\in(0,\infty)$, there exist positive constants $\alpha_{(p)}$, $C_{(p)}$ and $c_{(p)}$, depending on p, such that*

$$\begin{aligned}\left\{\int_{\mathbb{R}^n}|\nabla K_t(y,x)|^p\,e^{\alpha_{(p)}\frac{|y-x|^2}{t}}\,dy\right\}^{1/p}\\ \le \frac{C_{(p)}}{t^{1/2+n/(2p')}}\exp\left\{-c_{(p)}\left(1+t[m(x,V)]^2\right)^\delta\right\},\end{aligned}$$

where $m(\cdot,V)$ and δ are, respectively, as in (2.1) and Proposition 2.2.

To prove Lemma 2.5, we need the following boundedness of Riesz transforms $\nabla L^{-1/2}$, associated with L, on $L^p(\mathbb{R}^n)$.

Lemma 2.6. *Let L and q_+ be as in Proposition 2.2. Then, for all $p\in(1,2q_+)$, there exists a positive constant $C_{(p)}$ such that, for all $f\in L^p(\mathbb{R}^n)$,*

$$\left\|\nabla L^{-1/2}(f)\right\|_{L^p(\mathbb{R}^n)}\le C_{(p)}\|f\|_{L^p(\mathbb{R}^n)}.$$

To give out the proof of Lemma 2.6, we need the boundedness of second order Riesz transforms ∇^2L^{-1} on $L^p(\mathbb{R}^n)$, which is also very useful for the proof of (2.4).

Lemma 2.7. *Let L and q_+ be as in Proposition 2.2.*

(i) *If A in (1.4) satisfies (A_1), then for any $p\in[1,q_+)$, there exists a positive constant $C_{(p)}$ such that, for all $f\in L^p(\mathbb{R}^n)$, $\|VL^{-1}(f)\|_{L^p(\mathbb{R}^n)}\le C_{(p)}\|f\|_{L^p(\mathbb{R}^n)}$.*

(ii) *If A in (1.4) satisfies (A_1), (A_2) and (A_3), then for any $p\in(1,q_+)$, there exists a positive constant $C_{(p)}$ such that, for all $f\in L^p(\mathbb{R}^n)$,*

$$\left\|\nabla^2L^{-1}(f)\right\|_{L^p(\mathbb{R}^n)}\le C_{(p)}\|f\|_{L^p(\mathbb{R}^n)}.$$

Proof. The proof of (i) is similar to that of [33, Theorem 3.1] and we omit the details here.

Now we prove (ii). Let $L_0:=-\mathrm{div}(A\nabla)$. It was proved by Avellaneda and Lin in [4, Theorem B] that, for all $p\in(1,\infty)$ and $f\in L^p(\mathbb{R}^n)$, $\|\nabla^2L_0^{-1}(f)\|_{L^p(\mathbb{R}^n)}\lesssim$

$\|f\|_{L^p(\mathbb{R}^n)}$. From this and the conclusion of (i), we deduce that, for all $f \in L^p(\mathbb{R}^n)$ with $p \in (1, q_+)$,

$$\left\|\nabla^2 L^{-1}(f)\right\|_{L^p(\mathbb{R}^n)} \lesssim \left\|L_0 L^{-1}(f)\right\|_{L^p(\mathbb{R}^n)} \sim \left\|(L-V)L^{-1}(f)\right\|_{L^p(\mathbb{R}^n)} \lesssim \|f\|_{L^p(\mathbb{R}^n)}.$$

This finishes the proof of (ii) and hence Lemma 2.7. □

Now we prove Lemma 2.6 via Lemma 2.7.

Proof of Lemma 2.6. It is well-known that, for all $y \in \mathbb{R}$, L^{iy} is bounded on $L^p(\mathbb{R}^n)$ with $p \in (1, \infty)$, where i denotes the *imaginary unit* (see, for example, [10]). From this, Lemma 2.7(ii) and the Stein interpolation theorem for families of operators (see, for example, [34, Theorem 4.1, p. 205]), similar to the proof in [1, pp. 1990-1991], it follows that, for all $p \in (1, 2q_+)$, $\nabla L^{-1/2}$ is bounded on $L^p(\mathbb{R}^n)$. This finishes the proof of Lemma 2.6. □

Now we prove Lemma 2.5 by using Lemmas 2.4 and 2.6.

Proof of Lemma 2.5. By using Lemmas 2.4 and 2.6, and the definition of the operator L, similar to the proof of [28, (3.9), p. 48] or [8, Lemma 2.5], we prove Lemma 2.5. We omit the details here, which completes the proof of Lemma 2.5. □

Moreover, via Lemmas 2.4, 2.5 and 2.7, and Leibniz's rule for distributional derivative, similar to [28, Proposition 3.7] or [8, Lemma 2.7], we obtain the following Lemma 2.8. The details be omitted here.

Lemma 2.8. *Let L, q_+ and K_t be as in Proposition 2.2.*

(i) *If A in (1.4) satisfies (A_1), (A_2) and (A_3), then for all $p \in [1, q_+)$, $x \in \mathbb{R}^n$ and $t \in (0, \infty)$, there exist positive constants $\beta_{(p)}$, $C_{(p)}$ and $c_{(p)}$, depending on p, such that*

$$\left\{\int_{\mathbb{R}^n} \left|\nabla^2 K_t(y,x)\right|^p e^{\beta_{(p)} \frac{|y-x|^2}{t}}\, dy\right\}^{1/p} \le \frac{C_{(p)}}{t^{1+n/(2p')}} \exp\left\{-c_{(p)}(1 + t[m(x,V)]^2)^\delta\right\},$$

here and hereafter, $m(\cdot, V)$ and δ are, respectively, as in (2.1) and Proposition 2.2.

(ii) *If A in (1.4) satisfies (A_1), then for all $p \in [1, q_+)$, $x \in \mathbb{R}^n$ and $t \in (0, \infty)$, there exist positive constants $\beta_{(p)}$, $C_{(p)}$ and $c_{(p)}$, depending on p, such that*

$$\begin{aligned}\left\{\int_{\mathbb{R}^n} |V(y)K_t(y,x)|^p e^{\beta_{(p)} \frac{|y-x|^2}{t}}\, dy\right\}^{1/p}\\ \le \frac{C_{(p)}}{t^{1+n/(2p')}} \exp\left\{-c_{(p)}(1 + t[m(x,V)]^2)^\delta\right\}.\end{aligned}$$

Now we prove Lemma 2.3 by using Lemmas 2.5 and 2.8.

Proof of Lemma 2.3. From the commutative property of the semigroup $\{e^{-tL}\}_{t>0}$, it follows that, for any $k \in \mathbb{N}$ and $t \in (0, \infty)$,

$$\frac{\partial^k}{\partial t^k} e^{-2tL} = (-2L)^k e^{-2tL} = 2^k e^{-tL} \frac{\partial^k}{\partial t^k} e^{-tL}.$$

By this and the estimates obtained in Lemmas 2.5 and 2.7, via an argument similar to that used in the proof of [28, Proposition 7.7] (or [27, Proposition 3.3]), we obtain Lemma 2.3, the details being omitted. This finishes the proof of Lemma 2.3. $\square$

3. Proof of Theorem 1.3

In this section, we give out the proof of Theorem 1.3. We begin with some useful auxiliary conclusions. We first recall the definition of $(\varphi,\, q,\, M)_L$-atoms and the atomic Musielak–Orlicz–Hardy space $H^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$ introduced in [6, Definitions 5.2 and 5.8].

Definition 3.1. Let L and φ be, respectively, as in (1.4) and Definition 1.2. Assume that $q,\, s\in(1,\infty)$, $M\in\mathbb{N}$ and $B\subset\mathbb{R}^n$ is a ball.

(I) Let $\mathcal{D}(L^M)$ be the domain of L^M. A function $\alpha\in L^q(\mathbb{R}^n)$ is called a $(\varphi,\, q,\, M)_L$*-atom* associated with the ball B, if there exists a function $b\in\mathcal{D}(L^M)$ such that

(i) $\alpha=L^M b$;
(ii) for all $j\in\{0,\,1,\,\ldots,\,M\}$, $\operatorname{supp}(L^j b)\subset B$;
(iii) $\|(r_B^2L)^j b\|_{L^q(\mathbb{R}^n)}\le r_B^{2M}|B|^{1/q}\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}$, where r_B denotes the radius of B and $j\in\{0,\,1,\,\ldots,\,M\}$.

(II) For $f\in L^2(\mathbb{R}^n)$,

$$f=\sum_j\lambda_j\alpha_j \tag{3.1}$$

is called an *atomic* $(\varphi,\, q,\, s,\, M)_L$*-representation* if, for all j, α_j is a $(\varphi,\, q,\, M)_L$-atom associated with some ball $B_j\subset\mathbb{R}^n$, the summation (3.1) converges in $L^s(\mathbb{R}^n)$ and $\{\lambda_j\}_j\subset\mathbb{C}$ satisfies that $\sum_j\varphi(B_j,|\lambda_j|\|\chi_{B_j}\|^{-1}_{L^\varphi(\mathbb{R}^n)})<\infty$. Let

$$\widetilde{H}^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n):=\left\{f\in L^2(\mathbb{R}^n):\ f\text{ has an atomic }(\varphi,\,q,\,s,\,M)_L\text{-representation}\right\}$$

with the *quasi-norm*

$$\|f\|_{H^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)}:=\inf\left\{\Lambda(\{\lambda_j\alpha_j\}_j):\ \sum_j\lambda_j\alpha_j\text{ is a }(\varphi,\,q,\,s,\,M)_L\text{-representation of }f\right\},$$

where the infimum is taken over all the atomic $(\varphi,\, q,\, s,\, M)_L$-representations of f as above and

$$\Lambda(\{\lambda_j\alpha_j\}_j):=\inf\left\{\lambda\in(0,\infty):\ \sum_j\varphi\left(B_j,\frac{|\lambda_j|}{\lambda\|\chi_{B_j}\|_{L^\varphi(\mathbb{R}^n)}}\right)\le1\right\}. \tag{3.2}$$

The *atomic Musielak–Orlicz–Hardy space* $H^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$ is then defined as the completion of the set $\widetilde{H}^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$ with respect to the quasi-norm $\|\cdot\|_{H^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)}$.

In what follows, when $s = 2$, we denote the space $H^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$ simply by $H^{M,\,q}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$.

Then we have the following atomic characterization of $H_{\varphi,\,L}(\mathbb{R}^n)$, which is just a corollary of [6, Theorems 5.4 and 5.9].

Lemma 3.2. *Let L and φ be, respectively, as in (1.4) and Definition 1.2. Assume that Assume that $M \in \mathbb{N} \cap (\frac{nq(\varphi)}{2i(\varphi)}, \infty)$, $s \in (1,\infty)$ and $q \in ([r(\varphi)]'I(\varphi),\infty)$, where $q(\varphi)$, $i(\varphi)$, $I(\varphi)$ and $r(\varphi)$ are, respectively, as in (1.7), (1.6), (1.5) and (1.8). Then the spaces $H_{\varphi,\,L}(\mathbb{R}^n)$ and $H^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$ coincide with equivalent quasi-norms.*

Moreover, we also need some properties of φ in Definition 1.2. In what follows, for any measurable subset $E \subset \mathbb{R}^n$ and $t \in [0,\infty)$, let $\varphi(E,t) := \int_E \varphi(x,t)\,dx$. Then we have the following properties for φ from [6, Lemma 2.5], based on the corresponding results of [24, 15].

Lemma 3.3. *Let the function φ be as in Definition 1.2.*

(i) *There exists a positive constant C such that, for all $(x,t_j) \in \mathbb{R}^n \times [0,\infty)$ with $j \in \mathbb{N}$, $\varphi(x, \sum_{j=1}^\infty t_j) \le C \sum_{j=1}^\infty \varphi(x,t_j)$.*

(ii) *$\mathbb{A}_1(\mathbb{R}^n) \subset \mathbb{A}_p(\mathbb{R}^n) \subset \mathbb{A}_q(\mathbb{R}^n)$ for $1 \le p \le q < \infty$.*

(iii) *$\mathbb{RH}_\infty(\mathbb{R}^n) \subset \mathbb{RH}_p(\mathbb{R}^n) \subset \mathbb{RH}_q(\mathbb{R}^n)$ for $1 < q \le p \le \infty$.*

(iv) *$\mathbb{A}_\infty(\mathbb{R}^n) = \cup_{p\in[1,\infty)} \mathbb{A}_p(\mathbb{R}^n) = \cup_{q\in(1,\infty]} \mathbb{RH}_q(\mathbb{R}^n)$.*

(v) *If $\varphi \in \mathbb{A}_p(\mathbb{R}^n)$ with $p \in [1,\infty)$, then there exists a positive constant C such that, for all balls B_1, $B_2 \subset \mathbb{R}^n$ with $B_1 \subset B_2$ and $t \in (0,\infty)$, $\frac{\varphi(B_2,t)}{\varphi(B_1,t)} \le C[\frac{|B_2|}{|B_1|}]^p$.*

Furthermore, we need the following estimates for the potential V, which were established in [33, Lemma 1.2].

Lemma 3.4. *Let $V \in RH_{q_0}(\mathbb{R}^n)$ with $q_0 \in [n/2,\infty)$. Then there exists a positive constant C such that, for all $x \in \mathbb{R}^n$ and $0 < r < R < \infty$,*

$$\frac{1}{r^{n-2}} \int_{B(x,r)} V(y)\,dy \le C \left[\frac{R}{r}\right]^{\frac{n}{q_0}-2} \frac{1}{R^{n-2}} \int_{B(x,R)} V(y)\,dy.$$

Moreover, if $r := [m(x,V)]^{-1}$ with $x \in \mathbb{R}^n$, then $\frac{1}{r^{n-2}} \int_{B(x,r)} V(y)\,dy = 1$.

Furthermore, to prove that the operator $V^{1/2}\nabla L^{-1}$ is bounded from $H_{\varphi,\,L}(\mathbb{R}^n)$ to $L^\varphi(\mathbb{R}^n)$, we need the following boundedness of $V^{1/2}\nabla L^{-1}$ on $L^p(\mathbb{R}^n)$ with $p \in (1,\infty)$, whose proof is similar to that of [33, Theorem 4.13].

Lemma 3.5. *Let L be as in (1.4) with A satisfying (A_1) and (A_2) and $q_+ \in (n/2,\infty)$ with q_+ as in (1.3). Assume that $p_+ \in (1,\infty)$ given by $\frac{1}{p_+} := \frac{3}{2q_+} - \frac{1}{n}$ when $q_+ \in (n/2,n]$ and $p_+ := 2q_+$ when $q_+ \in (n,\infty)$. Then, for all $p \in [1,p_+)$, there exists a positive constant $C_{(p)}$ such that, for all $f \in L^p(\mathbb{R}^n)$,*

$$\left\|V^{1/2}\nabla L^{-1}(f)\right\|_{L^p(\mathbb{R}^n)} \le C_{(p)}\|f\|_{L^p(\mathbb{R}^n)}.$$

Now we prove Theorem 1.3 by using Lemmas 3.2 through 3.5.

Proof of Theorem 1.3. We first prove (i) of Theorem 1.3. From the assumption $q_+ > I(\varphi)[r(\varphi)]'$, we deduce that there exist $q \in (I(\varphi)[r(\varphi)]', q_+)$. Let $s \in (1,q_+)$,

$M \in \mathbb{N} \cap (\frac{nq(\varphi)}{2i(\varphi)}, \infty)$ and $f \in \widetilde{H}^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$. By this and Lemma 3.2, we know that there exist $\{\lambda_j\}_j \subset \mathbb{C}$ and a sequence $\{\alpha_j\}_j$ of $(\varphi,\, q,\, M)_L$-atoms, associated with the balls $\{B_j\}_j$, such that

$$f = \sum_j \lambda_j \alpha_j \text{ in } L^s(\mathbb{R}^n) \text{ and } \|f\|_{H_{\varphi,\,L}(\mathbb{R}^n)} \sim \Lambda(\{\lambda_j\alpha_j\}_j). \tag{3.3}$$

To finish the proof of the boundedness of VL^{-1} from $H_{\varphi,\,L}(\mathbb{R}^n)$ to $L^\varphi(\mathbb{R}^n)$, it suffices to prove that, for all $\lambda \in \mathbb{C}$ and $(\varphi,\, q,\, M)_L$-atoms α associated with $B := B(x_0, r_0)$ for some $x_0 \in \mathbb{R}^n$ and $r_0 \in (0,\, \infty)$,

$$\int_{\mathbb{R}^n} \varphi\left(x, \left|VL^{-1}(\lambda\alpha)(x)\right|\right)\, dx \lesssim \varphi\left(B, |\lambda| \|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\right). \tag{3.4}$$

If (3.4) holds true, from this, (3.3) and Lemmas 3.3(i), 3.2 and 2.7(i), it follows that, for all $\lambda \in (0, \infty)$,

$$\begin{aligned}\int_{\mathbb{R}^n} \varphi\left(x, \frac{|VL^{-1}(f)(x)|}{\lambda}\right) dx &\lesssim \sum_j \int_{\mathbb{R}^n} \varphi\left(x, \frac{|VL^{-1}(\lambda_j\alpha_j)(x)|}{\lambda}\right) dx \\ &\lesssim \sum_j \varphi\left(B_j, \frac{|\lambda_j|}{\lambda\|\chi_{B_j}\|_{L^\varphi(\mathbb{R}^n)}}\right),\end{aligned}$$

which, together with (3.3), implies that $\|VL^{-1}(f)\|_{L^\varphi(\mathbb{R}^n)} \lesssim \|f\|_{H^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)}$. By this and the fact that $\widetilde{H}^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$ is dense in $H^{M,\,q,\,s}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$ and Lemma 3.2, we further conclude that VL^{-1} is bounded from $H_{\varphi,\,L}(\mathbb{R}^n)$ to $L^\varphi(\mathbb{R}^n)$.

Now we prove (3.4). We first write

$$\begin{aligned}\int_{\mathbb{R}^n} \varphi\left(x, |VL^{-1}(\lambda\alpha)(x)|\right) dx &= \sum_{j=0}^\infty \int_{S_j(B)} \varphi\left(x, |VL^{-1}(\lambda\alpha)(x)|\right) dx \\ &=: \sum_{j=0}^\infty \mathrm{I}_j. \end{aligned}\tag{3.5}$$

By the choice of q, we see that there exists $p_1 \in (I(\varphi), 1]$ such that φ is of uniformly upper type p_1 and $(q/p_1)' < r(\varphi)$, which, combined with the definition of $r(\varphi)$, implies that $\varphi \in \mathbb{RH}_{(q/p_1)'}(\mathbb{R}^n)$. Moreover, from the assumption $M > \frac{nq(\varphi)}{2i(\varphi)}$ and the definitions of $q(\varphi)$ and $i(\varphi)$, we deduce that there exist $\widetilde{q} \in (q(\varphi), \infty)$ and $p_0 \in (0, i(\varphi)]$ such that φ is of uniformly lower type p_0, $\varphi \in \mathbb{A}_{\widetilde{q}}(\mathbb{R}^n)$ and $M > \frac{n\widetilde{q}}{2p_0}$. When $j \in \{0,\, 1,\, \ldots,\, 4\}$, by the uniformly upper type p_1 and lower type p_0 properties of φ, Hölder's inequality, Lemma 2.7(i), $p_0 \le p_1$, $\varphi \in \mathbb{RH}_{(q/p_1)'}(\mathbb{R}^n) \subset$

$\mathbb{RH}_{(q/p_0)'}(\mathbb{R}^n)$ and Lemma 3.3(v), we conclude that

$$\begin{aligned}
\mathrm{I}_j &\lesssim \sum_{k=0}^{1} \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{p_k} \int_{S_j(B)} \varphi\left(x, |\lambda|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right) \left|VL^{-1}(\alpha)(x)\right|^{p_k}\,dx\\
&\lesssim \sum_{k=0}^{1} \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{p_k} \left\|VL^{-1}(\alpha)\right\|_{L^q(S_j(B))}^{p_k} \left\|\varphi\left(\cdot, |\lambda|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right)\right\|_{L^{(q/p_k)'}(S_j(B))}\\
&\lesssim \sum_{k=0}^{1} \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{p_k} \|\alpha\|_{L^q(\mathbb{R}^n)}^{p_k} |2^{j+1}B|^{-p_k/q} \varphi\left(2^{j+1}B, |\lambda|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right)\\
&\lesssim \varphi\left(B, |\lambda|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right). \qquad (3.6)
\end{aligned}$$

When $j \in \mathbb{N}$ and $j \geq 5$, from the uniformly upper type p_1 and lower type p_0 properties of φ, it follows that

$$\mathrm{I}_j \lesssim \sum_{k=0}^{1} \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{p_k} \int_{S_j(B)} \varphi\left(x, |\lambda|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right) \left|VL^{-1}(\alpha)(x)\right|^{p_k}\,dx. \qquad (3.7)$$

To estimate the terms $\mathrm{I}_{1,j}$ and $\mathrm{I}_{2,j}$, we first estimate $\|VL^{-1}(\alpha)\|_{L^q(S_j(B))}$. By the functional calculus $L^{-1} = \int_0^\infty e^{-tL}\,dt$ and Minkowski's inequality, we see that

$$\begin{aligned}
\left\|VL^{-1}(\alpha)\right\|_{L^q(S_j(B))} &\leq \int_0^{r_B^2} \left\|Ve^{-tL}\alpha\right\|_{L^q(S_j(B))}\,dt + \int_{r_B^2}^\infty \cdots\\
&=: \mathrm{E}_j + \mathrm{F}_j. \qquad (3.8)
\end{aligned}$$

Moreover, it is easy to see that, when $j \geq 5$,

$$\operatorname{dist}(S_j(B), B) \gtrsim 2^{j-1}r_B - r_B \gtrsim 2^{j-2}r_B, \qquad (3.9)$$

which, together with Minkowski's inequality, (2.3) and Hölder's inequality, implies that

$$\begin{aligned}
\left\|Ve^{-tL}(\alpha)\right\|_{L^q(S_j(B))} &\leq \int_B |\alpha(y)| \left\{\int_{\{x\in\mathbb{R}^n:\,|x-y|\geq 2^{j-2}r_B\}} |V(x)K_t(x,y)|^q\,dx\right\}^{1/q} dy\\
&\lesssim \|\alpha\|_{L^1(\mathbb{R}^n)} \frac{1}{t^{1+n/(2q')}} e^{-\xi_{(0,\,q)}\frac{4^j r_B^2}{t}}\\
&\lesssim |B|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1} \frac{1}{t^{1+n/(2q')}} e^{-\xi_{(0,\,q)}\frac{4^j r_B^2}{t}}, \qquad (3.10)
\end{aligned}$$

where $\xi_{(0,\,q)}$ is as in (2.3). Furthermore, $M > \frac{n\widetilde{q}}{2p_0}$ further implies that there exists $s \in (n/(2q'), n/(2q') + M)$ satisfying $s > \frac{n\widetilde{q}}{2p_0}$. Then it follows, from (3.10) and Minkowski's inequality, that

$$\begin{aligned}
\mathrm{E}_j &\lesssim |B|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1} \int_0^{r_B^2} \frac{1}{t^{1+n/(2q')}} e^{-\xi_{(0,\,q)}\frac{4^j r_B^2}{t}}\,dt\\
&\lesssim |B|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1} \int_0^{r_B^2} \left[\frac{t}{4^j r_B^2}\right]^s \frac{1}{t^{1+n/(2q')}}\,dt\\
&\sim 2^{-2sj}|B|^{1/q}\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}. \qquad (3.11)
\end{aligned}$$

Now we estimate the term F_j. By the definition of $(\varphi,\, q,\, M)_L$-atoms, we know that there exists $b \in \mathcal{D}(L^M)$ such that $a = L^M b$, $\operatorname{supp}(L^j b) \subset B$ and $\|(r_B^2 L)^j b\|_{L^q(\mathbb{R}^n)} \le r_B^{2M}|B|^{1/q}\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}$ for all $j \in \{0,\, 1,\, \ldots,\, M\}$. From this and the fact that $\frac{\partial^M}{\partial t^M} e^{-tL} = (-1)^M L^M e^{-tL}$, we deduce that

$$e^{-tL}\alpha = e^{-tL}L^M b = L^M e^{-tL} b = (-1)^M \frac{\partial^M}{\partial t^M} e^{-tL} b,$$

which, combined with Minkowski's inequality, (3.9), (2.3) and Hölder's inequality, implies that

$$\begin{aligned}
&\left\|V e^{-tL}(\alpha)\right\|_{L^q(S_j(B))}\\
&\quad= \left\|V \frac{\partial^M}{\partial t^M} e^{-tL}(b)\right\|_{L^q(S_j(B))}\\
&\quad\le \int_B |b(y)| \left\{\int_{\{x\in\mathbb{R}^n:\,|x-y|\ge 2^{j-2}r_B\}} \left|V(x)\frac{\partial^M K_t(x,y)}{\partial t^M}\right|^q \,dx\right\}^{1/q} dy\\
&\quad\lesssim \|b\|_{L^1(\mathbb{R}^n)} \frac{1}{t^{M+1+n/(2q')}} e^{-\xi_{(M,\,q)}\frac{4^j r_B^2}{t}}\\
&\quad\lesssim |B|^{1+\frac{2M}{n}} \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1} \frac{1}{t^{M+1+n/(2q')}} e^{-\xi_{(M,\,q)}\frac{4^j r_B^2}{t}}.
\end{aligned} \tag{3.12}$$

Then by (3.12) and Minkowski's inequality, we conclude that

$$\begin{aligned}
\mathrm{F}_j &\lesssim |B|^{1+\frac{2M}{n}} \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1} \int_{r_B^2}^\infty \frac{1}{t^{M+1+n/(2q')}} e^{-\xi_{(M,\,q)}\frac{4^j r_B^2}{t}}\,dt\\
&\lesssim |B|^{1+\frac{2M}{n}} \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1} \int_{r_B^2}^\infty \left[\frac{t}{4^j r_B^2}\right]^s \frac{1}{t^{M+1+n/(2q')}}\,dt\\
&\sim 2^{-2sj}|B|^{1/q}\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}.
\end{aligned} \tag{3.13}$$

Thus, it follows from (3.8), (3.11) and (3.13) that, for any $j \in \mathbb{N}$ with $j \ge 5$,

$$\left\|VL^{-1}(\alpha)\right\|_{L^q(S_j(B))} \lesssim 2^{-2sj}|B|^{1/q}\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}.$$

This, combined with (3.7), Hölder's inequality, $p_0 \le p_1$,

$$\varphi \in \mathbb{RH}_{(q/p_1)'}(\mathbb{R}^n) \subset \mathbb{RH}_{(q/p_0)'}(\mathbb{R}^n)$$

and Lemma 3.3(v), implies that

$$\begin{aligned}
\mathrm{I}_j &\lesssim \sum_{k=0}^1 \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{p_k} \left\|VL^{-1}(\alpha)\right\|_{L^q(S_j(B))}^{p_k} \left\|\varphi\left(\cdot, |\lambda|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right)\right\|_{L^{(q/p_k)'}(S_j(B))}\\
&\lesssim \sum_{k=0}^1 2^{-2sp_k j}|B|^{p_k/q}|2^{j+1}B|^{-p_k/q}\varphi\left(2^{j+1}B, |\lambda|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right)\\
&\lesssim 2^{-[2s+\frac{n}{q}-\frac{n\widetilde{q}}{p_0}]p_0 j}\varphi\left(B, |\lambda|\|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right),
\end{aligned}$$

which, together with (3.5), (3.7) and $s > \frac{n\widetilde{q}}{2p_0}$, implies that

$$\sum_{j=5}^{\infty} \mathrm{I}_j \lesssim \sum_{j=5}^{\infty} 2^{-[2s+\frac{n}{q}-\frac{n\widetilde{q}}{p_0}]p_0 j} \varphi\left(B, |\lambda| \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right) \lesssim \varphi\left(B, |\lambda| \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right). \tag{3.14}$$

From this, (3.5) and (3.6), it follows that (3.4) holds true.

Now we prove (ii) of Theorem 1.3. The proof of (ii) is similar to that of (i). Here we give out the main sketch for this proof and omit some similar details. By the assumption $q_+ > I(\varphi)[r(\varphi)]'$, we could take $q \in (I(\varphi)[r(\varphi)]', q_+)$. Let $M \in \mathbb{N} \cap (\frac{nq(\varphi)}{2i(\varphi)}, \infty)$. Similar the proof of (i), it suffices to prove that, for all $\lambda \in \mathbb{C}$ and $(\varphi, q, M)_L$-atoms α associated with the ball B,

$$\int_{\mathbb{R}^n} \varphi\left(x, \left|V^{1/2}\nabla L^{-1}(\lambda\alpha)(x)\right|\right) dx \lesssim \varphi\left(B, |\lambda| \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right). \tag{3.15}$$

Assume that α is a $(\varphi, q, M)_L$-atom associated with the ball B and $\lambda \in \mathbb{C}$. For $j \in \mathbb{Z}_+$, let

$$\mathrm{II}_j := \int_{S_j(B)} \varphi\left(x, \left|V^{1/2}\nabla L^{-1}(\lambda\alpha)(x)\right|\right) dx.$$

Moreover, let p_1 be as in (3.6). Then $\varphi \in \mathbb{RH}_{(q/p_1)'}(\mathbb{R}^n)$ and $q < q_+ < \frac{2nq_+}{3n-2q_+} = p_+$ when $q_+ \in (n/2, n]$, which, together with Lemma 3.5, further implies that $V^{1/2}\nabla L^{-1}$ is bounded on $L^q(\mathbb{R}^n)$. From this, $\varphi \in \mathbb{RH}_{(q/p_1)'}(\mathbb{R}^n)$ and Lemma 3.3(v), similar to the proof of (3.6), we deduce that for $j \in \{0, 1, \ldots, 4\}$,

$$\mathrm{II}_j \lesssim \varphi\left(B, |\lambda| \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right). \tag{3.16}$$

For $j \geq 5$, by using Hölder's inequality, Lemma 3.4 and (2.2), we obtain an estimate similar to (2.2) for $[\int_{\{x\in\mathbb{R}^n:\,|x-y|\geq 2^{j-2}r_B\}} |V^{1/2}\nabla K_t(x,y)|^q\,dx]^{1/q}$ with any $y \in B$. From this and similar to the proof of (3.14), we deduce that

$$\sum_{j=5}^{\infty} \mathrm{II}_j \lesssim \varphi\left(B, |\lambda| \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}\right),$$

which, together with (3.16), implies that (3.15) holds true and hence finishes the proof of Theorem 1.3(ii).

The proof of (iii) is absolutely similar to that of (i), the details being omitted here. This finishes the proof of (iii) and hence Theorem 1.3. □

4. Proof of Theorem 1.6

In this section, we give out the proof of Theorem 1.6. To this end, we need a kind atomic Musielak–Orlicz–Hardy space $H^{q,\varepsilon}_{\varphi,L}(\mathbb{R}^n)$ as follows.

Definition 4.1. Let φ be as in Definition 1.2, $q \in (1, \infty)$ and $\varepsilon \in (0, \infty)$. A function $a \in L^q(\mathbb{R}^n)$ is called a $(\varphi, q, \varepsilon)_L$-*atom* associated with the ball $B := B(x_0, r_0)$, if

(i) $\operatorname{supp}(a) \subset B$;
(ii) $\|a\|_{L^q(\mathbb{R}^n)} \leq |B|^{1/q} \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1}$;
(iii) $\left|\int_B a(x)\,dx\right| \leq |B| \|\chi_B\|_{L^\varphi(\mathbb{R}^n)}^{-1} [r_0 m(x_0, V)]^\varepsilon$, where $m(\cdot, V)$ is as in (2.1).

The *Musielak–Orlicz–Hardy space* $H^{q,\,\varepsilon}_{\varphi,\,L}(\mathbb{R}^n)$ is defined via replacing $(\varphi,\,q,\,M)_L$-atoms by $(\varphi,\,q,\,\varepsilon)_L$-atoms in the definition of the space $H^{M,\,q}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$.

Remark 4.2. Let φ and $m(\cdot, V)$ be, respectively, as in Definition 1.2 and (2.1), and $q \in (1, \infty]$.

(I) Let $\varepsilon_1 \in (0, \infty)$. By Definition 4.1, we see that, for any $(\varphi,\,q,\,\varepsilon_1)_L$-atom a, a is also a $(\varphi,\,q,\,\varepsilon)_L$-atom for any $\varepsilon \in (0, \varepsilon_1]$.

(II) A function a on $\mathbb{R}^n$ is called a $(\varphi, q)_m$*-atom* associated with the ball $B := B(x_0, r_0)$, if

- (i) $\mathrm{supp}\,(a) \subset B$;
- (ii) $\|a\|_{L^q(\mathbb{R}^n)} \le |B|^{1/q}\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}$;
- (iii) $\int_{\mathbb{R}^n} a(x)\,dx = 0$ if $r_0 < [m(x_0, V)]^{-1}$.

It is easy to see that, for any $(\varphi,\,q)_m$-atom a and $\varepsilon \in (0, \infty)$, a is a $(\varphi,\,q,\,\varepsilon)_L$-atom.

(III) The *Musielak–Orlicz–Hardy space* $H^{\varphi,\,q}_m(\mathbb{R}^n)$ (which was introduced in [7, Definition 2.2]) is defined via replacing $(\varphi,\,q,\,M)_L$-atoms by $(\varphi, q)_m$-atoms in the definition of the space $H^{M,\,q}_{\varphi,\,L,\,\mathrm{at}}(\mathbb{R}^n)$.

Now we establish the inclusion relation $H^{q,\,\varepsilon}_{\varphi,\,L}(\mathbb{R}^n) \subset H_{\varphi,\,L}(\mathbb{R}^n)$, which is motivated by [26].

Lemma 4.3. *Let L and φ be, respectively, as in (1.4) and Definition 1.2, σ_0 as in (1.10) and $\varepsilon \in (0, \infty)$. Assume that A in (1.4) satisfies (A_1), $q \in (I(\varphi)[r(\varphi)]', \infty)$, $\frac{n+\min\{\sigma_0,\varepsilon\}}{n} > \frac{q(\varphi)}{i(\varphi)}$. Then $H^{q,\,\varepsilon}_{\varphi,\,L}(\mathbb{R}^n) \subset H_{\varphi,\,L}(\mathbb{R}^n)$ and there exists a positive constant C such that, for all $f \in H^{q,\,\varepsilon}_{\varphi,\,L}(\mathbb{R}^n)$, $\|f\|_{H_{\varphi,\,L}(\mathbb{R}^n)} \le C\|f\|_{H^{q,\,\varepsilon}_{\varphi,\,L}(\mathbb{R}^n)}$.*

As a corollary of Lemma 4.3 and [40, Theorem 2.3], we have the following conclusion.

Corollary 4.4. *Let φ and L be, respectively, as in Definition 1.2 and (1.4). Assume that A in (1.4) satisfies (A_1), $i(\varphi)$, $q(\varphi)$, $r(\varphi)$ and σ_0 are, respectively, as in (1.6), (1.7), (1.8) and (1.10). Let $q \in ([r(\varphi)]', \infty)$ satisfy $\sigma_0 + n/q > \frac{nq(\varphi)}{i(\varphi)}$ and $\varepsilon \in [\sigma_0, \infty)$. Then the spaces $H^{q,\,\varepsilon}_{\varphi,\,L}(\mathbb{R}^n)$ and $H_{\varphi,\,L}(\mathbb{R}^n)$ coincide with equivalent quasi-norms.*

To prove Lemma 4.3, we need the following Lemma 4.6, which is just [40, Lemma 2.6].

Lemma 4.5. *Let L be as in (1.4) with A satisfying (A_1) and K_t the kernel of e^{-tL}. Assume that σ_0 is as in (1.10).*

(i) *For each $t \in (0, \infty)$ and any $N \in \mathbb{N}$, there exist positive constants $C_{(N)}$, depending on N, and α such that, for almost every $(x, y) \in \mathbb{R}^n \times \mathbb{R}^n$,*

$$0 \le K_t(x, y) \le \frac{C_{(N)}}{t^{n/2}} e^{-\frac{\alpha|x-y|^2}{t}} \left\{1 + \sqrt{t}m(x, V) + \sqrt{t}m(y, V)\right\}^{-N}.$$

(ii) *For each $y \in \mathbb{R}^n$ and $t \in (0, \infty)$, any $N \in \mathbb{N}$ and $\mu \in (0, \sigma_0)$, there exist positive constants $C_{(N,\,\mu)}$, depending on N and μ, and α such that, for all*

$x,\ x+h,\ y\in\mathbb{R}^n$ *satisfying* $|h|\le\sqrt{t}$,

$$\begin{aligned}&|K_t(x+h,y)-K_t(x,y)|+|K_t(y,x+h)-K_t(y,x)|\\&\quad\le\frac{C_{(N,\mu)}}{t^{n/2}}\left[\frac{|h|}{\sqrt{t}}\right]^{\mu}e^{-\frac{\alpha|x-y|^2}{t}}\left\{1+\sqrt{t}m(x,V)+\sqrt{t}m(y,V)\right\}^{-N}.\end{aligned}$$

Proof of Lemma 4.3. For $f\in L^2(\mathbb{R}^n)$ and $x\in\mathbb{R}^n$, defined the *radial maximal function* of f, associated with $\{e^{-tL}\}_{t>0}$, by setting

$$\mathcal{R}_h(f)(x):=\sup_{t\in(0,\infty)}\left|e^{-tL}(f)(x)\right|.$$

Let

$$\widetilde{H}_{\varphi,\mathcal{R}_h}(\mathbb{R}^n):=\left\{f\in L^2(\mathbb{R}^n):\ \mathcal{R}_h(f)\in L^{\varphi}(\mathbb{R}^n)\right\}$$

with $\|f\|_{H_{\varphi,\mathcal{R}_h}(\mathbb{R}^n)}:=\|\mathcal{R}_h(f)\|_{L^{\varphi}(\mathbb{R}^n)}$. Then the space $H_{\varphi,\mathcal{R}_h}(\mathbb{R}^n)$ is defined as the *completion* of the set $\widetilde{H}_{\varphi,\mathcal{R}_h}(\mathbb{R}^n)$ with respect to the quasi-norm $\|\cdot\|_{H_{\varphi,\mathcal{R}_h}(\mathbb{R}^n)}$.

Let $\widetilde{\nabla}:=(\nabla,\frac{\partial}{\partial t})$ be the gradient operator on $\mathbb{R}^{n+1}_+$ and

$$\widetilde{A}:=\begin{pmatrix}1&0\\0&A\end{pmatrix}$$

be a partitioned matrix. Then we define the Schrödinger type operator $\widetilde{L}$ on $\mathbb{R}^{n+1}_+$ by

$$\widetilde{L}:=\widetilde{L}_0+V:=-\mathrm{div}(\widetilde{A}\widetilde{\nabla})+V,$$

where $0\le V\in L^1_{\mathrm{loc}}(\mathbb{R}^n)$. Let $u\in L^2_{\mathrm{loc}}(\mathbb{R}^{n+1}_+)$ be the weak solution of $\widetilde{L}u=0$ in the ball $B(X_0,2r)\subset\mathbb{R}^{n+1}_+$ with $X_0\in\mathbb{R}^{n+1}_+$ and $r\in(0,\infty)$. Then similar to [16, Lemma 8.4], we could verify that $\widetilde{L}_0|u|^2\le 0$ in the sense of weak solution. From this and De Giogi-Nash-Moser estimates (see, for example, [29]), we further deduce that, for any $p\in(0,\infty)$, there exists a positive constant $C_{(n,p)}$, depending only on n and p, such that

$$\sup_{X\in B(X_0,r)}|u(X)|\le C_{(n,p)}\left\{\frac{1}{r^{n+1}}\int_{B(X_0,2r)}|u(Y)|^p\,dY\right\}^{1/p}.$$

Via this estimate and similar to [6, Theorem 8.3], we obtain that $H_{\varphi,L}(\mathbb{R}^n)=H_{\varphi,\mathcal{R}_h}(\mathbb{R}^n)$ with equivalent quasi-norms.

Let $q\in(I(\varphi)[r(\varphi)]',\infty)$. Furthermore, by the assumption $\frac{n+\min\{\sigma_0,\varepsilon\}}{n}>\frac{q(\varphi)}{i(\varphi)}$, we see that there exist $\mu_0\in(0,\sigma_0)$, $p_0\in(0,i(\varphi)]$ and $\widetilde{q}\in(q(\varphi),\infty)$ such that $\frac{n+\min\{\mu_0,\varepsilon\}}{n}>\frac{\widetilde{q}}{p_0}$, $\varphi\in\mathbb{A}_{\widetilde{q}}(\mathbb{R}^n)$ and φ is of uniformly lower type p_0. Then to prove Lemma 4.3, it suffices to prove that, for all $(\varphi,\,q,\,\varepsilon)_L$-atom a, supported in $B:=B(x_0,r_0)$, and $\lambda\in\mathbb{C}$,

$$\int_{\mathbb{R}^n}\varphi\left(x,\mathcal{N}_h(\lambda a)(x)\right)\,dx\lesssim\varphi\left(B,|\lambda|\|\chi_B\|^{-1}_{L^{\varphi}(\mathbb{R}^n)}\right).\tag{4.1}$$

Now we prove (4.1). We first write

$$\int_{\mathbb{R}^n}\varphi\left(x,\mathcal{N}_h(\lambda a)(x)\right)\,dx=\sum_{j=0}^{\infty}\int_{S_j(B)}\varphi\left(x,\mathcal{N}_h(\lambda a)(x)\right)\,dx=:\sum_{j=0}^{\infty}\mathrm{I}_j.\tag{4.2}$$

Denote by $\mathcal{M}$ the classical *Hardy-Littlewood maximal operator* on $\mathbb{R}^n$. Then from the $L^p(\mathbb{R}^n)$-boundedness of $\mathcal{M}$ with $p \in (1, \infty)$ and the pointwise inequality $\mathcal{N}_h(a) \lesssim \mathcal{M}(a)$, we deduce that $\|\mathcal{N}_h(a)\|_{L^q(\mathbb{R}^n)} \lesssim \|a\|_{L^q(\mathbb{R}^n)}$. By this and Lemma 3.3(v), similar to the proof of (3.6), we conclude that, for $j \in \{0, 1, \ldots, 4\}$,

$$\mathrm{I}_j \lesssim \varphi\left(B, |\lambda|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\right). \tag{4.3}$$

When $j \geq 5$, for any $x \in S_j(B)$, from Hölder's inequality and Lemma 4.5, it follows that, for any $t \in (0, \infty)$,

$$\begin{aligned}
\left|e^{-tL}(a)(x)\right| &= \left|\int_B K_t(x,y)a(y)\,dy\right| \\
&\leq \left|\int_B [K_t(x,y) - K_t(x,x_0)]\,a(y)\,dy\right| + |K_t(x,x_0)|\left|\int_B a(y)\,dy\right| \\
&\lesssim \frac{r_0^{\mu_0}}{|x-x_0|^{n+\mu_0}}\|a\|_{L^1(B)} \\
&\quad + \frac{1}{t^{n/2}}e^{-\frac{\alpha|x-x_0|^2}{t}}\left[1+\sqrt{t}m(x_0,V)\right]^{-\varepsilon}|B|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}[r_0 m(x_0,V)]^\varepsilon \\
&\lesssim \frac{r_0^{\min\{\mu_0,\,\varepsilon\}}}{|x-x_0|^{n+\min\{\mu_0,\,\varepsilon\}}}|B|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)},
\end{aligned}$$

which, together with the fact that $|x - x_0| \sim 2^j r_0$ for any $x \in S_j(B)$, further implies that

$$\mathcal{N}_h(a)(x) \lesssim \frac{r_0^{\min\{\mu_0,\,\varepsilon\}}}{|x-x_0|^{n+\min\{\mu_0,\,\varepsilon\}}}|B|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)} \sim 2^{-(n+\min\{\mu_0,\,\varepsilon\})j}\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}.$$

By this, the uniformly lower type p_0 property of φ and Lemma 3.3(v), we see that

$$\begin{aligned}
\mathrm{I}_j &\lesssim \int_{S_j(B)} \varphi\left(x, 2^{-(n+\min\{\mu_0,\,\varepsilon\})j}|\lambda|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\right) \\
&\lesssim 2^{-(n+\min\{\mu_0,\,\varepsilon\})jp_0}\varphi\left(2^{j+1}B, |\lambda|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\right) \\
&\lesssim 2^{(n+\min\{\mu_0,\,\varepsilon\}-n\widetilde{q}/p_0)p_0 j}\varphi\left(B, |\lambda|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\right),
\end{aligned}$$

which, combined with $n + \min\{\mu_0,\, \varepsilon\} > n\widetilde{q}/p_0$, further concludes that

$$\begin{aligned}
\sum_{j=5}^\infty \mathrm{I}_j &\lesssim \sum_{j=5}^\infty 2^{(n+\min\{\mu_0,\,\varepsilon\}-n\widetilde{q}/p_0)p_0 j}\varphi\left(B, |\lambda|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\right) \\
&\lesssim \varphi\left(B, |\lambda|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\right).
\end{aligned}$$

This, together with (4.2) and (4.3), proves (4.1), which completes the proof of Lemma 4.3. □

Furthermore, as a corollary of Lemma 2.7, we have the following conclusion, whose proof is similar to that of [1, Corollary 1.3] and the details is omitted here.

Lemma 4.6. *Let L and φ be, respectively, as in (1.4) and Definition 1.2. Assume that A in (1.4) satisfies (A_1), (A_2) and (A_3), and $q_+ \in (n/2, \infty)$ with q_+ as in (1.3). Then for any $p \in (1, q_+)$, the m-accretive extension on $L^p(\mathbb{R}^n)$ of $L := -\mathrm{div}(A\nabla) + V$ defined on $C_c^\infty(\mathbb{R}^n)$ has domain $\mathcal{D}_p(L) = W^{2,p}(\mathbb{R}^n) \cap L^p_{V^p}(\mathbb{R}^n)$, where*

$$L^p_{V^p}(\mathbb{R}^n) := \left\{ f \in L^1_{\mathrm{loc}}(\mathbb{R}^n) : \ \|f\|_{L^p_{V^p}(\mathbb{R}^n)} := \left[\int_{\mathbb{R}^n} |f(x)V(x)|^p \, dx \right]^{1/p} < \infty \right\}.$$

Moreover, to prove Theorem 1.6(iv), we need the molecular characterization of $H_\varphi(\mathbb{R}^n)$ established in [18, Theorem 4.13]. To state the molecular characterization of the space $H_\varphi(\mathbb{R}^n)$, we first recall the definitions of $(\varphi,\, q,\, s,\, \varepsilon)$-molecules and molecular Musielak–Orlicz–Hardy spaces $H^{q,\,s,\,\varepsilon}_{\varphi,\,\mathrm{mol}}(\mathbb{R}^n)$.

Definition 4.7. Let φ be as in Definition 1.2, $q \in (1, \infty)$, $s \in \mathbb{Z}_+$ and $\varepsilon \in (0, \infty)$.

(I) A function $\alpha \in L^q(\mathbb{R}^n)$ is called a $(\varphi,\, q,\, s,\, \varepsilon)$-*molecule* associated with the ball B, if

(i) for each $j \in \mathbb{Z}_+$, $\|\alpha\|_{L^q(S_j(B))} \le 2^{-j\varepsilon} |2^j B|^{1/q} \|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}$;

(ii) $\int_{\mathbb{R}^n} \alpha(x) x^\beta \, dx = 0$ for all $\beta \in \mathbb{Z}^n_+$ with $|\beta| \le s$.

(II) The *molecular Musielak–Orlicz–Hardy space*, $H^{q,\,s,\,\varepsilon}_{\varphi,\,\mathrm{mol}}(\mathbb{R}^n)$, is defined to be the space of all $f \in \mathcal{S}'(\mathbb{R}^n)$ satisfying that $f = \sum_j \lambda_j \alpha_j$ in $\mathcal{S}'(\mathbb{R}^n)$, where $\{\lambda_j\}_j \subset \mathbb{C}$, $\{\alpha_j\}_j$ is a sequence of $(\varphi,\, q,\, s,\, \varepsilon)$-molecules, respectively, associated to the balls $\{B_j\}_j$, and

$$\sum_j \varphi\left(B_j,\, |\lambda_j| \|\chi_{B_j}\|^{-1}_{L^\varphi(\mathbb{R}^n)} \right) < \infty.$$

Moreover, define $\|f\|_{H^{q,\,s,\,\varepsilon}_{\varphi,\,\mathrm{mol}}(\mathbb{R}^n)} := \inf\{\Lambda(\{\lambda_j \alpha_j\}_j)\}$, where the infimum is taken over all the decompositions of f as above and $\Lambda(\{\lambda_j \alpha_j\}_j)$ is as in (3.2).

For any $s \in \mathbb{R}$, denote by $\lfloor s \rfloor$ the maximal integer k such that $k \le s$. Then we have the following conclusion, which is just [18, Theorem 4.13].

Lemma 4.8. *Let φ be as in Definition 1.2. Assume that $s \in \mathbb{Z}_+$ with $s \ge \lfloor n(q(\varphi)/i(\varphi) - 1) \rfloor$, $\epsilon \in (\max\{n + s, nq(\varphi)/i(\varphi)\}, \infty)$ and $p \in (q(\varphi)[r(\varphi)]', \infty)$, where $q(\varphi)$, $i(\varphi)$ and $r(\varphi)$ are, respectively, as in (1.6), (1.7) and (1.8). Then $H_\varphi(\mathbb{R}^n)$ and $H^{p,\,s,\,\epsilon}_{\varphi,\,\mathrm{mol}}(\mathbb{R}^n)$ coincide with equivalent quasi-norms.*

Now we prove Theorem 1.6 by using Lemmas 3.2, 4.3, 4.6 and 4.8.

Proof of Theorem 1.6. We first prove (i) of this theorem. By the assumption $\frac{n+\sigma_0}{n} > \frac{q(\varphi)}{i(\varphi)}$ and $\sigma_0 \le 2 - \frac{n}{q_+}$, we know that there exist $\varepsilon_0 \in (0, \sigma_0)$ and $q_1 \in (1, q_+)$ such that

$$2 - \frac{n}{q_1} > \varepsilon_0 \quad \text{and} \quad \frac{n + \varepsilon_0}{n} > \frac{q(\varphi)}{i(\varphi)},$$

which further implies that there exist $\widetilde{q} \in (q(\varphi), \infty)$ and $p_0 \in (0, i(\varphi))$ such that

$$n + \varepsilon_0 > \frac{n\widetilde{q}}{p_0},$$

$V\in RH_{q_1}(\mathbb{R}^n)$, $\varphi\in\mathbb{A}_{\widetilde{q}}(\mathbb{R}^n)$ and φ is of uniformly lower type p_0. Let $M\in\mathbb{N}$ satisfying $M>\frac{nq(\varphi)}{2i(\varphi)}$ and $q\in(\max\{q_1', I(\varphi)[r(\varphi)]'\},\infty)$. From this and the assumption $I(\varphi)[r(\varphi)]'<q_+$, we deduce that there exists $p_1\in(I(\varphi)[r(\varphi)]',\min\{q,q_+\})$. By Lemmas 3.2 and 4.3, we only need to prove that, for all $(\varphi,\,q,\,M)_L$-atoms α, $VL^{-1}(\alpha)$ is a $(\varphi,\,p_1,\,\varepsilon_0)_L$-atom up to a harmless constant multiple.

Via the definition of α, we see that there exists $b\in D(L)$ such that $\alpha=Lb$, $\operatorname{supp}(b)\subset B$ and $\|b\|_{L^q(\mathbb{R}^n)}\le r_0^2|B|^{1/q}\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}$. First, it follows from $\operatorname{supp}(b)\subset B$ and $\alpha=Lb$ that

$$\operatorname{supp}(VL^{-1}(\alpha))=\operatorname{supp}(Vb)\subset B. \tag{4.4}$$

Moreover, by Hölder's inequality and Lemma 2.7(i), we conclude that

$$\left\|VL^{-1}(\alpha)\right\|_{L^{p_1}(B)}\lesssim|B|^{\frac{1}{p_1}-\frac{1}{q}}\|\alpha\|_{L^q(B)}\lesssim|B|^{1/p_1}\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}. \tag{4.5}$$

Now we estimate $|\int_B VL^{-1}(\alpha)\,dx|$ by considering the following two cases.

Case 1) $r_0\in[[m(x_0,V)]^{-1},\infty)$. In this case, from Hölder's inequality, (4.5) and $r_0m(x_0,V)\ge1$, we deduce that

$$\begin{aligned}\left|\int_B VL^{-1}(\alpha)(x)\,dx\right|&\le\left\|VL^{-1}(\alpha)\right\|_{L^{p_1}(B)}|B|^{1/p_1'}\\&\lesssim|B|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\left[r_0m(x_0,V)\right]^{\varepsilon_0}.\end{aligned} \tag{4.6}$$

Case 2) $r_0\in(0,[m(x_0,V)]^{-1})$. In this case, by Hölder's inequality, $V\in RH_{q_1}(\mathbb{R}^n)$, $q>q_1'$, Lemma 3.4, $2-n/q_1>\varepsilon_0$ and $r_0m(x_0,V)\in(0,1)$, we see that

$$\begin{aligned}\left|\int_B VL^{-1}(\alpha)(x)\,dx\right|&\le\|Vb\|_{L^1(B)}\le\|V\|_{L^{q_1}(B)}\|b\|_{L^{q_1'}(B)}\\&\lesssim r_0^2\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\int_B V(x)\,dx\\&\lesssim|B|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\left[r_0m(x_0,V)\right]^{2-\frac{n}{q_1}}\\&\lesssim|B|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\left[r_0m(x_0,V)\right]^{\varepsilon_0}.\end{aligned}$$

From this and (4.6), it follows that

$$\left|\int_B VL^{-1}(\alpha)(x)\,dx\right|\lesssim|B|\|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}\left[r_0m(x_0,V)\right]^{\varepsilon_0},$$

which, together with (4.4) and (4.5), implies that $VL^{-1}(\alpha)$ is a $(\varphi,\,p_1,\,\varepsilon_0)_L$-atom up to a harmless constant multiple. This finishes the proof of Theorem 1.6(i).

Now we prove (ii). By the assumption $\frac{n+\sigma_0/2}{n}>\frac{q(\varphi)}{i(\varphi)}$ and $\sigma_0\le2-\frac{n}{q_+}$, we know that there exist $\varepsilon_1\in(0,\sigma_0)$, $q_2\in(1,q_+)$, $\widetilde{q}\in(q(\varphi),\infty)$ and $p_0\in(0,i(\varphi))$ such that

$$2-\frac{n}{q_2}>\varepsilon_1\quad\text{and}\quad n+\frac{\varepsilon_1}{2}>\frac{n\widetilde{q}}{p_0},$$

$V\in RH_{q_2}(\mathbb{R}^n)$, $\varphi\in\mathbb{A}_{\widetilde{q}}(\mathbb{R}^n)$ and φ is of uniformly lower type p_0. Let $M\in\mathbb{N}\cap(\frac{nq(\varphi)}{2i(\varphi)},\infty)$, $q\in(\max\{q_2', I(\varphi)[r(\varphi)]'\},\infty)$ and $p_2\in(I(\varphi)[r(\varphi)]',\min\{q,q_+\})$.

Similar to the proof of (i), we only need to show that, for all $(\varphi,\, q,\, M)_L$-atoms α, $V^{1/2}\nabla L^{-1}(\alpha)$ is a $(\varphi,\, p_2,\, \varepsilon_1/2)_L$-atom up to a harmless constant multiple.

Let α be a $(\varphi,\, q,\, M)$-atom associated with $B := B(x_0, r_0)$. Then there exists $b \in L^q(\mathbb{R}^n) \cap D(L)$ such that $\alpha = Lb$, $\operatorname{supp}(b) \subset B$ and $\|b\|_{L^q(\mathbb{R}^n)} \le r_0^2 |B|^{1/q} \|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}$. Furthermore, it follows from Lemma 4.6 that $b \in W^{2,q}(\mathbb{R}^n) \cap L^q_{V^q}(\mathbb{R}^n)$, which, together with $\operatorname{supp}(b) \subset B$, implies that $\operatorname{supp}(\nabla b) \subset B$. By this, we see that

$$\operatorname{supp}(V^{1/2}\nabla L^{-1}(\alpha)) = \operatorname{supp}(V^{1/2}\nabla b) = \operatorname{supp}(\nabla b) \subset B. \tag{4.7}$$

Moreover, from Hölder's inequality and the $L^q(\mathbb{R}^n)$-boundedness of $V^{1/2}\nabla L^{-1}$, we deduce that

$$\begin{aligned}\left\|V^{1/2}\nabla L^{-1}(\alpha)\right\|_{L^{p_2}(\mathbb{R}^n)} &\le |B|^{\frac{1}{p_2}-\frac{1}{q}} \left\|V^{1/2}\nabla L^{-1}(\alpha)\right\|_{L^q(\mathbb{R}^n)} \\ &\lesssim |B|^{\frac{1}{p_2}-\frac{1}{q}} \|\alpha\|_{L^q(\mathbb{R}^n)} \lesssim |B|^{1/p_2} \|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}.\end{aligned} \tag{4.8}$$

Now we estimate $|\int_B V^{1/2}\nabla L^{-1}(\alpha)\,dx|$ by considering the following two cases.

Case 1) $r_0 \in [[m(x_0,V)]^{-1}, \infty)$. In this case, similar to (4.6), we conclude that

$$\begin{aligned}\left|\int_B V^{1/2}\nabla L^{-1}(\alpha)(x)\,dx\right| &\le \left\|V^{1/2}\nabla L^{-1}(\alpha)\right\|_{L^{p_2}(B)} |B|^{1/p_2'} \\ &\lesssim |B| \|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)} [r_0 m(x_0,V)]^{\varepsilon_1/2}.\end{aligned} \tag{4.9}$$

Case 2) $r_0 \in (0, [m(x_0,V)]^{-1})$. In this case, it follows from Hölder's inequality and the Sobolev imbedding theorem (see, for example, [14, Theorem 7.10]) that, for any $p \in (1, q_+)$ with $p \ne n$,

$$\begin{aligned}\|\nabla b\|_{L^p(B)} &\lesssim \left\|\nabla^2 b\right\|_{L^p(B)} |B|^{1/n} \sim \left\|\nabla^2 L^{-1}(\alpha)\right\|_{L^p(B)} |B|^{1/n} \\ &\lesssim |B|^{1/n+1/p} \|\chi_B\|^{-1}_{L^\varphi(B)},\end{aligned} \tag{4.10}$$

which, together with Hölder's inequality, $V \in RH_{q_2}(\mathbb{R}^n)$, $q_+ > q_2' > (2q_2)'$, Lemma 3.4, $2 - n/q_2 > \varepsilon_1$ and $r_0 m(x_0,V) \in (0,1)$, further implies that

$$\begin{aligned}\left|\int_B V^{1/2}\nabla L^{-1}(\alpha)(x)\,dx\right| &\le \left\{\int_B [V(x)]^{q_2}\,dx\right\}^{1/(2q_2)} \left\{\int_B |\nabla b(x)|^{(2q_2)'}\,dx\right\}^{1/(2q_2)'} \\ &\lesssim |B|^{-1/2q_2'} \left[\int_B V(y)\,dy\right]^{1/2} |B|^{\frac{1}{(2q_2)'}+\frac{1}{n}} \|\chi_B\|^{-1}_{L^\varphi(B)} \\ &\lesssim |B| \|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)} [r_0 m(x_0,V)]^{1-\frac{n}{2q_2}} \\ &\lesssim |B| \|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)} [r_0 m(x_0,V)]^{\varepsilon_1/2}.\end{aligned}$$

This, combined with (4.7), (4.8) and (4.9), further implies that $V^{1/2}\nabla L^{-1}(\alpha)$ is a $(\varphi,\, p_2,\, \varepsilon_1/2)_L$-atom up to a harmless constant multiple, which completes the proof of Theorem 1.6(ii).

Now we prove (iii) of Theorem 1.6. Let $M \in \mathbb{N}$ satisfying $M > \frac{nq(\varphi)}{2i(\varphi)}$ and $q \in (I(\varphi)[r(\varphi)]', q_+)$. Similar to the proof of (i), we only need to show that, for all $(\varphi,\, q,\, M)_L$-atoms α, $\nabla^2 L^{-1}(\alpha)$ is a $(\varphi,\, q,\, \varepsilon)_L$-atom for any $\varepsilon \in (0,\infty)$ up to a harmless constant multiple.

Let α be a $(\varphi,\, q,\, M)_L$-atom associated with B. Then there exists $b \in L^q(\mathbb{R}^n) \cap D(L)$ such that $\alpha = Lb$ and $\operatorname{supp}(b) \subset B$ and $\|b\|_{L^q(\mathbb{R}^n)} \le r_0^2 |B|^{1/q} \|\chi_B\|^{-1}_{L^\varphi(\mathbb{R}^n)}$. Furthermore, it follows from Lemma 4.6 that $b \in W^{2,q}(\mathbb{R}^n) \cap L^q_{V^q}(\mathbb{R}^n)$, which, together with $\operatorname{supp}(b) \subset B$, implies that $\operatorname{supp}(\nabla^2 b) \subset B$. Thus,

$$\operatorname{supp}(\nabla^2 L^{-1}(\alpha)) \subset B.$$

Moreover, by Lemma 2.7(ii), we conclude that

$$\left\|\nabla^2 L^{-1}(\alpha)\right\|_{L^q(\mathbb{R}^n)} \lesssim \|\alpha\|_{L^q(B)} \lesssim |B|^{1/q} \|\chi_B\|^{-1}_{L^\varphi(B)}. \tag{4.11}$$

For the above $b \in \mathcal{D}(L)$, from (4.10) and Hölder's inequality, we deduce that $\nabla b \in L^1(\mathbb{R}^n)$. Furthermore, by (4.11), Hölder's inequality and $\alpha = Lb$, we further know that $\nabla^2 b \in L^1(\mathbb{R}^n)$. Take $\psi \in C_c^\infty(\mathbb{R}^n)$ such that $\operatorname{supp}(\psi) \subset 2B$ and $\psi \equiv 1$ on B. Then via the divergence theorem, we see that, for all $i,\, j \in \{1,\, \dots,\, n\}$,

$$\int_{\mathbb{R}^n} \frac{\partial^2 b(x)}{\partial x_i \partial x_j}\, dx = \int_{\mathbb{R}^n} \frac{\partial^2 b(x)}{\partial x_i \partial x_j} \psi(x)\, dx = -\int_{\mathbb{R}^n} \frac{\partial b(x)}{\partial x_j} \frac{\partial \psi(x)}{\partial x_i}\, dx = 0,$$

which further implies that

$$\int_{\mathbb{R}^n} \nabla^2 L^{-1}(\alpha)(x)\, dx = 0. \tag{4.12}$$

Thus, $\nabla^2 L^{-1}(\alpha)$ is a $(\varphi,\, q,\, \varepsilon)_L$-atom for any $\varepsilon \in (0, \infty)$ up to a harmless constant multiple.

Finally, we prove (iv). By the assumption $q(\varphi)[r(\varphi)]' < q_+$, we see that there exists $q \in (q(\varphi)[r(\varphi)]', q_+)$. Let M be as the proof of (iii) and α a $(\varphi,\, q,\, M)_L$-atom associated with B. Moreover, from $\operatorname{supp}(\nabla^2 L^{-1}(\alpha)) \subset B$, (4.11) and (4.12), it follows that $\nabla^2 L^{-1}(\alpha)$ is a $(\varphi,\, q,\, 0,\, \varepsilon)$-molecule for any $\varepsilon \in (0, \infty)$ up to a harmless constant multiple. By this and Lemmas 3.2 and 4.8, we conclude that $\nabla^2 L^{-1}$ is bounded from $H_{\varphi,\, L}(\mathbb{R}^n)$ to $H_\varphi(\mathbb{R}^n)$, which completes the proof of Theorem 1.6(iv) and hence Theorem 1.6. □

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