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THE L^q ESTIMATES OF RIESZ TRANSFORMS ASSOCIATED TO SCHRÖDINGER OPERATORS

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Abstract

Let $H = -\Delta + V$ be a Schrödinger operator with some general signed potential V. This paper is mainly devoted to establishing the L^q-boundedness of the Riesz transform $\nabla H^{-1/2}$ for $q > 2$. We mainly prove that under certain conditions on V, the Riesz transform $\nabla H^{-1/2}$ is bounded on L^q for all $q \in [2, p_0)$ with a given $2 < p_0 < n$. As an application, the main result can be applied to the operator $H = -\Delta + V_+ - V_-$, where V_+ belongs to the reverse Hölder class B_θ and $V_- \in L^{n/2,\infty}$ with a small norm. In particular, if $V_- = -\gamma|x|^{-2}$ for some positive number γ, $\nabla H^{-1/2}$ is bounded on L^q for all $q \in [2, n/2)$ and $n > 4$.

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1. Introduction

Let $H = -\Delta + V$ be a Schrödinger operator on $\mathbb{R}^n$, where Δ is the Laplace operator and V is a real-valued signed potential. Denote $V = V_+ - V_-$, where V_+ and V_- are the positive and negative parts of V, respectively. It is well known that there exist many interesting works about the L^q boundedness of the Riesz transform $\nabla H^{-1/2}$ associated to H. Let us recall some important progresses by the following Table 1. We first introduce some notation for the table: $P(x)$ is a nonnegative polynomial, K_n^∞ denotes the local Kato class potential (see also [24]) and $L^{r,\infty}$ $(1 \le r < \infty)$ denotes the weak $L^r(\mathbb{R}^n)$ space, that is,

$$L^{r,\infty} = \Big\{ f : \|f\|_{L^{r,\infty}} = \sup_{\gamma>0} \gamma |\{x \in \mathbb{R}^n ; |f(x)| > \gamma\}|^{1/r} < \infty \Big\}.$$

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TABLE 1. The L^q boundedness for Riesz transforms.

Potentials	Results	Papers
$V = \|x\|^2$	$\mathcal{R}_j = H^{-1/2}A_j$ and $\mathcal{R}_j^* = H^{-1/2}A_j^*$ ($j = 1, \ldots, n$) are bounded on L^q for $1 < q < \infty$, where $A_j = \partial_{x_j} + x_j$ and $A_j^* = -\partial_{x_j} + x_j$.	[25]
$V = P(x)$	$\nabla H^{-1/2}$ is bounded on L^q for $1 < q < \infty$.	[26, 28]
$V \in B_\theta$ and $n \geq 3$	$\nabla H^{-1/2}$ is bounded on L^q for $1 < q \leq n\theta/(n-\theta)$ if $n/2 \leq \theta < n$ and for $1 < q < \infty$ if $\theta = n$.	[22]
$0 \leq V \in L^1_{\mathrm{loc}}$	$\nabla H^{-1/2}$ is of weak-type $(1, 1)$ and is bounded on L^q for $1 < q \leq 2$.	[11, 18, 23]
$V \in B_\theta$ and $n \geq 1$	Let $\theta > 1$ and $\theta \geq n/2$. $\nabla H^{-1/2}$ is bounded on L^q for $1 < q < n\theta/(n-\theta) + \varepsilon$ for some $\varepsilon > 0$ if $\theta < n$ and for $1 < q < \infty$ if $\theta \geq n$.	[4]
$V \leq 0$ satisfies (A_1)	$\nabla H^{-1/2}$ is bounded on L^q for $p'_\mu < q \leq 2$ and for $1 < q < n$ if further $V \in L^{n/2,\infty} \cap K_n^\infty$.	[1]
$V = -\mu(n-2)^2\|x\|^{-2}/4$ and $n \geq 3$	$\nabla H^{-1/2}$ is bounded on L^q for $p'_\mu < q < np_\mu/(n + p_\mu)$.	[14]

Also, B_θ denotes the reverse Hölder class for some $\theta \in (1, \infty)$, which consists of a nonnegative locally integrable function w satisfying

$$\left(\frac{1}{|B|}\int_B |w(x)|^\theta \, dx\right)^{1/\theta} \leq C\left(\frac{1}{|B|}\int_B |w(x)| \, dx\right)$$

for every ball $B \subset \mathbb{R}^n$ and some constant $C > 0$ independent of θ and the ball B. For a real number $\mu > 0$, the index p_μ is defined by

$$p_\mu = \begin{cases} 2n/(n-2)(1-\sqrt{1-\mu}) & \text{if } n \geq 3, \\ \infty & \text{if } n = 1, 2. \end{cases} \tag{1.1}$$

By reviewing Table 1 above, although much progress has been made, yet for a signed potential or the cases $q > 2$, it seems that there is still room for further investigation. It is well known that the space $L^{n/2,\infty}$ plays an important role in many studies of Schrödinger operators with critical potentials (see [5, 13]). A typical example is the inverse square potential $V(x) = -\mu(n-2)^2|x|^{-2}/4 \in L^{n/2,\infty}$, which is

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widely studied in modern mathematical physics and quantum mechanics (see for example [7, 12, 19–21, 27] and references therein). Notice that the inverse square potential does not belong to the Kato class K_n^∞ and hence we could not apply [1, Theorem 4.1] to determine whether the Riesz transform of $H = -\Delta + V$ with signed potential $V \in L^{n/2,\infty}$ is bounded on L^q for any $q > 2$ or not. In the present paper, we are mainly devoted to the L^q boundedness of the Riesz transform $\nabla H^{-1/2}$ for $q > 2$ with such kind of critical potentials.

To this end, in the following we need to introduce some new conditions on V. First of all, a real-valued potential $V = V_+ - V_-$ is said to satisfy (A_1) (which is also called the *strongly subcritical condition*) if there exists $\mu \in (0, 1)$ such that for all $f \in W^{1,2}(\mathbb{R}^n)$ satisfying $\int_{\mathbb{R}^n} V_+|f|^2\,dx < \infty$, the following inequality holds:

$$(A_1): \quad \int_{\mathbb{R}^n} V_-(x)|f(x)|^2\,dx \le \mu\Big(\int_{\mathbb{R}^n} |\nabla f(x)|^2\,dx + \int_{\mathbb{R}^n} V_+(x)|f(x)|^2\,dx\Big).$$

If V satisfies (A_1), the forms

$$Q(f, g) = Q_+(f, g) - \int_{\mathbb{R}^n} V_-(x) f(x)\overline{g}(x)\,dx \tag{1.2}$$

with

$$Q_+(f, g) = \int_{\mathbb{R}^n} \nabla f(x)\overline{\nabla g}(x)\,dx + \int_{\mathbb{R}^n} V_+(x) f(x)\overline{g}(x)\,dx \tag{1.3}$$

are well defined and closed on the domain

$$D(Q) = D(Q_+) = \Big\{f \in W^{1,2}(\mathbb{R}^n);\ \int_{\mathbb{R}^n} V_+(x)|f(x)|^2\,dx < \infty\Big\}.$$

Thus, $H_+ := -\Delta + V_+$ and $H := -\Delta + V$ are nonnegative self-adjoint operators associated with the forms Q_+ and Q, respectively. Denote by $D(H_+)$ and $D(H)$ their domains.

Next, the potential V is said to satisfy (A_2) and (A_3) for some $p_0 > 2$, respectively, if there exists a constant $p_0 > 2$ such that

$$(A_2): \quad \|\nabla H_+^{-1/2}\|_{L^{p_0}-L^{p_0}} < \infty$$

and

$$(A_3): \quad \|V_-(I + H_+)^{-1}\|_{L^{p_0}-L^{p_0}} < \infty,$$

where H_+ with domain $D_{p_0}(H_+)$ is the generator of the Schrödinger semigroup e^{-tH_+} on L^{p_0} (see Lemma 3.1 in Section 3 below). It should be emphasized that our conditions are satisfied by a large class of signed potentials V with certain nonzero positive part V_+ (see Remark 1.2 below), whereas assumptions in Assaad [1] are only considered for $V \le 0$ or for $|V|$ in Assaad and Ouhabaz [2].

Our main result in this paper is as follows.

Theorem 1.1. *Let $n \geq 3$ and $H = -\Delta + V$ and $V_\pm$ be the positive and negative parts of V, respectively. Assume that (A_1) holds for some $\mu \in (0,1)$ and (A_2) and (A_3) hold for some $2 < p_0 < n$. Then there exists a constant δ_{p_0} depending on p_0 such that when*

$$\|V_-\|_{L^{n/2,\infty}} \leq \delta_{p_0}, \tag{1.4}$$

the Riesz transform $\nabla H^{-1/2}$ is bounded on $L^q(\mathbb{R}^n)$ for all $q \in (p'_\mu, p_0)$ with p_μ defined by (1.1).

Before we prove Theorem 1.1, several remarks about (A_2) and (A_3) are given as follows.

Remark 1.2. Let $V = V_+ - V_-$, where $V_\pm$ denote the positive and negative parts of V.

(i) It follows from Table 1 that $\nabla H_+^{-1/2}$ is of weak type (1, 1), which, combined with (A_2), implies that it is bounded on $L^p(\mathbb{R}^n)$ for all $1 < p \leq p_0$. On the other hand, (A_3) is actually equivalent to the following perturbation inequality:

$$\|V_- f\|_{L^{p_0}} \leq a\|H_+ f\|_{L^{p_0}} + b\|f\|_{L^{p_0}}, \quad f \in D_{p_0}(H_+) \tag{1.5}$$

with some positive constants $a, b > 0$. This is because

$$\begin{aligned}\|V_- f\|_{L^{p_0}} &\leq \|V_-(I + H_+)^{-1}(I + H_+) f\|_{L^{p_0}} \\ &\leq \|V_-(I + H_+)^{-1}\|_{L^{p_0} - L^{p_0}} (\|H_+ f\|_{L^{p_0}} + \|f\|_{L^{p_0}})\end{aligned}$$

and

$$\begin{aligned}\|V_-(I + H_+)^{-1} f\|_{L^{p_0}} &\leq a\|H_+(I + H_+)^{-1} f\|_{L^{p_0}} + b\|(I + H_+)^{-1} f\|_{L^{p_0}} \\ &\leq C\|f\|_{L^{p_0}},\end{aligned}$$

where $H_+(I + H_+)^{-1}$ and $(I + H_+)^{-1}$ are bounded on L^{p_0} by bounded functional calculus.

(ii) If $V_+ = 0$, clearly, the classical Riesz transform $\nabla(-\Delta)^{-1/2}$ is bounded on L^p for all $1 < p < \infty$ and then (A_2) holds for all $2 < p_0 < \infty$. Moreover, let $V_- \in L^{n/2,\infty}$; it follows from the weak-type Hölder inequality (3.3) and Sobolev's embedding theorem that for $1 < p < n/2$,

$$\|V_- f\|_{L^p} \leq C\|V_-\|_{L^{n/2,\infty}} \|\Delta f\|_{L^p}. \tag{1.6}$$

Therefore, if $V_+ = 0$, $V_- \in L^{n/2,\infty}$ and $n > 4$, (1.5) and (1.6) imply that (A_3) can hold for all $2 < p_0 < n/2$.

(iii) If $V_+ \neq 0$, then there exist several important nonnegative potential classes such that (A_2) holds. Let $n \geq 3$, $V_+ \in B_\theta$ for some $\theta \geq n/2$ and

$$\theta^* = \begin{cases} n\theta/(n - \theta) & \text{if } n/2 \leq \theta < n, \\ \infty & \text{if } \theta \geq n. \end{cases}$$

It follows from [22] and [4] that (A_2) holds for all $2 < p_0 < \theta^*$. In particular, if V_+ is a positive polynomial, (A_2) holds for all $2 < p_0 < \infty$. Moreover, if $V_+ \in B_\theta$ with $\theta \geq n/2 > 2$ and $V_- \in L^{n/2,\infty}$, we have that (A_3) holds for $2 < p_0 < n/2$ (see Lemma 4.4 below).

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Notice that if V_+ belongs to some reverse Hölder class B_θ and $V_- \in L^{n/2,\infty}$, then (A_2) and (A_3) hold for some $q_0 > 2$. Therefore, we have the following conclusion.

Theorem 1.3. *Let $n > 4$ and $H = -\Delta + V_+ - V_-$. If V_+ satisfies (B_θ) for $\theta \geq n/2$, then there exists a constant $\delta > 0$ such that when*

$$\|V_-\|_{L^{n/2,\infty}} \leq \delta,$$

the Riesz transform $\nabla H^{-1/2}$ is bounded on L^q for all $q \in (p'_\mu, n/2)$.

Now we consider the Schrödinger operator with inverse square potential $|x|^{-2}$. By applying Theorem 1.3, the following corollary holds.

Corollary 1.4. *Let $n > 4$ and $H = -\Delta + V_+ - \gamma(n-2)^2|x|^{-2}/4$ with $V_+ \in B_\theta$ for $\theta \geq n/2$. Then there exists a constant $\delta \in (0, 1)$ such that when $0 < \gamma < \delta$, the Riesz transform $\nabla H^{-1/2}$ is bounded on L^q for all $q \in (p'_\gamma, n/2)$.*

Remark 1.5. Let $V_+ = 0$ in Corollary 1.4. Recently, Hassell and Lin [14] have obtained the sharp interval for the boundedness of $\nabla H^{-1/2}$ on L^q based on a different method. Compared with their work, we here deal with a class of potentials V with nonzero positive parts V_+.

The paper is organized as follows. In Section 2, we establish the off-diagonal estimates for some families of operators related to the Schrödinger semigroup e^{-tH}. As an application, we prove that the Riesz transform $\nabla H^{-1/2}$ is of weak-type (1, 1) when $n = 1$. Section 3 is devoted to the study of the L^q regularity of $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ for $q > 2$. In Section 4, we will give the proofs of Theorem 1.1, Theorem 1.3 and Corollary 1.4.

2. The off-diagonal estimates and their application

2.1. The off-diagonal estimates. Let us begin with the definitions of the L^p–L^q estimates and the L^p–L^q off-diagonal estimates for a general family of operators.

Definition 2.1 (L^p–L^q off-diagonal estimates for a family of operators). We say that the family of operators $\{S_t\}_{t>0}$ satisfies the L^p–L^q off-diagonal estimates for some $p, q \in [1, \infty)$ with $p \leq q$ if there exist constants $C, c, \beta > 0$ such that for all closed sets $E, F \subset \mathbb{R}^n$, $t > 0$ and $f \in L^2 \cap L^p$ supported in E, the following estimate holds:

$$\|S_t f\|_{L^q(F)} \leq C t^{n/2q - n/2p} e^{-d^2(E,F)/ct} \|f\|_{L^p(E)}, \tag{2.1}$$

where, and in the sequel, $d(E, F)$ denotes the semidistance induced on sets by the Euclidean distance. In particular, if (2.1) holds for $p = q$, then we say that $\{S_t\}_{t>0}$ satisfies the L^p off-diagonal estimates.

Definition 2.2 (L^p–L^q estimates for a family of operators). We say that the family of operators $\{S_t\}_{t>0}$ satisfies the L^p–L^q estimates for some $p, q \in [1, \infty)$ with $p \leq q$ if

$$\|S_t f\|_{L^q} \leq C t^{n/2q - n/2p} \|f\|_{L^p},$$

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where $C > 0$, independent of t, and $f \in L^2 \cap L^p$. Obviously, if $\{S_t\}_{t>0}$ satisfies the L^p–L^p estimate, $\{S_t\}_{t>0}$ is bounded on L^p uniformly in t. In this case, we say that S_t is bounded on L^p.

The following lemma is due to Auscher [3].

Lemma 2.3. *If $\{T_t\}_{t>0}$ satisfies L^p–L^q estimates and $\{S_t\}_{t>0}$ satisfies L^q–L^r estimates, then $\{S_tT_t\}_{t>0}$ satisfies L^p–L^r estimates.*

The statement of the lemma remains valid with 'estimates' replaced by 'off-diagonal estimates'.

As we know, the off-diagonal estimates play an essential role in the studying of the Riesz transforms associated to operators. For the Schrödinger operators we considered, Assaad [1] and Assaad and Ouhabaz [2] have investigated the off-diagonal estimates (see Theorem A); one can also see the results for second and higher order elliptic operators in divergence form in [3] and [10], respectively.

Theorem A. *Let $H = -\Delta + V$, where $V_+ \in L^1_{\text{loc}}(\mathbb{R}^n)$ and V satisfies (A_1).*

(i) *$\{e^{-tH}\}_{t>0}$, $\{tHe^{-tH}\}_{t>0}$ and $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfy the L^2 off-diagonal estimates.*
(ii) *$\{e^{-tH}\}_{t>0}$, $\{tHe^{-tH}\}_{t>0}$ and $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfy the L^q–L^2 estimates and the L^q–L^2 off-diagonal estimates for all $q \in (p'_\mu, 2]$, where p_μ is given by (1.1).*
(iii) *$\{e^{-tH}\}_{t>0}$ and $\{tHe^{-tH}\}_{t>0}$ satisfy the L^2–L^q estimates and the L^2–L^q off-diagonal estimates for all $q \in [2, p_\mu)$.*
(iv) *$\{e^{-tH}\}_{t>0}$ are uniformly bounded on L^q for all $q \in (p'_\mu, p_\mu)$.*

For the family $\{tHe^{-tH}\}_{t>0}$, we build a bridge connecting the L^q boundedness, L^q–L^2 estimates and the L^q–L^2 off-diagonal estimates by the following proposition.

Proposition 2.4. *Let $q \in [1, 2)$ and $H = -\Delta + V$, where $V_+ \in L^1_{\text{loc}}(\mathbb{R}^n)$ and V satisfies (A_1).*

(i) *If $\{tHe^{-tH}\}_{t>0}$ is bounded on L^q, then it satisfies the L^q–L^2 estimates.*
(ii) *If $\{tHe^{-tH}\}_{t>0}$ satisfies the L^q–L^2 estimates, then, for all $r \in (q, 2)$, it satisfies the L^r–L^2 off-diagonal estimates.*
(iii) *If $\{tHe^{-tH}\}_{t>0}$ satisfies the L^q–L^2 off-diagonal estimates, then it is bounded on L^q.*

Moreover, The statements (i), (ii) and (iii) still hold when $2 \le q < \infty$, replacing L^q–L^2 by L^2–L^q everywhere.

Proof. We first consider the statement (i). Recall the Gagliardo–Nirenberg inequality

$$\|f\|^2_{L^2} \le C\|\nabla f\|^{2\alpha}_{L^2}\|f\|^{2\beta}_{L^q},$$

where $\alpha + \beta = 1$ and $(1 + \gamma_q)\alpha = \gamma_q$ with $\gamma_q = n/q - n/2$. On the other hand, it follows from the analyticity of e^{-tH} on L^2 that $e^{-tH}f \in D(H^2)$ for all $f \in L^2$, which means that $He^{-tH}f \in D(H) \subset W^{1,2}$. Thus,

$$\|He^{-tH}f\|^2_{L^2} \le C\|\nabla He^{-tH}f\|^{2\alpha}_{L^2}\|He^{-tH}f\|^{2\beta}_{L^q} \tag{2.2}$$

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holds for all $t > 0$ and $f \in L^2 \cap L^q$. By the condition (A_1) and (1.2),

$$\|\nabla He^{-tH} f\|_{L^2}^2 \le 1/(1-\mu)\,\langle HHe^{-tH} f, He^{-tH} f\rangle$$
$$= -1/(2-2\mu)\,\frac{d}{dt}\|He^{-tH} f\|_{L^2}^2. \tag{2.3}$$

Assume that $f \in L^2 \cap L^q$ with $\|f\|_{L^q} = 1$. Then it follows from the L^q boundedness of tHe^{-tH}, (2.2) and (2.3) that

$$\varphi(t) \le -C\varphi'(t)^{\alpha} t^{-2\beta}, \tag{2.4}$$

where $\varphi(t) = \|He^{-tH} f\|_{L^2}^2$. Notice that by (2.4),

$$\frac{d}{dt}[\varphi(t)^{1-1/\alpha}] \ge Ct^{2\beta/\alpha}.$$

Integrating between t and $2t$, we find that $\varphi(t) \le Ct^{-2-\gamma_q}$, which implies the statement (i).

By interpolating the L^q–L^2 estimates with the L^2 off-diagonal estimates, we can prove (ii) immediately.

The proof of (iii) can be concluded by invoking Auscher [3, Lemma 4.3]. Hence, we finish the proof of Proposition 2.4. □

Now let us focus on the off-diagonal estimates for $n = 1$. It has been proved in Assaad and Ouhabaz [2] that e^{-tH} satisfies the L^p–L^2 off-diagonal estimates for all $p \in (1, 2]$. Here, we can obtain the L^1–L^2 off-diagonal estimates for e^{-tH}, tHe^{-tH} and $\sqrt{t}\nabla e^{-tH}$, which will be useful for the boundedness of $\nabla H^{-1/2}$ on $L^1(\mathbb{R})$.

Proposition 2.5. *Let $H = -\Delta + V$, where $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R})$ and V satisfies (A_1).*

(i) *$\{e^{-tH}\}_{t>0}$, $\{tHe^{-tH}\}_{t>0}$ and $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfy the L^q–L^2 estimates and the L^q–L^2 off-diagonal estimates for all $q \in [1, 2]$.*

(ii) *$\{e^{-tH}\}_{t>0}$ and $\{tHe^{-tH}\}_{t>0}$ satisfy the L^2–L^q estimates and the L^2–L^q off-diagonal estimates for all $q \in [2, \infty]$.*

Proof. We first prove (ii). Let $\lambda > 0$ and $\mathcal{E}(\mathbb{R})$ be a set consisting of all bounded Lipschitz functions ϕ on $\mathbb{R}$ satisfying $\|\nabla\phi\|_{L^\infty} \le 1$. Let $H_{\lambda\phi} := e^{\lambda\phi} He^{-\lambda\phi}$ be the operator associated to

$$Q_{\lambda\phi}(f, g) := Q(e^{-\lambda\phi} f, e^{\lambda\phi} g), \quad f, g \in D(Q),$$

where Q is defined by (1.2). Since V_- satisfies (A_1),

$$(\lambda^2 + Q_{\lambda\phi})(f, f) \ge Q(f, f) \ge \|\nabla f\|_{L^2}^2.$$

Thus, $H_{\lambda\phi}$ generates an analytic semigroup on L^2 and

$$\|(tH_{\lambda\phi})^k e^{-tH_{\lambda\phi}}\|_{L^2-L^2} \le Ce^{c\lambda^2 t}$$

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for all $k \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$. Notice that for all $f \in L^2(\mathbb{R})$, $f_t := e^{-tH_{\lambda\phi}} f \in D(H_{\lambda\phi}) = D(H) \subset W^{1,2}(\mathbb{R})$ and the embedding inequality

$$\|u\|_{L^q} \le C\|(-\Delta)^{1/2}u\|_{L^2}^{\theta}\|u\|_{L^2}^{1-\theta}$$

holds for all $u \in W^{1,2}(\mathbb{R})$, where $\theta = 1/2 - 1/q$ and $2 \le q \le \infty$. Then, for $2 \le q \le \infty$,

$$\begin{aligned}\|f_t\|_{L^q} &\le C\|(-\Delta)^{1/2}f_t\|_{L^2}^{\theta}\|f_t\|_{L^2}^{1-\theta} \le C(\lambda^2\langle f_t, f_t\rangle + \langle H_{\lambda\phi}f_t, f_t\rangle)^{\theta/2}\|f_t\|_{L^2}^{1-\theta}\\ &\le Ct^{-(1/4-1/2q)}e^{c\lambda^2 t}\|f\|_{L^2},\end{aligned}$$

which means that

$$\|e^{-tH_{\lambda\phi}}f\|_{L^q} \le Ct^{-(1/4-1/2q)}e^{c\lambda^2 t}\|f\|_{L^2} \tag{2.5}$$

for all $2 \le q \le \infty$.

Now, for any compact subsets $E, F \subset \mathbb{R}$, and $f \in L^2$ supported in F, we choose $\phi(x) = d(x, F)$ in (2.5) to obtain that

$$\|e^{-tH}f\|_{L^q(E)} \le Ct^{-(1/4-1/2q)}e^{-\lambda d(E,F)+c\lambda^2 t}\|f\|_{L^2(F)},$$

which implies that

$$\|e^{-tH}f\|_{L^q(E)} \le At^{-(1/4-1/2q)}e^{-d^2(E,F)/at}\|f\|_{L^2(F)} \tag{2.6}$$

for some constants $A, a > 0$. For arbitrary closed sets $E, F \subset \mathbb{R}$, since $E = \bigcup_{\ell=1}^{\infty} E_\ell$ and $F = \bigcup_{\ell=1}^{\infty} E_\ell$, where both $\{E_\ell\}_{\ell=1}^{\infty}$ and $\{F_\ell\}_{\ell=1}^{\infty}$ are increasing monotone sets of sequences and then by a limitation procedure, it is easy to see that (2.6) holds for an arbitrary closed set. Hence, we prove that e^{-tH} satisfies he L^2–L^q off-diagonal estimates for all $q \in [2, \infty]$. The results for $\{tHe^{-tH}\}_{t>0}$ and $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ can be obtained by the following identities:

$$\sqrt{t}\nabla e^{-tH} = \sqrt{t}\nabla e^{-tH/2}e^{-tH/2}, \quad tHe^{-tH} = tHe^{-tH/2}e^{-tH/2}$$

and Lemma 2.3.

We turn to prove (i). In fact, by using duality and the above identities again, (i) can be easily concluded. Hence, we finish the whole proof. □

REMARK 2.6.

(i) It follows from the proof of Proposition 2.2 in [1] that all conclusions of Proposition 2.4 also hold for the operator e^{-tH}. Moreover, Proposition 2.4 is still true for e^{-tL} if L denotes the homogeneous elliptic operator in divergence form with second and higher orders, respectively (see [3] and [10]).

(ii) When $n = 1$, by the Sobolev embedding theorem and duality, we can show that e^{-tH} satisfies the L^1–L^2 estimates, which, combined with the L^2 off-diagonal estimates of e^{-tH} and [8, Theorem 4.2], would also imply the L^1–L^2 off-diagonal estimates for e^{-tH}.

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2.2. The weak-type (1, 1) estimate of the Riesz transform when $n = 1$. An important application of the L^q–L^2 off-diagonal estimates is to show the boundedness of Riesz transforms $\nabla H^{-1/2}$ on L^q for $q \leq 2$. In fact, Assaad [1] and Assaad and Ouhabaz [2] proved the following theorem.

Theorem B. *Let $H = -\Delta + V$, where $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$ and V satisfies (A_1). Then $\nabla H^{-1/2}$ is bounded on L^q for all $q \in (p'_\mu, 2]$, where p_μ is defined by (1.1).*

It was also mentioned in [1] that the lower bound p'_μ in Theorem B is sharp; it is of interest to concern the boundedness of $\nabla H^{-1/2}$ on $L^{p'_\mu}$. When $n = 1$, by using the L^1–L^2 off-diagonal estimates for e^{-tH} (see Proposition 2.5), we can prove that $\nabla H^{-1/2}$ is of weak-type (1, 1). However, it is not clear to us what would happen on $L^{p'_\mu}$ when $n \geq 2$.

Theorem 2.7. *Let $n = 1$ and $H = -\Delta + V$, where $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R})$ and V satisfies (A_1). Then $\nabla H^{-1/2}$ is of weak-type (1, 1).*

Proof. By Proposition 2.5, we know that the families of operators $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ and $\{e^{-tH}\}_{t>0}$ satisfy L^1–L^2 estimates and L^1–L^2 off-diagonal estimates when $n = 1$. Thus, Theorem 2.7 follows trivially from the same procedure which was involved in the proof of [1, Theorem 3.2]. □

3. The L^p-regularity of $\sqrt{t}\nabla e^{-tH}$

Before studying the family of operators $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$, we give a quick comment on the regularity of the semigroup e^{-tH}. Denote by Σ_μ the open sector $\{z \in \mathbb{C}\backslash\{0\} : |\arg z| < \mu\}$ for $\mu \in [0, \pi)$ and by $H^\infty(\Sigma_\nu)$ the space of all bounded holomorphic functions on Σ_μ. Since H_+ is a nonnegative self-adjoint operator associated to Q_+ defined by (1.3), it is well known that its heat kernel $K(t, x, y)$ is nonnegative and satisfies the Gaussian upper bound (see [18]). That is,

$$0 \leq K(t, x, y) \leq (4\pi t)^{-n/2} e^{-|x-y|^2/4t}.$$

Moreover, we have the following lemma (see [6, 15–18] and so on).

Lemma 3.1. *Let H_+ be the nonnegative self-adjoint operator associated to Q_+ defined by (1.3). Then we have the following statements.*

(i) *The positive contractive semigroup e^{-tH_+} on L^2 has an analytic extension $\{e^{-zH_+}\}_{z\in\Sigma_{\pi/2}}$.*

(ii) *e^{-tH_+} extends to an analytic semigroup on L^q for all $1 \leq q < \infty$. Let $H_{+,q}$ be its generator; then $H_{+,q}$ is densely defined and closed on L^q with domain $D_q(H_{+,q})$. Furthermore, the sector of analyticity and the spectrum of the generator $H_{+,q}$ are q-independent for $1 \leq q < \infty$.*

(iii) *For all $\nu \in [0, \pi)$ and $1 < q < \infty$, H_+ has an $H^\infty(\Sigma_\nu)$ calculus on L^q. That is, there exists a constant $c_{\nu,q} > 0$ such that for all $F \in H^\infty(\Sigma_\nu)$,*

$$\|F(H_+)\|_{L^q-L^q} \leq c_{\nu,q}\|F\|_{L^\infty(\Sigma_\nu)}. \tag{3.1}$$

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Remark 3.2. By (ii) of Lemma 3.1, it is easy to see that $e^{-tH_{+,q}}$ are consistent for all $q \in [1, \infty)$ on $\mathscr{S}(\mathbb{R}^n)$ (Schwartz function spaces). Thus, for the sake of convenience, we denote H_+ and e^{-tH_+} for all $q \in [1, \infty)$.

In the sequel, we denote by $q^* = nq/(n-q)$ the Sobolev embedding index of q for $q \in (1, n)$.

Lemma 3.3. *Let $n \geq 3$ and $H = -\Delta + V$, where V satisfies (A_1) for some $\mu \in (0, 1)$. Assume that the family $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ is bounded on L^p for some $2 \leq p < n$. Then $\{e^{-tH}\}_{t>0}$ is bounded on L^q for all $2 \leq q < p^*$.*

Proof. For given $2 \leq p < n$ as in the assumption, interpolating by the Riesz–Thorin theorem the L^p and L^2 boundedness of $\sqrt{t}\nabla e^{-tH}$, we have that $\sqrt{t}\nabla e^{-tH}$ is bounded on L^r for all $2 \leq r \leq p$; it then follows from Sobolev's embedding theorem that

$$\|e^{-tH}\|_{L^r - L^{r^*}} \leq Ct^{-1/2}, \quad 2 \leq r \leq p. \tag{3.2}$$

Noticing that there exist constants $n_0 \in \mathbb{N}$ and $2 \leq p_0 < p_\mu$ such that $p^* = np_0/(n - n_0 p_0) < \infty$ and e^{-tH} satisfies L^2–L^{p_0} estimates (see Theorem A), let $p_k = (p_{k-1})^*$ $(k = 1, 2, \ldots, n_0)$; by (3.2),

$$\begin{aligned}\|e^{-(n_0+1)tH}\|_{L^2 - L^{p^*}} &\leq \|e^{-tH}\|_{L^2 - L^{p_0}}\|e^{-tH}\|_{L^{p_0} - L^{p_1}} \cdots \|e^{-tH}\|_{L^{p_{n_0-1}} - L^{p_{n_0}}} \\ &\leq Ct^{-(n/4 - n/2p^*)},\end{aligned}$$

which, combined with (i) of Remark 2.6, can finish the proof. □

Before proving the main theorem of this paper, we introduce the Sobolev constant and the weak-type Hölder constant in the following ways. Let s_p $(1 \leq p < n)$ be the constant such that

$$\|f\|_{L^{np/n-p}} \leq s_p\|\nabla f\|_{L^p}.$$

Let $h_{p,q,r}$ be the constant such that the weak-type Hölder inequality (see [1, Lemma 4.1])

$$\|fg\|_{L^p} \leq h_{p,q,r}\|f\|_{L^{r,\infty}}\|g\|_{L^q} \tag{3.3}$$

holds, where $f \in L^{r,\infty}$, $g \in L^q$ and $1/p = 1/q + 1/r$ for all $r, p, q \in (1, \infty)$.

Remark 3.4. Notice that if $V_+ \in L^1_{\text{loc}}(\mathbb{R}^n)$ and V_- satisfies the assumption (1.4), then, by (3.3), we have for $f \in D(Q)$ and $n \geq 3$,

$$\begin{aligned}\int_{\mathbb{R}^n} V_-(x)|f(x)|^2\,dx &\leq \|V_-^{1/2} f\|_{L^2}\|V_-^{1/2} f\|_{L^2} \leq h^2\|V_-^{1/2}\|^2_{L^{n,\infty}}\|f\|^2_{L^{2n/n-2}} \\ &\leq h^2 s_2^2\|V_-\|_{L^{n/2,\infty}}\|\nabla f\|^2_{L^2} \leq h^2 s_2^2 \delta_{p_0} Q_+(f, f),\end{aligned} \tag{3.4}$$

where $h = h_{2,2n/n-2,n}$ in (3.3). Equation (3.4) implies that V satisfies (A_1) with $\mu < \widetilde{\mu} := \delta_{p_0} h^2 s_2^2 \in (0, 1)$ if $\delta_{p_0} < (hs_2)^{-2}$. Thus, the constant μ in condition (A_1) can be understood as the best constant such that (A_1) holds.

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Now we study the L^p boundedness of $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ for some $p > 2$. Note that if the potential V satisfies the condition (A_1) only, the possible interval for L^p $(p > 2)$ boundedness of $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ is $[2, np_\mu/(n - p_\mu))$ $(n \geq 3)$, which is not confirmed yet. However, if extra conditions (A_2) and (A_3) are satisfied, we can prove the following result.

Proposition 3.5. *Let $n \geq 3$ and $H = -\Delta + V$ with $V \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$. Assume that (A_1) holds for some $\mu \in (0, 1)$ and (A_2) and (A_3) hold for some $2 < p_0 < n$. Then there exists a constant $\delta_{p_0} > 0$ such that when*

$$\|V_-\|_{L^{n/2,\infty}} \leq \delta_{p_0},$$

we have that $\sqrt{t}\nabla e^{-tH}$ is bounded on $L^{p_0}(\mathbb{R}^n)$.

Proof. Let H_+ be defined as in Lemma 3.1. We first show that both $V_-^{1/2}(\mathbf{I} + tH_+)^{-1/2}$ and $(\mathbf{I} + tH_+)^{-1/2}V_-^{1/2}$ are bounded operators on L^{p_0}. To this end, notice that for all $t > 0$, let $F_t(z) = \sqrt{tz/1 + tz}$ with $\Re z \geq 0$ and $\nu = \pi/2$; by (iii) of Lemma 3.1, we have $F_z \in H^\infty(\Sigma_\nu)$ and

$$\|F_z(H_+)\|_{L^{p_0}-L^{p_0}} = \|H_+^{1/2}(t^{-1} + H_+)^{-1/2}\|_{L^{p_0}-L^{p_0}} \leq c_{p_0}\|F_z\|_{L^\infty} \leq c_{p_0}, \tag{3.5}$$

where $c_{p_0} = c_{\pi/2,p_0}$ in (3.1). Then it follows from (3.5) and the weak-type Hölder inequality that

$$\begin{aligned}\|V_-^{1/2}(t^{-1} + H_+)^{-1/2}\|_{L^{p_0}-L^{p_0}} &\leq \|V_-^{1/2}H_+^{-1/2}\|_{L^{p_0}-L^{p_0}}\|H_+^{1/2}(t^{-1} + H_+)^{-1/2}\|_{L^{p_0}-L^{p_0}}\\ &\leq c_{p_0}\|V_-^{1/2}H_+^{-1/2}\|_{L^{p_0}-L^{p_0}}\\ &\leq c_{p_0}h_{p_0}\|V_-^{1/2}\|_{L^{n/2,\infty}}\|H_+^{-1/2}\|_{L^{p_0}-L^{np_0/n-p_0}}\\ &\leq c_{p_0}h_{p_0}s_{p_0}\delta_{p_0}^{1/2}\|\nabla H_+^{-1/2}\|_{L^p-L^p} \leq C_{p_0}\delta_{p_0}^{1/2},\end{aligned}$$

where $\alpha_{p_0} := \|\nabla H_+^{-1/2}\|_{L^{p_0}-L^{p_0}}$, $h_{p_0} = h_{p_0,np_0/n-p_0,n}$ and $C_{p_0} = c_{p_0}h_{p_0}s_{p_0}\alpha_{p_0}$. Let $1/p_0 + 1/p_0' = 1$; by (i) of Remark 1.2, we have that $\nabla H_+^{-1/2}$ is bounded on $L^{p_0'}$. Then the same procedure above can be applied to obtain

$$\begin{aligned}\|V_-^{1/2}(t^{-1} + H_+)^{-1/2}\|_{L^{p_0'}-L^{p_0'}} &\leq \|V_-^{1/2}H_+^{-1/2}\|_{L^{p_0'}-L^{p_0'}}\|H_+^{1/2}(t^{-1} + H_+)^{-1/2}\|_{L^{p_0'}-L^{p_0'}}\\ &\leq C_{p_0'}\delta_{p_0}^{1/2}\end{aligned}$$

and

$$\begin{aligned}\|V_-^{1/2}(\mathbf{I} + tH_+)^{-1/2}\|_{L^{p_0'}-L^{p_0'}} &\leq \|V_-^{1/2}H_+^{-1/2}\|_{L^{p_0'}-L^{p_0'}}\|H_+^{1/2}(I + tH_+)^{-1/2}\|_{L^{p_0'}-L^{p_0'}}\\ &\leq C_{p_0'}\delta_{p_0}^{1/2}t^{-1/2},\end{aligned}$$

where $\alpha_{p_0'} := \|\nabla H_+^{-1/2}\|_{L^{p_0'}-L^{p_0'}}$, $h_{p_0'} = h_{p_0',np_0'/n-p_0',n}$ and $C_{p_0'} = c_{p_0'}h_{p_0'}s_{p_0'}\alpha_{p_0'}$. By duality,

$$\|(\mathbf{I} + tH_+)^{-1/2}V_-^{1/2}\|_{L^{p_0}-L^{p_0}} = \|V_-^{1/2}(I + tH_+)^{-1/2}\|_{L^{p_0'}-L^{p_0'}} \leq C_{p_0'}\delta_{p_0}^{1/2}t^{-1/2}$$

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and

$$\|(t^{-1}+H_+)^{-1/2}V_-^{1/2}\|_{L^{p_0}-L^{p_0}} = \|V_-^{1/2}(t^{-1}+H_+)^{-1/2}\|_{L^{p_0'}-L^{p_0'}} \le C_{p_0'}\delta_{p_0}^{1/2}.$$

We denote $A = \mathbf{I} - V_-(t^{-1}+H_+)^{-1}$. It is easy to see that the operator A is well defined on L^{p_0} by (A_3). Let

$$I_k = (\mathbf{I}+tH_+)^{-1/2}(V_-(t^{-1}+H_+)^{-1})^k$$

and $J_k = I_k A$. Notice that for each k,

$$\begin{aligned} I_k &= (\mathbf{I}+tH_+)^{-1/2}(V_-(t^{-1}+H_+)^{-1})\cdots(V_-(t^{-1}+H_+)^{-1}) \\ &= (\mathbf{I}+tH_+)^{-1/2}V_-^{1/2}V_-^{1/2}(t^{-1}+H_+)^{-1/2}\cdots \\ &\quad \cdots((t^{-1}+H_+)^{-1/2}V_-^{1/2}V_-^{1/2}(t^{-1}+H_+)^{-1/2})\cdots \\ &\quad \cdots((t^{-1}+H_+)^{-1/2}V_-^{1/2}V_-^{1/2}(t^{-1}+H_+)^{-1/2})(t^{-1}+H_+)^{-1/2}. \end{aligned}$$

Thus,

$$\begin{aligned} \|I_k\|_{L^{p_0}-L^{p_0}} &\le \|(\mathbf{I}+tH_+)^{-1/2}V_-^{1/2}\|_{L^{p_0}-L^{p_0}}\|V_-^{1/2}(t^{-1}+H_+)^{-1/2}\|^k_{L^{p_0}-L^{p_0}} \\ &\quad \times\|(t^{-1}+H_+)^{-1/2}V_-^{1/2}\|^{k-1}_{L^{p_0}-L^{p_0}}\|(t^{-1}+H_+)^{-1/2}\|_{L^{p_0}-L^{p_0}}. \end{aligned} \tag{3.6}$$

Similarly to (3.5),

$$\|(t^{-1}+H_+)^{-1/2}\|_{L^{p_0}-L^{p_0}} \le c_p t^{1/2}. \tag{3.7}$$

Thus, it follows from (3.6) and (3.7) that

$$\|I_k\|_{L^{p_0}-L^{p_0}} \le c_{p_0}(C_{p_0'}C_{p_0}\delta_{p_0})^k, \tag{3.8}$$

which means that $\sum_{k=0}^{\ell} I_k$ converges to an operator T on L^{p_0} if we choose $\delta_{p_0} < (C_{p_0'}C_{p_0})^{-1}$. That is, $T = \sum_{k=0}^{\infty} I_k$ in the sense of L^{p_0}. Thus,

$$\Big\|TAf - \sum_{k=0}^{\ell} J_k f\Big\|_{L^{p_0}} = \Big\|\Big(T - \sum_{k=0}^{\ell} I_k\Big)Af\Big\|_{L^{p_0}} \le \Big\|T - \sum_{k=0}^{\ell} I_k\Big\|_{L^{p_0}-L^{p_0}}\|Af\|_{L^{p_0}}$$

for all $f \in L^{p_0}$, which implies that $TAf = \lim_{\ell\to\infty}\sum_{k=0}^{\ell} J_k f$. On the other hand, for every $f \in L^{p_0}$, it follows from (3.8) that

$$\begin{aligned} \Big\|\sum_{k=0}^{\ell} J_k f - (\mathbf{I}+tH_+)^{-1/2}f\Big\|_{L^{p_0}} &= \|I_{\ell+1}f\|_{L^{p_0}} \\ &\le c_{p_0}(C_{p_0'}C_{p_0}\delta_{p_0})^{\ell+1}\|f\|_{L^{p_0}}. \end{aligned} \tag{3.9}$$

Then, by choosing $\delta_{p_0} < (C_{p_0'}C_{p_0})^{-1}$ in (3.9),

$$(\mathbf{I}+tH_+)^{-1/2}f = \lim_{\ell\to\infty}\sum_{k=0}^{\ell} J_k f$$

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in the sense of L^{p_0}, which leads to the fact that $(\mathbf{I}+tH_+)^{-1/2}f = TAf$ for all $f \in L^{p_0}$. Thus, we can write

$$\begin{aligned}\nabla(\mathbf{I}+tH)^{-1} &= \nabla(\mathbf{I}+tH_+-tV_-)^{-1}\\ &= \nabla(\mathbf{I}+tH_+)^{-1/2}(\mathbf{I}+tH_+)^{-1/2}(\mathbf{I}-V_-(t^{-1}+H_+)^{-1})^{-1}\\ &= \nabla(\mathbf{I}+tH_+)^{-1/2}TA(\mathbf{I}-V_-(t^{-1}+H_+)^{-1})^{-1}\\ &= \nabla(\mathbf{I}+tH_+)^{-1/2}\sum_{k=0}^{\infty} I_k. \end{aligned} \tag{3.10}$$

It follows from (3.5) and (A_2) that

$$\begin{aligned}\|\nabla(\mathbf{I}+tH_+)^{-1/2}\|_{L^{p_0}-L^{p_0}} &\le \|\nabla H_+^{-1/2}\|_{L^{p_0}-L^{p_0}}\|H_+^{1/2}(\mathbf{I}+tH_+)^{-1/2}\|_{L^{p_0}-L^{p_0}}\\ &\le c_{p_0}\alpha_{p_0}t^{-1/2}. \end{aligned}\tag{3.11}$$

Thus, by (3.10), (3.11) and choosing $\delta_{p_0} < (C_{p_0'}C_{p_0})^{-1}$ in (3.8),

$$\|\nabla(\mathbf{I}+tH)^{-1}\|_{L^{p_0}-L^{p_0}} \le Ct^{-1/2}. \tag{3.12}$$

If $p_\mu > p_0$, it follows from (3.12), Theorem A and Proposition 2.4 that

$$\|\nabla e^{-tH}\|_{L^{p_0}-L^{p_0}} \le \|\nabla(\mathbf{I}+tH)^{-1}\|_{L^{p_0}-L^{p_0}}\|(\mathbf{I}+tH)e^{-tH}\|_{L^{p_0}-L^{p_0}} \le Ct^{-1/2}.$$

However, when $p_\mu < p_0$, we need a more sophisticated discussion. First of all, it follows from the fact that $\nabla H^{-1/2}$ is bounded on L^2 and the functional calculi of H on L^2 that

$$\begin{aligned}\|\nabla(\mathbf{I}+tH)^{-1}\|_{L^2-L^2} &\le \|\nabla H^{-1/2}\|_{L^2-L^2}\|H^{1/2}(\mathbf{I}+tH)^{-1}\|_{L^2-L^2}\\ &\le Ct^{-1/2}. \end{aligned}\tag{3.13}$$

By interpolating (3.12) with (3.13),

$$\|\nabla(\mathbf{I}+tH)^{-1}\|_{L^r-L^r} \le Ct^{-1/2}, \quad 2 \le r \le p_0. \tag{3.14}$$

Notice that both e^{-tH} and tHe^{-tH} are bounded on L^r for all $2 \le r < p_\mu$ (see Theorem A); then, for $2 \le r < p_\mu < p_0$,

$$\|\nabla e^{-tH}\|_{L^r-L^r} \le \|\nabla(\mathbf{I}+tH)^{-1}\|_{L^r-L^r}\|(I+tH)e^{-tH}\|_{L^r-L^r} \le Ct^{-1/2},$$

which, combined with Theorem A and Lemma 3.3, implies that e^{-tH} is bounded on L^r for all $2 \le r < p_\mu^*$. Moreover, by (i) of Remark 2.6, Proposition 2.4 and the identity $tHe^{-tH} = e^{-tH/2}tHe^{-tH/2}$, we have that tHe^{-tH} is bounded on L^r for all $2 \le r < p_\mu^*$. Therefore, for all $2 \le r < p_\mu^*$ (we assume that $p_\mu^* < p_0$, otherwise the proof would be concluded), it follows from (3.14) that

$$\|\nabla e^{-tH}\|_{L^r-L^r} \le \|\nabla(\mathbf{I}+tH)^{-1}\|_{L^r-L^r}\|(I+tH)e^{-tH}\|_{L^r-L^r} \le Ct^{-1/2}.$$

Now let $r_0 \in (2, p_\mu)$ be chosen later and $r_k = r_{k-1}^* = nr_{k-1}/(n-r_{k-1})$; we can find a suitable $r_0 \in (2, p_\mu)$ and a integer k_0 such that $p_0 = r_{k_0} < n$. Then, by applying the same argument as above, we obtain that tHe^{-tH} and e^{-tH} are bounded on L^r for all $2 \le r < p_0^*$, which, combined with (3.14), again implies that $\sqrt{t}\nabla e^{-tH}$ is bounded on L^{p_0}. Hence, we finish the proof. □

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REMARK 3.6. It follows from the proof above that the constant δ_{p_0} can be expressed explicitly by $\delta_{p_0} < (C_{p_0'}C_{p_0})^{-1}$, where

$$C_{p_0'} = c_{p_0'}h_{p_0',np_0'/n-p_0',n}s_{p_0'}\alpha_{p_0'} \quad \text{and} \quad C_{p_0} = c_{p_0}h_{p_0,np_0/n-p_0,n}s_{p_0}\alpha_{p_0}.$$

Moreover, C_p $(p \in (p_0', p_0))$ can be obtained by interpolating all the constants in $C_{p_0'}$ and C_{p_0}.

4. The L^q boundedness of the Riesz transform for $q > 2$

4.1. The proof of Theorem 1.1. Let $H = -\Delta + V$ satisfy (A_1)–(A_3) and $V_- \in L^{n/2,\infty}$; we will study the Riesz transform $\nabla H^{-1/2}$ on L^q for $q > 2$. To do this, we first introduce the following theorem which deals with general Calderón–Zygmund operators. For a ball $B \subset \mathbb{R}^n$ and $\lambda > 0$, we denote by $\lambda(B)$ the ball with the same center and radius λ times that of B and set

$$S_1(B) = 4B, \quad S_j(B) = 2^{j+1}B \setminus 2^jB \quad \text{for} \ \ j \geq 2.$$

Denote by $\mathcal{M}$ the Hardy–Littlewood maximal operator

$$\mathcal{M}(f)(x) = \sup_{x \in B} \frac{1}{|B|}\int_B |f(y)|\,dy,$$

where B ranges over all open balls (or cubes) containing x.

THEOREM C (Auscher–Coulhon–Duong–Hofmann). *Let $q_0 \in [2, \infty)$. Suppose that T is a sublinear operator acting on $L^2(\mathbb{R}^n)$ and $\{A_r\}_{r>0}$ is a family of linear operators acting on $L^2(\mathbb{R}^n)$. Also, assume that*

$$\left(\frac{1}{|B|}\int_B |T(\mathbf{I} - A_{r(B)})f(x)|^2\,dx\right)^{1/2} \leq C(\mathcal{M}(|f|^2))^{1/2}(y) \tag{4.1}$$

and

$$\left(\frac{1}{|B|}\int_B |TA_{r(B)}f(x)|^{q_0}\,dx\right)^{1/q_0} \leq C(\mathcal{M}(|Tf|^2))^{1/2}(y) \tag{4.2}$$

for all $f \in L^2$, all balls B and all $y \in B$, where $r(B)$ is the radius of B. Then, if $2 < q < q_0$ and $Tf \in L^q$ as $f \in L^q$, T is of strong type (q, q). That is, $\|Tf\|_{L^q} \leq c\|f\|_{L^q}$ for all $f \in L^2 \cap L^q$, where c depends only on n, q, q_0 and C.

LEMMA 4.1. *Assume that $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfy L^2 off-diagonal estimates. Then there exists a constant $C > 0$ such that for all balls B with radius $r > 0$, $f \in L^2(\mathbb{R}^n)$ with $\mathrm{supp} f \in S_j(B)$ and $j \geq 2$,*

$$\|\nabla H^{-1/2}(\mathbf{I} - e^{-r^2H})^M f\|_{L^2(B)} \leq C2^{-2Mj}\|f\|_{L^2(S_j(B))}.$$

PROOF. The proof for the operator $\nabla H^{-1/2}(\mathbf{I} - e^{-r^2H})^M$ is exactly the same as the one with $p = 2$ in Auscher [3, Lemma 5.4], where the only fact involved in the proof is that $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfy L^p–L^2 off-diagonal estimates. One can also see the proof in Assaad [1, Theorem 3.1] and Assaad and Ouhabaz [2, Theorem 3.6]. □

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Now we investigate the L^2–L^q $(q \geq 2)$ off-diagonal estimates of the family $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$, which essentially connect the L^q boundedness of the Riesz transform for $q > 2$.

Proposition 4.2. *Let $p \in (2, \infty)$ and $n \geq 3$. Assume that $H = -\Delta + V$, where $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$ and V satisfies (A_1) for some $\mu \in (0, 1)$. Then the following statements hold.*

(i) *If $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ is bounded on L^p, then it satisfies the L^2–L^p estimates.*
(ii) *If $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfies the L^2–L^p estimates, then it satisfies the L^2–L^q off-diagonal estimates for $2 < q < p$.*
(iii) *If $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfies the L^2–L^p off-diagonal estimates, then it is bounded on L^p.*

Proof. The proof is based on the idea described in Auscher [3, Proposition 3.9]; we omit the details. □

Proposition 4.3. *Let $H = -\Delta + V$, where $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$ and V satisfies (A_1) for some $\mu \in (0, 1)$.*

(i) *If $\nabla H^{-1/2}$ is bounded on L^p for $2 < p < \infty$, then $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfies the L^2–L^q off-diagonal estimates for all $2 < q < p$.*
(ii) *If $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfies the L^2–L^p off-diagonal estimates for $2 < p < \infty$ and $n \geq 3$, then $\nabla H^{-1/2}$ is bounded on L^q with $2 < q < p$.*

Proof. We first prove (i). By the assumptions, it is easy to see that $\nabla H^{-1/2}$ is bounded on L^r for all $2 \leq r \leq p$, which, combined with Sobolev's embedding theorem, implies that

$$\|H^{-1/2} f\|_{L^{r^*}} \leq C\|\nabla H^{-1/2} f\|_{L^r} \leq C\|f\|_{L^r}, \quad 2 \leq r \leq p,\ r < n. \tag{4.3}$$

We choose constants $k_0 \in \mathbb{N}$ and $2 \leq r_0 < p_\mu$ such that $p = nr_0/(n - k_0 r_0)$ and let $r_k = (r_{k-1})^*$ for $k = 1, 2, \ldots, k_0$; it follows from (4.3) that

$$H^{-k_0/2} : \quad L^{r_0} \to L^{r_{k_0}}. \tag{4.4}$$

Now write

$$e^{-tH} = H^{-k_0/2} e^{-tH/2} (H^{k_0/2} e^{-tH/2}). \tag{4.5}$$

Notice that $H^{k_0/2} e^{-tH/2}$ is bounded on L^2 with bound $Ct^{-k_0/2}$ and $e^{-tH/2}$ satisfies the L^2–L^{r_0} estimates (see Theorem A); then, by (4.4) and (4.5), we obtain that e^{-tH} satisfies the L^2–L^p estimates. Write

$$\nabla e^{-tH} = \nabla H^{-1/2} e^{-tH/2} (H^{1/2} e^{-tH/2});$$

it follows that $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfies the L^2–L^p estimates. By applying (ii) of Proposition 4.2, we conclude that $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfies the L^2–L^q off-diagonal estimates for all $2 < q < p$. Hence, we finish the proof of (i).

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We turn to prove (ii). For given $2 < p < \infty$, let B be an open ball and $r = r(B)$ its radius and $A_r = \mathbf{I} - (\mathbf{I} - e^{-r^2 H})^M$, where $M \in \mathbb{N}$ with $M > n/4$. By applying Theorem C, we need to show that (4.1) and (4.2) hold for $T = \nabla H^{-1/2}$ and q_0, where q_0 satisfies $2 < q < q_0 < p$. We will finish the proof in the following two steps.

Step 1. Note that $M > n/4$; to get (4.1), it suffices to show that for $f \in L^{q_0}(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$,

$$\|\nabla H^{-1/2}(\mathbf{I} - e^{-r^2 H})^M f\|_{L^2(B)} \le C|B|^{1/2} \sum_{j\ge1} g(j)\Big(\frac{1}{|2^{j+1}B|}\int_{2^{j+1}B}|f|^2\,dx\Big)^{1/2} \tag{4.6}$$

with $g(j) = 2^{j(n/2-2M)}$. Let $S_j(B)$ $(j \ge 1)$ be defined as in Theorem C; by Minkowski's inequality,

$$\|\nabla H^{-1/2}(\mathbf{I} - e^{-r^2 H})^M f\|_{L^2(B)} \le \sum_{j\ge1}\|\nabla H^{-1/2}(\mathbf{I} - e^{-r^2 H})^M(\chi_{S_j(B)}f)\|_{L^2(B)}.$$

For $j = 1$, by the L^2 boundedness of $\nabla H^{-1/2}$ and e^{-tH},

$$\|\nabla H^{-1/2}(\mathbf{I} - e^{-r^2 H})^M(\chi_{S_1(B)}f)\|_{L^2(B)} \le C|4B|^{1/2}\Big(\frac{1}{|4B|}\int_{4B}|f|^2\,dx\Big)^{1/2}.$$

When $j \ge 2$, since H is the operator defined in Theorem 1.1, it follows that $\sqrt{t}\nabla e^{-tH}$ satisfies the L^2 off-diagonal estimate. Thus, Lemma 4.1 can be applied to get

$$\|\nabla H^{-1/2}(\mathbf{I} - e^{-r^2 H})^M(\chi_{S_j(B)}f)\|_{L^2(B)} \le C2^{-2Mj}\|f\|_{L^2(S_j(B))},$$

which implies (4.6) immediately.

Step 2. Notice that $A_r = \sum_{\ell=1}^{M} C_{M,\ell}e^{-\ell r^2 H}$. We first prove that

$$\Big(\frac{1}{|B|}\int_B|\nabla e^{-\ell r^2 H}f(x)|^{q_0}\,dx\Big)^{1/q_0} \le C\sum_{j\ge1} g(j)\Big(\frac{1}{|2^{j+1}B|}\int_{2^{j+1}B}|\nabla f(x)|^2\,dx\Big)^{1/2} \tag{4.7}$$

for all $\ell = 1, \ldots, M$ with $\sum g(j) < \infty$. Let $S_j(B)$ $(j \ge 1)$ be defined as in Theorem C. For $j = 1$, by Propositions 3.5 and 4.2, we have that $\sqrt{t}\nabla e^{-tH}$ also satisfies the L^2–L^p estimate. Thus,

$$\Big(\frac{1}{|B|}\int_B\Big|\nabla e^{-\ell r^2 H}(\chi_{S_1(B)}f)(x)\Big|^{q_0}\,dx\Big)^{1/q_0} \le C|B|^{-1/q_0}r^{-1+(n/q_0-n/2)}\|f\|_{L^2(4B)}.$$

When $j \ge 2$, by Propositions 3.5 and 4.2 again, we have the L^2–L^p off-diagonal estimate for $\sqrt{t}\nabla e^{-tH}$, which leads to

$$\Big(\frac{1}{|B|}\int_B\Big|\nabla e^{-\ell r^2 H}(\chi_{S_j(B)}f)(x)\Big|^{q_0}\,dx\Big)^{1/q_0} \le C|B|^{-1/q_0}r^{-1+(n/q_0-n/2)}e^{-2^{2j}}\|f\|_{L^2(S_j(B))}.$$

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On the other hand, for every $j \geq 1$, by Hardy's inequality, we have for $n > 2$,

$$\begin{aligned}\Big(\int_{S_j(B)} |f(x)|^2\,dx\Big)^{1/2} &\leq 2^j r\Big(\frac{1}{(2^j r)^2}\int_{S_j(B)} |f(x)|^2\,dx\Big)^{1/2}\\ &\leq C2^j r\Big(\int_{\mathbb{R}^n} |\chi_{S_j(B)} f(x)|^2/|x|^2\,dx\Big)^{1/2}\\ &\leq C2^j r\|\nabla f\|_{L^2(S_j(B))}.\end{aligned}$$

Thus,

$$\Big(\frac{1}{|B|}\int_B \big|\nabla e^{-\ell r^2 H} f\big|^{q_0}\,dx\Big)^{1/q_0} \leq C\sum_{j\geq 1} 2^{-2Mj+j+Nj/2}\Big(\frac{1}{|2^{j+1}B|}\int_{2^{j+1}B} |\nabla f(x)|^2\,dx\Big)^{1/2},$$

which implies (4.7) by choosing large enough M. Now this applied to $f = H^{-1/2}g$ gives us (4.2). □

The proof of Theorem 1.1. The proof for $q \in (p'_\mu, 2]$ is essentially the same as the one in [2] (see also [1, 3]), where the L^p–L^2 off-diagonal estimates for $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ and $\{e^{-tH}\}_{t>0}$ are involved. Thus, we consider the case for $2 < q < p_0$ only. It follows from Proposition 3.5 that the family $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ is bounded on L^{p_0} for the given p_0 in Theorem 1.1, which, combined with Proposition 4.2, means that $\{\sqrt{t}\nabla e^{-tH}\}_{t>0}$ satisfies the $L^2 - L^r$ off-diagonal estimates for all $2 < r < p_0$. Thus, we can finish the proof of Theorem 1.1 by applying Proposition 4.3.

4.2. Applications. In this section, we will give the proofs of Theorem 1.3 and Corollary 1.4, which are actually important applications of Theorem 1.1. First of all, we consider Theorem 1.3. Let us begin with the following lemma.

Lemma 4.4. *Let $n > 4$ and $H = -\Delta + V_+ - V_-$, where $V_+ \in B_\theta$ for $\theta \geq n/2$ and $V_- \in L^{n/2,\infty}$. Then the condition (A_3) holds for all $2 < p_0 < n/2$.*

Proof. It was proved in Shen [22, Theorem 0.3] that if $V_+ \in B_\theta$ with $\theta \geq n/2$, then, for all $1 < p \leq \theta$,

$$\|\Delta(-\Delta + V_+)^{-1} f\|_{L^p - L^p} \leq \overline{C}_p, \tag{4.8}$$

where the constant $\overline{C}_p$ depends on n, p and the constant in the reverse Hölder inequality of V_+. Then it follows from (1.6) and (4.8) that for all $1 < p < n/2$,

$$\begin{aligned}\|V_- f\|_{L^p} \leq C\|V_-\|_{L^{n/2,\infty}}\|\Delta f\|_{L^p} &\leq C\|V_-\|_{L^{n/2,\infty}}\|\Delta(-\Delta + V_+)^{-1}(-\Delta + V_+) f\|_{L^p}\\ &\leq C\|(-\Delta + V_+) f\|_{L^p},\end{aligned}$$

which, combined with (1.5), implies that (A_3) holds for all $2 < p_0 < n/2$. □

The proof of Theorem 1.3. For the Schrödinger operator H defined as in Theorem 1.3, by Remark 3.4, it is easy to see that there exists $\mu \in (0, 1)$ such that (A_1) holds if we choose suitable δ_{p_0}. Moreover, by the results in [4], we know that $\nabla H_+^{-1/2}$ is bounded on L^p for all $1 < p < n\theta/(n-\theta) + \varepsilon$ for some $\varepsilon > 0$ as $n/2 \le \theta < n$ and for $1 < p < \infty$ as $\theta \ge n$ (see also Table 1 above), which means that (A_2) holds for all $2 < p_0 < n/2$. Thus, by Lemma 4.4 and Theorem 1.1, $\nabla H^{-1/2}$ is bounded on L^q for all $q \in (p'_\mu, n/2)$ if we choose δ_{p_0} in (1.4) appropriately.

It remains to show that the constant δ_{p_0} is bounded uniformly for all $2 < p_0 < n/2$. In fact, it follows from the proof of Proposition 3.5 that $\delta_{p_0} < (C_{p'_0} C_{p_0})^{-1}$, where

$$C_{p'_0} = c_{p'_0} h_{p'_0, np'_0/n-p'_0, n} s_{p'_0} \alpha_{p'_0} \quad \text{and} \quad C_{p_0} = c_{p_0} h_{p_0, np_0/n-p_0, n} s_{p_0} \alpha_{p_0}.$$

On the other hand, it is easy to see that C_2 and $C_{n/2}$ are finite. Then, by Remark 3.6, we have that δ_{p_0} is uniformly bounded for all $2 < p_0 < n/2$, which finishes the proof.

The proof of Corollary 1.4. If $V_+ \in B_\theta$ and $V_- = \gamma(n-2)^2|x|^{-2}/4$, then, by Hardy's inequality (see [9]),

$$(n-2)^2/4 \int_{\mathbb{R}^n} |x|^{-2}|f(x)|^2\, dx \le \int_{\mathbb{R}^n} |\nabla f(x)|^2\, dx \le Q_+(f, f),$$

which means that the potential V satisfies (A_1) for $\mu = \gamma \in (0, 1)$. Then, by using Theorem 1.3, there exists a constant $\bar{\delta} > 0$ independent of p_0 such that when

$$\|V_-\|_{L^{n/2,\infty}} = \gamma(n-2)^2/4 \big\||x|^{-2}\big\|_{L^{n/2,\infty}} = \gamma(n-2)^2 d_n^{n/2}/4 < \bar{\delta},$$

that is, $\gamma < \delta := 4d_n^{-2/n}\bar{\delta}/(n-2)^2$, where d_n denotes the volume of the unit ball in $\mathbb{R}^n$, the Riesz transform $\nabla H^{-1/2}$ is bounded on L^q for all $q \in (p'_\gamma, n/2)$.

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