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Boundedness of spectral multipliers for Schrödinger operators on open sets

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Abstract. Let H_V be a self-adjoint extension of the Schrödinger operator $-\Delta + V(x)$ with the Dirichlet boundary condition on an arbitrary open set Ω of $\mathbb{R}^d$, where $d \geq 1$ and the negative part of potential V belongs to the Kato class on Ω. The purpose of this paper is to prove L^p-L^q-estimates and gradient estimates for an operator $\varphi(H_V)$, where φ is an arbitrary rapidly decreasing function on $\mathbb{R}$, and $\varphi(H_V)$ is defined via the spectral theorem.

1. Introduction and main results

Let Ω be an open set of $\mathbb{R}^d$, with $d \geq 1$. We consider the Schrödinger operator

$$-\Delta + V(x) = -\sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} + V(x)$$

with the Dirichlet boundary condition. Here $V(x)$ is a real-valued measurable function on Ω. If the negative part of potential V is assumed to be of Kato class on Ω, then the operator $-\Delta + V(x)$ defined on $C_0^\infty(\Omega)$ is uniquely extended to a semi-bounded self-adjoint operator H_V with domain

$$\mathcal{D}(H_V) = \big\{ u \in H_0^1(\Omega) \,\big|\, \sqrt{V_+}u \in L^2(\Omega),\ H_V u \in L^2(\Omega) \big\}$$

such that

$$\big\langle H_V u, v \big\rangle_{L^2(\Omega)} = \int_\Omega \nabla u(x) \cdot \overline{\nabla v(x)}\, dx + \int_\Omega V(x)\, u(x)\, \overline{v(x)}\, dx$$

for any $u \in \mathcal{D}(H_V)$ and $v \in H_0^1(\Omega)$ with $\sqrt{V_+}v \in L^2(\Omega)$ (see Proposition 2.1 in Section 2), where V_+ is the positive part of V, $\big\langle H_V u, v \big\rangle_{L^2(\Omega)}$ stands for the

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inner product of $H_V u$ and v in $L^2(\Omega)$, and $H_0^1(\Omega)$ is the completion of $C_0^\infty(\Omega)$ with respect to $H^1(\Omega)$-norm. Let $\{E_{H_V}(\lambda)\}_{\lambda\in\mathbb{R}}$ be the spectral resolution of the identity for H_V, where the resolution $\{E_{H_V}(\lambda)\}_{\lambda\in\mathbb{R}}$ is uniquely determined for H_V by the spectral theorem. Then for any Borel measurable function φ on $\mathbb{R}$, an operator $\varphi(H_V)$ is defined by letting

$$\varphi(H_V) = \int_{-\infty}^{\infty} \varphi(\lambda)\, dE_{H_V}(\lambda)$$

with domain

$$\mathcal{D}(\varphi(H_V)) = \Big\{ f \in L^2(\Omega) \;\Big|\; \int_{-\infty}^{\infty} |\varphi(\lambda)|^2\, d\langle E_{H_V}(\lambda)f, f\rangle_{L^2(\Omega)} < \infty \Big\}.$$

In this paper we study functional calculus of $\varphi(\theta H_V)$ for $\theta > 0$.

We suppose that the potential V satisfies the following condition:

Assumption A. *V is a real-valued measurable function on Ω, and is decomposed as $V = V_+ - V_-$ such that $V_\pm \geq 0$, $V_+ \in L^1_{\mathrm{loc}}(\Omega)$ and $V_- \in K_d(\Omega)$, where $K_d(\Omega)$ is the Kato class of potentials.*

Following Simon (see Section A.2 in [22]), let us give the definition of $K_d(\Omega)$ as follows.

Definition. We say that V_- belongs to the class $K_d(\Omega)$ if

$$\begin{cases} \displaystyle\lim_{r\to 0} \sup_{x\in\Omega} \int_{\Omega\cap\{|x-y|<r\}} \frac{V_-(y)}{|x-y|^{d-2}}\, dy = 0, & d \geq 3, \\ \displaystyle\lim_{r\to 0} \sup_{x\in\Omega} \int_{\Omega\cap\{|x-y|<r\}} \log(|x-y|^{-1}) V_-(y)\, dy = 0, & d = 2, \\ \displaystyle\sup_{x\in\Omega} \int_{\Omega\cap\{|x-y|<1\}} V_-(y)\, dy < \infty, & d = 1. \end{cases}$$

The aim of this paper is to show L^p-L^q-estimates and gradient estimates for spectral multipliers $\varphi(H_V)$ on Ω. The motivation of the problem in this paper comes from the point of view of harmonic analysis and PDEs. For instance, the spectral multiplier is a generalization of Fourier multiplier in the following sense: When $\Omega = \mathbb{R}^d$ and $H_V = -\Delta$ is the free Hamiltonian on $\mathbb{R}^d$, the spectral multiplier coincides with the Fourier multiplier, i.e.,

$$\varphi(-\Delta) = \mathscr{F}^{-1}\big[\varphi(|\cdot|^2)\mathscr{F}\big],$$

where $\mathscr{F}$ and $\mathscr{F}^{-1}$ denote the Fourier transform and inverse Fourier transform, respectively. We also show uniform estimates for $\varphi(\theta H_V)$ with respect to a parameter θ. These estimates play a fundamental role in studying Hardy spaces, BMO spaces, Besov spaces and Triebel–Lizorkin spaces generated by the Schrödinger operator (see [1], [5], [7], [10], [14], [17], [25]). The theory of spectral multipliers is also related to the study of convergence of the Riesz means or convergence of eigenfunction expansion of self-adjoint operators (see, e.g., Chapter IX in Stein [23]).

In this paper we denote by $\mathscr{B}(X,Y)$ the space of all bounded linear operators from a Banach space X to another one Y. When $X=Y$, we denote by $\mathscr{B}(X)=\mathscr{B}(X,X)$. We use the notation $\mathcal{D}(T)$ for the domain of an operator T. We denote by $\mathscr{S}(\mathbb{R})$ the space of rapidly decreasing functions on $\mathbb{R}$.

We shall prove the following.

Theorem 1.1. *Let $\varphi \in \mathscr{S}(\mathbb{R})$. Suppose that the potential V satisfies assumption* A. *Let $1 \le p \le q \le \infty$. Then $\varphi(H_V)$ is extended to a bounded linear operator from $L^p(\Omega)$ to $L^q(\Omega)$. Furthermore, the following assertions hold*:

(i) *There exists a constant $C>0$ such that*

$$\|\varphi(\theta H_V)\|_{\mathscr{B}(L^p(\Omega),L^q(\Omega))} \le C\,\theta^{-(d/2)(1/p-1/q)} \tag{1.1}$$

for any $0<\theta\le 1$.

(ii) *Assume further that V_- satisfies*

$$\begin{cases} \sup_{x\in\Omega}\int_\Omega \dfrac{V_-(y)}{|x-y|^{d-2}}\,dy < \dfrac{\pi^{d/2}}{\Gamma(d/2-1)}, & \text{if } d\ge 3,\\ V_- = 0, & \text{if } d=1,2. \end{cases} \tag{1.2}$$

Then the estimate (1.1) *holds for any $\theta>0$.*

Theorem 1.2. *Let $\varphi \in \mathscr{S}(\mathbb{R})$. Suppose that the potential V satisfies assumption* A. *Let $1\le p\le 2$. Then $\varphi(H_V)$ is extended to a bounded linear operator from $L^p(\Omega)$ to $W^{1,p}(\Omega)$. Furthermore, the following assertions hold*:

(i) *There exists a constant $C>0$ such that*

$$\|\nabla\varphi(\theta H_V)\|_{\mathscr{B}(L^p(\Omega))} \le C\,\theta^{-1/2} \tag{1.3}$$

for any $0<\theta\le 1$.

(ii) *Assume further that V_- satisfies* (1.2). *Then the estimate* (1.3) *holds for any $\theta>0$.*

In the rest of this section, let us give some remarks on Theorems 1.1 and 1.2. In the setting of Euclidean spaces, there are many results on L^p-estimates for $\varphi(\theta H_V)$ under the assumption that the potential is non-negative on $\mathbb{R}^d$ (see, e.g., [10], [13], [25]). On the other hand, when the potentials are admitted to be negative, there are several known results; Jensen and Nakamura dealt with the Schrödinger operator with potential whose negative part is of Kato class (see [14] and [15]), and then D'Ancona and Pierfelice also dealt with the same type of potentials satisfying (1.2) (see [5]). Furthermore, Jensen and Nakamura proved L^p-L^q-estimates for $\varphi(\theta H_V)$ (see [14], [15]). As is already mentioned before, it would be very important to derive L^p-estimates for $\varphi(H_V)$ on open sets of $\mathbb{R}^d$.

There are several studies on L^p-estimates for more general operators $\varphi(L)$, where L is a non-negative self-adjoint operator having the property that the integral kernel of semigroup $\{e^{-tL}\}_{t>0}$ has a Gaussian upper bound (see [6], [12], [17], [18]). Among other things, there is a result on the estimates involving a parameter $\theta > 0$; Duong, Ouhabaz and Sikora proved uniform L^p-estimates for $\varphi(\theta L)$ with respect to $\theta > 0$, where φ is in $H^s(\mathbb{R})$ $(s > d/2)$ with compact support (see [6]). Here, we note in Theorem 1.1 that φ can be taken as functions in the weighted Sobolev spaces. For more detail, one can refer to some remarks in Section 8. As to Theorem 1.2, the problem is closely related to L^p-boundedness of operators ∇e^{-tH_V} and $\nabla H_V^{-1/2}$. When V is non-negative, the results of [4], [18] imply the estimate (1.3) for $p \le 2$. On the other hand, the situation of the case $p > 2$ is more complicated (see [2], [4], [8], [16], [18], [21]).

One of the main ingredients of this paper is to reveal that we are able to deal with a potential satisfying (1.2) in the setting of open sets. In fact, to the best of our knowledge, L^p-estimates for $\varphi(\theta H_V)$ are known for operators H_V with the Gaussian upper bounds for e^{-tH_V} (see [6]) and we prove upper bounds of this type in Proposition 3.1 below. The advantage of this paper is to provide a unified treatment of the proof of Theorems 1.1 and 1.2. For this purpose, we introduce amalgam spaces on Ω and apply the Gaussian upper bounds and commutator estimates. This idea comes from Jensen and Nakamura ([14], [15]).

Let us introduce some notations used in this paper. We denote by χ_E the characteristic function of a measurable set E. The convolution of measurable functions f and g on $\mathbb{R}^d$ is defined by letting

$$(f * g)(x) = \int_{\mathbb{R}^d} f(x-y)\, g(y)\, dy.$$

For a self-adjoint operator T on a Hilbert space, we denote by $\sigma(T)$ the spectrum of T.

This paper is organized as follows. In Section 2 the self-adjointness of operator H_V is shown. In Section 3 we prepare the pointwise estimate for the kernel of e^{-tH_V}. Section 4 is devoted to proving the uniform estimates in scaled amalgam spaces for the resolvent of H_V. In Section 5 some commutator estimates are derived. In Section 6 L^p-estimates for $\varphi(\theta H_V)$ are proved. Based on these estimates, the proof of Theorems 1.1 and 1.2 are given in Section 7.

2. Self-adjointness of H_V

In this section we show self-adjointness of Schrödinger operators with the Dirichlet boundary condition under assumption A by using the theory of quadratic forms.

Our purpose in this section is to prove the following.

Proposition 2.1. *Suppose that the potential V satisfies assumption* A. *Then the following assertions hold*:

(i) *There exists a unique semi-bounded self-adjoint operator H_V on $L^2(\Omega)$ with domain*

$$\mathcal{D}(H_V) = \big\{u \in H_0^1(\Omega) \,\big|\, \sqrt{V_+}u \in L^2(\Omega),\ H_V u \in L^2(\Omega)\big\} \tag{2.1}$$

such that

$$\langle H_V u, v\rangle_{L^2(\Omega)} = \int_\Omega \nabla u(x)\cdot\overline{\nabla v(x)}\,dx + \int_\Omega V(x)\,u(x)\,\overline{v(x)}\,dx \tag{2.2}$$

for any $u \in \mathcal{D}(H_V)$ and $v \in H_0^1(\Omega)$ with $\sqrt{V_+}v \in L^2(\Omega)$.

(ii) *Assume further that V_- satisfies*

$$\begin{cases} \sup\limits_{x\in\Omega}\displaystyle\int_\Omega \frac{V_-(y)}{|x-y|^{d-2}}\,dy < \frac{4\pi^{d/2}}{\Gamma(d/2-1)}, & \text{if } d\ge 3,\\ V_- = 0, & \text{if } d = 1,2. \end{cases} \tag{2.3}$$

Then H_V is non-negative on $L^2(\Omega)$.

We recall a notion of quadratic forms on Hilbert spaces (see p. 276 in Reed and Simon [19]).

Definition. Let $\mathscr{H}$ be a Hilbert space with the norm $\|\cdot\|$. A quadratic form is a map

$$q : \mathcal{Q}(q)\times\mathcal{Q}(q) \to \mathbb{C},$$

where $\mathcal{Q}(q)$ is a dense linear subset of $\mathscr{H}$ called the form domain, such that $q(\cdot, v)$ is linear and $q(u,\cdot)$ is conjugate linear for $u, v \in \mathcal{Q}(q)$. A quadratic form q is called semi-bounded if

$$q(u,u) \ge -M\|u\|^2$$

for some real number M, and in particular, q is called non-negative if

$$q(u,u)\ge 0$$

for any $u \in \mathcal{Q}(q)$. We say that a semi-bounded quadratic form q is closed if $\mathcal{Q}(q)$ is complete with respect to the norm:

$$\|u\|_{+1} := \sqrt{q(u,u) + (M+1)\|u\|^2}. \tag{2.4}$$

The proof of Proposition 2.1 is done by using the following two lemmas.

Lemma 2.2. *Let $\mathscr{H}$ be a Hilbert space with the inner product $\langle\cdot,\cdot\rangle$, and let*

$$q : \mathcal{Q}(q)\times\mathcal{Q}(q)\to\mathbb{C}$$

be a densely defined semi-bounded closed quadratic form. Then there exists a semi-bounded self-adjoint operator T on $\mathscr{H}$ uniquely such that

$$\begin{cases} \mathcal{D}(T) = \big\{u\in\mathcal{Q}(q) \,|\, \exists\, w_u \in \mathscr{H} \text{ such that } q(u,v) = \langle w_u, v\rangle \text{ for all } v\in\mathcal{Q}(q)\big\},\\ Tu = w_u, \quad u\in\mathcal{D}(T). \end{cases}$$

We note that $\mathcal{D}(T)$ can be simply written as

$$\mathcal{D}(T) = \{u \in \mathcal{Q}(q) \,|\, Tu \in \mathscr{H}\}.$$

For the proof of Lemma 2.2, see Theorem VIII.15 in [19] (see also Section 1.2.3 in Ouhabaz [18] and Theorem 5.37 in Weidmann [24]).

The following lemma states that the negative part of the potential is relatively form-bounded with respect to the Dirichlet Laplacian.

Lemma 2.3. *Suppose that the negative part V_- of the potential V belongs to $K_d(\Omega)$. Then the following assertions hold*:

(i) *For any $\varepsilon > 0$, there exists a constant $b_\varepsilon > 0$ such that*

$$\int_\Omega V_-(x)\,|u(x)|^2\,dx \le \varepsilon\,\|\nabla u\|^2_{L^2(\Omega)} + b_\varepsilon\|u\|^2_{L^2(\Omega)} \tag{2.5}$$

for any $u \in H^1_0(\Omega)$.

(ii) *Let $d \ge 3$. Assume further that V_- satisfies*

$$\|V_-\|_{K_d(\Omega)} := \sup_{x\in\Omega}\int_\Omega \frac{V_-(y)}{|x-y|^{d-2}}\,dy < \infty. \tag{2.6}$$

Then

$$\int_\Omega V_-(x)\,|u(x)|^2\,dx \le \frac{\Gamma(d/2-1)\|V_-\|_{K_d(\Omega)}}{4\pi^{d/2}}\,\|\nabla u\|^2_{L^2(\Omega)} \tag{2.7}$$

for any $u \in H^1_0(\Omega)$.

Proof. The proof is done by reducing the problem to the whole space case, and by the similar argument of Lemma 3.1 from D'Ancona and Pierfelice [5] who treated mainly three dimensional case.

First we show the assertion (i). Let $u \in C_0^\infty(\Omega)$, and let $\tilde{u}$ and $\tilde{V}_-$ be the zero extensions of u and V_- to $\mathbb{R}^d$, respectively. We prove that for any $\varepsilon > 0$, there exists a constant $b_\varepsilon > 0$ such that

$$\int_{\mathbb{R}^d} \tilde{V}_-(x)|\tilde{u}(x)|^2\,dx \le \varepsilon\,\|\nabla\tilde{u}\|^2_{L^2(\mathbb{R}^d)} + b_\varepsilon\|\tilde{u}\|^2_{L^2(\mathbb{R}^d)}. \tag{2.8}$$

The inequality (2.8) is equivalent to

$$\int_{\mathbb{R}^d} \tilde{V}_-(x)\,|\tilde{u}(x)|^2\,dx \le \varepsilon\,\langle \tilde{u}, -\Delta\tilde{u}\rangle_{L^2(\mathbb{R}^d)} + b_\varepsilon\|\tilde{u}\|^2_{L^2(\mathbb{R}^d)} = \varepsilon\left\|\left(H_0 + \frac{b_\varepsilon}{\varepsilon}\right)^{1/2}\tilde{u}\right\|^2_{L^2(\mathbb{R}^d)},$$

where $H_0 = -\Delta$ is the self-adjoint operator with domain $H^2(\mathbb{R}^d)$. Put

$$v = \left(H_0 + \frac{b_\varepsilon}{\varepsilon}\right)^{1/2}\tilde{u}.$$

Then the inequality (2.8) takes the following form:

$$\Big\| \tilde{V}_-^{1/2} \Big(H_0 + \frac{b_\varepsilon}{\varepsilon} \Big)^{-1/2} v \Big\|_{L^2(\mathbb{R}^d)}^2 \le \varepsilon \, \|v\|_{L^2(\mathbb{R}^d)}^2.$$

This estimate can be obtained if we show that

$$\|TT^*\|_{\mathscr{B}(L^2(\mathbb{R}^d))} \le \varepsilon, \tag{2.9}$$

where we set

$$T := \tilde{V}_-^{1/2} \Big(H_0 + \frac{b_\varepsilon}{\varepsilon} \Big)^{-1/2}.$$

Thus, our goal is to show that for any $\varepsilon > 0$, there exists a constant $b_\varepsilon > 0$ such that the estimate (2.9) holds.

Let $\varepsilon > 0$ be fixed arbitrarily, and let $b > 0$. Let $G_0(x-y; M)$ be the kernel of $(H_0 + M)^{-1}$ for $M \ge 0$. By the definition of G_0 and the Schwarz inequality, we estimate

$$\begin{aligned}
\|TT^* v\|_{L^2(\mathbb{R}^d)}^2 &= \Big\| \tilde{V}_-^{1/2} \Big(H_0 + \frac{b}{\varepsilon} \Big)^{-1} \tilde{V}_-^{1/2} v \Big\|_{L^2(\mathbb{R}^d)}^2 \\
&= \int_{\mathbb{R}^d} \tilde{V}_-(x) \Big| \int_{\mathbb{R}^d} G_0\Big(x-y; \frac{b}{\varepsilon}\Big) \tilde{V}_-^{1/2}(y) v(y)\, dy \Big|^2 dx \\
&\le \int_{\mathbb{R}^d} \tilde{V}_-(x) \Big(\int_{\mathbb{R}^d} G_0\Big(x-y; \frac{b}{\varepsilon}\Big) \tilde{V}_-(y)\, dy \Big) \Big(\int_{\mathbb{R}^d} G_0\Big(x-y; \frac{b}{\varepsilon}\Big) |v(y)|^2\, dy \Big) dx \\
&\le \Big\| \Big(H_0 + \frac{b}{\varepsilon} \Big)^{-1} \tilde{V}_- \Big\|_{L^\infty(\mathbb{R}^d)} \int_{\mathbb{R}^d} \tilde{V}_-(x) \Big(\int_{\mathbb{R}^d} G_0\Big(x-y; \frac{b}{\varepsilon}\Big) |v(y)|^2\, dy \Big) dx.
\end{aligned}$$

Applying the Fubini–Tonelli theorem to the integral on the right, we estimate

$$\begin{aligned}
&\int_{\mathbb{R}^d} \tilde{V}_-(x) \Big(\int_{\mathbb{R}^d} G_0\Big(x-y; \frac{b}{\varepsilon}\Big) |v(y)|^2\, dy \Big) dx \\
&\qquad = \int_{\mathbb{R}^d} \Big(\int_{\mathbb{R}^d} G_0\Big(x-y; \frac{b}{\varepsilon}\Big) \tilde{V}_-(x)\, dx \Big) |v(y)|^2\, dy \\
&\qquad \le \Big\| \Big(H_0 + \frac{b}{\varepsilon} \Big)^{-1} \tilde{V}_- \Big\|_{L^\infty(\mathbb{R}^d)} \|v\|_{L^2(\mathbb{R}^d)}^2.
\end{aligned}$$

Combining the above two estimates, we obtain

$$\|TT^* v\|_{L^2(\mathbb{R}^d)}^2 \le \Big\| \Big(H_0 + \frac{b}{\varepsilon} \Big)^{-1} \tilde{V}_- \Big\|_{L^\infty(\mathbb{R}^d)}^2 \|v\|_{L^2(\mathbb{R}^d)}^2.$$

Using the fact that $V \in K_d(\mathbb{R}^d)$ is equivalent to

$$\lim_{M \to \infty} \big\| (H_0 + M)^{-1} |V| \big\|_{L^\infty(\mathbb{R}^d)} = 0$$

(see Proposition A.2.3 in [22]), we see that there exists a constant $b_\varepsilon > 0$ such that

$$\Big\| \Big(H_0 + \frac{b_\varepsilon}{\varepsilon} \Big)^{-1} \tilde{V}_- \Big\|_{L^\infty(\mathbb{R}^d)} \le \varepsilon, \tag{2.10}$$

since $\tilde{V}_- \in K_d(\mathbb{R}^d)$, which implies (2.9). Hence (2.8) is proved.

Now the required inequality (2.5) follows from (2.8). In fact, we estimate, by using (2.8),

$$\int_\Omega V_-(x)\,|u(x)|^2\,dx = \int_{\mathbb{R}^d} \tilde{V}_-(x)|\tilde{u}(x)|^2\,dx$$
$$\le \varepsilon\,\|\nabla\tilde{u}\|^2_{L^2(\mathbb{R}^d)} + b_\varepsilon\|\tilde{u}\|^2_{L^2(\mathbb{R}^d)} = \varepsilon\,\|\nabla u\|^2_{L^2(\Omega)} + b_\varepsilon\|u\|^2_{L^2(\Omega)}.$$

As a consequence, by density argument, the inequality (2.5) is proved.

Next we show the assertion (ii). The proof of (2.7) is almost identical to that of (2.5) by regarding b_ε as 0. The only difference is the estimate (2.10). We use the following pointwise estimate:

$$0 < G_0(x;0) \le \frac{\Gamma(d/2-1)}{4\pi^{d/2}}\,\frac{1}{|x|^{d-2}}, \quad x \ne 0$$

for $d \ge 3$. Instead of (2.10), we can apply the following estimate:

$$\|H_0^{-1}\tilde{V}_-\|_{L^\infty(\mathbb{R}^d)} = \sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d} G_0(x-y;0)\,\tilde{V}_-(y)\,dy$$
$$\le \frac{\Gamma(d/2-1)}{4\pi^{d/2}}\sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d}\frac{\tilde{V}_-(y)}{|x-y|^{d-2}}\,dy = \frac{\Gamma(d/2-1)\|V_-\|_{K_d(\Omega)}}{4\pi^{d/2}},$$

whence the argument in (2.5) works well in this case, and we get (2.7). The proof of Lemma 2.3 is complete. □

We are now in a position to prove Proposition 2.1.

Proof of Proposition 2.1. Let q be a quadratic form defined by letting

$$q(u,v) = \int_\Omega \left(\nabla u(x)\cdot\overline{\nabla v(x)} + V(x)\,u(x)\,\overline{v(x)}\,\right)dx, \quad u,v \in \mathcal{Q}(q),$$

where

$$\mathcal{Q}(q) = \left\{u \in H_0^1(\Omega)\,\middle|\,\sqrt{V_+}u \in L^2(\Omega)\right\}.$$

It is clear that q is densely defined on $L^2(\Omega)$. Moreover, q is semi-bounded. In fact, it follows from the inequality (2.5) for $\varepsilon = 1$ that

$$q(u,u) \ge \|\nabla u\|^2_{L^2(\Omega)} - \int_\Omega V_-(x)\,|u(x)|^2\,dx \ge -b_1\|u\|^2_{L^2(\Omega)} \tag{2.11}$$

for any $u \in \mathcal{Q}(q)$. Hence, if we show that q is closed, then Lemma 2.2 ensures the unique existence of the semi-bounded self-adjoint operator H_V on $L^2(\Omega)$ satisfying (2.1) and (2.2).

We show that q is closed. Put

$$q_1(u,v) = \int_\Omega \left(\nabla u(x)\cdot\overline{\nabla v(x)} - V_-(x)u(x)\overline{v(x)}\,\right)dx, \quad u,v \in \mathcal{Q}_1(q) := H_0^1(\Omega),$$
$$q_2(u,v) = \int_\Omega V_+(x)u(x)\overline{v(x)}\,dx, \quad u,v \in \mathcal{Q}_2(q) := \left\{u \in L^2(\Omega)\,\middle|\,\sqrt{V_+}u \in L^2(\Omega)\right\}.$$

Then we have

$$q(u,v) = q_1(u,v) + q_2(u,v), \quad u,v \in \mathcal{Q}_1(q) \cap \mathcal{Q}_2(q).$$

Since the sum of two closed quadratic forms is also closed, it suffices to show that q_1 and q_2 are closed. First we show that q_1 is closed. All we have to do is to show that the norm $\|\cdot\|_{+1}$ is equivalent to that of $H_0^1(\Omega)$, where $\|\cdot\|_{+1}$ is defined in (2.4), i.e.,

$$\|u\|_{+1} = \sqrt{q_1(u,u) + (b_1+1)\|u\|^2_{L^2(\Omega)}}.$$

Since $V_- \geq 0$, we see that

$$\|u\|^2_{+1} \leq \|\nabla u\|^2_{L^2(\Omega)} + (b_1+1)\|u\|^2_{L^2(\Omega)} \leq (b_1+1)\|u\|^2_{H^1(\Omega)}$$

for any $u \in H_0^1(\Omega)$, and by using the inequality (2.5), we have

$$\begin{aligned}\|u\|^2_{+1} &= \|\nabla u\|^2_{L^2(\Omega)} - \int_\Omega V_-(x)|u(x)|^2\,dx + (b_1+1)\|u\|^2_{L^2(\Omega)} \\ &\geq (1-\varepsilon)\|\nabla u\|^2_{L^2(\Omega)} + (b_1 - b_\varepsilon + 1)\|u\|^2_{L^2(\Omega)}\end{aligned}$$

for any $u \in H_0^1(\Omega)$, where we choose $\varepsilon \in (0,1)$ and b_ε such that $b_1 < b_\varepsilon < b_1+1$. The above two inequalities imply that $\|\cdot\|_{+1}$ is equivalent to $\|\cdot\|_{H^1(\Omega)}$. Hence q_1 is closed.

Next we show that q_2 is closed. Put $q_2(u) = q_2(u,u)$ for simplicity. Assume that

$$u \in L^2(\Omega), \quad u_j \in \mathcal{Q}(q_2), \quad q_2(u_j - u_k) \to 0, \quad \|u_j - u\|_{L^2(\Omega)} \to 0 \quad \text{as } j,k \to \infty,$$

and we prove that

$$u \in \mathcal{Q}(q_2) \quad \text{and} \quad q_2(u_j - u) \to 0 \quad \text{as } j \to \infty. \tag{2.12}$$

Since $\{\sqrt{V_+}u_j\}_{j=1}^\infty$ is a Cauchy sequence in $L^2(\Omega)$, there exists $v \in L^2(\Omega)$ such that

$$\sqrt{V_+}u_j \to v \quad \text{in } L^2(\Omega).$$

Hence the sequence $\{\sqrt{V_+}u_j\}_{j=1}^\infty$ converges to v almost everywhere along a subsequence denoted by the same, namely,

$$\sqrt{V_+}u_j(x) \to v(x) \quad \text{a.e.}\, x \in \Omega \text{ as } j \to \infty.$$

On the other hand, since any convergent sequence in $L^2(\Omega)$ contains a subsequence which converges almost everywhere in Ω, it follows that

$$\sqrt{V_+}u_j(x) \to \sqrt{V_+}u(x) \quad \text{a.e.}\, x \in \Omega \text{ as } j \to \infty.$$

Summarizing the three convergences obtained now, we get

$$\sqrt{V_+}u = v \in L^2(\Omega).$$

This proves (2.12). Thus q is closed.

Finally, we prove the assertion (ii). We estimate by using the inequality (2.7) from Lemma 2.3 and assumption (2.3) of V_-,

$$\begin{aligned}\langle H_V u, u\rangle_{L^2(\Omega)} &\geq \|\nabla u\|^2_{L^2(\Omega)} - \int_\Omega V_-(x)\,|u(x)|^2\,dx \\ &\geq \Big(1 - \frac{\Gamma(d/2-1)\|V_-\|_{K_d(\Omega)}}{4\pi^{d/2}}\Big)\|\nabla u\|^2_{L^2(\Omega)} \geq 0\end{aligned}$$

for any $u \in \mathcal{D}(H_V)$. Hence H_V is non-negative on $L^2(\Omega)$. The proof of Proposition 2.1 is complete. □

3. L^p-L^q-estimates and pointwise estimates for e^{-tH_V}

In this section we shall prove L^p-L^q-estimates for semigroup $\{e^{-tH_V}\}_{t>0}$ generated by H_V, and pointwise estimates for the kernel of e^{-tH_V}. Throughout this section we use the following notation:

$$\gamma_d = \frac{\pi^{d/2}}{\Gamma(d/2-1)} \quad \text{for } d \geq 3.$$

Recalling the quantity

$$\|V_-\|_{K_d(\Omega)} = \sup_{x\in\Omega}\int_\Omega \frac{V_-(y)}{|x-y|^{d-2}}\,dy$$

(see (2.6)), we have the following.

Proposition 3.1. *Let p and q be such that $1 \leq p \leq q \leq \infty$. Suppose that the potential V satisfies assumption* A. *Then e^{-tH_V} is extended to a bounded linear operator from $L^p(\Omega)$ to $L^q(\Omega)$ for each $t > 0$. Furthermore, the following assertions hold*:

(i) *There exist two constants $\omega \geq -\inf\sigma(H_V)$ and $C_1 > 0$ such that*

$$\big\|e^{-tH_V} f\big\|_{L^q(\Omega)} \leq C_1 t^{-(d/2)(1/p-1/q)} e^{\omega t}\|f\|_{L^p(\Omega)} \tag{3.1}$$

for any $t > 0$ and $f \in L^p(\Omega)$.

(ii) *There exist two constants $\omega \geq -\inf\sigma(H_V)$ and $C_2 > 0$ such that the kernel $K(t,x,y)$ of e^{-tH_V} fulfills with the following estimate*:

$$0 \leq K(t,x,y) \leq C_2 t^{-d/2} e^{\omega t} e^{-\frac{|x-y|^2}{8t}} \quad a.e.\ x,y \in \Omega \tag{3.2}$$

for any $t > 0$.

(iii) *Assume further that V_- satisfies*

$$\begin{cases} \|V_-\|_{K_d(\Omega)} < 2\gamma_d, & \text{if } d \geq 3, \\ V_- = 0, & \text{if } d = 1,2. \end{cases} \tag{3.3}$$

Then

$$\left\|e^{-tH_V}f\right\|_{L^q(\Omega)} \le \begin{cases} \dfrac{(2\pi t)^{-(d/2)(1/p-1/q)}}{\left(1-\|V_-\|_{K_d(\Omega)}/2\gamma_d\right)^2}\|f\|_{L^p(\Omega)}, & \text{if } d \ge 3,\\ (4\pi t)^{-(d/2)(1/p-1/q)}\|f\|_{L^p(\Omega)}, & \text{if } d = 1,2 \end{cases} \tag{3.4}$$

for any $t > 0$ and $f \in L^p(\Omega)$.

(iv) *If V_- is restricted to* (1.2), *i.e.,*

$$\begin{cases} \|V_-\|_{K_d(\Omega)} < \gamma_d, & \text{if } d \ge 3,\\ V_- = 0, & \text{if } d = 1,2, \end{cases}$$

then

$$0 \le K(t,x,y) \le \begin{cases} \dfrac{(2\pi t)^{-d/2}}{1-\|V_-\|_{K_d(\Omega)}/\gamma_d}\, e^{-\frac{|x-y|^2}{8t}} & \text{if } d \ge 3,\\ (4\pi t)^{-d/2}e^{-\frac{|x-y|^2}{4t}} & \text{if } d = 1,2, \end{cases} \tag{3.5}$$

a.e. $x, y \in \Omega$, for any $t > 0$.

The following lemma is crucial in the proof of Proposition 3.1.

Lemma 3.2. *Suppose that the potential V satisfies assumption* A. *Let $\tilde V$ and $\tilde V_-$ be the zero extensions of V and V_- to $\mathbb{R}^d$, respectively. Let $\tilde H_{\tilde V}$ and $\tilde H_{\tilde V_-}$ be the self-adjoint extensions of $-\Delta + \tilde V$ and $-\Delta - \tilde V_-$ on $L^2(\mathbb{R}^d)$, respectively. Then for any non-negative function $f \in L^2(\Omega)$, the following estimates hold*:

$$\left(e^{-tH_V}f\right)(x) \ge 0, \quad a.e.\ \ x \in \Omega, \tag{3.6}$$

$$\left(e^{-tH_V}f\right)(x) \le \left(e^{-t\tilde H_{\tilde V}}\tilde f\right)(x), \quad a.e.\ \ x \in \Omega, \tag{3.7}$$

$$\left(e^{-t\tilde H_{\tilde V}}\tilde f\right)(x) \le \left(e^{-t\tilde H_{\tilde V_-}}\tilde f\right)(x), \quad a.e.\ \ x \in \Omega, \tag{3.8}$$

for any $t > 0$, where $\tilde f$ is the zero extension of f to $\mathbb{R}^d$.

The proof of Lemma 3.2 is rather long, and will be postponed.

Let us prove Proposition 3.1.

Proof of Proposition 3.1. The assertion (i) is an immediate consequence of the assertion (ii) and Young's inequality. Hence we concentrate on proving the assertion (ii). We adopt a sequence $\{j_\varepsilon(x)\}_{\varepsilon>0}$ of functions on $\mathbb{R}^d$ defined by letting

$$j_\varepsilon(x) := \frac{1}{\varepsilon^d}\, j\Big(\frac{x}{\varepsilon}\Big), \quad x \in \mathbb{R}^d, \tag{3.9}$$

where

$$j(x) = \begin{cases} A_d\, e^{-\frac{1}{1-|x|^2}}, & \text{for } |x| < 1,\\ 0, & \text{for } |x| \ge 1 \end{cases}$$

with

$$A_d := \Big(\int_{|x|<1} e^{-\frac{1}{1-|x|^2}}\, dx \Big)^{-1}.$$

As is well known, the sequence $\{j_\varepsilon(x)\}_{\varepsilon>0}$ enjoys the following property:

$$j_\varepsilon(\cdot - y) \to \delta_y \quad \text{in } \mathscr{S}'(\mathbb{R}^d) \text{ as } \varepsilon \to 0, \tag{3.10}$$

where δ_y is the Dirac delta function at $y \in \Omega$. Let $y \in \Omega$ be fixed, and let $\tilde{K}(t,x,y)$ be the kernel of $e^{-t\tilde{H}_{\tilde{V}}}$. Taking $\varepsilon > 0$ sufficiently small so that $\operatorname{supp} j_\varepsilon(\cdot - y) \Subset \Omega$, and applying (3.6) and (3.7) from Lemma 3.2 to both f and $\tilde{f}$ replaced by $j_\varepsilon(\cdot - y)$, we get

$$0 \le \int_\Omega K(t,x,z)\, j_\varepsilon(z-y)\, dz \le \int_{\mathbb{R}^d} \tilde{K}(t,x,y)\, j_\varepsilon(z-y)\, dz \quad \text{a.e. } x \in \Omega.$$

Noting (3.10) and taking the limit of the previous inequality as $\varepsilon \to 0$, we get

$$0 \le K(t,x,y) \le \tilde{K}(t,x,y) \quad \text{a.e. } x, y \in \Omega$$

for any $t > 0$. Finally, by using the pointwise estimates:

$$\tilde{K}(t,x,y) \le C\, t^{-d/2}\, e^{\omega t}\, e^{-\frac{|x-y|^2}{8t}} \quad \text{a.e. } x, y \in \Omega \tag{3.11}$$

for any $t > 0$ (see Proposition B.6.7 in [22]), we obtain the estimate (3.2), as desired. Thus the assertion (ii) is proved.

Finally, we prove the estimates (3.4) in (iii) and (3.5) in (iv). We recall, Proposition 5.1 in [5], that if $d \ge 3$, then

$$\big\| e^{-t\tilde{H}_{\tilde{V}}} |\tilde{f}| \big\|_{L^q(\mathbb{R}^d)} \le \frac{(2\pi t)^{-(d/2)(1/p-1/q)}}{\big(1 - \|\tilde{V}_-\|_{K_d(\mathbb{R}^d)}/2\gamma_d\big)^2} \|\tilde{f}\|_{L^p(\mathbb{R}^d)}$$

for any $t > 0$, and

$$\tilde{K}(t,x,y) \le \frac{(2\pi t)^{-d/2}}{1 - \|\tilde{V}_-\|_{K_d(\mathbb{R}^d)}/\gamma_d} e^{-\frac{|x-y|^2}{8t}} \Big(= \frac{(2\pi t)^{-d/2}}{1 - \|V_-\|_{K_d(\Omega)}/\gamma_d} e^{-\frac{|x-y|^2}{8t}} \Big)$$

for a.e. $x, y \in \Omega$ and any $t > 0$. When $d = 1, 2$, we have

$$\big\| e^{-t\tilde{H}_{\tilde{V}}} |\tilde{f}| \big\|_{L^q(\mathbb{R}^d)} \le (4\pi t)^{-(d/2)(1/p-1/q)} \|\tilde{f}\|_{L^p(\mathbb{R}^d)},$$
$$\tilde{K}(t,x,y) \le (4\pi t)^{-d/2} e^{-\frac{|x-y|^2}{4t}} \quad \text{a.e. } x, y \in \Omega$$

for any $t > 0$. Then, applying the above estimates to the argument of the derivations of (3.1) and (3.2), we conclude (3.4) and (3.5). The proof of Proposition 3.1 is finished. □

In the rest of this section we shall prove Lemma 3.2. For this purpose, we need further the following two lemmas. The first one is concerned with the existence and uniqueness of solutions for evolution equations in abstract setting.

Lemma 3.3. *Let $\mathscr{H}$ be a Hilbert space with norm $\|\cdot\|$. Assume that A is a non-negative self-adjoint operator on $\mathscr{H}$. Let $\{T(t)\}_{t\geq 0}$ be the semigroup generated by A, and let $f \in \mathscr{H}$ and $u(t) = T(t)f$. Then u is a unique solution of the following problem*:

$$\begin{cases} u \in C([0,\infty);\mathscr{H}) \cap C((0,\infty);\mathcal{D}(A)) \cap C^1((0,\infty);\mathscr{H}), \\ u'(t) + Au(t) = 0, \quad t > 0, \\ u(0) = f, \end{cases}$$

where $\mathcal{D}(A)$ means the Banach space with graph norm $\|\cdot\| + \|A\cdot\|$.

Remark. It is known that for any non-negative self-adjoint operator on a Hilbert space, its domain is a Banach space with respect to the graph norm of its operator (see Corollary 2.2.9 in Cazenave and Haraux [3]).

For the proof of Lemma 3.3, see, e.g., Theorem 3.2.1 in [3].

The second one is about the differentiability properties for composite functions of Lipschitz continuous functions and $W^{1,p}$-functions.

Lemma 3.4. *Consider the positive and negative parts of a real-valued function $u \in W^{1,p}(\Omega)$ for $1 \leq p \leq \infty$*:

$$u^+ = \chi_{\{u>0\}}u \quad \textit{and} \quad u^- = -\chi_{\{u<0\}}u.$$

Then $u^\pm \in W^{1,p}(\Omega)$ and

$$\partial_{x_j}u^+ = \chi_{\{u>0\}}\partial_{x_j}u, \quad \partial_{x_j}u^- = -\chi_{\{u<0\}}\partial_{x_j}u \quad (j = 1, 2, \dots, d),$$

where $\partial_{x_j} = \partial/\partial x_j$. Furthermore, if $u \in W_0^{1,p}(\Omega)$ for $1 \leq p < \infty$, then

$$u^\pm \in W_0^{1,p}(\Omega), \tag{3.12}$$

where $W_0^{1,p}(\Omega)$ is the completion of $C_0^\infty(\Omega)$ with respect to $W^{1,p}(\Omega)$-norm.

Proof. Since the first part of the lemma is well known, we omit the proof. For the proof, see Lemma 7.6 in Gilbarg and Trudinger [11]. Hence we prove only the latter part.

Since $u \in W_0^{1,p}(\Omega)$ with $1 \leq p < \infty$, there exists a sequence $\{\varphi_n\}_n$ in $C_0^\infty(\Omega)$ such that

$$\varphi_n \to u \quad \text{in } W^{1,p}(\Omega) \text{ as } n \to \infty. \tag{3.13}$$

Let us take a non-negative function $\psi \in C^\infty(\mathbb{R})$ as

$$\psi(x) \begin{cases} = -x, & \text{if } x \leq -1, \\ \leq -x, & \text{if } -1 < x < 0, \\ = 0, & \text{if } x \geq 0, \end{cases}$$

and put

$$\psi_n(x) := \frac{1}{n}\,\psi(nx), \quad n = 1, 2, \dots \tag{3.14}$$

Then there exists a constant $C_0 > 0$ such that

$$|\psi_n'(x)| \le C_0, \quad n = 1, 2, \dots \tag{3.15}$$

Let us consider two kinds of composite functions $\psi_n \circ \varphi_n$ and $\psi_n \circ u$. We show that

$$\psi_n \circ \varphi_n - \psi_n \circ u \to 0 \quad \text{in } W^{1,p}(\Omega), \tag{3.16}$$

$$\psi_n \circ u - u^- \to 0 \quad \text{in } W^{1,p}(\Omega) \tag{3.17}$$

as $n \to \infty$. In fact, noting (3.15), we deduce from the mean value theorem that

$$\begin{aligned} \|\psi_n \circ \varphi_n - \psi_n \circ u\|_{L^p(\Omega)} &= \Big\| \int_0^1 \psi_n'\big(\theta\varphi_n + (1-\theta)u\big)(\varphi_n - u)\, d\theta \Big\|_{L^p(\Omega)} \\ &\le C_0\, \|\varphi_n - u\|_{L^p(\Omega)}. \end{aligned} \tag{3.18}$$

As to the derivatives of $\psi_n \circ \varphi_n - \psi_n \circ u$, we write

$$\begin{aligned} &\|\partial_{x_j}(\psi_n \circ \varphi_n - \psi_n \circ u)\|_{L^p(\Omega)} \\ &\qquad = \|\psi_n'(\varphi_n)\partial_{x_j}\varphi_n - \psi_n'(u)\partial_{x_j}u\|_{L^p(\Omega)} \\ &\qquad \le \|\psi_n'(\varphi_n)(\partial_{x_j}\varphi_n - \partial_{x_j}u)\|_{L^p(\Omega)} + \|\,[\psi_n'(\varphi_n) - \psi_n'(u)]\,\partial_{x_j}u\|_{L^p(\Omega)} \\ &\qquad \le C_0\,\|\partial_{x_j}\varphi_n - \partial_{x_j}u\|_{L^p(\Omega)} + \|\,[\psi_n'(\varphi_n) - \psi_n'(u)]\,\partial_{x_j}u\|_{L^p(\Omega)}, \end{aligned} \tag{3.19}$$

where we used again (3.15) in the last step. Noting the pointwise convergence and uniform boundedness with respect to n:

$$\begin{aligned} &[\psi_n'(\varphi_n)(x) - \psi_n'(u)(x)]\,\partial_{x_j}u(x) \to 0 \quad \text{a.e. } x \in \Omega \text{ as } n \to \infty, \\ &\big|[\psi_n'(\varphi_n)(x) - \psi_n'(u)(x)]\,\partial_{x_j}u(x)\big| \le 2\,C_0\,\big|\partial_{x_j}u(x)\big| \in L^p(\Omega), \end{aligned}$$

we can apply Lebesgue's dominated convergence theorem to obtain

$$\big\|[\psi_n'(\varphi_n) - \psi_n'(u)]\,\partial_{x_j}u\big\|_{L^p(\Omega)} \to 0 \quad \text{as } n \to \infty. \tag{3.20}$$

Hence, summarizing (3.13) and (3.18)-(3.20), we obtain (3.16).

As to the latter convergence (3.17), since

$$\big|(\psi_n \circ u)(x) - u^-(x)\big| \le 2\,|u(x)| \in L^p(\Omega),$$

$$\big|\partial_{x_j}(\psi_n \circ u)(x) - \partial_{x_j}u^-(x)\big| \le (C_0 + 1)\,\big|\partial_{x_j}u(x)\big| \in L^p(\Omega),$$

and since

$$(\psi_n \circ u)(x) - u^-(x) \to 0, \quad \text{a.e. } x \in \Omega,$$

$$\partial_{x_j}(\psi_n \circ u)(x) - \partial_{x_j}u^-(x) = [\psi_n'(u) - \chi_{\{u<0\}}]\,\partial_{x_j}u(x) \to 0, \quad \text{a.e. } x \in \Omega$$

as $n \to \infty$, Lebesgue's dominated convergence theorem allows us to conclude (3.17).

It follows from (3.16) and (3.17) that

$$\psi_n \circ \varphi_n - u^- \to 0 \quad \text{in } W^{1,p}(\Omega) \text{ as } n \to \infty.$$

Since $\{\psi_n \circ \varphi_n\}$ is a sequence in $C_0^\infty(\Omega)$, we conclude (3.12) from the above convergence. The proof of Lemma 3.4 is finished. □

Proof of Lemma 3.2. We start by proving (3.6). Let M be a real number satisfying

$$M > -\inf \sigma(H_V).$$

Then $H_V + M$ is the non-negative self-adjoint operator on $L^2(\Omega)$ with domain

$$\mathcal{D}(H_V + M) = \left\{u \in H_0^1(\Omega) \,\middle|\, \sqrt{V_+}u \in L^2(\Omega),\ H_V u \in L^2(\Omega)\right\}.$$

Put

$$u(t) = e^{-t(H_V+M)}f, \quad t \geq 0$$

for a non-negative function $f \in L^2(\Omega)$. Lemma 3.3 implies that $u(t)$ satisfies

$$\begin{cases} u \in C([0,\infty); L^2(\Omega)) \cap C([0,\infty); \mathcal{D}(H_V + M)) \cap C^1((0,\infty); L^2(\Omega)), \\ \partial_t u(t) + (H_V + M)u(t) = 0, \quad t > 0, \\ u(0) = f. \end{cases}$$

If we show that

(3.21) $\qquad \|u^-(t)\|^2_{L^2(\Omega)}$ is monotonically decreasing with respect to $t \geq 0$,

then we obtain

$$u^-(t,x) = 0 \quad \text{a.e. } x \in \Omega$$

for each $t > 0$, since

$$u^-(0,x) = f^-(x) = 0 \quad \text{a.e. } x \in \Omega.$$

This means that

$$u(t,x) \geq 0 \quad \text{a.e. } x \in \Omega$$

for each $t > 0$; thus we conclude (3.6). Now the assertion (3.21) is an immediate consequence of the following:

$$\frac{d}{dt}\int_\Omega (u^-)^2\,dx \leq 0. \tag{3.22}$$

Hence we pay attention to prove (3.22). Here and below, the time variable t may be omitted, since no confusion arises.

By the definition of u^+, we have

$$\partial_t u^+(t,x) = 0 \quad \text{for } x \in \{u < 0\} \text{ and each } t > 0.$$

We compute

$$\begin{aligned}\frac{d}{dt}\int_\Omega \left(u^-\right)^2 dx &= 2\int_\Omega u^-\partial_t u^-\,dx = 2\int_{\{u<0\}} u^-\partial_t\left(u^+ - u\right)dx \\ &= -2\int_{\{u<0\}} u^-\partial_t u\,dx = 2\int_\Omega \left[(H_V+M)u\right]u^-\,dx\end{aligned} \tag{3.23}$$

where we use the equation

$$\partial_t u + (H_V + M)u = 0$$

in the last step. Since $u^- \in H^1_0(\Omega)$ and $\sqrt{V_+}u^- \in L^2(\Omega)$ by Lemma 3.4 and $\sqrt{V_+}u \in L^2(\Omega)$, we have, by going back to (2.2) in the definition of H_V,

$$\int_\Omega \left[(H_V+M)u\right]u^-\,dx = \int_\Omega \nabla u\cdot\nabla u^-\,dx + \int_\Omega Vuu^-\,dx + \int_\Omega Muu^-\,dx. \tag{3.24}$$

Here we see from Lemma 3.4 that

$$\nabla u^- = -\chi_{\{u<0\}}\nabla u,$$

and hence, the first term on the right of (3.24) is written as

$$\int_\Omega \nabla u\cdot\nabla u^-\,dx = -\int_\Omega |\nabla u^-|^2\,dx.$$

As to the second, by the estimate (2.5) for $\varepsilon = 1$ from Lemma 2.3, we have

$$\int_\Omega Vuu^-\,dx = -\int_\Omega V|u^-|^2\,dx \le \int_\Omega V_-|u^-|^2\,dx \le \|u^-\|^2_{L^2(\Omega)} + b_1\|\nabla u^-\|^2_{L^2(\Omega)};$$

thus, by choosing M as

$$M > b_1\,(\ge -\inf\sigma(H_V)), \tag{3.25}$$

we find that

$$\int_\Omega \left[(H_V+M)u\right]u^-\,dx \le (b_1 - M)\|\nabla u^-\|^2_{L^2(\Omega)} \le 0.$$

Hence, combining this inequality and (3.23), we conclude (3.22).

Next, we prove (3.7). Let us define two functions $v^{(1)}(t)$ and $v^{(2)}(t)$ as follows:

$$v^{(1)}(t) := e^{-t(\tilde H_{\tilde V}+M)}\tilde f \quad\text{and}\quad v^{(2)}(t) := e^{-t(H_V+M)}f$$

for $t \ge 0$. Then it follows from Lemma 3.3 that $v^{(1)}$ and $v^{(2)}$ satisfy

$$\begin{cases} v^{(1)} \in C([0,\infty);L^2(\mathbb{R}^d)) \cap C((0,\infty);\mathcal{D}(\tilde H_{\tilde V}+M)) \cap C^1((0,\infty);L^2(\mathbb{R}^d)), \\ \partial_t v^{(1)}(t) + (\tilde H_{\tilde V}+M)v^{(1)}(t) = 0, \quad t>0, \\ v^{(1)}(0) = \tilde f \end{cases} \tag{3.26}$$

and

$$
(3.27) \quad \begin{cases} v^{(2)} \in C([0,\infty); L^2(\Omega)) \cap C((0,\infty); \mathcal{D}(H_V + M)) \cap C^1((0,\infty); L^2(\Omega)), \\ \partial_t v^{(2)}(t) + (H_V + M) v^{(2)}(t) = 0, \quad t > 0, \\ v^{(2)}(0) = f \end{cases}
$$

for each $t > 0$, respectively. We define a new function v as

$$
v(t) := v^{(1)}(t)|_\Omega - v^{(2)}(t)
$$

for $t \geq 0$, where $v^{(1)}(t)|_\Omega$ is the restriction of $v^{(1)}(t)$ to Ω. Let us consider the negative part of v:

$$
v^- = -\chi_{\{v<0\}} v.
$$

Then, thanks to (3.26) and (3.27), we have

$$
v^- \in C([0,\infty); L^2(\Omega)) \cap C^1((0,\infty); L^2(\Omega)).
$$

Moreover, we have $v^- \in H^1(\Omega)$ by using Lemma 3.4, since $v \in H^1(\Omega)$, and we immediately have $\sqrt{V_+} v^- \in L^2(\Omega)$, since $\sqrt{V_+} v \in L^2(\Omega)$. Once we prove that

$$
(3.28) \qquad v^- \in H_0^1(\Omega),
$$

we get, by the previous argument,

$$
(3.29) \qquad \frac{d}{dt} \int_\Omega (v^-)^2 \, dx \leq 0.
$$

In fact, by the definition of v^-, we have

$$
\begin{aligned}
\frac{d}{dt} \int_\Omega (v^-)^2 \, dx &= -2 \int_{\{v<0\}} v^- \partial_t v^{(1)} \, dx + 2 \int_{\{v<0\}} v^- \partial_t v^{(2)} \, dx \\
&= 2 \int_{\mathbb{R}^d} \{(\tilde{H}_{\tilde{V}} + M) v^{(1)}\} \tilde{v}^- \, dx - 2 \int_\Omega \{(H_V + M) v^{(2)}\} v^- \, dx,
\end{aligned}
$$

where $\tilde{v}^-$ is the zero extension of v^- to $\mathbb{R}^d$, and we used equations

$$
\partial_t v^{(1)} + (\tilde{H}_{\tilde{V}} + M) v^{(1)} = 0 \quad \text{and} \quad \partial_t v^{(2)} + (H_V + M) v^{(2)} = 0
$$

in the last step. Since $v^- \in H_0^1(\Omega)$ and $\sqrt{V_+} v^- \in L^2(\Omega)$ by (3.28), we have, by definitions of $\tilde{H}_{\tilde{V}}$ and H_V,

$$
\begin{aligned}
&\int_{\mathbb{R}^d} \left[(\tilde{H}_{\tilde{V}} + M) v^{(1)}\right] \tilde{v}^- \, dx - \int_\Omega \left[(H_V + M) v^{(2)}\right] v^- \, dx \\
&\quad = \int_{\mathbb{R}^d} \nabla v^{(1)} \cdot \nabla \tilde{v}^- \, dx + \int_{\mathbb{R}^d} \tilde{V} v^{(1)} \tilde{v}^- \, dx + \int_{\mathbb{R}^d} M v^{(1)} \tilde{v}^- \, dx \\
&\qquad - \int_\Omega \nabla v^{(2)} \cdot \nabla v^- \, dx - \int_\Omega V v^{(2)} v^- \, dx - \int_\Omega M v^{(2)} v^- \, dx \\
&\quad = \int_\Omega \nabla v \cdot \nabla v^- \, dx + \int_\Omega V v v^- \, dx + \int_\Omega M v v^- \, dx \leq (b_1 - M) \|v^-\|_{L^2(\Omega)}^2 \leq 0,
\end{aligned}
$$

since M is chosen as in (3.25). Hence we obtain (3.29), which implies the required inequality (3.7).

We have to prove (3.28). The proof is similar to that of Lemma 3.4. Since $v^{(2)}(t) \in H_0^1(\Omega)$ for each $t > 0$ by (3.27), there exists a sequence $\{\varphi_n(t)\}$ in $C_0^\infty(\Omega)$ such that

$$\varphi_n(t) \to v^{(2)}(t) \quad \text{in } H^1(\Omega) \text{ as } n \to \infty$$

for each $t > 0$. Put

$$v_n(t) := v^{(1)}(t)|_\Omega - \varphi_n(t), \quad n = 1, 2, \dots$$

Let $\{\psi_n\}$ be the sequence as in (3.14). As in the proof of Lemma 3.4, we can show that

$$\psi_n \circ v_n^- \to v^- \quad \text{in } H^1(\Omega) \text{ as } n \to \infty.$$

Since v_n^- have compact supports in $\operatorname{supp}\varphi_n$ by $v^{(1)} \geq 0$ on Ω, it follows that the functions $\psi_n \circ v_n^-$ also have compact supports in Ω. Let $(\psi_n \circ v_n^-)\tilde{}$ be the zero extension of $\psi_n \circ v_n^-$ to $\mathbb{R}^d$, and $j_\varepsilon(x)$ be the functions defined in (3.9). Taking ε along a sequence $\{\varepsilon_n\}$ such that

$$\varepsilon_n \searrow 0 \quad \text{and} \quad \operatorname{supp} j_{\varepsilon_n} * (\psi_n \circ v_n^-)\tilde{} \Subset \Omega \text{ for any } n,$$

we have

$$j_{\varepsilon_n} * (\psi_n \circ v_n^-)\tilde{}\,\big|_\Omega \in C_0^\infty(\Omega) \quad \text{for any } n.$$

Since

$$j_{\varepsilon_n} * (\psi_n \circ v_n^-)\tilde{}\,\big|_\Omega \to v^- \quad \text{in } H^1(\Omega) \text{ as } n \to \infty,$$

we conclude (3.28).

Finally, as to the inequality (3.8), letting $f \in L^2(\Omega)$ be non-negative, we put

$$w^{(1)}(t) := e^{-t(\tilde{H}_{\tilde{V}_-}+M)}\tilde{f}, \quad w^{(2)}(t) := e^{-t(\tilde{H}_{\tilde{V}}+M)}\tilde{f}, \quad w(t) := w^{(1)}(t) - w^{(2)}(t)$$

for $t \geq 0$. Noting that $w^{(1)}(t) \in \mathcal{D}(\tilde{H}_{\tilde{V}_-})$ and $w^{(2)}(t) \in \mathcal{D}(\tilde{H}_{\tilde{V}})$, it suffices to show that

$$\frac{d}{dt}\int_\Omega (w^-)^2\,dx \leq 0. \tag{3.30}$$

We prove (3.30). Since we have $w^- \in H_0^1(\Omega)$ in a similar way to (3.28), we estimate

$$\begin{aligned}
\frac{d}{dt}\int_\Omega (w^-)^2\,dx &= -2\int_\Omega (\partial_t w) w^-\,dx \\
&= 2\int_\Omega \left[(\tilde{H}_{\tilde{V}_-}+M)w^{(1)}\right] w^-\,dx - 2\int_\Omega \left[(\tilde{H}_{\tilde{V}}+M)w^{(2)}\right] w^-\,dx \\
&= 2\int_\Omega \left\{\nabla w^{(1)}\cdot\nabla w^- - (\tilde{V}_- w^{(1)})w^- + Mw^{(1)}w^-\right\} dx \\
&\quad - 2\int_\Omega \left\{\nabla w^{(2)}\cdot\nabla w^- + (\tilde{V}_+ w^{(2)})w^- - (\tilde{V}_- w^{(2)})w^- + Mw^{(2)}w^-\right\} dx \\
&= -2\int_\Omega \left(|\nabla w^-|^2 - \tilde{V}_-|w^-|^2 + M|w^-|^2\right) dx - 2\int_\Omega (\tilde{V}_+ w^{(2)})w^-\,dx \\
&\leq -2\int_\Omega (\tilde{V}_+ w^{(2)})w^-\,dx,
\end{aligned}$$

where we used the inequality (2.5) in the last step. Since $w^{(2)}(t) \geq 0$ by (3.6) and (3.7), we conclude the required inequality (3.30), which proves the inequality (3.8). The proof of Lemma 3.2 is complete. □

4. L^p-L^q-estimates for the resolvent of θH_V

In this section we shall prove the boundedness of resolvent of θH_V in scaled amalgam spaces. The result in this section plays an important role in the proof of Theorem 1.1.

Following Fournier and Stewart (see [9]), let us give the definition of scaled amalgam spaces on Ω as follows.

Definition. Let $1 \leq p, q \leq \infty$ and $\theta > 0$. The space $l^p(L^q)_\theta$ is defined by letting

$$l^p(L^q)_\theta = l^p(L^q)_\theta(\Omega) := \big\{ f \in L^q_{\mathrm{loc}}(\overline{\Omega}) \,\big|\, \|f\|_{l^p(L^q)_\theta} < \infty \big\},$$

with norm

$$\|f\|_{l^p(L^q)_\theta} = \begin{cases} \Big(\displaystyle\sum_{n \in \mathbb{Z}^d} \|f\|^p_{L^q(C_\theta(n))} \Big)^{1/p} & \text{for } 1 \leq p < \infty, \\ \displaystyle\sup_{n \in \mathbb{Z}^d} \|f\|_{L^q(C_\theta(n))} & \text{for } p = \infty, \end{cases}$$

where $C_\theta(n)$ is the cube centered at $\theta^{1/2} n \in \theta^{1/2}\mathbb{Z}^d$ with side length $\theta^{1/2}$:

$$C_\theta(n) = \Big\{ x = (x_1, x_2, \dots, x_d) \in \Omega \,\Big|\, \max_{j=1,\dots,d} |x_j - \theta^{1/2} n_j| \leq \frac{\theta^{1/2}}{2} \Big\}.$$

Here we adopt the Euclidean norm for $n = (n_1, n_2, \dots, n_d) \in \mathbb{Z}^d$:

$$|n| = \sqrt{n_1^2 + n_2^2 + \cdots + n_d^2}.$$

Let us give a remark on the properties of $l^p(L^q)_\theta$-spaces. The spaces $l^p(L^q)_\theta$ are complete with respect to the norm $\|\cdot\|_{l^p(L^q)_\theta}$, and have the property that

$$l^p(L^q)_\theta \hookrightarrow L^p(\Omega) \cap L^q(\Omega)$$

for any $\theta > 0$, provided $1 \leq p \leq q \leq \infty$.

The goal in this section is to prove the following.

Proposition 4.1. *Let $1 \leq p \leq q \leq \infty$, and β be such that*

$$\beta > \frac{d}{2}\Big(\frac{1}{p} - \frac{1}{q}\Big). \tag{4.1}$$

Suppose that the potential V satisfies assumption A. *Let $z \in \mathbb{C}$ with*

$$\mathrm{Re}(z) < \min\{-\omega, 0\}, \tag{4.2}$$

where ω is the constant as in Proposition 3.1. Then $(H_V - z)^{-\beta}$ is extended to a bounded linear operator from $L^p(\Omega)$ to $l^p(L^q)_\theta$ with $\theta = 1$. Furthermore, the following assertions hold:

(i) *There exists a constant C depending on d, p, q, β and z such that*

$$\big\|(\theta H_V - z)^{-\beta}\big\|_{\mathscr{B}(L^p(\Omega), L^q(\Omega))} \le C\,\theta^{-(d/2)(1/p-1/q)}, \tag{4.3}$$

$$\big\|(\theta H_V - z)^{-\beta}\big\|_{\mathscr{B}(L^p(\Omega), l^p(L^q)_\theta)} \le C\,\theta^{-(d/2)(1/p-1/q)} \tag{4.4}$$

for any $0 < \theta \le 1$.

(ii) *Assume further that V_- satisfies*

$$\begin{cases} \displaystyle\sup_{x\in\Omega} \int_\Omega \frac{V_-(y)}{|x-y|^{d-2}}\,dy < \frac{2\pi^{d/2}}{\Gamma(d/2-1)}, & \text{if } d \ge 3,\\ V_- = 0, & \text{if } d = 1, 2. \end{cases}$$

Let $z \in \mathbb{C}$ be such that

$$\operatorname{Re}(z) < 0.$$

Then the estimate (4.3) holds for any $\theta > 0$. Moreover, if V_- satisfies

$$\begin{cases} \displaystyle\sup_{x\in\Omega} \int_\Omega \frac{V_-(y)}{|x-y|^{d-2}}\,dy < \frac{\pi^{d/2}}{\Gamma(d/2-1)}, & \text{if } d \ge 3,\\ V_- = 0, & \text{if } d = 1, 2, \end{cases}$$

then the estimate (4.4) holds for any $\theta > 0$.

Proof. First we prove (4.3). Let $0 < \theta \le 1$. We use the following formula:

$$(H_V - z)^{-\beta} = \frac{1}{\Gamma(\beta)} \int_0^\infty t^{\beta-1} e^{zt} e^{-tH_V}\,dt \tag{4.5}$$

for any $z \in \mathbb{C}$ with $\operatorname{Re}(z) < \inf \sigma(H_V)$ and $\beta > 0$. Thanks to (4.5) and L^p-L^q-estimates (3.1) for $e^{-t\theta H_V}$ in Proposition 3.1, we estimate

$$\begin{aligned} &\big\|(\theta H_V - z)^{-\beta} f\big\|_{L^q(\Omega)} \\ &\quad\le \frac{1}{\Gamma(\beta)} \int_0^\infty t^{\beta-1} e^{\operatorname{Re}(z)t} \big\|e^{-t\theta H_V} f\big\|_{L^q(\Omega)}\,dt \\ &\quad\le C\,\theta^{-(d/2)(1/p-1/q)} \Big(\int_0^\infty t^{\beta-1} e^{[\operatorname{Re}(z) - \min\{-\omega, 0\}]t}\, t^{-(d/2)(1/p-1/q)}\,dt \Big) \|f\|_{L^p(\Omega)} \end{aligned}$$

for any $f \in L^p(\Omega)$ provided $1 \le p \le q \le \infty$, where C is the positive constant independent of θ. Here, let us take z as in (4.2). Then the integral on the right is absolutely convergent, since β satisfies the inequality (4.1). This proves (4.3).

Let us turn to the proof of (4.4). If we prove that there exists a constant $C > 0$ such that

$$
\begin{aligned}
(4.6)\quad & \|e^{-t\theta H_V} f\|_{l^p(L^q)_\theta} \\
& \leq C\,\theta^{-(d/2)(1/p-1/q)}\{t^{-(d/2)(1/p-1/q)} + 1\}e^{-\min\{-\omega,0\}t}\|f\|_{L^p(\Omega)}
\end{aligned}
$$

for any $t > 0$ and $f \in L^p(\Omega)$ provided $1 \leq p \leq q \leq \infty$, then the estimate (4.4) is obtained by combining (4.5) and (4.6). In fact, by using (4.5), we estimate

$$
\begin{aligned}
& \|(\theta H_V - z)^{-\beta} f\|_{l^p(L^q)_\theta} \\
& \leq \frac{1}{\Gamma(\beta)}\int_0^\infty t^{\beta-1}e^{\mathrm{Re}(z)t}\|e^{-t\theta H_V} f\|_{l^p(L^q)_\theta}\,dt \\
& \leq C\,\theta^{-(d/2)(1/p-1/q)} \\
& \qquad \times \Big(\int_0^\infty t^{\beta-1}e^{\{\mathrm{Re}(z)-\min\{-\omega,0\}\}t}\{t^{-(d/2)(1/p-1/q)} + 1\}\,dt\Big)\|f\|_{L^p(\Omega)}.
\end{aligned}
$$

Here the integral on the right is absolutely convergent, since z satisfies the inequality (4.2) and β satisfies the inequality (4.1). This proves (4.4). Therefore, all we have to do is to prove the estimate (4.6).

To this end, we recall the estimate (3.2) from Proposition 3.1. We define the right member of (3.2) as $K_0(t, x - y)$, i.e.,

$$
K_0(t,x) = C_2\,t^{-d/2}e^{\omega t}e^{-\frac{|x|^2}{8t}} \quad t > 0, \quad x \in \mathbb{R}^d.
$$

Now, letting $1 \leq r \leq \infty$, we prove that

$$
(4.7)\qquad \|K_0(\theta t,\cdot)\|_{l^1(L^r)_\theta} \leq C\,\theta^{-(d/2)(1-1/r)}\{t^{-(d/2)(1-1/r)} + 1\}e^{-\min\{-\omega,0\}t}
$$

for any $t > 0$, where $C > 0$ is independent of θ. We estimate $L^r(C_\theta(n))$-norms of $K_0(\theta t,\cdot)$ for the case $n = 0$ and $n \neq 0$, separately.

The case $n = 0$. When $1 \leq r < \infty$, we estimate

$$
\begin{aligned}
\|K_0(\theta t,\cdot)\|_{L^r(C_\theta(0))} & \leq C_2\,(\theta t)^{-d/2}e^{-\min\{-\omega,0\}\theta t}\Big(\int_{\mathbb{R}^d} e^{-\frac{r|x|^2}{8\theta t}}\,dx\Big)^{1/r} \\
& = C_2\,(\theta t)^{-d/2}e^{-\min\{-\omega,0\}\theta t}\Big(\int_{\mathbb{R}^d} e^{-\frac{r|x|^2}{8}}(\theta t)^{d/2}\,dx\Big)^{1/r} \\
& \leq C_2\,(\theta t)^{-(d/2)(1-1/r)}e^{-\min\{-\omega,0\}t}\Big(\int_{\mathbb{R}^d} e^{-\frac{r|x|^2}{8}}\,dx\Big)^{1/r} \\
& = \frac{(8\pi)^{d/(2r)}C_2}{r^{d/(2r)}}\,(\theta t)^{-(d/2)(1-1/r)}\,e^{-\min\{-\omega,0\}t}.
\end{aligned} \tag{4.8}
$$

When $r = \infty$, we estimate

$$
\begin{aligned}
(4.9)\qquad \|K_0(\theta t,\cdot)\|_{L^\infty(C_\theta(0))} & = C_2\,(\theta t)^{-d/2}e^{-\min\{-\omega,0\}\theta t}\big(\sup_{x\in C_\theta(0)} e^{-\frac{|x|^2}{8\theta t}}\big) \\
& \leq C_2\,(\theta t)^{-d/2}e^{-\min\{-\omega,0\}t}.
\end{aligned}
$$

The case $n \neq 0$. We estimate

$$\begin{aligned}\sum_{n\neq 0} &\|K_0(\theta t,\cdot)\|_{L^r(C_\theta(n))}\\ &\le \sum_{n\neq 0}\|K_0(\theta t,\cdot)\|_{L^\infty(C_\theta(n))}|C_\theta(n)|^{1/r}\\ &= C_2\,(\theta t)^{-d/2}e^{-\min\{-\omega,0\}\theta t}\sum_{n\neq 0}\Big(\sup_{x\in C_\theta(n)} e^{-\frac{|x|^2}{8\theta t}}\Big)\cdot|C_\theta(n)|^{1/r}.\end{aligned} \tag{4.10}$$

Here, observing that

$$\frac{|\theta^{1/2}n|}{2}\le |x|\,(\le 2|\theta^{1/2}n|),\quad x\in C_\theta(n),$$

we can estimate the right member of (4.10) as

$$C_2\,(\theta t)^{-d/2}e^{-\min\{-\omega,0\}t}\Big(\sum_{n\neq 0}e^{-\frac{|n|^2}{32t}}\Big)(\theta^{d/2})^{1/r},$$

and hence, we get

$$\sum_{n\neq 0}\|K_0(\theta t,\cdot)\|_{L^r(C_\theta(n))}\le C_2\,(\theta t)^{-d/2}e^{-\min\{-\omega,0\}t}\Big(\sum_{n\neq 0}e^{-\frac{|n|^2}{32t}}\Big)(\theta^{d/2})^{1/r}.$$

Here, by an explicit calculation, we see that

$$\begin{aligned}\sum_{n\neq 0}e^{-\frac{|n|^2}{32t}} &= \sum_{n\neq 0}e^{-\frac{n_1^2+n_2^2+\cdots+n_d^2}{32t}} = 2^d\Big(\sum_{j=1}^\infty e^{-\frac{j^2}{32t}}\Big)^d\\ &\le 2^d\Big(\int_0^\infty e^{-\frac{\sigma^2}{32t}}\,d\sigma\Big)^d = (8\sqrt{2})^d\,\pi^{d/2}\,t^{d/2}.\end{aligned}$$

Summarizing the estimates obtained now, we conclude that

$$\begin{aligned}\sum_{n\neq 0}&\|K_0(\theta t,\cdot)\|_{L^r(C_\theta(n))}\\ &\le C_2\,(\theta t)^{-d/2}\,e^{-\min\{-\omega,0\}t}\cdot(8\sqrt{2})^d\,\pi^{d/2}\,t^{d/2}\cdot(\theta^{d/2})^{1/r}\\ &= (8\sqrt{2})^d\,\pi^{d/2}\,C_2\,\theta^{-(d/2)(1-1/r)}e^{-\min\{-\omega,0\}t}\end{aligned} \tag{4.11}$$

for any $r\in[1,\infty]$.

Combining the estimates (4.8), (4.9) and (4.11), we get (4.7), as desired.

We are now in a position to prove the key estimate (4.6). Let $f\in L^p(\Omega)$ and $\tilde{f}$ be a zero extension of f to $\mathbb{R}^d$. Thanks to the estimate (3.2) from Proposition 3.1, i.e.,

$$0\le K(t,x,y)\le K_0(t,x-y)\quad \text{a.e.}\,x,y\in\Omega$$

for any $t > 0$, we estimate

$$\begin{aligned}\|e^{-t\theta H_V} f\|_{l^p(L^q)_\theta} &= \Big\| \int_\Omega K(\theta t, \cdot, y) f(y)\, dy \Big\|_{l^p(L^q)_\theta} \\ &\le \Big\| \int_\Omega K(\theta t, \cdot, y)|f(y)|\, dy \Big\|_{l^p(L^q)_\theta} \le \Big\| \int_{\mathbb{R}^d} K_0(\theta t, \cdot - y)|\tilde{f}(y)|\, dy \Big\|_{l^p(L^q)_\theta(\mathbb{R}^d)}.\end{aligned}$$

Applying the Young inequality (A.1) (see Appendix A) to the right member, and using the inequality (4.7), we deduce that

$$\begin{aligned}\|e^{-t\theta H_V} f\|_{l^p(L^q)_\theta} &\le 3^d \|K_0(\theta t, \cdot)\|_{l^1(L^r)_\theta(\mathbb{R}^d)} \|\tilde{f}\|_{l^p(L^p)_\theta(\mathbb{R}^d)} \\ &\le C\, \theta^{-(d/2)(1-1/r)} \big\{ t^{-(d/2)(1-1/r)} + 1 \big\}\, e^{-\min\{-\omega,0\}t} \|\tilde{f}\|_{L^p(\mathbb{R}^d)} \\ &= C\, \theta^{-(d/2)(1/p-1/q)} \big\{ t^{-(d/2)(1/p-1/q)} + 1 \big\}\, e^{-\min\{-\omega,0\}t} \|f\|_{L^p(\Omega)},\end{aligned}$$

provided that p, q, r satisfy $1 \le p, q, r \le \infty$ and $1/p + 1/r - 1 = 1/q$. This proves (4.6).

Finally, the proof of the assertion (ii) is done by the same argument as in (i), if we apply (3.4) and (3.5) to the identity (4.5). So we may omit the details. The proof of Proposition 4.1 is finished. □

5. Commutator estimates

In this section we shall prepare commutator estimates. These estimates will be also an important tool in the proof of Theorem 1.1. Among other things, we introduce operators $\mathrm{Ad}^k(L)$ for some operator L as follows.

Definition. Let X and Y be topological vector spaces, and let A and B be continuous linear operators from X and Y into themselves, respectively. For a continuous linear operator L from X into Y, the operators $\mathrm{Ad}^k(L)$ from X into Y, $k = 0, 1, \ldots$, are successively defined by

$$\mathrm{Ad}^0(L) = L, \quad \mathrm{Ad}^k(L) = \mathrm{Ad}^{k-1}(BL - LA), \quad k \ge 1.$$

The result in this section is concerned with L^2-boundedness for $\mathrm{Ad}^k(e^{-itR_{V,\theta}})$, where $R_{V,\theta}$ is the resolvent operator defined by letting

$$R_{V,\theta} := (\theta H_V + M)^{-1}, \quad \theta > 0$$

for a fixed constant M with

$$M > \max\{-\inf \sigma(H_V), 0\}.$$

Hereafter, operators A and B are taken as

$$A = B = x_j - \theta^{1/2} n_j \quad \text{for some } j \in \{1, \ldots, d\}. \tag{5.1}$$

Then we shall prove here the following.

Proposition 5.1. *Suppose that the potential V satisfies assumption* A. *Let A and B be the operators as in* (5.1). *Then for any non-negative integer k, the following assertions hold:*

(i) *There exists a constant $C > 0$ depending on d, k and M such that*

$$\left\|\mathrm{Ad}^k(e^{-itR_{V,\theta}})\right\|_{\mathscr{B}(L^2(\Omega))} \le C\,\theta^{k/2}(1+|t|)^k \tag{5.2}$$

for any $t \in \mathbb{R}$ and $0 < \theta \le 1$.

(ii) *Assume further that V_- satisfies*

$$\begin{cases} \sup\limits_{x\in\Omega} \displaystyle\int_\Omega \frac{V_-(y)}{|x-y|^{d-2}}\,dy < \frac{4\pi^{d/2}}{\Gamma(d/2-1)}, & \text{if } d \ge 3, \\ V_- = 0, & \text{if } d = 1, 2. \end{cases}$$

Then the estimate (5.2) *holds for any $t \in \mathbb{R}$ and $\theta > 0$.*

First, we prepare L^2-boundedness for $R_{V,\theta}$ and $\partial_{x_j} R_{V,\theta}$ to prove Proposition 5.1.

Lemma 5.2. *Suppose that the potential V satisfies assumption* A. *Then the following assertions hold:*

(i) *There exists a constant $C > 0$ such that*

$$\|R_{V,\theta}\|_{\mathscr{B}(L^2(\Omega))} \le \frac{1}{M + \min\{\inf\sigma(H_V), 0\}}, \tag{5.3}$$

$$\|\nabla R_{V,\theta}\|_{\mathscr{B}(L^2(\Omega))} \le C\,\theta^{-1/2} \tag{5.4}$$

for any $0 < \theta \le 1$.

(ii) *Assume further that V_- satisfies*

$$\begin{cases} \sup\limits_{x\in\Omega} \displaystyle\int_\Omega \frac{V_-(y)}{|x-y|^{d-2}}\,dy < \frac{4\pi^{d/2}}{\Gamma(d/2-1)}, & \text{if } d \ge 3, \\ V_- = 0, & \text{if } d = 1, 2. \end{cases} \tag{5.5}$$

Then

$$\|R_{V,\theta}\|_{\mathscr{B}(L^2(\Omega))} \le M^{-1}, \tag{5.6}$$

and

$$\|\nabla R_{V,\theta}\|_{\mathscr{B}(L^2(\Omega))} \le M^{-1/2}\Big(1 - \frac{\Gamma(d/2-1)\|V_-\|_{K_d(\Omega)}}{4\pi^{d/2}}\Big)^{-1/2}\theta^{-1/2} \tag{5.7}$$

for any $\theta > 0$.

Proof. First we prove the assertion (i). Since H_V is the self-adjoint operator on $L^2(\Omega)$, we obtain (5.3), (5.4), (5.6) and (5.7) by the spectral resolution. In fact, we have

$$\begin{aligned}\|R_{V,\theta}f\|^2_{L^2(\Omega)} &= \int_{\inf\sigma(H_V)}^{\infty} \frac{1}{(\theta\lambda+M)^2}\, d\|E_{H_V}(\lambda)f\|^2_{L^2(\Omega)}\\ &\le \begin{cases} \dfrac{1}{M^2}\|f\|^2_{L^2(\Omega)}, & \text{if } \inf\sigma(H_V)\ge 0,\\ \dfrac{1}{[M+\inf\sigma(H_V)]^2}\|f\|^2_{L^2(\Omega)}, & \text{if } \inf\sigma(H_V)<0\end{cases}\end{aligned}$$

for any $f \in L^2(\Omega)$, since $0<\theta\le 1$. This proves (5.3).

Next we consider the estimate for $\nabla R_{V,\theta}f$. Since $R_{V,\theta}f \in \mathcal{D}(H_V)$ for any $f\in L^2(\Omega)$, we estimate

$$\begin{aligned}\|\nabla R_{V,\theta}f\|^2_{L^2(\Omega)} &= \int_\Omega \left(\nabla R_{V,\theta}f\cdot\nabla R_{V,\theta}f + V|R_{V,\theta}f|^2 - V|R_{V,\theta}f|^2\right)dx\\ &= \langle H_V R_{V,\theta}f, R_{V,\theta}f\rangle_{L^2(\Omega)} + \int_\Omega (V_- - V_+)|R_{V,\theta}f|^2\,dx\\ &\le \langle H_V R_{V,\theta}f, R_{V,\theta}f\rangle_{L^2(\Omega)} + \int_\Omega V_-|R_{V,\theta}f|^2\,dx =: I + II.\end{aligned}$$

Then we estimate the first term I as

$$\begin{aligned} I &= \int_{\inf\sigma(H_V)}^{\infty}\frac{\lambda}{(\theta\lambda+M)^2}\,d\|E_{H_V}(\lambda)f\|^2_{L^2(\Omega)}\\ &\le \int_{\max\{\inf\sigma(H_V),0\}}^{\infty}\theta^{-1}\cdot\frac{\theta\lambda}{\theta\lambda+M}\cdot\frac{1}{\theta\lambda+M}\,d\|E_{H_V}(\lambda)f\|^2_{L^2(\Omega)}\\ &\le M^{-1}\theta^{-1}\int_{\inf\sigma(H_V)}^{\infty} d\,\|E_{H_V}(\lambda)f\|^2_{L^2(\Omega)} = M^{-1}\theta^{-1}\|f\|^2_{L^2(\Omega)}.\end{aligned}$$

As to the second term II, by using the inequality (2.5) for $\varepsilon\in(0,1)$ from Lemma 2.3 and estimate (5.3), we have

$$\begin{aligned} II &\le \varepsilon\,\|\nabla R_{V,\theta}f\|^2_{L^2(\Omega)} + b_\varepsilon\|R_{V,\theta}f\|^2_{L^2(\Omega)}\\ &\le \varepsilon\,\|\nabla R_{V,\theta}f\|^2_{L^2(\Omega)} + C\,b_\varepsilon\,\theta^{-1}\|f\|^2_{L^2(\Omega)},\end{aligned}\tag{5.8}$$

since $0<\theta\le 1$. Combining the above three estimates, we conclude the estimate (5.4).

We now turn to the proof of (ii). In this case we have $\inf\sigma(H_V)\ge 0$. It is sufficient to prove only the estimate (5.7) for $\nabla R_{V,\theta}f$, since the proof of (5.6) is similar to (5.3). If V_- satisfies assumption (5.5), then we have, by using the inequality (2.7) from Lemma 2.3,

$$II \le \frac{\Gamma(d/2-1)\|V_-\|_{K_d(\Omega)}}{4\pi^{d/2}}\,\|\nabla R_{V,\theta}f\|^2_{L^2(\Omega)}.$$

Using this estimate instead of (5.8), the estimate (5.7) is proved for any $\theta>0$ in the same way as (5.4). The proof of Lemma 5.2 is complete. □

We are now in a position to prove Proposition 5.1.

Proof of Proposition 5.1. Let us denote by $\mathscr{D}(\Omega)$ the totality of the test functions on Ω, and by $\mathscr{D}'(\Omega)$ its dual space. We regard X as $\mathscr{D}(\Omega)$ and Y as $\mathscr{D}'(\Omega)$ in the definition of operator Ad. Then we have, by Lemma B.2 in appendix B,

$$\mathrm{Ad}^0(R_{V,\theta}) = R_{V,\theta}, \quad \mathrm{Ad}^1(R_{V,\theta}) = -2\theta R_{V,\theta}\partial_{x_j} R_{V,\theta}, \tag{5.9}$$

$$\mathrm{Ad}^k(R_{V,\theta}) = \theta\big\{-2k\mathrm{Ad}^{k-1}(R_{V,\theta})\partial_{x_j}R_{V,\theta} + k(k-1)\mathrm{Ad}^{k-2}(R_{V,\theta})R_{V,\theta}\big\} \tag{5.10}$$

for $k \ge 2$.

First we prove the assertion (i). Let $0 < \theta \le 1$. Since $R_{V,\theta}$ and $\partial_{x_j}R_{V,\theta}$ are bounded on $L^2(\Omega)$ by (5.3) and (5.4) from Lemma 5.2, operators $\mathrm{Ad}^k(R_{V,\theta})$ are also bounded on $L^2(\Omega)$ for each $k \ge 0$. Before going to prove the estimates (5.2), we prepare the following estimates for $\mathrm{Ad}^k(R_{V,\theta})$: let k be a non-negative integer. Then there exists a constant $C_k > 0$ such that

$$\|\mathrm{Ad}^k(R_{V,\theta})\|_{\mathscr{B}(L^2(\Omega))} \le C_k\theta^{k/2} \tag{5.11}$$

for any $0 < \theta \le 1$. We prove (5.11) by induction. For $k = 0, 1$, we have, by using the identity (5.9) and estimates (5.3) and (5.4) from Lemma 5.2,

$$\|\mathrm{Ad}^0(R_{V,\theta})\|_{\mathscr{B}(L^2(\Omega))} = \|R_{V,\theta}\|_{\mathscr{B}(L^2(\Omega))} \le C_0,$$
$$\|\mathrm{Ad}^1(R_{V,\theta})\|_{\mathscr{B}(L^2(\Omega))} = 2\theta\,\|R_{V,\theta}\partial_{x_j}R_{V,\theta}\|_{\mathscr{B}(L^2(\Omega))} \le C\,\theta\cdot\theta^{-1/2} = C_1\,\theta^{1/2}.$$

Let us suppose that (5.11) is true for $k \in \{0, 1, \dots, l\}$. Combining identities (5.10) and estimates (5.3) and (5.7) from Lemma 5.2, we get (5.11) for $k = l + 1$:

$$\begin{aligned}
&\big\|\mathrm{Ad}^{l+1}(R_{V,\theta})\big\|_{\mathscr{B}(L^2(\Omega))}\\
&\quad = \big\|\theta\big\{-2(l+1)\mathrm{Ad}^l(R_{V,\theta})\partial_{x_j}R_{V,\theta} + l(l+1)\mathrm{Ad}^{l-1}(R_{V,\theta})R_{V,\theta}\big\}\big\|_{\mathscr{B}(L^2(\Omega))}\\
&\quad \le 2l(l+1)\,\theta\,\big\{\|\mathrm{Ad}^l(R_{V,\theta})\|_{\mathscr{B}(L^2(\Omega))}\|\partial_{x_j}R_{V,\theta}\|_{\mathscr{B}(L^2(\Omega))}\\
&\qquad\qquad + \|\mathrm{Ad}^{l-1}(R_{V,\theta})\|_{\mathscr{B}(L^2(\Omega))}\|R_{V,\theta}\|_{\mathscr{B}(L^2(\Omega))}\big\}\\
&\quad \le C_{l+1}\,\theta\,\big\{\theta^{l/2}\cdot\theta^{-1/2} + \theta^{(l-1)/2}\big\} \le C_{l+1}\,\theta^{(l+1)/2}.
\end{aligned}$$

Thus (5.11) is true for any $k \ge 0$.

We prove (5.2) also by induction. Clearly, (5.2) is true for $k = 0$. As to the case $k = 1$, by using the estimate (5.11) and the formula (B.7) from Lemma B.3 in appendix B:

$$\mathrm{Ad}^1(e^{-itR_{V,\theta}}) = -i\int_0^t e^{-isR_{V,\theta}}\,\mathrm{Ad}^1(R_{V,\theta})\,e^{-i(t-s)R_{\theta,V}}\,ds$$

for each $t \in \mathbb{R}$, we have

$$\begin{aligned}
&\big\|\mathrm{Ad}^1(e^{-itR_{V,\theta}})\big\|_{\mathscr{B}(L^2(\Omega))}\\
&\quad \le \int_0^{|t|}\big\|e^{-isR_{V,\theta}}\big\|_{\mathscr{B}(L^2(\Omega))}\big\|\mathrm{Ad}^1(R_{V,\theta})\big\|_{\mathscr{B}(L^2(\Omega))}\big\|e^{-i(t-s)R_{V,\theta}}\big\|_{\mathscr{B}(L^2(\Omega))}\,ds\\
&\quad \le C_1\int_0^{|t|}\theta^{1/2}\,ds \le C_1\,\theta^{1/2}(1+|t|)
\end{aligned}$$

for any $t \in \mathbb{R}$. Hence, (5.2) is true for $k = 1$. Let us suppose that (5.2) holds for $k \in \{0, 1, \dots, \ell\}$. Then, by using the estimate (5.11) and the formula (B.8) from Lemma B.3:

$$\begin{aligned}
&\mathrm{Ad}^{l+1}(e^{-itR_{V,\theta}}) \\
&\quad = -i \int_0^t \sum_{l_1+l_2+l_3=l} \Gamma(l_1, l_2, l_3)\, \mathrm{Ad}^{l_1}(e^{-isR_{\theta,V}})\, \mathrm{Ad}^{l_2+1}(R_{V,\theta})\, \mathrm{Ad}^{l_3}(e^{-i(t-s)R_{V,\theta}})\, ds,
\end{aligned}$$

where constants $\Gamma(l_1, l_2, l_3)$ are trinomial coefficients:

$$\Gamma(l_1, l_2, l_3) = \frac{l!}{l_1!\, l_2!\, l_3!},$$

we estimate

$$\begin{aligned}
&\big\|\mathrm{Ad}^{l+1}(e^{-itR_{V,\theta}})\big\|_{\mathscr{B}(L^2(\Omega))} \\
&\quad \le C_{l+1} \int_0^t \sum_{l_1+l_2+l_3=l} \big\|\mathrm{Ad}^{l_1}(e^{-isR_{V,\theta}})\big\|_{\mathscr{B}(L^2(\Omega))} \big\|\mathrm{Ad}^{l_2+1}(R_{V,\theta})\big\|_{\mathscr{B}(L^2(\Omega))} \\
&\qquad\qquad \times \big\|\mathrm{Ad}^{l_3}(e^{-i(t-s)R_{V,\theta}})\big\|_{\mathscr{B}(L^2(\Omega))}\, ds \\
&\quad \le C_{l+1} \int_0^t \sum_{l_1+l_2+l_3=l} \theta^{l_1/2}(1+|s|)^{l_1} \cdot \theta^{(l_2+1)/2} \cdot \theta^{l_3/2}(1+|t-s|)^{l_3}\, ds \\
&\quad \le C_{l+1}\, \theta^{(l+1)/2}(1+|t|)^{l+1}
\end{aligned}$$

for any $t \in \mathbb{R}$. Hence (5.2) is true for $k = l + 1$. Thus (5.2) holds for any $k \ge 0$.

The assertion (ii) is proved in the same way as assertion (i) by using the estimate (5.7) from Lemma 5.2 instead of (5.4). The proof of Proposition 5.1 is complete. □

6. L^p-estimates for $\varphi(\theta H_V)$

In this section we prove L^p-boundedness of $\varphi(\theta H_V)$. The goal in this section is the following:

Theorem 6.1. *Let $\varphi \in \mathscr{S}(\mathbb{R})$. Suppose that the potential V satisfies assumption* A. *Let $1 \le p \le \infty$. Then $\varphi(H_V)$ is extended to a bounded linear operator on $L^p(\Omega)$. Furthermore, the following assertions hold:*

(i) *There exists a constant $C > 0$ such that*

$$\|\varphi(\theta H_V)\|_{\mathscr{B}(L^p(\Omega))} \le C \tag{6.1}$$

for any $0 < \theta \le 1$.

(ii) *Assume further that* V_- *satisfies*

$$\begin{cases} \sup_{x\in\Omega} \int_\Omega \frac{V_-(y)}{|x-y|^{d-2}}\,dy < \frac{\pi^{d/2}}{\Gamma(d/2-1)}, & \text{if } d \geq 3, \\ V_- = 0, & \text{if } d = 1, 2. \end{cases}$$

Then the estimate (6.1) *holds for any* $\theta > 0$.

To begin with, let us introduce a family $\mathscr{A}_\alpha$ of operators, which is useful to prove the theorem.

Definition. Let $\alpha > 0$ and $\theta > 0$. We say that $L \in \mathscr{A}_\alpha (= \mathscr{A}_{\alpha,\theta})$ if $L \in \mathscr{B}(L^2(\Omega))$ and

$$\|\!|L|\!\|_\alpha := \sup_{n\in\mathbb{Z}^d} \big\| |\cdot - \theta^{1/2} n|^\alpha L \chi_{C_\theta(n)} \big\|_{\mathscr{B}(L^2(\Omega))} < \infty. \tag{6.2}$$

First we prepare two lemmas.

Lemma 6.2. *Let* $\theta > 0$, *and let* $L \in \mathscr{A}_\alpha$ *for some* $\alpha > d/2$. *Then there exists a constant* $C > 0$ *depending only on* α *and* d *such that*

$$\|Lf\|_{l^1(L^2)_\theta} \leq C\big(\|L\|_{\mathscr{B}(L^2(\Omega))} + \theta^{-d/4} \|\!|L|\!\|_\alpha^{d/2\alpha} \|L\|_{\mathscr{B}(L^2(\Omega))}^{1-d/2\alpha}\big) \|f\|_{l^1(L^2)_\theta} \tag{6.3}$$

for any $f \in l^1(L^2)_\theta$.

Proof. If we prove that

$$\sum_{m\in\mathbb{Z}^d} \big\|\chi_{C_\theta(m)} L \chi_{C_\theta(n)} f\big\|_{L^2(\Omega)} \leq C\big(\|L\|_{\mathscr{B}(L^2(\Omega))} + \theta^{-d/4} \|\!|L|\!\|_\alpha^{d/2\alpha} \|L\|_{\mathscr{B}(L^2(\Omega))}^{1-d/2\alpha}\big) \|\chi_{C_\theta(n)} f\|_{L^2(\Omega)} \tag{6.4}$$

for any $\theta > 0$ and $n \in \mathbb{Z}^d$, then, summing up (6.4) with respect to $n \in \mathbb{Z}^d$, we conclude the required estimate (6.3):

$$\begin{aligned} \|Lf\|_{l^1(L^2)_\theta} &\leq \sum_{n\in\mathbb{Z}^d} \sum_{m\in\mathbb{Z}^d} \big\|\chi_{C_\theta(m)} L \chi_{C_\theta(n)} f\big\|_{L^2(\Omega)} \\ &\leq C\big(\|L\|_{\mathscr{B}(L^2(\Omega))} + \theta^{-d/4} \|\!|L|\!\|_\alpha^{d/2\alpha} \|L\|_{\mathscr{B}(L^2(\Omega))}^{1-d/2\alpha}\big) \|f\|_{l^1(L^2)_\theta} \end{aligned}$$

for any $\theta > 0$ and $f \in l^1(L^2)_\theta$. Hence we have only to prove the estimate (6.4).

Let $n \in \mathbb{Z}^d$ be fixed. For any $\omega > 0$, we write

$$\begin{aligned} &\sum_{m\in\mathbb{Z}^d} \big\|\chi_{C_\theta(m)} L \chi_{C_\theta(n)} f\big\|_{L^2(\Omega)} \\ &= \sum_{|m-n|>\omega} |\theta^{1/2} m - \theta^{1/2} n|^{-\alpha} |\theta^{1/2} m - \theta^{1/2} n|^\alpha \big\|\chi_{C_\theta(m)} L \chi_{C_\theta(n)} f\big\|_{L^2(\Omega)} \\ &\quad + \sum_{|m-n|\leq\omega} \big\|\chi_{C_\theta(m)} L \chi_{C_\theta(n)} f\big\|_{L^2(\Omega)} \\ &=: I(n) + II(n). \end{aligned}$$

By using the Schwarz inequality we estimate $I(n)$ as

$$
\begin{aligned}
I(n) \le \theta^{-\alpha/2}\Big(\sum_{|m-n|>\omega} |m-n|^{-2\alpha}\Big)^{1/2} \\
\times \Big(\sum_{|m-n|>\omega} |\theta^{1/2}m-\theta^{1/2}n|^{2\alpha} \left\|\chi_{C_\theta(m)} L \chi_{C_\theta(n)} f\right\|^2_{L^2(\Omega)}\Big)^{1/2}.
\end{aligned}
\tag{6.5}
$$

The first factor of (6.5) is estimated as

$$
\sum_{|m-n|>\omega} |m-n|^{-2\alpha} = \sum_{|m|>\omega} |m|^{-2\alpha} \le C(d,\alpha)\,\omega^{-2\alpha+d}. \tag{6.6}
$$

In fact, since $\alpha > d/2$, the right member of (6.6) is estimated as

$$
\begin{aligned}
\sum_{|m|>\omega} |m|^{-2\alpha} &\le \prod_{j=1}^{d} \sum_{|m_j|>\omega/\sqrt{d}} |m_j|^{-2\alpha/d} \le C(d,\alpha) \prod_{j=1}^{d} \sum_{|m_j|>\omega/\sqrt{d}} (1+|m_j|)^{-2\alpha/d} \\
&\le C(d,\alpha) \prod_{j=1}^{d} \int_{\{\sigma>\omega/\sqrt{d}\}} \sigma^{-2\alpha/d}\, d\sigma \le C(d,\alpha) \prod_{j=1}^{d} \omega^{-2\alpha/d+1} = C(d,\alpha)\omega^{-2\alpha+d},
\end{aligned}
$$

which implies (6.6). As to the second factor of (6.5), noting that

$$
\frac{|\theta^{1/2}m-\theta^{1/2}n|}{2} \le |x-\theta^{1/2}n|
$$

for any $x \in C_\theta(m)$, we estimate as

$$
\begin{aligned}
&\sum_{|m-n|>\omega} |\theta^{1/2}m-\theta^{1/2}n|^{2\alpha} \left\|\chi_{C_\theta(m)} L \chi_{C_\theta(n)} f\right\|^2_{L^2(\Omega)} \\
&\qquad = \sum_{|m-n|>\omega} |\theta^{1/2}m-\theta^{1/2}n|^{2\alpha} \int_{C_\theta(m)} |L\chi_{C_\theta(n)} f|^2\, dx \\
&\qquad \le 2^{2\alpha} \sum_{|m-n|>\omega} \int_{C_\theta(m)} \left|\, |x-\theta^{1/2}n|^{\alpha} L\chi_{C_\theta(n)} f\right|^2 dx.
\end{aligned}
$$

Moreover, by the definition (6.2) of $|\!|\!| L |\!|\!|_\alpha$, we estimate as

$$
\begin{aligned}
\sum_{|m-n|>\omega} \int_{C_\theta(m)} \left|\, |x-\theta^{1/2}n|^{\alpha} L\chi_{C_\theta(n)} f\right|^2 dx &\le \left\| |\cdot-\theta^{1/2}n|^{\alpha} L\chi_{C_\theta(n)} f\right\|^2_{L^2(\Omega)} \\
&\le |\!|\!| L |\!|\!|^2_\alpha \left\|\chi_{C_\theta(n)} f\right\|^2_{L^2(\Omega)}.
\end{aligned}
$$

Hence, summarizing the above two estimates, we deduce that

$$
\sum_{|m-n|>\omega} |\theta^{1/2}m-\theta^{1/2}n|^{2\alpha} \left\|\chi_{C_\theta(m)} L \chi_{C_\theta(n)} f\right\|^2_{L^2(\Omega)} \le 2^{2\alpha} |\!|\!| L |\!|\!|^2_\alpha \left\|\chi_{C_\theta(n)} f\right\|^2_{L^2(\Omega)}. \tag{6.7}
$$

Thus we find from (6.5)-(6.7) that

$$I(n) \le C(d,\alpha)\,\theta^{-\alpha/2}\,\omega^{-(\alpha-d/2)}\,|||L|||_\alpha\,\big\|\chi_{C_\theta(n)}f\big\|_{L^2(\Omega)}. \tag{6.8}$$

Let us turn to the estimation of $II(n)$. It is readily to see that

$$II(n) \le \Big(\sum_{|m-n|\le\omega} 1\Big)^{1/2}\Big(\sum_{|m-n|\le\omega} \big\|\chi_{C_\theta(m)}L\chi_{C_\theta(n)}f\big\|^2_{L^2(\Omega)}\Big)^{1/2}.$$

Since

$$\sum_{|m-n|\le\omega} 1 \le 1+\omega^d,$$

we deduce from the same argument as in $I(n)$ that

$$\begin{aligned} II(n) &\le (1+\omega^{d/2})\Big(\sum_{|m-n|\le\omega} \big\|\chi_{C_\theta(m)}L\chi_{C_\theta(n)}f\big\|^2_{L^2(\Omega)}\Big)^{1/2} \\ &\le (1+\omega^{d/2})\,\big\|L\chi_{C_\theta(n)}f\big\|_{L^2(\Omega)} \le (1+\omega^{d/2})\|L\|_{\mathscr{B}(L^2(\Omega))}\,\big\|\chi_{C_\theta(n)}f\big\|_{L^2(\Omega)}. \end{aligned} \tag{6.9}$$

Combining the estimates (6.8) and (6.9), we get

$$\begin{aligned} &\sum_{m\in\mathbb{Z}^d} \|\chi_{C_\theta(m)}L\chi_{C_\theta(n)}f\|_{L^2(\Omega)} \\ &\quad \le C(d,\alpha)\big\{\theta^{-\alpha/2}\omega^{-(\alpha-d/2)}|||L|||_\alpha + (1+\omega^{d/2})\|L\|_{\mathscr{B}(L^2(\Omega))}\big\}\big\|\chi_{C_\theta(n)}f\big\|_{L^2(\Omega)}. \end{aligned}$$

Finally, taking

$$\omega = (|||L|||_\alpha/\|L\|_{\mathscr{B}(L^2(\Omega))})^{1/\alpha}\cdot\theta^{-1/2},$$

we obtain the required estimate (6.4). The proof of Lemma 6.2 is complete. □

Lemma 6.3. *Let $\varphi \in \mathscr{S}(\mathbb{R})$. Suppose that the potential V satisfies assumption* A. *Let $\alpha > 0$. Then the following assertions hold:*

(i) *The operator $\varphi(\theta H_V)$ belongs to $\mathscr{A}_\alpha$ for any $0<\theta\le 1$. Furthermore, there exist a constant $C>0$ such that*

$$|||\varphi(\theta H_V)|||_\alpha \le C\theta^{\alpha/2} \tag{6.10}$$

for any $0<\theta\le 1$.

(ii) *Assume further that V_- satisfies*

$$\begin{cases} \sup_{x\in\Omega}\displaystyle\int_\Omega \frac{V_-(y)}{|x-y|^{d-2}}\,dy < \frac{4\pi^{d/2}}{\Gamma(d/2-1)}, & \text{if } d\ge 3, \\ V_- = 0, & \text{if } d=1,2. \end{cases}$$

Then the same conclusion as in the assertion (i) *holds for any $\theta>0$.*

Proof. To begin with, we prove the assertion (i). Let $0<\theta\le 1$ and M be a real number such that

$$M>\max\{-\inf\sigma(H_V),0\}. \tag{6.11}$$

We may assume that $\mathrm{supp}\varphi\subset[-M,\infty)$ without loss of generality. Let us choose $\psi\in C_0^\infty(\mathbb{R})$ such that

$$\psi(\mu)=\chi(\mu)\,\varphi(\mu^{-1}-M),$$

where χ is a smooth function on $\mathbb{R}$ such that

$$\chi(\mu)=\begin{cases}1 & \text{for } 0\le\mu\le\dfrac{1}{M+\inf\sigma(H_V)}+1,\\ 0 & \text{for } \mu\le -1 \text{ and } \mu\ge\dfrac{1}{M+\inf\sigma(H_V)}+2.\end{cases} \tag{6.12}$$

When we consider the operator θH_V for $0<\theta\le 1$, it is possible to take, independently of θ, the real number M satisfying (6.11). Then we write

$$\psi(R_{V,\theta})=\psi\big((\theta H_V+M)^{-1}\big)=\varphi(\theta H_V).$$

In order to prove the estimate (6.10), it suffices to show that

$$\|\!|\psi(R_{V,\theta})|\!\|_\alpha\le C\,\theta^{\alpha/2}\int_{-\infty}^{\infty}(1+|t|)^\alpha\,|\hat\psi(t)|\,dt, \tag{6.13}$$

where $\hat\psi$ is the Fourier transform of ψ on $\mathbb{R}$ and the integral on the right is absolutely convergent, since $\hat\psi\in\mathscr{S}(\mathbb{R})$. The proof is based on the formula:

$$\psi(R_{V,\theta})=(2\pi)^{-1/2}\int_{-\infty}^{\infty}e^{-itR_{V,\theta}}\,\hat\psi(t)\,dt. \tag{6.14}$$

Applying the formula (6.14), we obtain

$$\begin{aligned}\|\!|\psi(R_{V,\theta})|\!\|_\alpha &= \sup_{n\in\mathbb{Z}^d}\big\||\cdot-\theta^{1/2}n|^\alpha\psi(R_{V,\theta})\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))}\\ &\le(2\pi)^{-1/2}\sup_{n\in\mathbb{Z}^d}\int_{-\infty}^{\infty}\big\||\cdot-\theta^{1/2}n|^\alpha e^{-itR_{V,\theta}}\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))}\,|\hat\psi(t)|\,dt.\end{aligned}$$

Let N be a positive integer. Thanks to Lemma B.1 for $A=B=x_j-\theta^{1/2}n_j$ and $L=e^{-itR_{V,\theta}}$, we find from the assertion (i) in Proposition 5.1 that

$$\begin{aligned}&\big\||\cdot-\theta^{1/2}n|^N e^{-itR_{V,\theta}}\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))}\\ &\quad\le\sum_{k=0}^N C(N,k)\big\|\mathrm{Ad}^k(e^{-itR_{V,\theta}})\big\|_{\mathscr{B}(L^2(\Omega))}\big\||\cdot-\theta^{1/2}n|^{N-k}\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))}\\ &\quad\le\sum_{k=0}^N C(N,k)\,\theta^{k/2}(1+|t|)^k\,\theta^{(N-k)/2}\le C\,\theta^{N/2}(1+|t|)^N.\end{aligned}$$

Now, it follows from the Calderón–Lions interpolation theorem (see Theorem IX.20 in Reed and Simon [20]) that

$$\big\| \, | \cdot - \theta^{1/2} n|^\alpha \, e^{-itR_{V,\theta}} \chi_{C_\theta(n)} \big\|_{\mathscr{B}(L^2(\Omega))} \le C \, \theta^{\alpha/2} (1+|t|)^\alpha$$

for any $\alpha > 0$ and $t \in \mathbb{R}$. Thus we conclude (6.13), which proves (6.10).

As to the assertion (ii), noting that $\inf \sigma(H_V) \ge 0$, we can prove the estimate (6.10) for any $\theta > 0$ in the same way as assertion (i) by using the assertion (ii) in Proposition 5.1 instead of assertion (i) in Proposition 5.1. The proof of Lemma 6.3 is finished. □

We are now in a position to prove Theorem 6.1.

Proof of Theorem 6.1. First we prove the assertion (i). Let $0 < \theta \le 1$. It suffices to show L^1-estimate for $\varphi(\theta H_V)$. In fact, if L^1-estimate is proved, then L^∞-estimate is also obtained by duality argument, and hence, the Riesz–Thorin interpolation theorem allows us to conclude L^p-estimates (6.1) for $1 \le p \le \infty$.

Let us proceed the proof of L^1-estimate. Going back to the definition of $l^1(L^2)_\theta$, we estimate

$$\begin{aligned} \|\varphi(\theta H_V) f\|_{L^1(\Omega)} &= \sum_{n \in \mathbb{Z}^d} \|\varphi(\theta H_V) f\|_{L^1(C_\theta(n))} \\ &\le \sum_{n \in \mathbb{Z}^d} |C_\theta(n)|^{1/2} \|\varphi(\theta H_V) f\|_{L^2(C_\theta(n))} \le \theta^{d/4} \, \|\varphi(\theta H_V) f\|_{l^1(L^2)_\theta}, \end{aligned} \tag{6.15}$$

where we used the inequality

$$|C_\theta(n)|^{1/2} \le \theta^{d/4}.$$

Here, given a positive real number β, we choose $\tilde{\varphi} \in \mathscr{S}(\mathbb{R})$ as

$$\tilde{\varphi}(\lambda) = (\lambda + M)^\beta \varphi(\lambda) \quad \text{for } \lambda \in \sigma(H_V), \tag{6.16}$$

where M is a real number such that

$$M > \max\{\omega, 0\},$$

where ω is the constant in Proposition 3.1. Then we write

$$\begin{aligned} \|\varphi(\theta H_V) f\|_{l^1(L^2)_\theta} &= \big\|\varphi(\theta H_V)(\theta H_V + M)^\beta (\theta H_V + M)^{-\beta} f\big\|_{l^1(L^2)_\theta} \\ &= \big\|\tilde{\varphi}(\theta H_V)(\theta H_V + M)^{-\beta} f\big\|_{l^1(L^2)_\theta}. \end{aligned}$$

Applying $\tilde{\varphi}(\theta H_V)$ to the operator A in Lemma 6.2, we get

$$\begin{aligned} &\big\|\tilde{\varphi}(\theta H_V)(\theta H_V + M)^{-\beta} f\big\|_{l^1(L^2)_\theta} \\ &\le C\big(\|\tilde{\varphi}(\theta H_V)\|_{\mathscr{B}(L^2(\Omega))} + \theta^{-d/4} |||\tilde{\varphi}(\theta H_V)|||_\alpha^{d/2\alpha} \|\tilde{\varphi}(\theta H_V)\|_{\mathscr{B}(L^2(\Omega))}^{1-d/2\alpha}\big) \\ &\quad \times \big\|(\theta H_V + M)^{-\beta} f\big\|_{l^1(L^2)_\theta}, \end{aligned} \tag{6.17}$$

where $\alpha > d/2$. Thanks to (6.10) from Lemma 6.3 and (4.4) from Theorem 4.1, the right-hand side of the above inequality is estimated as

$$C\big\{1+\theta^{-d/4}\cdot(\theta^{\alpha/2})^{d/2\alpha}\big\}\,\theta^{-d/4}\,\|f\|_{L^1(\Omega)} = 2C\,\theta^{-d/4}\|f\|_{L^1(\Omega)}.$$

Summarizing the estimates obtained now, we find that

$$\|\varphi(\theta H_V)f\|_{l^1(L^2)_\theta} \le C\,\theta^{-d/4}\|f\|_{L^1(\Omega)}. \tag{6.18}$$

Therefore, combining the estimates (6.15) and (6.18), we conclude that

$$\|\varphi(\theta H_V)f\|_{L^1(\Omega)} \le C\,\|f\|_{L^1(\Omega)}$$

for any $0<\theta\le 1$ and $f\in L^1(\Omega)$.

The assertion (ii) is proved in the same way as assertion (i) by using assertions (ii) in Proposition 4.1 and Lemma 6.3 instead of assertions (i) in Proposition 4.1 and Lemma 6.3, respectively. The proof of Theorem 6.1 is complete. □

7. Proof of Theorems 1.1 and 1.2

This section is devoted to proving the main theorems.

Proof of Theorem 1.1. We prove only the assertion (i), since the assertion (ii) is proved in the same way as assertion (i). Let $0<\theta\le 1$. Let M be a real number such that

$$M > \max\{\omega, 0\},$$

where ω is the constant in Proposition 3.1. Given a positive real number β satisfying

$$\beta > \frac{d}{2}\Big(\frac{1}{p}-\frac{1}{q}\Big),$$

we choose $\tilde\varphi\in\mathscr{S}(\mathbb{R})$ as

$$\tilde\varphi(\lambda) = (\lambda+M)^\beta\varphi(\lambda) \quad \text{for } \lambda\in\sigma(H_V).$$

By using Proposition 4.1 and Theorem 6.1, we estimate

$$\begin{aligned}\|\varphi(\theta H_V)\|_{\mathscr{B}(L^p(\Omega),L^q(\Omega))} &= \|\varphi(\theta H_V)(\theta H_V+M)^\beta(\theta H_V+M)^{-\beta}\|_{\mathscr{B}(L^p(\Omega),L^q(\Omega))}\\ &\le \|\tilde\varphi(\theta H_V)\|_{\mathscr{B}(L^q(\Omega))}\|(\theta H_V+M)^{-\beta}\|_{\mathscr{B}(L^p(\Omega),L^q(\Omega))}\\ &\le C\,\theta^{-(d/2)(1/p-1/q)}\end{aligned}$$

for any p,q satisfying $1\le p\le q\le\infty$. The proof of Theorem 1.1 is complete. □

In the rest of this section we prove Theorem 1.2; L^p-estimates for $\nabla\varphi(\theta H_V)$. We recall the definition (6.2) of norms $|||L|||_\alpha$ of an operator L:

$$|||L|||_\alpha := \sup_{n\in\mathbb{Z}^d}\big\||\cdot-\theta^{1/2}n|^\alpha L\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} < \infty$$

for each $\theta>0$.

Lemma 7.1. *Let* $\varphi \in \mathscr{S}(\mathbb{R})$*. Suppose that the potential* V *satisfies assumption* A*. Let* $\alpha > 0$*. Then the following assertions hold*:

(i) *The operator* $\nabla\varphi(\theta H_V)$ *belongs to* $\mathscr{A}_\alpha$ *for any* $0 < \theta \le 1$*. Furthermore, there exist a constant* $C > 0$ *such that*

$$\|\nabla\varphi(\theta H_V)\|_{\mathscr{B}(L^2(\Omega))} \le C\theta^{-1/2}, \tag{7.1}$$

$$|||\nabla\varphi(\theta H_V)|||_\alpha \le C\theta^{(\alpha-1)/2} \tag{7.2}$$

for any $0 < \theta \le 1$*.*

(ii) *Assume further that* V_- *satisfies*

$$\begin{cases} \sup_{x\in\Omega} \int_\Omega \frac{V_-(y)}{|x-y|^{d-2}}\, dy < \frac{4\pi^{d/2}}{\Gamma(d/2-1)}, & \text{if } d \ge 3, \\ V_- = 0, & \text{if } d = 1, 2. \end{cases}$$

Then the same conclusion as in the assertion (i) *holds for any* $\theta > 0$*.*

Proof. First we prove the assertion (i). Let $0 < \theta \le 1$. We prove the estimate (7.1). Since $\varphi(\theta H_V)f \in \mathcal{D}(H_V)$ for any $f \in L^2(\Omega)$, we estimate

$$\begin{aligned} &\|\nabla\varphi(\theta H_V)f\|^2_{L^2(\Omega)} \\ &\quad= \int_\Omega \left(\nabla\varphi(\theta H_V)f \cdot \nabla\varphi(\theta H_V)f + V|\varphi(\theta H_V)f|^2 - V|\varphi(\theta H_V)f|^2\right) dx \\ &\quad= \langle H_V\varphi(\theta H_V)f, \varphi(\theta H_V)f\rangle_{L^2(\Omega)} + \int_\Omega (V_- - V_+)|\varphi(\theta H_V)f|^2\, dx \\ &\quad\le \langle H_V\varphi(\theta H_V)f, \varphi(\theta H_V)f\rangle_{L^2(\Omega)} + \int_\Omega V_-|\varphi(\theta H_V)f|^2\, dx \\ &\quad=: I + II. \end{aligned} \tag{7.3}$$

Then, applying Theorem 1.1 to $H_V\varphi(\theta H_V)f$ and $\varphi(\theta H_V)f$, we estimate I as

$$I \le \|H_V\varphi(\theta H_V)f\|_{L^2(\Omega)}\, \|\varphi(\theta H_V)f\|_{L^2(\Omega)} \le C\,\theta^{-1}\|f\|^2_{L^2(\Omega)}. \tag{7.4}$$

As to the second term II, by using the inequality (2.5) from Lemma 2.3, we have

$$II \le \varepsilon\, \|\nabla\varphi(\theta H_V)f\|^2_{L^2(\Omega)} + b_\varepsilon\, \|\varphi(\theta H_V)f\|^2_{L^2(\Omega)}$$

for any $\varepsilon > 0$. Noting the trivial inequality $\theta^{-1} > 1$, and using (6.1) from Theorem 6.1, we get

$$b_\varepsilon\, \|\varphi(\theta H_V)f\|^2_{L^2(\Omega)} \le C\, b_\varepsilon\, \theta^{-1}\|f\|^2_{L^2(\Omega)};$$

whence

$$II \le \varepsilon\, \|\nabla\varphi(\theta H_V)f\|^2_{L^2(\Omega)} + Cb_\varepsilon\, \theta^{-1}\|f\|^2_{L^2(\Omega)}. \tag{7.5}$$

Here we choose ε as $0 < \varepsilon < 1$. Then, combining the estimates (7.3)–(7.5), we conclude the estimate (7.1).

Next we prove the estimate (7.2). Let M be a real number such that

$$M > \max\{-\inf \sigma(H_V), 0\}.$$

We may assume that $\operatorname{supp} \varphi \subset [-M, \infty)$ without loss of generality. Let us choose $\psi \in C_0^\infty(\mathbb{R})$ such that

$$\psi(\mu) = \chi(\mu)\, \mu^{-1} \varphi(\mu^{-1} - M), \tag{7.6}$$

where χ is a smooth function on $\mathbb{R}$ satisfying (6.12). Then we write

$$\nabla \varphi(\theta H_V) = \nabla R_{V,\theta} \psi(R_{V,\theta}).$$

Hence we have only to show that there exists a constant $C > 0$ such that

$$\left\|\!\left|\nabla R_{V,\theta} \psi(R_{V,\theta})\right|\!\right\|_\alpha \le C\, \theta^{(\alpha-1)/2} \tag{7.7}$$

for any $0 < \theta \le 1$.

It suffices to show the estimate (7.7) for positive integers α by using the Calderón–Lions interpolation theorem. We prove (7.7) only for $\alpha = 1$, since the cases $\alpha \ge 2$ are proved by the induction with Lemmas B.2 and B.3. Let $j \in \{1, 2, \dots, d\}$ be fixed. By the formula (6.14), we have

$$\begin{aligned}
&\left\|\!\left|\partial_{x_j} R_{V,\theta} \psi(R_{V,\theta})\right|\!\right\|_1 \\
&\qquad = \sup_{n \in \mathbb{Z}^d} \left\| |\cdot - \theta^{1/2} n|\, \partial_{x_j} R_{V,\theta} \psi(R_{V,\theta}) \chi_{C_\theta(n)} \right\|_{\mathscr{B}(L^2(\Omega))} \\
&\qquad \le \sup_{n \in \mathbb{Z}^d} (2\pi)^{-1/2} \int_{-\infty}^{\infty} \left\| |\cdot - \theta^{1/2} n|\, \partial_{x_j} R_{V,\theta}\, e^{-itR_\theta} \chi_{C_\theta(n)} \right\|_{\mathscr{B}(L^2(\Omega))} |\hat{\psi}(t)|\, dt.
\end{aligned} \tag{7.8}$$

If we show that

$$\left\| |\cdot - \theta^{1/2} n|\, \partial_{x_j} R_{V,\theta}\, e^{-itR_\theta} \chi_{C_\theta(n)} \right\|_{\mathscr{B}(L^2(\Omega))} \le C(1 + |t|) \tag{7.9}$$

for any $t \in \mathbb{R}$ and $n \in \mathbb{Z}^d$, then we conclude from (7.8) that

$$\left\|\!\left|\partial_{x_j} R_{V,\theta} \psi(R_{V,\theta})\right|\!\right\|_1 \le C (2\pi)^{-1/2} \int_{-\infty}^{\infty} (1 + |t|)\, |\hat{\psi}(t)|\, dt \left(= C\, \theta^{(1-1)/2} \right)$$

for all $j = 1, 2, \dots, d$, which is the estimate (7.7) for $\alpha = 1$. Hence we pay attention to prove (7.9). Writing

$$\begin{aligned}
&(x_k - \theta^{1/2} n_k)\, \partial_{x_j} R_{V,\theta}\, e^{-itR_{V,\theta}} \\
&\quad = \partial_{x_j} \left[(x_k - \theta^{1/2} n_k) R_{V,\theta}\, e^{-itR_{V,\theta}} \right] - \delta_{jk}\, R_{V,\theta}\, e^{-itR_{V,\theta}} \\
&\quad = \partial_{x_j} R_{V,\theta} (x_k - \theta^{1/2} n_k)\, e^{-itR_{V,\theta}} + \partial_{x_j} \mathrm{Ad}^1(R_{V,\theta}) e^{-itR_{V,\theta}} - \delta_{jk}\, R_{V,\theta}\, e^{-itR_{V,\theta}} \\
&\quad = \partial_{x_j} R_{V,\theta}\, e^{-itR_{V,\theta}} (x_k - \theta^{1/2} n_k) + \partial_{x_j} R_{V,\theta} \mathrm{Ad}^1(e^{-itR_{V,\theta}}) \\
&\qquad + \partial_{x_j} \mathrm{Ad}^1(R_{V,\theta}) e^{-itR_{V,\theta}} - \delta_{jk}\, R_{V,\theta}\, e^{-itR_{V,\theta}}
\end{aligned}$$

for all $k = 1, 2, \dots, d$, where we have chosen A and B in the operators $\mathrm{Ad}^1(R_{V,\theta})$ and $\mathrm{Ad}^1(e^{-itR_{V,\theta}})$ as

$$A = B = x_k - \theta^{1/2} n_k,$$

and δ_{jk} is Kronecker's delta, we estimate

$$\begin{aligned}
&\big\|(x_k - \theta^{1/2}n_k)\partial_{x_j} R_{V,\theta}\, e^{-itR_\theta} \chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} \\
&\le \big\|\partial_{x_j} R_{V,\theta}\, e^{-itR_{V,\theta}} (x_k - \theta^{1/2}n_k)\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} \\
&\quad + \big\|\partial_{x_j} R_{V,\theta} \mathrm{Ad}^1(e^{-itR_{V,\theta}})\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} \\
&\quad + \big\|\partial_{x_j} \mathrm{Ad}^1(R_{V,\theta}) e^{-itR_{V,\theta}}\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} + \big\|\delta_{jk} R_{V,\theta}\, e^{-itR_{V,\theta}}\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} \\
&=: I + II + III + IV
\end{aligned}$$

for all $k = 1, 2, \dots, d$. Noting that there exists a constant $C > 0$ such that

$$\big\|(x_k - \theta^{1/2}n_k)\chi_{C_\theta(n)} f\big\|_{L^2(\Omega)} \le C\,\theta^{1/2}\|f\|_{L^2(\Omega)} \tag{7.10}$$

for any $\theta > 0$ and $n \in \mathbb{Z}^d$, we use the estimate (5.4) on $\nabla R_{V,\theta}$ from Lemma 5.2 to deduce that

$$\begin{aligned}
I &\le \big\|\partial_{x_j} R_{V,\theta}\big\|_{\mathscr{B}(L^2(\Omega))} \|e^{-itR_{V,\theta}}\|_{\mathscr{B}(L^2(\Omega))} \big\|(x_k - \theta^{1/2}n_k)\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} \\
&\le C\,\theta^{-1/2}\cdot\theta^{1/2} = C\,.
\end{aligned}$$

As to the second term II, we estimate by using (5.2) for $k = 1$ from Proposition 5.1 and (5.4) from Lemma 5.2:

$$\begin{aligned}
II &\le \big\|\partial_{x_j} R_{V,\theta}\big\|_{\mathscr{B}(L^2(\Omega))} \big\|\mathrm{Ad}^1(e^{-itR_{V,\theta}})\big\|_{\mathscr{B}(L^2(\Omega))} \big\|\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} \\
&\le C\,\theta^{-1/2}\cdot\theta^{1/2}(1 + |t|) = C\,(1 + |t|).
\end{aligned}$$

As to the third term III, we use (B.3) from Lemma B.2:

$$\mathrm{Ad}^1(R_{V,\theta}) = -2\theta R_{V,\theta}\,\partial_{x_k} R_{V,\theta}.$$

Then we estimate, by using (5.4) from Lemma 5.2,

$$\begin{aligned}
III &= 2\theta\,\big\|\partial_{x_j} R_{V,\theta}\partial_{x_k} R_{V,\theta}\, e^{-itR_{V,\theta}}\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} \\
&\le 2\theta\,\big\|\partial_{x_j} R_{V,\theta}\big\|_{\mathscr{B}(L^2(\Omega))} \big\|\partial_{x_k} R_{V,\theta}\big\|_{\mathscr{B}(L^2(\Omega))} \big\|e^{-itR_{V,\theta}}\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} \\
&\le C\,\theta\cdot\theta^{-1/2}\cdot\theta^{-1/2} = C\,.
\end{aligned}$$

As to the fourth term IV, we readily see that

$$IV \le \big\|R_{V,\theta}\big\|_{\mathscr{B}(L^2(\Omega))} \big\|e^{-itR_{V,\theta}}\big\|_{\mathscr{B}(L^2(\Omega))} \big\|\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} \le C\,.$$

Combining all the above estimates, we arrive at the following:

$$\big\|(x_k - \theta^{1/2}n_k)\partial_{x_j} R_{V,\theta}\, e^{-itR_\theta}\chi_{C_\theta(n)}\big\|_{\mathscr{B}(L^2(\Omega))} \le C\,(1 + |t|)$$

for all $k = 1, 2, \dots, d$, which imply the estimate (7.9). The assertion (ii) is proved in the similar way to assertion (i). In fact, we have only to use the inequality (2.7) instead of (2.5), and assertions (ii) instead of assertions (i) from Lemmas 5.2 and 6.3. Thus the proof of Lemma 7.1 is finished. □

Proof of Theorem 1.2. We prove only the assertion (i), since the assertion (ii) is proved in the same way as assertion (i). Let $0 < \theta \le 1$. It suffices to show L^1-estimate for $\nabla\varphi(\theta H_V)$, since L^2-estimate has been already proved in (7.1) and L^p-estimates are proved by the Riesz–Thorin interpolation theorem.

Going back to the definition of $l^1(L^2)_\theta$, we estimate

$$\begin{aligned}\big\|\nabla\varphi(\theta H_V)f\big\|_{L^1(\Omega)} &= \sum_{n\in\mathbb{Z}^d}\|\nabla\varphi(\theta H_V)f\|_{L^1(C_\theta(n))}\\ &\le \sum_{n\in\mathbb{Z}^d}|C_\theta(n)|^{1/2}\|\nabla\varphi(\theta H_V)f\|_{L^2(C_\theta(n))} \le \theta^{d/4}\|\nabla\varphi(\theta H_V)f\|_{l^1(L^2)_\theta},\end{aligned} \tag{7.11}$$

where we used

$$|C_\theta(n)|^{1/2} \le \theta^{d/4}.$$

Let M be a real number such that

$$M > \max\{\omega, 0\},$$

where ω is the constant in Proposition 3.1. Here, given a positive real number β, we choose $\tilde\varphi \in \mathscr{S}(\mathbb{R})$ as

$$\tilde\varphi(\lambda) = (\lambda + M)^\beta\varphi(\lambda) \quad \text{for } \lambda \in \sigma(H_V).$$

Then we write

$$\|\nabla\varphi(\theta H_V)f\|_{l^1(L^2)_\theta} = \big\|\nabla\tilde\varphi(\theta H_V)(\theta H_V + M)^{-\beta}f\big\|_{l^1(L^2)_\theta}.$$

Applying $\nabla\tilde\varphi(\theta H_V)$ to the operator A in Lemma 6.2, we get

$$\begin{aligned}&\big\|\nabla\tilde\varphi(\theta H_V)(\theta H_V + M)^{-\beta}f\big\|_{l^1(L^2)_\theta}\\ &\quad\le C\big(\|\nabla\tilde\varphi(\theta H_V)\|_{\mathscr{B}(L^2(\Omega))} + \theta^{-d/4}|\!|\!|\nabla\tilde\varphi(\theta H_V)|\!|\!|_\alpha^{d/2\alpha}\|\nabla\tilde\varphi(\theta H_V)\|_{\mathscr{B}(L^2(\Omega))}^{1-d/2\alpha}\big)\\ &\qquad\times\big\|(\theta H_V + M)^{-\beta}f\big\|_{l^1(L^2)_\theta}\end{aligned}$$

for any $\alpha > d/2$. Thanks to Lemma 7.1 and (4.4) from Theorem 4.1, the right-hand side of the above inequality is estimated as

$$\begin{aligned}&C\big\{\theta^{-1/2} + \theta^{-d/4}\cdot(\theta^{(\alpha-1)/2})^{d/2\alpha}\cdot(\theta^{-1/2})^{1-d/2\alpha}\big\}\theta^{-d/4}\|f\|_{L^1(\Omega)}\\ &\qquad\qquad\le C\,\theta^{-d/4-1/2}\|f\|_{L^1(\Omega)},\end{aligned}$$

provided $\beta > d/4$. Summarizing the estimates obtained now, we find that

$$\|\nabla\varphi(\theta H_V)f\|_{l^1(L^2)_\theta} \le C\,\theta^{-d/4-1/2}\|f\|_{L^1(\Omega)}. \tag{7.12}$$

Therefore, combining the estimates (7.11) and (7.12), we conclude that

$$\|\nabla\varphi(\theta H_V)f\|_{L^1(\Omega)} \le C\,\theta^{-1/2}\|f\|_{L^1(\Omega)}$$

for any $0 < \theta \le 1$ and $f \in L^1(\Omega)$. The proof of Theorem 1.2 is complete. □

8. Final remarks

In this section we shall give two remarks on the estimates for the operator $\varphi(H_V)$; the first remark is to weaken the assumption that $\varphi \in \mathscr{S}(\mathbb{R})$ in Theorems 1.1 and 1.2, and the second one is about the estimates for the operators $H_V^m \varphi(\theta H_V)$ for an integer m.

First, the function φ in Theorems 1.1 and 1.2 can be taken from the weighted Sobolev spaces. In fact, let m be an integer with $m > (d+1)/2$, and β a real number with $\beta > d/4 + (d/2)(1/p - 1/q)$. If the measurable potential V satisfies assumption A, then there exists a constant $C_0 > 0$, independent of φ, such that

$$\|\varphi(\theta H_V)\|_{\mathscr{B}(L^p(\Omega), L^q(\Omega))} \le C_0 \big\|(1+|\cdot|^2)^{(\beta+m)/2}\varphi\big\|_{H^m(\mathbb{R})} \tag{8.1}$$

for any $0 < \theta \le 1$. Needless to say, once the estimate (8.1) is established for $0 < \theta \le 1$, after some trivial changes, if we further assume (1.2) on V, then the estimate (8.1) holds for any $\theta > 0$. We prove this estimate only for $0 < \theta \le 1$. To begin with, we show (8.1) for $p = q$. Let us define $\tilde{\varphi}$ as in (6.16):

$$\tilde{\varphi}(\lambda) = (\lambda + M)^\beta \varphi(\lambda) \quad \text{for } \lambda \in \sigma(H_V),$$

where $\beta > d/4$. We note that

$$\|\tilde{\varphi}(\theta H_V)\|_{\mathscr{B}(L^2(\Omega))} \le \|\tilde{\varphi}\|_{L^\infty(\mathbb{R})}$$

for any $0 < \theta \le 1$. Indeed, we have:

$$\|\tilde{\varphi}(\theta H_V) f\|^2_{L^2(\Omega)} = \int_{\inf \sigma(H_V)}^\infty |\tilde{\varphi}(\theta\lambda)|^2 \, d\|E_{H_V}(\lambda) f\|^2_{L^2(\Omega)} \le \|\tilde{\varphi}\|^2_{L^\infty(\mathbb{R})} \|f\|^2_{L^2(\Omega)}$$

for any $0 < \theta \le 1$. Then, following the proof of Theorem 6.1, we estimate

$$\|\varphi(\theta H_V)\|_{\mathscr{B}(L^p(\Omega))} \le C\big(\|\tilde{\varphi}\|_{L^\infty(\mathbb{R})} + \theta^{-d/4} \|\!|\tilde{\varphi}(\theta H_V)|\!\|_\alpha^{d/2\alpha} \|\tilde{\varphi}\|^{1-d/2\alpha}_{L^\infty(\mathbb{R})}\big) \tag{8.2}$$

for any $\alpha > d/2$ and $0 < \theta \le 1$. To estimate the quantity $\|\!|\tilde{\varphi}(\theta H_V)|\!\|_\alpha$, let us choose ψ such that

$$\psi(\mu) = \chi(\mu)\, \tilde{\varphi}(\mu^{-1} - M), \tag{8.3}$$

where χ is a smooth function on $\mathbb{R}$ satisfying (6.12). Then we write

$$\tilde{\varphi}(\theta H_V) = \psi(R_{V,\theta}).$$

From the estimate (6.13) in the proof of Theorem 6.1, we get, by using Schwarz' inequality and Plancherel's identity,

$$\begin{aligned} \|\!|\tilde{\varphi}(\theta H_V)|\!\|_\alpha &\le C\,\theta^{\alpha/2} \int_{-\infty}^\infty (1+|t|)^\alpha |\hat{\psi}(t)|\, dt, \\ &\le C\,\theta^{\alpha/2} \big\|(1+|\cdot|)^{\alpha-m}\big\|_{L^2(\mathbb{R})} \big\|(1+|\cdot|)^m \hat{\psi}\big\|_{L^2(\mathbb{R})} = C\,\theta^{\alpha/2} \|\psi\|_{H^m(\mathbb{R})}, \end{aligned}$$

provided that the integer m satisfies

$$m > \alpha + \frac{1}{2} > \frac{d+1}{2}.$$

Hence, noting from the definition (8.3) of ψ that

$$\begin{aligned}
\|\psi\|^2_{H^m(\mathbb{R})} &= \sum_{k=0}^{m} \int_{\mathbb{R}} \Big| \frac{d^k}{d\mu^k}\{\chi(\mu)\tilde{\varphi}(\mu^{-1} - M)\}\Big|^2 d\mu \\
&\le C\Big\{ \int_{\inf \sigma(H_V)}^{\infty} |\tilde{\varphi}(\lambda)|^2 (\lambda + M)^{-2} d\lambda + \sum_{k=1}^{m} \int_{\inf \sigma(H_V)}^{\infty} \Big| \frac{d^k}{d\lambda^k}\{(\lambda+M)^k \tilde{\varphi}(\lambda)\}\Big|^2 d\lambda \Big\} \\
&\le C \big\|(1 + |\cdot|^2)^{m/2} \tilde{\varphi}\big\|^2_{H^m(\mathbb{R})} \le C \big\|(1 + |\cdot|^2)^{(\beta+m)/2} \varphi\big\|^2_{H^m(\mathbb{R})},
\end{aligned}$$

we obtain

$$\|\!|\!|\tilde{\varphi}(\theta H_V)|\!|\!|_{\alpha} \le C\, \theta^{\alpha/2} \big\|(1 + |\cdot|^2)^{(\beta+m)/2} \varphi\big\|_{H^m(\mathbb{R})}. \tag{8.4}$$

Furthermore, by using Sobolev's inequality, we have

$$\|\tilde{\varphi}\|_{L^\infty(\mathbb{R})} = \big\|(\cdot + M)^\beta \varphi\big\|_{L^\infty(\mathbb{R})} \le C \big\|(1 + |\cdot|)^\beta \varphi\big\|_{H^1(\mathbb{R})}. \tag{8.5}$$

Therefore, applying (8.4) and (8.5) to (8.2), we conclude that

$$\big\|\varphi(\theta H_V)\big\|_{\mathscr{B}(L^p(\Omega))} \le C_0 \big\|(1 + |\cdot|^2)^{(\beta+m)/2} \varphi\big\|_{H^m(\mathbb{R})},$$

which implies (8.1) for $p = q$.

In the case when $p < q$, we can also prove (8.1) by the same way as above, if φ in the above argument is replaced by $(\lambda + M)^{\beta'}\varphi$ for $\beta' > (d/2)(1/p - 1/q)$.

Secondly, in the proof of Theorem 1.1, if we choose $\tilde{\varphi} \in \mathscr{S}(\mathbb{R})$ as

$$\tilde{\varphi}(\lambda) = \lambda^m (\lambda + M)^\beta \varphi(\lambda) \quad \text{for } \lambda \in \sigma(H_V),$$

the argument is effective also for the operators $H_V^m \varphi(H_V)$. More precisely, we have:

Theorem 8.1. *Let $\varphi \in \mathscr{S}(\mathbb{R})$. Suppose that the potential V satisfies assumption* A. *Let m be a non-negative integer, and let $1 \le p \le q \le \infty$. Then the following assertions hold*:

(i) *There exists a constant $C > 0$ such that*

$$\big\|H_V^m \varphi(\theta H_V)\big\|_{\mathscr{B}(L^p(\Omega), L^q(\Omega))} \le C\, \theta^{-(d/2)(1/p-1/q)-m} \tag{8.6}$$

for any $0 < \theta \le 1$.

(ii) *Assume further that V_- satisfies*

$$\begin{cases} \sup_{x\in\Omega} \int_{\Omega} \frac{V_-(y)}{|x-y|^{d-2}}\, dy < \frac{\pi^{d/2}}{\Gamma(d/2-1)}, & \text{if } d \ge 3, \\ V_- = 0, & \text{if } d = 1, 2. \end{cases}$$

Then the estimate (8.6) holds for any $\theta > 0$.

We note that the estimates (8.6) are useful to discuss several properties of Besov spaces generated by H_V. This topic will be done elsewhere.

A. The Young inequality

In this appendix we introduce the Young inequality for scaled amalgam spaces.

Lemma A.1. *Let $d \geq 1$, and let $1 \leq p, p_1, p_2, q, q_1, q_2 \leq \infty$ be such that*

$$\frac{1}{p_1} + \frac{1}{p_2} - 1 = \frac{1}{p} \quad \text{and} \quad \frac{1}{q_1} + \frac{1}{q_2} - 1 = \frac{1}{q}.$$

If $f \in l^{p_1}(L^{q_1})_\theta(\mathbb{R}^d)$ and $g \in l^{p_2}(L^{q_2})_\theta(\mathbb{R}^d)$, then $f * g \in l^p(L^q)_\theta(\mathbb{R}^d)$ and

$$\|f * g\|_{l^p(L^q)_\theta(\mathbb{R}^d)} \leq 3^d \|f\|_{l^{p_1}(L^{q_1})_\theta(\mathbb{R}^d)} \|g\|_{l^{p_2}(L^{q_2})_\theta(\mathbb{R}^d)}. \tag{A.1}$$

For the proof of Lemma A.1, see Fournier and Stewart [9] (see also [15]).

B. Recursive formula of operators

In this appendix we shall introduce some formulas on the operator Ad.

Lemma B.1 (Lemma 3.1 in [15])**.** *Let X and Y be topological vector spaces, and let A and B be continuous linear operators from X and Y into themselves, respectively. If L is a continuous linear operator from X into Y, then there exists a set of constants $\{C(n,m) \,|\, n \geq 0,\, 0 \leq m \leq n\}$ such that*

$$B^n L = \sum_{m=0}^{n} C(n,m)\, \mathrm{Ad}^m(L)\, A^{n-m}. \tag{B.1}$$

We shall derive two kind of recursive formulas of operator

$$R_{V,\theta} = (\theta H_V + M)^{-1}, \quad \theta > 0, \tag{B.2}$$

where M is a certain large constant. Hereafter we put

$$X = \mathscr{D}(\Omega), \quad Y = \mathscr{D}'(\Omega),$$

where we denote by $\mathscr{D}(\Omega)$ the totality of the test functions on Ω, and by $\mathscr{D}'(\Omega)$ its dual space, and we take

$$A = B = x_j - \theta^{1/2} n_j \quad \text{for some } j \in \{1, \dots, d\}.$$

Lemma B.2. *Let V be a measurable function on Ω such that H_V is a self-adjoint operator on $L^2(\Omega)$ whose domain is given by*

$$\mathcal{D}(H_V) = \{u \in H_0^1(\Omega) \,|\, \sqrt{V_+}u \in L^2(\Omega),\ H_V u \in L^2(\Omega)\}.$$

Let M be an element of resolvent set of $-\theta H_V$, and let us denote by $R_{V,\theta}$ the resolvent operator defined by (B.2). Then the sequence $\{\mathrm{Ad}^k(R_{V,\theta})\}_{k=0}^{\infty}$ of operators satisfies the following recursive formula:

$$\mathrm{Ad}^0(R_{V,\theta}) = R_{V,\theta}, \quad \mathrm{Ad}^1(R_{V,\theta}) = -2\theta R_{V,\theta}\,\partial_{x_j} R_{V,\theta}, \tag{B.3}$$

and for $k \geq 2$,

$$\mathrm{Ad}^k(R_{V,\theta}) = \theta\big\{-2k\mathrm{Ad}^{k-1}(R_{V,\theta})\partial_{x_j} R_{V,\theta} + k(k-1)\mathrm{Ad}^{k-2}(R_{V,\theta})R_{V,\theta}\big\}. \tag{B.4}$$

Proof. When $k = 0$, the first equation in (B.3) is trivial. Hence it is sufficient to prove the case when $k > 0$. For the sake of simplicity, we perform a formal argument without considering the domain of operators. The rigorous argument is given in the final part.

Let us introduce the generalized binomial coefficients $\Gamma(k,m)$ as follows:

$$\Gamma(k,m) = \begin{cases} \dfrac{k!}{(k-m)!\,m!}, & k \geq m \geq 0, \\ 0, & k < m \text{ or } k < 0. \end{cases}$$

Once the following recursive formula is established:

$$\mathrm{Ad}^k(R_{V,\theta}) = -\sum_{m=0}^{k-1} \Gamma(k,m)\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{k-m}(\theta H_V)R_{V,\theta}, \quad k = 1, 2, \dots, \tag{B.5}$$

identities (B.3) and (B.4) are an immediate consequence of (B.5), since

$$\mathrm{Ad}^1(\theta H_V) = 2\theta\partial_{x_j}, \quad \mathrm{Ad}^2(\theta H_V) = -2\theta, \quad \mathrm{Ad}^k(\theta H_V) = 0, \quad k \geq 3.$$

Hence, all we have to do is to prove (B.5). We proceed the argument by induction. For $k = 1$, it can be readily checked that

$$\begin{aligned}\mathrm{Ad}^1(R_{V,\theta}) &= x_j R_{V,\theta} - R_{V,\theta}x_j = R_{V,\theta}(\theta H_V + M)x_j R_{V,\theta} - R_{V,\theta}x_j(\theta H_V + M)R_{V,\theta} \\ &= R_{V,\theta}\left(\theta H_V x_j - x_j \cdot \theta H_V\right) R_{V,\theta} = -R_{V,\theta}\mathrm{Ad}^1(\theta H_V)R_{V,\theta} \\ &= -\Gamma(1,0)\mathrm{Ad}^0(R_{V,\theta})\mathrm{Ad}^1(\theta H_V)R_{V,\theta}.\end{aligned}$$

Hence (B.5) is true for $k = 1$. For $l = 1, 2, \dots$, let us suppose that (B.5) holds for $k = 1, \dots, l$. Writing

$$\mathrm{Ad}^{l+1}(R_{V,\theta}) = x_j\mathrm{Ad}^l(R_{V,\theta}) - \mathrm{Ad}^l(R_{V,\theta})x_j, \tag{B.6}$$

we see that the first term becomes

$$\begin{aligned}x_j\mathrm{Ad}^l(R_{V,\theta}) &= x_j\Big\{-\sum_{m=0}^{l-1}\Gamma(l,m)\,\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l-m}(\theta H_V)\Big\}R_{V,\theta} \\ &= -\sum_{m=0}^{l-1}\Gamma(l,m)\big\{\mathrm{Ad}^{m+1}(R_{V,\theta})\mathrm{Ad}^{l-m}(\theta H_V) + \mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l-m+1}(\theta H_V)\big\}R_{V,\theta} \\ &\quad -\sum_{m=0}^{l-1}\Gamma(l,m)\,\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l-m}(\theta H_V)x_j R_{V,\theta} \\ &=: I_1 + I_2.\end{aligned}$$

Here I_1 is written as

$$\begin{aligned}
I_1 &= -\sum_{m=1}^{l} \Gamma(l,m-1)\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l-m+1}(\theta H_V)R_{V,\theta} \\
&\quad - \sum_{m=0}^{l-1} \Gamma(l,m)\,\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l-m+1}(\theta H_V)R_{V,\theta} \\
&= -\sum_{m=0}^{l} \Gamma(l,m-1)\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l+1-m}(\theta H_V)R_{V,\theta} \\
&\quad - \sum_{m=0}^{l} \Gamma(l,m)\,\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l-m+1}(\theta H_V)R_{V,\theta} + \mathrm{Ad}^l(R_{V,\theta})\mathrm{Ad}^1(\theta H_V)R_{V,\theta} \\
&= -\sum_{m=0}^{l} \Gamma(l+1,m)\,\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l+1-m}(\theta H_V)R_{V,\theta} + \mathrm{Ad}^l(R_{V,\theta})\mathrm{Ad}^1(\theta H_V)R_{V,\theta},
\end{aligned}$$

where we used

$$\Gamma(l,m-1) + \Gamma(l,m) = \Gamma(l+1,m)$$

in the last step. As to I_2, we write as

$$\begin{aligned}
I_2 &= -\Big\{ \sum_{m=0}^{l-1} \Gamma(l,m)\,\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l-m}(\theta H_V)R_{V,\theta} \Big\}(\theta H_V + M)\, x_j R_{V,\theta} \\
&= \mathrm{Ad}^l(R_{V,\theta})(\theta H_V + M)\, x_j R_{V,\theta}.
\end{aligned}$$

Hence, summarizing the previous equations, we get

$$\begin{aligned}
x_j \mathrm{Ad}^l(R_{V,\theta}) = -&\sum_{m=0}^{l} \Gamma(l+1,m)\,\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l+1-m}(\theta H_V) \\
&+ \mathrm{Ad}^l(R_{V,\theta})\left\{\mathrm{Ad}^1(\theta H_V) + (\theta H_V + M)x_j\right\} R_{V,\theta}.
\end{aligned}$$

Therefore, going back to (B.6), and noting

$$\mathrm{Ad}^1(\theta H_V) + (\theta H_V + M)x_j = x_j(\theta H_V + M),$$

we conclude that

$$\begin{aligned}
\mathrm{Ad}^{l+1}(R_{V,\theta}) &= -\sum_{m=0}^{l} \Gamma(l+1,m)\,\mathrm{Ad}^m(R_{V,\theta})\,\mathrm{Ad}^{l+1-m}(\theta H_V) \\
&\quad + \mathrm{Ad}^l(R_{V,\theta})\left\{\mathrm{Ad}^1(\theta H_V) + (\theta H_V + M)\, x_j\right\} R_{V,\theta} - \mathrm{Ad}^l(R_{V,\theta})\, x_j \\
&= -\sum_{m=0}^{l} \Gamma(l+1,m)\,\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l+1-m}(\theta H_V) \\
&\quad + \mathrm{Ad}^l(R_{V,\theta})\, x_j(\theta H_V + M)R_{V,\theta} - \mathrm{Ad}^l(R_{V,\theta})\, x_j \\
&= -\sum_{m=0}^{l} \Gamma(l+1,m)\,\mathrm{Ad}^m(R_{V,\theta})\mathrm{Ad}^{l+1-m}(\theta H_V).
\end{aligned}$$

Hence (B.5) is true for $k = l+1$.

The above proof is formal in the sense that the domain of operators is not taken into account in the argument. In fact, even for $f \in C_0^\infty(\Omega)$, each $x_j R_{V,\theta} f$ does not necessarily belong to the domain of H_V, since we only know the fact that

$$R_{V,\theta} f \in \mathcal{D}(H_V) = \big\{ u \in H_0^1(\Omega) \,\big|\, \sqrt{V_+}u \in L^2(\Omega),\ H_V u \in L^2(\Omega) \big\}.$$

Therefore, we should perform the argument by using a duality pair ${}_{\mathscr{D}'(\Omega)}\langle \cdot, \cdot \rangle_{\mathscr{D}(\Omega)}$ of $\mathscr{D}'(\Omega)$ and $\mathscr{D}(\Omega)$ in a rigorous way. We may prove the lemma only for $k = 1$. For, as to the case $k > 1$, the argument is done in a similar manner. Now we write

$${}_{\mathscr{D}'(\Omega)}\langle \mathrm{Ad}^1(R_{V,\theta}) f, g \rangle_{\mathscr{D}(\Omega)} = \langle R_{V,\theta} f, x_j g \rangle_{L^2(\Omega)} - \langle x_j f, R_{V,\theta} g \rangle_{L^2(\Omega)} =: I - II$$

for $f, g \in C_0^\infty(\Omega)$. Since $R_{V,\theta} f, R_{V,\theta} g \in H_0^1(\Omega)$, there exist two sequences $\{f_n\}_n$, $\{g_m\}_m$ in $C_0^\infty(\Omega)$ such that

$$f_n \to R_{V,\theta} f \quad \text{and} \quad g_m \to R_{V,\theta} g \quad \text{in } H^1(\Omega) \text{ as } n, m \to \infty.$$

Hence we obtain by $x_j f_n, x_j g_m \in C_0^\infty(\Omega)$,

$$\begin{aligned}
I &= \lim_{n\to\infty} \langle f_n, x_j g \rangle_{L^2(\Omega)} \\
&= \lim_{n\to\infty} \langle x_j f_n, (\theta H_V + M) R_{V,\theta} g \rangle_{L^2(\Omega)} \\
&= \lim_{n\to\infty} \big\{ \theta \langle \nabla(x_j f_n), \nabla R_{V,\theta} g \rangle_{L^2(\Omega)} + \langle (\theta V + M) x_j f_n, R_{V,\theta} g \rangle_{L^2(\Omega)} \big\} \\
&= \lim_{n,m\to\infty} \big\{ \theta \langle \nabla(x_j f_n), \nabla g_m \rangle_{L^2(\Omega)} + \langle (\theta V + M) x_j f_n, g_m \rangle_{L^2(\Omega)} \big\} \\
&= \lim_{n,m\to\infty} \big\{ \theta \langle f_n, \partial_{x_j} g_m \rangle_{L^2(\Omega)} + \theta \langle x_j \nabla f_n, \nabla g_m \rangle_{L^2(\Omega)} + \langle (\theta V + M) x_j f_n, g_m \rangle_{L^2(\Omega)} \big\}
\end{aligned}$$

and

$$\begin{aligned}
II &= \lim_{m\to\infty} \langle x_j f, g_m \rangle_{L^2(\Omega)} \\
&= \lim_{m\to\infty} \langle (\theta H_V + M) R_{V,\theta} f, x_j g_m \rangle_{L^2(\Omega)} \\
&= \lim_{m\to\infty} \big\{ \theta \langle \nabla R_{V,\theta} f, \nabla(x_j g_m) \rangle_{L^2(\Omega)} + \langle (\theta V + M) x_j R_{V,\theta} f, g_m \rangle_{L^2(\Omega)} \big\} \\
&= \lim_{n,m\to\infty} \big\{ \theta \langle \nabla f_n, \nabla(x_j g_m) \rangle_{L^2(\Omega)} + \langle (\theta V + M) x_j f_n, g_m \rangle_{L^2(\Omega)} \big\} \\
&= \lim_{n,m\to\infty} \big\{ \theta \langle \partial_{x_j} f_n, g_m \rangle_{L^2(\Omega)} + \theta \langle x_j \nabla f_n, \nabla g_m \rangle_{L^2(\Omega)} \\
&\qquad\qquad + \langle (\theta V + M) x_j f_n, g_m \rangle_{L^2(\Omega)} \big\}.
\end{aligned}$$

Then, combining the above equations, we deduce that

$$\begin{aligned}
{}_{\mathscr{D}'(\Omega)}\langle \mathrm{Ad}^1(R_{V,\theta}) f, g \rangle_{\mathscr{D}(\Omega)} &= \lim_{n,m\to\infty} \theta \big\{ \langle f_n, \partial_{x_j} g_m \rangle_{L^2(\Omega)} - \langle \partial_{x_j} f_n, g_m \rangle_{L^2(\Omega)} \big\} \\
&= \lim_{n,m\to\infty} \theta \langle -2\partial_{x_j} f_n, g_m \rangle_{L^2(\Omega)} = \langle -2\theta \partial_{x_j} R_{V,\theta} f, R_{V,\theta} g \rangle_{L^2(\Omega)} \\
&= \langle -2\theta R_{V,\theta} \partial_{x_j} R_{V,\theta} f, g \rangle_{L^2(\Omega)}
\end{aligned}$$

for any $f, g \in C_0^\infty(\Omega)$. Thus (B.3) is valid in a distributional sense. In a similar way, (B.4) can be also shown in a distributional sense. The proof of Lemma B.2 is finished. □

Lemma B.3. *Assume that V satisfies the same assumption as in Lemma B.2. Let A, B and L be as in Lemma B.2. Then the following formula holds for each $t \in \mathbb{R}$:*

$$\mathrm{Ad}^1(e^{-itR_{V,\theta}}) = -i \int_0^t e^{-isR_{V,\theta}} \mathrm{Ad}^1(R_{V,\theta})\, e^{-i(t-s)R_{V,\theta}}\, ds. \tag{B.7}$$

Furthermore, the following formulas hold for $k > 1$:

$$\begin{aligned}&\mathrm{Ad}^{k+1}(e^{-itR_{V,\theta}}) \\ &= -i \int_0^t \sum_{k_1+k_2+k_3=k} \Gamma(k_1,k_2,k_3) \mathrm{Ad}^{k_1}(e^{-isR_{V,\theta}}) \mathrm{Ad}^{k_2+1}(R_{V,\theta}) \mathrm{Ad}^{k_3}(e^{-i(t-s)R_{V,\theta}})\, ds,\end{aligned} \tag{B.8}$$

where the constants $\Gamma(k_1,k_2,k_3)$ $(k_1,k_2,k_3 \geq 0)$ are trinomial coefficients:

$$\Gamma(k_1,k_2,k_3) = \frac{k!}{k_1!\,k_2!\,k_3!}.$$

Proof. It is sufficient to prove the lemma without taking account of the domain of operators as in the proof of Lemma B.2. We write

$$\begin{aligned}\mathrm{Ad}^1(e^{-itR_{V,\theta}}) &= x_j e^{-itR_{V,\theta}} - e^{-itR_{V,\theta}} x_j = -\int_0^t \frac{d}{ds}\Big(e^{-isR_{V,\theta}} x_j\, e^{-i(t-s)R_{V,\theta}}\Big)\, ds \\ &= -i \int_0^t e^{-isR_{V,\theta}} (x_j R_{V,\theta} - R_{V,\theta} x_j)\, e^{-i(t-s)R_{V,\theta}}\, ds \\ &= -i \int_0^t e^{-isR_{V,\theta}} \mathrm{Ad}^1(R_{V,\theta})\, e^{-i(t-s)R_{V,\theta}}\, ds.\end{aligned}$$

This proves (B.7). The proof of (B.8) is performed by induction argument. So we may omit the details. The proof of Lemma B.3 is complete. □

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