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Abstract

We consider the Schrödinger operator $H = -\Delta + V(|x|)$ with radial potential V which may have singularity at 0 and a quadratic decay at infinity. First, we study the structure of positive harmonic functions of H and give their precise behavior. Second, under quite general conditions we prove an upper bound for the correspond heat kernel $p(x, y, t)$ of the type

$$0 < p(x, y, t) \le C\, t^{-\frac{N}{2}} \frac{U(\min\{|x|, \sqrt{t}\})U(\min\{|y|, \sqrt{t}\})}{U(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right)$$

for all x, $y \in \mathbf{R}^N$ and $t > 0$, where U is a positive harmonic function of H. Third, if U^2 is an A_2 weight on $\mathbf{R}^N$, then we prove a lower bound of a similar type.

1 Introduction

Heat kernel bounds of differential operators on domains of $\mathbf{R}^N$ or Riemannian manifolds have attracted attention in recent years. We refer the reader for an account on this to the monographs of Davies [8], Grigor'yan [10] and Ouhabaz [25]. Typically, for a second order differential elliptic operator H, the associated heat kernel $p(x, y, t)$ (i.e. the integral kernel of the semigroup e^{-tH} generated by $-H$, or the fundamental solution to the heat equation associated with H) satisfies in many cases the following upper bound

$$|p(x, y, t)| \le \frac{C}{\sqrt{|B(x, \sqrt{t})|}\sqrt{|B(y, \sqrt{t})|}} e^{-\frac{|x-y|^2}{ct}},$$

where $|B(x, r)|$ denotes the volume of the open ball of the manifold with center x and radius r and $|x - y|$ denotes the Riemannian distance between the two points x and y. In the Euclidean setting (i.e. $\mathbf{R}^N$) the above estimate reduces to

$$|p(x, y, t)| \le Ct^{-N/2} e^{-\frac{|x-y|^2}{ct}}.$$

These bounds are referred to as Gaussian upper bounds for $p(x, y, t)$. Such bounds have been studied in many situations. They play an important role in several problems. For example, they are used in harmonic analysis in order to prove boundedness of some singular integral operators such as Riesz transforms or spectral multipliers, in spectral theory in order to prove p-independence of the spectrum, to prove maximal regularity for the

evolution equation, and so on. For all this we refer to Chapter 7 in [25] and references there.

There are however many cases where such upper bound cannot hold. A typical and important example is the Schrödinger operator with inverse square potential, i.e.,

$$H = -\Delta + \frac{\lambda}{|x|^2},$$

where $-(N-2)^2/4 \le \lambda < 0$. It is well known that the semigroup e^{-tH} does not act on $L^p(\mathbf{R}^N)$ for p outside a certain symmetric interval around 2 whose length depends on the constant λ. See Liskevich, Sobol and Vogt [20]. Therefore, the corresponding heat kernel $p(x,y,t)$ does not satisfy the above classical Gaussian bound. It was proved by Milman and Semenov [22], and later by Liskevich and Sobol [19] that the heat kernel satisfies

$$0 < p(x,y,t) \le C\, t^{-\frac{N}{2}+\sigma} (\min\{|x|, \sqrt{t}\})^{-\sigma} (\min\{|y|, \sqrt{t}\})^{-\sigma} \exp\left(-\frac{|x-y|^2}{Ct}\right)$$

for all x, $y \in \mathbf{R}^N$ and $t > 0$, where

$$\sigma = \frac{N-2}{2} - \frac{1}{2}\sqrt{(N-2)^2 + 4\lambda}.$$

See also Barbatis, Filippas and Tertikas [2]. The result in [19] deals with a more general class of operators in the sense that Δ is replaced by a divergence form operator with appropriate behavior of the coefficients. A lower bound of the same type was also proved in [21] and [22]. We observe that this upper bound can be rephrased as

$$0 < p(x,y,t) \le C\, t^{-\frac{N}{2}} \frac{U(\min\{|x|, \sqrt{t}\}) U(\min\{|y|, \sqrt{t}\})}{U(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right), \tag{1.1}$$

where $U(x) = |x|^{-\sigma}$ and it turns out that U is a positive harmonic function of H.

Our aim in this paper is to prove the bounds as in (1.1) for a wide class of potentials. Thus we are led to consider first existence and behavior of positive harmonic functions.

The behavior of positive harmonic functions for Schrödinger operators have been studied by Murata [24]. He studied the structure of all positive harmonic functions for the elliptic operator $-\Delta + V(x)$ in the case where $V \in L^p_{\mathrm{loc}}(\mathbf{R}^N)$ with some $p > N/2$ if $N \ge 2$ and $p > 1$ if $N = 1$. Furthermore, he classified the behavior of positive harmonic functions, in particular, in the case where V is a radially symmetric function on $\mathbf{R}^N$ (see [24, Section 3]). See also Remark 1.1.

In the present paper we consider a more general class of possibly negative potentials. We assume that $N \ge 2$ and the radial potential V is continuous on $(0,\infty)$ and satisfies

$$\begin{cases} \lim\limits_{r\to 0} r^{-\theta} \left|r^2 V(r) - \lambda_1\right| = 0, \quad \lim\limits_{r\to\infty} r^{\theta} \left|r^2 V(r) - \lambda_2\right| = 0, \\ \text{where } \lambda_1,\, \lambda_2 \in [\lambda_*, \infty) \text{ with } \lambda_* := -(N-2)^2/4, \end{cases} \tag{1.2}$$

for some $\theta > 0$. We also assume that the Schrödinger operator $H := -\Delta + V$ is nonnegative, that is

$$\int_{\mathbf{R}^N} \left[|\nabla\phi|^2 + V\phi^2\right] dx \ge 0 \quad \text{for all } \phi \in C_0^\infty(\mathbf{R}^N \setminus \{0\}).$$

We first study the behavior of positive harmonic functions in the light of Murata's paper [24]. The result will be then used to prove upper and lower estimate for the heat kernel $p(x,y,t)$. In order to state our results we introduce some definitions and notation.

We say that H is subcritical if, for any $W \in C_0^\infty(\mathbf{R}^N)$, $H - \epsilon W$ is nonnegative for small enough $\epsilon > 0$; H is critical if H is not subcritical. On the other hand, if H is not nonnegative, then H is said to be supercritical.

For any $\lambda \in [\lambda_*, \infty)$, let $A^\pm(\lambda)$ be roots of the algebraic equation $\alpha^2 + (N-2)\alpha - \lambda = 0$ such that $A^-(\lambda) \le A^+(\lambda)$, that is

$$A^\pm(\lambda) := \frac{-(N-2) \pm \sqrt{D_\lambda}}{2}, \quad \text{where} \quad D_\lambda := (N-2)^2 + 4\lambda \ge 0. \tag{1.3}$$

Then $v(r) := r^{A^\pm(\lambda)}$ satisfies

$$v'' + \frac{N-1}{r} v' - \frac{\lambda}{r^2} v = 0 \quad \text{in} \quad (0,\infty).$$

Furthermore, it follows that

$$A^-(\lambda) < -\frac{N-2}{2} < A^+(\lambda) \quad \text{if} \quad \lambda > \lambda_*, \quad A^\pm(\lambda) = -\frac{N-2}{2} \quad \text{if} \quad \lambda = \lambda_*. \tag{1.4}$$

For positive functions f and g defined on $(0,R)$ for some $R > 0$, we write

$$f(r) \sim g(r) \quad \text{as} \quad r \to 0 \quad \text{if} \quad \lim_{r\to 0} \frac{f(r)}{g(r)} = 1.$$

Similarly, for positive functions f and g defined on (R,∞) for some $R > 0$, we write

$$f(r) \sim g(r) \quad \text{as} \quad r \to \infty \quad \text{if} \quad \lim_{r\to \infty} \frac{f(r)}{g(r)} = 1.$$

Furthermore, for any two nonnegative functions f_1 and f_2 defined on a set D, we write

$$f_1(r) \asymp f_2(r) \quad \text{for} \quad r \in D$$

if there exists a positive constant C such that $C^{-1} f_2(r) \le f_1(r) \le C f_2(r)$ for all $r \in D$.

Now we are ready to state the main results of this paper. The first theorem ensures the existence of positive harmonic functions for the operator $H = -\Delta + V$ and classifies the behavior of positive harmonic functions.

Theorem 1.1 *Let $N \ge 2$. Let V be a continuous function on $(0,\infty)$ satisfying (1.2).*

(1) *There exists a unique solution U of*

$$U'' + \frac{N-1}{r} U' - V(r)\, U = 0 \quad \text{in} \quad (0,\infty), \tag{O}$$

with the property $U(r) \sim r^{A^+(\lambda_1)}$ as $r \to 0$.

(2) *For any solution w of* (O) *satisfying*

$$w(r) = o(r^{A^-(\lambda_1)}) \quad \text{if} \quad \lambda_1 > \lambda_*, \qquad w(r) = o\left(r^{-\frac{N-2}{2}}|\log r|\right) \quad \text{if} \quad \lambda_1 = \lambda_*,$$

as $r \to 0$, there exists a constant c such that $w(r) = cU(r)$ on $(0,\infty)$, where U is as in (1).

(3) *Assume that $H := -\Delta + V$ is nonnegative. Then $U(r) > 0$ on $(0,\infty)$ and*

(a) $U(r) \sim c_* r^{A^+(\lambda_2)}$ *as $r \to \infty$ if H is subcritical and $\lambda_2 > \lambda_*$,*

(b) $U(r) \sim c_* r^{A^-(\lambda_2)}$ *as $r \to \infty$ if H is critical and $\lambda_2 > \lambda_*$,*

(c) $U(r) \sim c_* r^{-\frac{N-2}{2}} \log r$ *as $r \to \infty$ if H is subcritical and $\lambda_2 = \lambda_*$,*

(d) $U(r) \sim c_* r^{-\frac{N-2}{2}}$ *as $r \to \infty$ if H is critical and $\lambda_2 = \lambda_*$,*

for some $c_* > 0$.

(4) *Assume that H is subcritical. Let $W \in C_0([0,\infty))$ be such that $W \geq 0$ and $W \not\equiv 0$ on $[0,\infty)$. Set $H_\mu := -\Delta + V - \mu W$ for $\mu \in \mathbf{R}$. Then there exists $\mu_* > 0$ such that*

(a) *H_μ is subcritical if $\mu < \mu_*$;*

(b) *H_μ is critical if $\mu = \mu_*$;*

(c) *H_μ is supercritical if $\mu > \mu_*$.*

Remark 1.1 *Let $N \geq 2$. Let V be a continuous function on $(0,\infty)$ satisfying* (1.2).

(i) *In the case of $\lambda_1 = 0$, we see that $V \in L^{p/2}_{\mathrm{loc}}(\mathbf{R}^N)$ for some $p > N/2$. Then Theorem* 1.1 *follows from Theorem* 3.1 *in* [24].

(ii) *If $V(r) \geq \lambda r^{-2}$ on $[0,\infty)$ for some $\lambda > \lambda_*$, then H is subcritical. This immediately follows from the Hardy inequality.*

The next results are concerned with upper and lower bounds for the heat kernel $p(x,y,t)$ of $H = -\Delta + V$. Recall that the heat kernel is the fundamental solution of

$$\partial_t u = \Delta u - V(|x|)u \quad \text{in} \quad \mathbf{R}^N \times (0,\infty). \tag{1.5}$$

We prove the following results.

Theorem 1.2 *Let $N \geq 2$. Let V be a continuous function on $(0,\infty)$ satisfying* (1.2) *and $p = p(x,y,t)$ the fundamental solution of* (1.5). *Assume that $H := -\Delta + V(|x|)$ is nonnegative and let U be as in Theorem* 1.1. *If $\omega(x) := U(|x|)^2$ is an A_2 weight on $\mathbf{R}^N$, then there exist positive constants C_1 and C_2 such that*

$$\frac{C_1 U(x)U(y)}{\sqrt{\omega(B(x,\sqrt{t}))}\sqrt{\omega(B(y,\sqrt{t}))}} \exp\left(-\frac{|x-y|^2}{C_1 t}\right) \leq p(x,y,t) \leq \frac{C_2 U(x)U(y)}{\sqrt{\omega(B(x,\sqrt{t}))}\sqrt{\omega(B(y,\sqrt{t}))}} \exp\left(-\frac{|x-y|^2}{C_2 t}\right)$$

for all x, $y \in \mathbf{R}^N$ and $t > 0$. Here $\omega(B(x,\sqrt{t})) := \int_{B(x,\sqrt{t})} \omega(z)\,dz$.

We shall see in the proof that the upper bound can be made slightly more precise in the sense that the constant C_2 could chosen to be arbitrary close to 4. Indeed we prove that

$$p(x,y,t) \le \frac{C_\epsilon U(x)U(y)}{\sqrt{\omega(B(x,\sqrt{t}))}\sqrt{\omega(B(y,\sqrt{t}))}} \exp\left(-\frac{|x-y|^2}{(4+\epsilon)t}\right).$$

for every $\epsilon > 0$. The constant C_ϵ is independent of x, y and t.

Note that in Theorem 1.2, $\omega \equiv U^2$ is an A_2 weight on $\mathbf{R}^N$ if $A^+(\lambda_1) < N/2$ and

$$C^{-1} r^{-A_1} \le U(r) \le C r^{-A_2}, \qquad r \ge 1,$$

for some A_1 and A_2 such that $-N/2 < A_2 \le A_1 < N/2$. Next we weaken the A_2-assumption on ω and obtain an upper Gaussian estimate for $p = p(x,y,t)$.

Theorem 1.3 *Let $N \ge 2$. Let V be a continuous function on $(0,\infty)$ satisfying (1.2). Assume that $H := -\Delta + V(|x|)$ is nonnegative and let U be as in Theorem 1.1. Furthermore, if H is critical, then we assume that*

$$A^-(\lambda_2) > -\frac{N}{2}.$$

Then there exists a positive constant C such that

$$0 < p(x,y,t) \le C\, t^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{t}\})U(\min\{|y|,\sqrt{t}\})}{U(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right) \tag{1.6}$$

for all x, $y \in \mathbf{R}^N$ and $t > 0$.

For the proof of Theorem 1.3, we apply a refinement of the technique developed in [11, 12, 15, 16] and construct supersolutions of (1.5). Furthermore, we combine the comparison principle with the standard arguments as given, for example, [26, Section 6], and prove Theorem 1.3.

The final result is an observation that for a non-necessarily radial positive potential V, if one knows that there exists a harmonic function U which behaves as a polynomial on the whole $\mathbf{R}^N$, then the Gaussian upper bound holds. More precisely,

Proposition 1.1 *Suppose that $V \ge 0$ and that H has a harmonic function U satisfying*

$$C_0\,|x|^\alpha \le U(x) \le C_0'\,|x|^\alpha, \qquad x \in \mathbf{R}^N,$$

for some $\alpha \ge 0$ and C_0, $C_0' > 0$. Then

$$p(x,y,t) \le C\, t^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{t}\})U(\min\{|y|,\sqrt{t}\})}{U(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right)$$

for all x, $y \in \mathbf{R}^N$ and $t > 0$.

The proof of the latter result uses the standard Caffarelli-Kohn-Nirenberg inequalities. The idea is classical and we work on the weighted space $L^2(\mathbf{R}^N, |x|^\alpha dx)$. Then the Sobolev inequality on this weighted space (which is the Caffarelli-Kohn-Nirenberg inequality) allows us to obtain an appropriate $L^2(\mathbf{R}^N, |x|^\alpha dx) - L^\infty(\mathbf{R}^N, |x|^\alpha dx)$ decay of the semigroup. The standard perturbation method allows then to convert this decay into a Gaussian bound. This reasoning has already appeared in [2] in the context of the Schrödinger operator $-\Delta + \frac{\lambda}{|x|^2}$.

Note that the above results extend the results from the papers [2], [19], [21] and [22] mentioned above which deal with the case where $V = \frac{\lambda}{|x|^2}$.

2 Preliminaries

In this section we recall some properties for parabolic equations with A_2 weight. Throughout this section and in the rest of the paper, we denote by C generic positive constants which may have different values even within the same line.

Let ω be a nonnegative measurable function on a domain $\Omega \subset \mathbf{R}^N$. Suppose that ω is an A_2 weight on Ω, that is ω, $\omega^{-1} \in L^1_{\rm loc}(\Omega)$ and

$$[\omega](\Omega) := \sup \left\{ \int_E \omega \, dz \int_E \omega^{-1} \, dz \Big/ \left(\int_E dz \right)^2 : E \text{ is a ball in } \Omega \right\} < \infty.$$

Then $\omega(z)\, dz$ is a measure on Ω with the doubling property, that is

$$\omega(B(x, 2r)) \le C\omega(B(x, r)) \tag{2.1}$$

holds for all $x \in \mathbf{R}^N$ and $r > 0$, where $\omega(B(x,r)) := \int_{B(x,r)} \omega(z)\, dz$. For further details on A_2 weights, see e.g., [27].

We denote by $L^p(\Omega, \omega\, dx)$ $(1 \le p < \infty)$ the usual Lebesgue spaces with norm

$$\|f\|_{p,\omega;\,\Omega} := \left(\int_\Omega |f(z)|^p \omega(z)\, dz \right)^{\frac{1}{p}}.$$

By $H^1(\Omega, \omega\, dx)$ we denote the Sobolev space defined as the completion of $C^\infty(\overline{\Omega})$ with respect to the norm

$$\left(\int_\Omega (|f(z)|^2 + |\nabla f(z)|^2) \omega(z)\, dz \right)^{\frac{1}{2}}.$$

Consider the degenerate parabolic equation

$$\partial_t v = \frac{1}{\omega} \mathrm{div}\, (\omega \nabla v) + cv \quad \text{in} \quad \Omega \times I, \tag{2.2}$$

where I is an open interval of $\mathbf{R}$ and $c \in L^\infty(I : L^\infty(\Omega))$. We say that a measurable function v on $\Omega \times I$ is a solution of (2.2) if

$$v \in L^\infty(I : L^2(\Omega), w\, dz)) \cap L^2(I : H^1(\Omega, w\, dz))$$

and v satisfies

$$\int_I \int_\Omega \{-v\partial_t\varphi + \nabla v \cdot \nabla\varphi - cv\varphi\}\,\omega\,dzdt = 0$$

for all $\varphi \in C_0^\infty(\Omega \times I)$. The following results hold (see [4] and also [13]).

Proposition 2.1 *Assume that ω is an A_2 weight on $B(0,1)$. Let v be a solution of (2.2) on $B(0,1)\times(0,1)$. Then there exists a constant γ_1 such that*

$$\|v\|_{L^\infty(B(0,1/2)\times(1/2,1))} \le \left(\frac{\gamma_1}{\omega(B(0,1))}\int_0^1 \int_{B(0,1)} v^2\omega\,dzdt\right)^{\frac{1}{2}}.$$

Here γ_1 depends only on N, $\omega(B(0,1))$ and $\|c\|_{L^\infty(0,1:L^\infty(B(0,1)))}$.

Proposition 2.2 *Assume that ω is an A_2 weight on $B(0,1)$. Let v be a nonnegative solution of (2.2) on $B(0,1)\times(-1,1)$. Then there exists a constant γ_2 such that*

$$\sup_{Q_-} v \le \gamma_2 \inf_{Q^+} v,$$

where

$$Q_- := B\left(0,\frac{1}{2}\right)\times\left(-\frac{3}{4},-\frac{1}{4}\right), \qquad Q_+ := B\left(0,\frac{1}{2}\right)\times\left(\frac{1}{4},\frac{3}{4}\right).$$

Here γ_2 depends only on N, $\omega(B(0,1))$ and $\|c\|_{L^\infty(0,1:L^\infty(B(0,1)))}$.

By Proposition 2.2 we have:

Lemma 2.1 *Let $R>0$ and w an A_2 weight on $B(0,R)$. Let v be a nonnegative solution of (2.2) on $B(0,R)\times(0,T)$, where $0<T<\infty$. Then there exists a positive constant C such that*

$$v(x_1,t_1) \le Cv(x_2,t_2)\exp\left(C\frac{|x_1-x_2|^2}{t_2-t_1}+\frac{t_2}{t_1}\right) \tag{2.3}$$

for all x_1, $x_2 \in B(0,R/2)$ and $0<t_1\le t_2\le T$. Here C depends on $\omega(B(0,R))$ and $\|c\|_{L^\infty(-1,1:L^\infty(B(0,1)))}$.

Proof. Let $x\in B(0,R/2)$ and $0<t<T$. Assume that

$$Q := B(x,r)\times(t-r^2,t+r^2) \subset B(0,R)\times(0,T)$$

for some $r>0$. Set

$$\tilde v(z,s) := v(x+rz,t+r^2s), \quad \tilde\omega(z) := \omega(x+rz), \quad \tilde c(z,s) := r^2c(x+rz,t+r^2s),$$

for $z\in B(0,1)$ and $s\in(-1,1)$. Then $\tilde v$ satisfies

$$\partial_s\tilde v = \frac{1}{\tilde\omega}\mathrm{div}_z\left(\tilde\omega(z)\nabla_z\tilde v\right) + \tilde c\tilde v \quad \text{in} \quad B(0,1)\times(-1,1).$$

Since $\tilde{\omega}(B(0,1)) = \omega(B(0,r)) \le \omega(B(0,R))$, by Proposition 2.2 we can find a positive constant c, independent of x, t and r, such that

$$\sup_{Q_-} \tilde{v} \le c \inf_{Q_+} \tilde{v},$$

where Q_+ and Q_- are as in Proposition 2.2. This implies that

$$\sup_{Q_-(x,t;r)} v \le c \inf_{Q_+(x,t;r)} v,$$

where

$$\begin{aligned} Q_-(x,t;r) :=& B\left(x, \frac{r}{2}\right) \times \left(t - \frac{3}{4}r^2, t - \frac{1}{4}r^2\right), \\ Q_+(x,t;r) :=& B\left(x, \frac{r}{2}\right) \times \left(t + \frac{1}{4}r^2, t + \frac{3}{4}r^2\right). \end{aligned}$$

Then, similarly to [1, Theorem E] and [23, Theorem 2], we obtain (2.3). (See also [17] and [18].) Thus Lemma 2.1 follows. □

3 Behavior of the harmonic function

In this section we study the behavior of positive harmonic functions for nonnegative Schrödinger operators and prove Theorem 1.1. In what follows, for $\lambda \in [\lambda_*, \infty)$, set $u_\lambda^\pm(r) := r^{A^\pm(\lambda)}$ if $\lambda > \lambda_*$ and

$$u_\lambda^+(r) := r^{-\frac{N-2}{2}}, \qquad u_\lambda^-(r) := r^{-\frac{N-2}{2}} |\log r|$$

if $\lambda = \lambda_*$. Furthermore, we put $V_\lambda(r) := V(r) - \lambda r^{-2}$.

We first study the behavior of solutions of (O) at $r = 0$ and $r = \infty$.

Lemma 3.1 *Let $V \in C((0,\infty))$. Assume that*

$$\lim_{r \to 0} r^{2-\theta} |V_{\lambda_1}(r)| = 0 \tag{3.1}$$

for some $\lambda_1 \in [\lambda_*, \infty)$ and $\theta > 0$. Then there exist solutions $U_*^\pm$ of (O) such that

$$\begin{aligned} U_*^\pm(r) &= u_{\lambda_1}^\pm(r) + O(r^{\theta'} u_{\lambda_1}^\pm(r)), \\ (U_*^\pm)'(r) &= (u_{\lambda_1}^\pm)'(r) + O(r^{-1+\theta'} u_{\lambda_1}^\pm(r)), \end{aligned} \tag{3.2}$$

as $r \to 0$, for some $\theta' \in (0, \theta]$. Furthermore, for any solution w of (O), there exist constants C_1 and C_2 such that

$$w(r) = C_1 U_*^+(r) + C_2 U_*^-(r), \qquad r > 0. \tag{3.3}$$

Proof. The proof is similar to [14, Section 3] but we give details for the sake of completeness. We write $u^{\pm} = u^{\pm}_{\lambda_1}$ for simplicity.

We first construct the solution U^+_* of (O). Set $U^+_1(r) := u^+(r)$ and define U^+_n $(n = 2, 3, \dots)$ inductively by

$$U^+_{n+1}(r) := u^+(r)(1 + F_n(r)), \tag{3.4}$$

where

$$F_n(r) := \int_0^r s^{1-N}[u^+(s)]^{-2} \left(\int_0^s \tau^{N-1} u^+(\tau) V_{\lambda_1}(\tau) U^+_n(\tau)\, d\tau \right) ds.$$

Let $0 < R < 1$ and assume that

$$|U^+_n(r)| \le 2u^+(r) \quad \text{in} \quad (0, R] \tag{3.5}$$

for some $n \in \{1, 2, \dots\}$. Then it follows from (1.3), (3.1) and (3.5) that

$$\begin{aligned} |F_n'(r)| &\le Cr^{1-N}[u^+(r)]^{-2} \int_0^r \tau^{N-1}\tau^{-2+\theta}[u^+(\tau)]^2\, d\tau \\ &= Cr^{-1-\sqrt{D_{\lambda_1}}} \int_0^r \tau^{-1+\theta+\sqrt{D_{\lambda_1}}}\, d\tau \le Cr^{-1+\theta} \end{aligned} \tag{3.6}$$

for $r \in (0, R]$. Taking a sufficiently small $R > 0$ if necessary, by (3.4) and (3.6) we have

$$|U^+_{n+1}(r) - u^+(r)| \le Cr^{\theta} u^+(r) \le u^+(r) \tag{3.7}$$

for $r \in (0, R]$. This implies that (3.5) holds for $n = 1, 2, \dots$. Furthermore, we see that (3.7) holds for $n = 1, 2, \dots$. Applying the successive approximation arguments on the existence of solutions to ordinary differential equations (see e.g., [5, Chapter 1]), we can find a function $U^+_* \in C((0, R])$ such that

$$|U^+_*(r) - u^+(r)| \le Cr^{\theta} u^+(r), \qquad U^+_*(r) = u^+(r)(1 + F(r)), \tag{3.8}$$

for $r \in (0, R]$, where

$$F(r) := \int_0^r s^{1-N}[u^+(s)]^{-2} \left(\int_0^s \tau^{N-1} u^+(\tau) V_{\lambda_1}(\tau) U^+_*(\tau)\, d\tau \right) ds.$$

Similarly to (3.6), it follows that $|F'(r)| \le Cr^{-1+\theta}$ on $(0, R]$, which implies that

$$(U^+_*)'(r) - (u^+)'(r) = (u^+)'(r)F(r) + u^+(r)F'(r) = O(r^{-1+\theta}u^+(r)) \tag{3.9}$$

as $r \to 0$. Furthermore, since

$$(U^+_*)'' + \frac{N-1}{r}(U^+_*)' - \frac{\lambda_1}{r^2}U^+_* = V_{\lambda_1}U^+_* \quad \text{in} \quad (0, R],$$

U^+_* satisfies (O) on $(0, R]$. By (3.8) and (3.9), extending U^+_* to the solution of (O) on $(0, \infty)$, we obtain the desired solution U^+_* of (O).

Next we construct the solution U^-_* in the case $\lambda_1 = \lambda_*$. We set $U^-_1(r) = u^-(r)$ and define U^-_n $(n = 2, 3, \dots)$ inductively by

$$U^-_{n+1}(r) := u^-(r) + u^+(r)\tilde{F}_n(r),$$

where

$$\tilde{F}_n(r) := \int_0^r s^{1-N}[u^+(s)]^{-2}\left(\int_0^s \tau^{N-1}u^+(\tau)V_{\lambda_1}(\tau)U_n^-(\tau)\,d\tau\right)ds.$$

Let $0 < R < 1$ and assume that

$$|U_n^-(r)| \le 2u^-(r) \quad \text{in} \quad (0,R] \tag{3.10}$$

for some $n \in \{1,2,\dots\}$. Similarly to (3.6), by (1.2) and (3.10) we have

$$\begin{aligned} |\tilde{F}_n'(r)| &\le Cr^{1-N}[u^+(r)]^{-2}\int_0^r \tau^{N-1}\tau^{-2+\theta}u^+(\tau)u^-(\tau)\,d\tau \\ &= Cr^{-1}\int_0^r \tau^{-1+\theta}|\log\tau|\,d\tau \le Cr^{-1+\theta}|\log r| \end{aligned} \tag{3.11}$$

for $r \in (0,R]$. This implies that

$$|\tilde{F}(r)| \le Cr^\theta|\log r|, \qquad u^+(r)|\tilde{F}(r)| \le Cr^{-\frac{N-2}{2}+\theta}|\log r| = Cr^\theta u^-(r)$$

for $r \in (0,R]$. Then, by a similar argument as in the construction of U_*^+ we can find the desired solution U_*^- in the case $\lambda = \lambda_*$.

Next we construct the solution U_*^- in the case $\lambda_1 > \lambda_*$. Let δ be a sufficiently small positive constant. We set $U_1^-(r) := u^-(r)$ and define U_n^- $(n = 2,3,\dots)$ inductively by

$$U_{n+1}^-(r) := u^-(r)(1 + G_n(r)),$$

where

$$G_n(r) := \int_0^r s^{1-N}[u^-(s)]^{-2}\left(\int_s^\delta \tau^{N-1}u^-(\tau)V_{\lambda_1}(\tau)U_n^-(\tau)\,d\tau\right)ds.$$

Similarly to (3.5), we assume

$$|U_n^-(r)| \le 2u^-(r) \quad \text{in} \quad (0,\delta] \tag{3.12}$$

for some $n \in \{1,2,\dots\}$. Since we can assume, without loss of generality, that $\theta < \sqrt{D_{\lambda_1}}$, by (1.2) and (3.12) we have

$$\begin{aligned} |G_n'(r)| &\le Cr^{1-N}[u^-(r)]^{-2}\int_r^\delta \tau^{N-1}\tau^{-2+\theta}[u^-(\tau)]^2\,d\tau \\ &= Cr^{-1+\sqrt{D_{\lambda_1}}}\int_r^\delta \tau^{-1+\theta-\sqrt{D_{\lambda_1}}}\,d\tau \le Cr^{-1+\theta} \end{aligned}$$

for $r \in (0,\delta]$. Then, taking a sufficiently small $\delta > 0$ if necessary, we obtain

$$|U_{n+1}^-(r) - u^-(r)| \le Cr^\theta u^-(r) \le u^-(r)$$

for $r \in (0,\delta]$. Repeating the above argument, we can find the desired solution U_*^- in the case $\lambda > \lambda_*$. Therefore, we obtain the desired solutions $U_*^\pm$ of (O). Furthermore, since $U_*^\pm$ are linearly independent, we see (3.3). Thus Lemma 3.1 follows. □

Lemma 3.2 *Let $V \in C((0,\infty))$. Assume that*

$$\lim_{r\to\infty} r^{2+\theta}\,|V_{\lambda_2}(r)| = 0 \tag{3.13}$$

for some $\lambda_2 \in [\lambda_*, \infty)$ and $\theta > 0$. Then there exist solutions $U^{\pm}_{**}$ of (O) *such that*

$$U^{\pm}_{**}(r) = u^{\pm}_{\lambda_2}(r) + O(r^{-\theta'} u^{\pm}_{\lambda_2}(r)) \tag{3.14}$$

as $r \to \infty$, for some $\theta' \in (0, \theta]$. Furthermore, for any solution w of (O)*, there exist constants C_1 and C_2 such that*

$$w(r) = C_1 U^{+}_{**}(r) + C_2 U^{-}_{**}(r), \qquad r > 0. \tag{3.15}$$

Proof. Let w be a solution of (O) on $(0,\infty)$. Set $\hat{w}(s) := s^{-N+2} w(s^{-1})$, which is the Kelvin transformation of w. Then $\hat{w}$ satisfies

$$\hat{w}'' + \frac{N-1}{s}\hat{w}' - \hat{V}(s)\hat{w} = 0 \quad \text{in} \quad (0,\infty), \tag{3.16}$$

where $\hat{V}(s) := s^{-4} V(s^{-1})$. It follows from (3.13) that

$$\lim_{s\to 0} s^{-\theta} |s^2 \hat{V}(s) - \lambda_2| = \lim_{r\to\infty} r^{2+\theta} |V_{\lambda_2}(r)| = 0.$$

Therefore, by Lemma 3.1 we can find solutions $W^{\pm}(r)$ of (3.16) such that

$$W^{\pm}(s) = u^{\pm}_{\lambda_2}(s) + O\left(s^{\theta'} u^{\pm}_{\lambda_2}(s)\right) \quad \text{as} \quad s \to 0, \tag{3.17}$$

for some $\theta' \in (0, \theta]$. Set $U^{\pm}_{**}(r) := r^{-N+2} W^{\mp}(r^{-1})$. Then $U^{\pm}_{**}(r)$ are solutions of (O) on $(0,\infty)$. Furthermore, it follows that

$$-A^{\pm}(\lambda_2) - N + 2 = \frac{-(N-2) \mp \sqrt{(N-2)^2 + 4\lambda_2}}{2} = A^{\mp}(\lambda_2),$$

which together with (3.17) implies (3.14). Furthermore, since $U^{\pm}_{**}$ are linearly independent, we obtain (3.15). Thus Lemma 3.2 follows. □

In what follows, we set

$$U(r) := U^{+}_{*}(r).$$

Next we show the positivity of U under the assumption that H is nonnegative.

Lemma 3.3 *Let $V \in C((0,\infty))$. Assume* (1.2) *and that H is nonnegative. Then $U(r) > 0$ on $(0,\infty)$.*

Proof. We consider the case $-\lambda_* \le \lambda_1 \le 0$. For $n = 1, 2, \ldots$, set

$$V_n(r) := \max\{-n, V(r)\}, \qquad H_n := -\Delta + V_n.$$

Since $V_n \in L^{\infty}(0,\infty)$ and H_n is nonnegative, by (ii) of Theorem 3.1 in [24] there exists a radially symmetric and bounded function $u_n = u_n(|x|) \in C^2(\mathbf{R}^N)$ such that

$$-\Delta u_n + V_n u_n = 0 \quad \text{in} \quad \mathbf{R}^N, \qquad u_n > 0 \quad \text{in} \quad \mathbf{R}^N. \tag{3.18}$$

In particular, it follows from the regularity of u_n that

$$u_n'(0) = 0. \tag{3.19}$$

By (3.2) we can find $R > 0$ such that $U(r) > 0$ on $(0, R]$. Set

$$U_n(r) := U(R)\frac{u_n(r)}{u_n(R)}.$$

Since U_n satisfies (3.18), we have

$$-\frac{1}{r^{N-1}}(r^{N-1}U_n')' + V_nU_n = 0 \quad \text{in} \quad (0,\infty),$$

which implies that

$$\begin{aligned} 0 &= \int_{r'}^{r} [-(s^{N-1}U_n')'U + s^{N-1}V_nU_nU]\,ds \\ &= \left[-s^{N-1}U_n'U\right]_{s=r'}^{s=r} + \int_{r'}^{r} [s^{N-1}U_n'U' + s^{N-1}V_nU_nU]\,ds \end{aligned} \tag{3.20}$$

for $0 < r' < r$. Similarly, since U is a solution of (O), we have

$$\begin{aligned} 0 &= \int_{r'}^{r} [-(s^{N-1}U')'U_n + s^{N-1}V(s)UU_n]\,ds \\ &= \left[-s^{N-1}U'U_n\right]_{s=r'}^{s=r} + \int_{r'}^{r} [s^{N-1}U'U_n' + s^{N-1}V(s)UU_n]\,ds \end{aligned} \tag{3.21}$$

for $0 < r' < r$. Since $U(r) > 0$, $U_n(r) > 0$ and $V(r) \le V_n(r)$ on $(0, R]$, we deduce from (3.20) and (3.21) that

$$\begin{aligned} &r^{N-1}[U'(r)U_n(r) - U(r)U_n'(r)] - (r')^{N-1}[U'(r')U_n(r') - U(r')U_n'(r')] \\ &= \int_{r'}^{r} s^{N-1}[V(s) - V_n(s)]UU_n\,ds \le 0 \end{aligned} \tag{3.22}$$

for $0 < r' < r \le R$. On the other hand, it follows from (3.2) that

$$\lim_{r'\to 0} (r')^{N-1}[U'(r')U_n(r') - U(r')U_n'(r')] = 0.$$

Taking $r' \to 0$ in (3.22) together with (3.19) implies that

$$0 \ge r^{N-1}[U'(r)U_n(r) - U(r)U_n'(r)] = r^{N-1}U_n(r)^2\left(\frac{U(r)}{U_n(r)}\right)', \qquad 0 < r \le R.$$

We deduce from $U_n(R) = U(R)$ that

$$\frac{U(r)}{U_n(r)} \ge \frac{U(R)}{U_n(R)} = 1, \qquad 0 < r \le R.$$

Therefore we obtain

$$0 < U_n(r) \le U(r), \qquad 0 < r \le R. \tag{3.23}$$

On the other hand, since $V \in C((0,\infty))$ and $U_n(R) = 1$, by the Harnack inequality and regularity theorems for elliptic equations in a similar way to the Perron method, we can find a function $\tilde{U} \in C^2((0,\infty))$ such that

$$\lim_{n\to\infty} \|U_n - \tilde{U}\|_{C^2(I)} = 0$$

for any compact set I in $(0,\infty)$. Then $\tilde{U}$ is a solution of (O) on $(0,\infty)$. Furthermore, by (3.23) we see that

$$\tilde{U}(r) \geq 0 \quad \text{in} \quad (0,\infty), \qquad \tilde{U}(r) \leq U(r) \quad \text{in} \quad (0,R], \qquad \tilde{U}(R) = U(R) > 0. \tag{3.24}$$

Using the Harnack inequality again, we obtain

$$\tilde{U}(r) > 0 \quad \text{in} \quad (0,\infty). \tag{3.25}$$

Furthermore, by Lemma 3.1 there exist constants C_1 and C_2 such that

$$\tilde{U}(r) = C_1 U_*^+(r) + C_2 U_*^-(r) \quad \text{in} \quad (0,\infty). \tag{3.26}$$

Since $A^-(\lambda_1) < A^+(\lambda_1)$, by (3.24) and (3.26) we see that $C_2 = 0$ and $C_1 = 1$, that is $\tilde{U}(r) = U_*^+(r) = U(r)$ on $(0,\infty)$. Therefore we deduce from (3.25) that $U(r) > 0$ on $(0,\infty)$.

It remains to consider the case $\lambda_1 > 0$. Let $k \in \{1,2,\dots\}$ be such that $\lambda_1 < \omega_k := k(N+k-2)$. For any $\phi \in C^\infty(\mathbf{R}^{N+2k} \setminus \{0\})$ and $\omega \in \mathbf{S}^{N+2k-1}$, set

$$\phi_\omega(r) := \phi(r\omega), \qquad \psi_\omega(r) := r^k \phi_\omega(r).$$

Since H is nonnegative, we have

$$\begin{aligned}
0 &\leq \frac{1}{|\mathbf{S}^{N-1}|} \int_{\mathbf{R}^N} \left[|\nabla \psi_\omega|^2 + V\psi_\omega^2 \right] dx = \int_0^\infty \left[|\psi_\omega'|^2 + V\psi_\omega^2 \right] r^{N-1}\, dr \\
&= \int_0^\infty \left[r^{2k}|\phi_\omega'|^2 + 2kr^{2k-1}\phi_\omega\phi_\omega' + k^2 r^{2k-2}\phi_\omega^2 + r^{2k}V\phi_\omega^2 \right] r^{N-1}\, dr \\
&= \int_0^\infty \left[|\phi_\omega'|^2 + k^2 r^{-2}\phi_\omega^2 + V\phi_\omega^2 \right] r^{N+2k-1}\, dr + \int_0^\infty kr^{N+2k-2}[(\phi_\omega)^2]'\, dr \\
&= \int_0^\infty \left[|\phi_\omega'|^2 + \tilde{V}\phi_\omega^2 \right] r^{N+2k-1}\, dr \leq |\mathbf{S}^{N+2k-1}|^{-1} \int_{\mathbf{R}^{N+2k}} \left[|\nabla\phi|^2 + \tilde{V}\phi^2 \right] dx,
\end{aligned}$$

where $\tilde{V}(r) := V(r) - \omega_k r^{-2}$. This means that $\tilde{H} := -\Delta_{N+2k} + \tilde{V}$ is nonnegative operator on $\mathbf{R}^{N+2k}$. Furthermore, (1.2) holds with λ_1 and λ_2 replaced by

$$\tilde{\lambda}_1 := \lambda_1 - \omega_k > -\frac{(N+2k-2)^2}{4} \quad \text{and} \quad \tilde{\lambda}_2 := \lambda_2 - \omega_k > -\frac{(N+2k-2)^2}{4},$$

respectively. Therefore, by Lemma 3.3 in the case $\lambda_* < \lambda_1 \leq 0$ we can find a solution $u = u(r)$ of

$$\begin{aligned}
&u'' + \frac{N+2k-1}{r}u' - \tilde{V}(r) = 0 \quad \text{in} \quad (0,\infty), \\
&u(r) > 0 \quad \text{in} \quad (0,\infty), \quad u(r) = r^a + O(r^{a+\theta}) \quad \text{as} \quad r \to 0,
\end{aligned}$$

where

$$a := \frac{-(N+2k-2)+\sqrt{(N+2k-2)^2+4(\lambda_1-\omega_k)}}{2} = -k + A^+(\lambda_1).$$

Then $\tilde{U}(r) := r^k u(r)$ is a solution of (O) and it satisfies

$$\tilde{U}(r) > 0 \quad \text{in} \quad (0,\infty), \qquad \tilde{U}(r) \sim r^{A^+(\lambda_1)} \quad \text{as} \quad r \to 0.$$

It follows from Lemma 3.1 that $U(r) = \tilde{U}(r) > 0$ on $(0,\infty)$. Thus Lemma 3.3 follows. □

Next we study the asymptotic behavior of $U(r)$ as $r \to \infty$.

Lemma 3.4 *Let $V \in C((0,\infty))$. Assume* (1.2) *and that $-\Delta + V(|x|) - W(|x|)$ is nonnegative for some $W \in C_0((0,\infty))$ with*

$$W \geq 0, \qquad W \not\equiv 0 \quad \text{in} \quad (0,\infty).$$

Then there exists a positive constant c such that

$$U(r) \sim c r^{A^+(\lambda_2)} \ \text{ if } \lambda_2 > \lambda_*, \qquad U(r) \sim c r^{-\frac{N-2}{2}} \log r \ \text{ if } \lambda_2 = \lambda_*,$$

as $r \to \infty$.

Proof. Since $-\Delta + V - W$ is nonnegative, by Lemmas 3.1 and 3.3 we can find a function $U_W \in C^2((0,\infty))$ satisfying

$$\begin{aligned} &U_W'' + \frac{N-1}{r} U_W' - (V(r) - W(r)) U_W = 0 \quad \text{in} \quad (0,\infty), \\ &U_W > 0 \quad \text{in} \quad (0,\infty), \qquad U_W(r) = r^{A^+(\lambda_1)}(1+o(1)) \quad \text{as} \quad r \to 0. \end{aligned} \tag{3.27}$$

On the other hand, U satisfies

$$U'' + \frac{N-1}{r} U' - (V(r) - W(r)) U = W(r) U \quad \text{in} \quad (0,\infty).$$

Define

$$\tilde{U}(r) = U_W(r)(1 + F_W(r)),$$

where

$$F_W(r) := \int_0^r s^{1-N} [U_W(s)]^{-2} \left(\int_0^s \tau^{N-1} U_W(\tau) W(\tau) U(\tau)\, d\tau \right) ds \geq 0.$$

Since W has a compact support, $F_W(r) = 0$ for all sufficiently small $r > 0$. Furthermore, by (3.27) we have

$$\tilde{U}'' + \frac{N-1}{r} \tilde{U}' - (V(r) - W(r)) \tilde{U} = WU \quad \text{in} \quad (0,\infty).$$

Then $\hat{U} := U - \tilde{U}$ satisfies

$$\begin{aligned} &\hat{U}'' + \frac{N-1}{r} \hat{U}' - (V(r) - W(r)) \hat{U} = 0 \quad \text{in} \quad (0,\infty), \\ &\hat{U}(r) = U(r) - U_W(r) = o\left(r^{A^+(\lambda_1)} \right) \quad \text{as} \quad r \to 0. \end{aligned}$$

This together with Lemma 3.1 imply that $\hat{U} = 0$ in $(0, \infty)$, that is,

$$U(r) = U_W(r)(1 + F_W(r)) \quad \text{in} \quad (0, \infty). \tag{3.28}$$

On the other hand, by Lemmas 3.2 and 3.3 we see that, either

$$\text{(a)} \quad U_W(r) \sim c_1 u^-_{\lambda_2}(r) \qquad \text{or} \qquad \text{(b)} \quad U_W(r) \sim c_2 u^+_{\lambda_2}(r)$$

as $r \to \infty$, where c_1 and c_2 are positive constants.

Consider the case $\lambda_2 > \lambda_1$. Assume that (a) holds. Since W has a compact support and $U > 0$ on $(0, \infty)$, we take a sufficiently large constant $R > 0$ so that

$$\begin{aligned} U_W(r)F_W(r) &\geq CU_W(r) \int_R^r s^{1-N}[U_W(s)]^{-2}\, ds \\ &\geq Cr^{\frac{-(N-2)-\sqrt{D(\lambda_2)}}{2}} \int_1^r s^{-1+\sqrt{D(\lambda_2)}}\, ds \geq Cr^{\frac{-(N-2)+\sqrt{D(\lambda_2)}}{2}} = Cr^{A^+(\lambda_2)} \end{aligned} \tag{3.29}$$

for all sufficiently large r. On the other hand, if (b) holds, then it follows from (3.28) that

$$U(r) \geq U_W(r) \geq Cr^{A^+(\lambda_2)} \tag{3.30}$$

for all sufficiently large r. In both cases of (a) and (b), $U(r) \geq Cr^{A^+(\lambda_2)}$ for all sufficiently large r. Then Lemma 3.4 in the case $\lambda_2 > \lambda_*$ follows from Lemma 3.2.

Consider the case $\lambda_2 = \lambda_*$. If (a) holds, then, similarly to (3.30), we have $U(r) \geq U_W(r) \geq Cr^{-\frac{N-2}{2}} \log r$ for all sufficiently large r. If (b) holds, then, similarly to (3.29), we have

$$U_W(r)F_W(r) \geq CU_W(r) \int_R^r s^{1-N}[U_W(s)]^{-2}\, ds \geq Cr^{-\frac{N-2}{2}} \int_1^r s^{-1}\, ds \geq Cr^{-\frac{N-2}{2}} \log r$$

for all sufficiently large r. In both cases of (a) and (b), $U(r) \geq Cr^{-\frac{N-2}{2}} \log r$ for all sufficiently large r. Then Lemma 3.4 in the case $\lambda_2 = \lambda_*$ follows from Lemma 3.2. Thus the proof of Lemma 3.4 is complete. □

Next we employ the arguments in [9, Lemma 6] and prove the following lemma.

Lemma 3.5 *Let $V \in C((0, \infty))$. Assume* (1.2) *and that H is nonnegative. If there exists a positive constant c such that*

$$U(r) \geq cr^{A^+(\lambda_2)} \quad \textit{if} \quad \lambda_2 > \lambda_*, \qquad U(r) \geq cr^{-\frac{N-2}{2}} \log r \quad \textit{if} \quad \lambda_2 = \lambda_*, \tag{3.31}$$

for all sufficiently large $r > 0$, then $H := -\Delta + V$ is subcritical.

Proof. Let $\phi \in C_0^\infty(\mathbf{R}^N \setminus \{0\})$. Set

$$\tilde{\phi}(x) := \phi(x)/U(|x|).$$

Then we have

$$\begin{aligned} |\nabla\tilde{\phi}|^2 &= \left|\frac{U\nabla\phi - \phi\nabla U}{U^2}\right|^2 = \frac{U^2|\nabla\phi|^2 - 2U\phi\nabla\phi\nabla U + \phi^2|\nabla U|^2}{U^4} \\ &= \frac{U^2|\nabla\phi|^2 - U\nabla|\phi|^2\nabla U + \phi^2|\nabla U|^2}{U^4}. \end{aligned}$$

This implies that

$$\begin{aligned}\int_{\mathbf{R}^N} |\nabla\tilde{\phi}|^2 U^2\,dx &= \int_{\mathbf{R}^N} \left[|\nabla\phi|^2 + \phi^2\nabla\left(\frac{\nabla U}{U}\right) + \frac{\phi^2|\nabla U|^2}{U^2}\right] U^2\,dx \\ &= \int_{\mathbf{R}^N} (|\nabla\phi|^2 + V\phi^2)\,dx.\end{aligned} \tag{3.32}$$

Let $\tilde{V}$ satisfy (1.2) and $\tilde{V}(r) > \lambda_* r^{-2}$ on $(0,\infty)$. Let $W \in C_0^\infty(\mathbf{R}^N)$ be such that $W \geq 0$ on $\mathbf{R}^N$. By the Hardy inequality there exists $\epsilon > 0$ such that

$$\int_{\mathbf{R}^N} \left[|\nabla\psi|^2 + (\tilde{V} - \epsilon W)\psi^2\right] dx \geq 0 \quad \text{for} \quad \psi \in C^\infty(\mathbf{R}^N \setminus \{0\}). \tag{3.33}$$

Furthermore, by Lemma 3.4 we can find a positive function $\tilde{U} \in C^2((0,\infty))$ such that

$$\begin{aligned}&\tilde{U}'' + \frac{N-1}{r}\tilde{U}' - \tilde{V}\tilde{U} = 0 \quad \text{in} \quad (0,\infty), \qquad \tilde{U}(r) \sim r^{A^+(\lambda_1)} \quad \text{as} \quad r \to 0, \\ &\tilde{U}(r) \sim c r^{A^+(\lambda_2)} \quad \text{as} \quad r \to \infty \quad \text{if} \quad \lambda > \lambda_*, \\ &\tilde{U}(r) \sim c r^{-\frac{N-2}{2}} \log r \quad \text{as} \quad r \to \infty \quad \text{if} \quad \lambda = \lambda_*,\end{aligned} \tag{3.34}$$

for some constant $c > 0$. Since $U(r) = r^{A^+(\lambda_1)}(1 + o(1))$ as $r \to 0$, it follows from (3.31) and (3.34) that $U(r) \geq C^{-1}\tilde{U}(r)$ on $(0,\infty)$. This together with (3.33) implies that

$$\begin{aligned}\int_{\mathbf{R}^N} |\nabla\tilde{\phi}|^2 U^2\,dx &\geq C\int_{\mathbf{R}^N} |\nabla\tilde{\phi}|^2\tilde{U}^2\,dx \\ &= C\int_{\mathbf{R}^N} (|\nabla\hat{\phi}|^2 + \tilde{V}\hat{\phi}^2)\,dx \geq C\epsilon\int_{\mathbf{R}^N} W\hat{\phi}^2\,dx,\end{aligned} \tag{3.35}$$

as in the same way as (3.32), where

$$\hat{\phi}(x) = \tilde{U}(|x|)\tilde{\phi}(x) = \frac{\tilde{U}(|x|)}{U(|x|)}\phi(x).$$

Since $U(r) \sim \tilde{U}(r)$ as $r \to 0$ and W has a compact support, we deduce from (3.32) and (3.35) that

$$\int_{\mathbf{R}^N} (|\nabla\phi|^2 + V\phi^2)\,dx \geq C\epsilon\int_{\mathbf{R}^N} W\hat{\phi}^2\,dx \geq C\epsilon\int_{\mathbf{R}^N} W\phi^2\,dx, \quad \phi \in C_0^\infty(\mathbf{R}^N \setminus \{0\}).$$

This means that H is subcritical. Thus Lemma 3.5 follows. □

Proof of Theorem 1.1. Assertions (1) and (2) follow from Lemma 3.1. Assertion (3) follows from Lemmas 3.2, 3.3 and 3.5.

It remains to prove assertion (4). Let $W \in C_0((0,\infty))$ be such that $W \geq 0$ and $W \not\equiv 0$ on $(0,\infty)$. Assume that H is nonnegative. For any $\mu \in \mathbf{R}$, let

$$H_\mu := -\Delta + V + \mu W.$$

Define

$$I := \{\mu \in \mathbf{R} \,:\, H_\mu \text{ is subcritical}\}, \qquad \mu_* := \inf_{\mu \in I} \mu.$$

It follows from Lemmas 3.4 and 3.5 that $I = (\mu_*, \infty)$ and $\mu_* \le 0$. Since H_{μ_*} is nonnegative, H_{μ_*} must be critical. Then assertion (4) follows. Therefore the proof of Theorem 1.1 is complete by replacing W in this proof by $-W$. $\square$

4 Proof of Theorem 1.2

Assume (1.2). Let $H := -\Delta + V$ be nonnegative and U the positive harmonic function given in Theorem 1.1. We define the unitary operator $\mathcal{U}$ by

$$\mathcal{U} \,:\, L^2(\mathbf{R}^N, dx) \ni f \;\longmapsto\; U^{-1} f \in L^2(\mathbf{R}^N, \omega(x)\, dx),$$

where $\omega(x) = U(|x|)^2$. Then the operator $L := \mathcal{U} H \mathcal{U}^{-1}$ is given by

$$Lv := -\frac{1}{\omega(x)} \mathrm{div}\,(\omega(x) \nabla v).$$

We denote by $p(x, y, t)$ and $G(x, y, t)$ the heat kernels of H and L, respectively. Then

$$p(x, y, t) = U(|x|) U(|y|) G(x, y, t) \tag{4.1}$$

for x, $y \in \mathbf{R}^N$ and $t > 0$. In this section we study upper and lower bounds of $G = G(x, y, t)$ and then obtain Theorem 1.2.

Lemma 4.1 *Let x, $y \in \mathbf{R}^N$ and $t > 0$. Assume that ω is an A_2 weight on $B(x, 2\sqrt{t}) \cup B(y, 2\sqrt{t})$. Then there exists a constant C such that*

$$G(x, y, t) \le \frac{C}{\sqrt{\omega(B(x, \sqrt{t}))}\sqrt{\omega(B(y, \sqrt{t}))}} \exp\left(-\frac{|x - y|^2}{Ct}\right) \tag{4.2}$$

for x, $y \in \mathbf{R}^N$ and $t > 0$, where $C = C_{x,y,t}$ depends on $[\omega](B(x, 2\sqrt{t}))$ and $[\omega](B(y, 2\sqrt{t}))$. In particular, C is independent of x, y and t if w is an A_2 weight on $\mathbf{R}^N$.

Proof. We obtain the upper bound of $G = G(x, y, t)$ by using the standard method as given, for example, [26, Section 6]. We give the proof for completeness of this paper.

We fix x, $y \in \mathbf{R}^N$ and $t > 0$. Let $\lambda \in \mathbf{R}$ and ψ be a bounded smooth function on $\mathbf{R}^N$ such that $|\nabla \psi| \le 1$ on $\mathbf{R}^N$. For $f_0 \in L^2(B(y, \sqrt{t}), \omega\, dz)$, we set

$$f(\xi, s) := \int_{B(y, \sqrt{t})} G(\xi, z, s) e^{-\lambda \psi(z)} f_0(z) \omega(z)\, dz, \quad F(\xi, s) := e^{\lambda \psi(\xi)} f(\xi, s). \tag{4.3}$$

Since $f = f(\xi, s)$ satisfies

$$\partial_s f = \frac{1}{\omega(\xi)} \mathrm{div}_\xi\,(\omega(\xi) \nabla_\xi f) \quad \text{in} \quad \mathbf{R}^N \times (0, \infty), \tag{4.4}$$

we have

$$\begin{aligned}\frac{d}{ds}\int_{\mathbf{R}^N} F(\xi,s)^2\omega\,d\xi &= 2\int_{\mathbf{R}^N} e^{2\lambda\psi(\xi)} f(\partial_s f)\omega\,d\xi \\ &= -2\int_{\mathbf{R}^N}\left[2\lambda e^{2\lambda\psi} f\,\nabla\psi\cdot\nabla f + e^{2\lambda\psi}|\nabla f|^2\right]\omega\,d\xi \\ &\le 2\lambda^2\int_{\mathbf{R}^N} e^{2\lambda\psi} f^2|\nabla\psi|^2\omega\,d\xi \ \le 2\lambda^2\int_{\mathbf{R}^N} F(\xi,s)^2\omega\,d\xi,\end{aligned}$$

which implies that

$$\int_{\mathbf{R}^N} F(\xi,s)^2\omega\,d\xi \le e^{2\lambda^2 s}\int_{\mathbf{R}^N} F(\xi,0)^2\omega\,d\xi = e^{2\lambda^2 s}\int_{B(y,\sqrt{t})} f_0(\xi)^2\omega\,d\xi, \quad s>0. \tag{4.5}$$

Let $0<\tau\le t$ and let $\tilde f(y,s) := f(x+\sqrt{\tau}y/2, 3\tau/4+\tau s/4)$ for $(y,s)\in B(0,1)\times(0,1)$. Then $\tilde f$ satisfies

$$\partial_s\tilde f = \frac{1}{\tilde\omega}\mathrm{div}\,(\tilde\omega\nabla\tilde f) \quad \text{in} \quad B(0,1)\times(0,1),$$

where $\tilde\omega(y) := \omega(x+\sqrt{\tau}y/2)$. Then, by Proposition 2.1 we obtain

$$\begin{aligned} f(x,\tau)^2 = \tilde f(0,0)^2 &\le \frac{C}{\tilde\omega(B(0,1))}\int_0^1\int_{B(0,1)}\tilde f(y,s)^2\tilde\omega\,dyds \\ &\le \frac{C}{\tau\omega(B(x,\sqrt{\tau}))}\int_{3\tau/4}^{\tau}\int_{B(x,\sqrt{\tau})} f(\xi,s)^2\omega\,d\xi ds.\end{aligned} \tag{4.6}$$

The constant C depends on $[\omega](B(x,2\sqrt{t}))$. Since $|\nabla\psi|\le 1$, by (2.1), (4.3), (4.5) and (4.6) we have

$$\begin{aligned} e^{2\lambda\psi(x)} f(x,\tau)^2 &\le \frac{C}{\tau\omega(B(x,\sqrt{t}))}\int_{3\tau/4}^{\tau}\int_{B(x,\sqrt{\tau})} e^{2\lambda(\psi(x)-\psi(\xi))}F(\xi,s)^2\omega\,d\xi ds \\ &\le \frac{Ce^{2\lambda\sqrt{t}}}{\omega(B(x,\sqrt{t}))}\sup_{0<s<t}\int_{\mathbf{R}^N} F(\xi,s)^2\omega\,d\xi \\ &\le \frac{Ce^{2\lambda\sqrt{t}}}{\omega(B(x,\sqrt{t}))}e^{2\lambda^2 t}\int_{B(y,\sqrt{t})} f_0(\xi)^2\omega\,d\xi\end{aligned} \tag{4.7}$$

for all $t/2\le\tau\le t$. Furthermore, by (4.3) we obtain

$$\begin{aligned} f(x,\tau) &= e^{-\lambda\psi(y)}\int_{B(y,\sqrt{t})} G(x,z,\tau)e^{-\lambda(\psi(z)-\psi(y))}f_0(z)\omega\,dz \\ &\ge e^{-\lambda\sqrt{t}}e^{-\lambda\psi(y)}\int_{B(y,\sqrt{t})} G(x,z,\tau)f_0(z)\omega\,dz\end{aligned}$$

for $\tau > 0$. This implies that

$$\begin{aligned}
&\left(\int_{B(y,\sqrt{t})} G(x,z,\tau)^2 \omega(z)\, dz \right)^{1/2} \\
&= \sup \Bigg\{ \int_{\mathbf{R}^N} G(x,z,\tau) f_0(z) \omega(z)\, dz \ : \\
&\qquad\qquad f_0 \in L^2(B(y,\sqrt{t}), \omega\, dz), \ \ \|f_0\|_{L^2(B(y,\sqrt{t}),\omega\, dz)} \le 1 \Bigg\} \\
&\le e^{\lambda\sqrt{t}} e^{\lambda\psi(y)} \sup \left\{ f(x,\tau) \ : \ f_0 \in L^2(B(y,\sqrt{t}), \omega\, dz), \ \ \|f_0\|_{L^2(B(y,\sqrt{t}),\omega\, dz)} \le 1 \right\},
\end{aligned}$$

which together with (4.7) yields

$$\begin{aligned}
&\int_{B(y,\sqrt{t})} G(x,z,\tau)^2 \omega(z)\, dz \\
&\le e^{2\lambda\sqrt{t}} e^{-2\lambda(\psi(x)-\psi(y))} \\
&\qquad \times \sup \left\{ e^{2\lambda\psi(x)} f(x,\tau)^2 \ : \ f_0 \in L^2(B(y,\sqrt{t}), \omega\, dz), \ \ \|f_0\|_{L^2(\mathbf{R}^N,\omega\, dz)} \le 1 \right\} \\
&\le e^{2\lambda\sqrt{t}} e^{-2\lambda(\psi(x)-\psi(y))} \frac{C e^{2\lambda\sqrt{t}}}{\omega(B(x,\sqrt{t}))} e^{2\lambda^2 t}
\end{aligned} \tag{4.8}$$

for all $t/2 \le \tau \le t$.

On the other hand, since $\tilde{g}(\xi, s) := G(x, \xi, s)$ is also a solution of (4.4), similarly to (4.6), we have

$$G(x,y,t)^2 \le \frac{C}{t\omega(B(y,\sqrt{t}))} \int_{3t/4}^{t} \int_{B(y,\sqrt{t})} G(x,z,\tau)^2 \omega(z)\, dz d\tau.$$

Then we deduce from (4.8) that

$$G(x,y,t)^2 \le \frac{C}{\omega(B(x,\sqrt{t}))\omega(B(y,\sqrt{t}))} e^{4\lambda\sqrt{t}+2\lambda^2 t-2\lambda(\psi(x)-\psi(y))}.$$

We choose $\lambda = \frac{\psi(x)-\psi(y)}{2t}$ and optimize over ψ with $|\nabla\psi| \le 1$. This gives (4.2), and the proof is complete. □

If w is an A_2 weight on $\mathbf{R}^N$, then we obtain upper estimate of Lemma 4.1. We mention that the proof actually gives the estimate

$$G(x,y,t) \le \frac{C_\epsilon}{\sqrt{\omega(B(x,\sqrt{t}))}\sqrt{\omega(B(y,\sqrt{t}))}} \exp\left(-\frac{|x-y|^2}{(4+\epsilon)t} \right)$$

for every $\epsilon > 0$ and all $x, y \in \mathbf{R}^N$ and $t > 0$. Here C_ϵ is a positive constant depending on ϵ. Therefore, by (4.1) we obtain the following upper estimate

$$p(x,y,t) \le \frac{C_\epsilon U(x) U(y)}{\sqrt{\omega(B(x,\sqrt{t}))}\sqrt{\omega(B(y,\sqrt{t}))}} \exp\left(-\frac{|x-y|^2}{(4+\epsilon)t} \right). \tag{4.9}$$

This shows the upper bound of Theorem 1.2.

Next, we prove the lower bound. In the rest of this section we assume that w is an A_2 weight on $\mathbf{R}^N$. The idea of proof is known and has been used in the context of Riemmannian manifolds, see, e.g., [6], [25, Chapter 7] and references therein.

It follows from the definition of the operator L and the fact that U is a harmonic function of H that $e^{-tL}\mathbf{1} = \mathbf{1}$. In other words,

$$\int_{\mathbf{R}^N} G(x, y, t)\omega(y)dy = 1.$$

This together with the doubling property (2.1) and the Gaussian upper bound (4.9) imply the diagonal lower bound

$$G(x, x, t) \geq \frac{C}{\omega(B(x, \sqrt{t}))} \tag{4.10}$$

for some constant $C > 0$. See, e.g., [6] and [25, Chapter 7]. Next, one extends this diagonal lower bound to x and y near the diagonal. In order to do this one needs the Hölder continuity of the heat kernel $G(t, x, y)$. This latter property follows from the Harnack inequality. The Hölder continuity is also proved in [7], namely

$$|G(x, x, t) - G(x, y, t)| \leq \frac{Ct^{-\eta/2}}{\omega(B(x, \sqrt{t}))}|x - y|^\eta \tag{4.11}$$

for some $\eta \in (0, 1)$ and all x, y and $t > 0$ such that $|x - y| \leq \frac{1}{2}\sqrt{t}$. Using (4.10) and (4.11) one obtains easily

$$G(x, y, t) \geq \frac{C}{\sqrt{\omega(B(x, \sqrt{t}))}\sqrt{\omega(B(y, \sqrt{t}))}}$$

for $x, y \in \mathbf{R}^N$ and $t > 0$ such that $|x - y| \leq \delta\sqrt{t}$ for some constant $\delta > 0$. Finally, the Gaussian lower bound

$$G(x, y, t) \geq \frac{C}{\sqrt{\omega(B(x, \sqrt{t}))}\sqrt{\omega(B(y, \sqrt{t}))}} \exp\left(-\frac{|x - y|^2}{Ct}\right)$$

follows by a chain argument and the semigroup property. See again, e.g., [6] and [25, Chapter 7]. The equality (4.1) gives the lower estimate of Theorem 1.2. Thus the proof of Theorem 1.2 is complete.

5 Non A_2 weight

In this section we study upper bounds of $p = p(x, y, t)$ without the assumption that U^2 is an A_2 weight on $\mathbf{R}^N$, and prove Theorem 1.3. In what follows, we set

$$d := A^+(\lambda_2) \quad \text{if } H \text{ is subcritical}, \qquad d := A^-(\lambda_2) \quad \text{if } H \text{ is critical}.$$

The first lemma follows from a similar argument as in the proof of Lemma 4.1.

Lemma 5.1 *Let V be a continuous function on $(0,\infty)$ satisfying (1.2). Assume that $H := -\Delta + V(|x|)$ is nonnegative and let U be as in Theorem 1.1. Then, for any $\epsilon \in (0,1]$, there exists a constant C such that*

$$p(x,y,t) \le Ct^{-\frac{N}{2}} \exp\left(-\frac{|x-y|^2}{Ct}\right) \tag{5.1}$$

for all x, $y \in \mathbf{R}^N \setminus B(0,\epsilon\sqrt{t})$ and $t > 0$. In particular,

$$p(x,y,t) \le Ct^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{t}\})U(\min\{|y|,\sqrt{t}\})}{U(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right) \tag{5.2}$$

for all x, $y \in \mathbf{R}^N \setminus B(0,\epsilon\sqrt{t})$ and $t > 0$.

Proof. Let $\epsilon \in (0,1]$, x, $y \in \mathbf{R}^N \setminus B(0,\epsilon\sqrt{t})$ and $t > 0$. Similarly to the proof of Lemma 4.1, let $\lambda \in \mathbf{R}$ and let ψ be a bounded smooth function ψ on $\mathbf{R}^N$ such that $|\nabla\psi| \le 1$ on $\mathbf{R}^N$. For any $f_0 \in L^2(B(y,\epsilon\sqrt{t}))$, set

$$f(\xi,s) := \int_{B(y,\epsilon\sqrt{t})} p(\xi,z,s)e^{-\lambda\psi(z)} f_0(z)\,dz, \quad F(\xi,s) := e^{\lambda\psi(\xi)} f(\xi,s).$$

Then it follows from the nonnegativity of H that

$$\begin{aligned}
&\frac{d}{ds}\int_{\mathbf{R}^N} F(\xi,s)^2\,d\xi \\
&= -2\int_{\mathbf{R}^N} e^{2\lambda\psi}\left[2\lambda f\,\nabla\psi\cdot\nabla f + |\nabla f|^2 + Vf^2\right]\,d\xi \\
&= -2\int_{\mathbf{R}^N}\left[|\nabla(e^{\lambda\psi}f)|^2 + V(e^{\lambda\psi}f)^2\right]\,d\xi + 2\lambda^2\int_{\mathbf{R}^N} e^{2\lambda\psi}f^2|\nabla\psi|^2\,d\xi \\
&\le 2\lambda^2\int_{\mathbf{R}^N} e^{2\lambda\psi}f^2|\nabla\psi|^2\,d\xi \le 2\lambda^2\int_{\mathbf{R}^N} F(\xi,s)^2\,d\xi,
\end{aligned}$$

which implies that

$$\int_{\mathbf{R}^N} F(\xi,s)^2\,d\xi \le e^{2\lambda^2 s}\int_{B(y,\sqrt{t})} f_0(\xi)^2\,d\xi.$$

Let $0 < \eta \le t$. Set

$$\tilde{f}(\xi,s) := f(x+\delta\epsilon\xi, \eta+\delta^2\epsilon^2 s) \quad \text{with} \quad \delta = \sqrt{\eta}/4, \qquad \tilde{V}(\xi) := \delta^2\epsilon^2 V(x+\delta\epsilon\xi).$$

Since f satisfies $\partial_s f = \Delta_\xi f - V(\xi)f$ on $\mathbf{R}^N \times (0,\infty)$, we have

$$\partial_s\tilde{f} = \Delta_\xi\tilde{f} - \tilde{V}(\xi)\tilde{f} \quad \text{in} \quad \mathbf{R}^N \times \left(-16\epsilon^{-2},\infty\right).$$

Furthermore,

$$|x+\delta\epsilon\xi| \ge |x| - \frac{\epsilon}{4}\sqrt{\eta}|\xi| \ge \epsilon\sqrt{t} - \frac{\epsilon}{4}\sqrt{t}|\xi| \ge \frac{\epsilon}{2}\sqrt{t} \ge \frac{\epsilon}{2}\sqrt{\eta} \tag{5.3}$$

for $x \in \mathbf{R}^N \setminus B(0,\epsilon\sqrt{t})$ and $\xi \in B(0,2)$. Since $|V(|x|)| \le C|x|^{-2}$ by (1.2), we deduce from (5.3) that

$$|\tilde{V}(\xi)| \le C\delta^2\epsilon^2|x+\delta\epsilon\xi|^{-2} \le C, \qquad \xi \in B(0,2).$$

Then it follows from Proposition 2.1 that

$$|\tilde{f}(0,0)|^2 \le C \int_{-1}^{0} \int_{B(0,1)} |\tilde{f}|^2 \, d\xi ds.$$

Since $\eta - \delta^2\epsilon^2 \ge 3\eta/4$ and $\delta\epsilon \le \epsilon\sqrt{t}$, it follows that

$$\begin{aligned} f(x,\eta)^2 &\le C(\delta\epsilon)^{-N-2} \int_{\eta-\delta^2\epsilon^2}^{\eta} \int_{B(x,\delta\epsilon)} |f(\xi,s)|^2 \, d\xi ds \\ &\le C\eta^{-\frac{N}{2}-1} \int_{3\eta/4}^{\eta} \int_{B(x,\epsilon\sqrt{t})} |f(\xi,s)|^2 \, d\xi ds \end{aligned}$$

for $x \in \mathbf{R}^N \setminus B(0,\epsilon\sqrt{t})$ and $0 < \eta \le t \le 1$. Then we apply a similar argument as in the proof of Lemma 4.1 to obtain (5.1). Furthermore, it follows from Theorem 1.1 that

$$U(\min\{|x|,\epsilon\sqrt{t}\}) \asymp U(\min\{|x|,\sqrt{t}\}) \quad \text{and} \quad U(\epsilon\sqrt{t}) \asymp U(\sqrt{t}) \tag{5.4}$$

for $x \in \mathbf{R}^N$ and $t > 0$. Then we deduce from (5.1) and (5.4) that

$$\begin{aligned} p(x,y,t) &\le Ct^{-\frac{N}{2}} \frac{U(\min\{|x|,\epsilon\sqrt{t}\})U(\min\{|y|,\epsilon\sqrt{t}\})}{U(\epsilon\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right) \\ &\le Ct^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{t}\})U(\min\{|y|,\sqrt{t}\})}{U(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right) \end{aligned}$$

for all x, $y \in \mathbf{R}^N \setminus B(0,\epsilon\sqrt{t})$ and $t > 0$. So we have (5.2), and the proof is complete. □

Combining Lemma 5.1 with Lemma 4.1, we obtain upper estimates of $p = p(x,y,t)$ in the case where $0 < t \le 1$ and $A^+(\lambda_1) < N/2$.

Lemma 5.2 *Assume the same conditions as in Theorem* 1.3 *and* $A^+(\lambda_1) < N/2$. *Then there exists a constant* C *such that*

$$p(x,y,t) \le Ct^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{t}\})U(\min\{|y|,\sqrt{t}\})}{U(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right) \tag{5.5}$$

for all x, $y \in \mathbf{R}^N$ *and* $0 < t \le 1$.

Proof. Let $G = G(x,y,t)$ be as in Section 4. Let $0 < t \le 1$. The proof is divided into the following four cases:

(i) $x, y \in \mathbf{R}^N \setminus B(0,\sqrt{t})$; (ii) $x, y \in B(0,\sqrt{t})$;

(iii) $x \in \mathbf{R}^N \setminus B(0,\sqrt{t})$, $y \in B(0,\sqrt{t})$; (iv) $x \in B(0,\sqrt{t})$, $y \in \mathbf{R}^N \setminus B(0,\sqrt{t})$.

In case (i) (5.5) follows from Lemma 5.1. So we have only to consider cases (ii), (iii) and (iv).

Consider case (ii). It follows from Theorem 1.1 that $U(|x|) \sim |x|^{A^+(\lambda_1)}$ as $|x| \to 0$. Combining (1.4) with the assumption $A^+(\lambda_1) < N/2$, we see that $A^+(\lambda_1) \in (-N/2, N/2)$,

which means that $\omega(x) = U(|x|)^2$ is an A_2 weight on $B(0,2)$. Then Lemma 4.1 implies that

$$G(x,y,t) \le \frac{C}{\sqrt{\omega(B(x,\sqrt{t}))}\sqrt{\omega(B(y,\sqrt{t}))}} \exp\left(-\frac{|x-y|^2}{Ct}\right). \tag{5.6}$$

Furthermore, it follows from Theorem 1.1 and (2.1) that

$$\omega(B(\xi,\sqrt{s})) \asymp \omega(B(\xi,2\sqrt{s})) \ge \omega(B(0,\sqrt{s})) \asymp s^{\frac{N}{2}+A^+(\lambda_1)} \asymp s^{\frac{N}{2}} U(\sqrt{s})^2 \tag{5.7}$$

for $\xi \in B(0,\sqrt{s})$ and $0 < s \le 1$. By (4.1), (5.6) and (5.7) we obtain

$$\begin{aligned} p(x,y,t) &\le \frac{CU(|x|)U(|y|)}{\sqrt{\omega(B(x,\sqrt{t}))}\sqrt{\omega(B(y,\sqrt{t}))}} \exp\left(-\frac{|x-y|^2}{Ct}\right) \\ &\le Ct^{-\frac{N}{2}} \frac{U(|x|)U(|y|)}{U(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right) \\ &= Ct^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{t}\})U(\min\{|y|,\sqrt{t}\})}{U(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right), \end{aligned}$$

which implies (5.5) in case (ii).

Consider case (iii). Set $\tilde{y} := \sqrt{2t}y/|y|$ and $g(\xi,s) := G(x,\xi,s)$. Recalling that w is A_2 weight on $B(0,2)$, we apply Lemma 2.1 to g to obtain

$$g(y,t) \le Cg(\tilde{y},2t) \exp\left(C\frac{|y-\tilde{y}|^2}{t}\right) \le Cg(\tilde{y},2t),$$

which together with (4.1) implies

$$p(x,y,t) \le C\frac{U(|y|)}{U(|\tilde{y}|)} p(x,\tilde{y},2t) = C\frac{U(|y|)}{U(\sqrt{2t})} p(x,\tilde{y},2t) \le C\frac{U(|y|)}{U(\sqrt{t})} p(x,\tilde{y},2t). \tag{5.8}$$

Since $|x| \ge \sqrt{t} = \epsilon\sqrt{2t}$ with $\epsilon = 1/\sqrt{2}$, applying Lemma 5.1, we have

$$\begin{aligned} p(x,\tilde{y},2t) &\le C(2t)^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{2t}\})U(\min\{|\tilde{y}|,\sqrt{2t}\})}{U(\sqrt{2t})^2} \exp\left(-\frac{|x-\tilde{y}|^2}{2Ct}\right) \\ &\le Ct^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{2t}\})}{U(\sqrt{2t})} \exp\left(-\frac{|x|^2}{Ct}\right) \\ &\le Ct^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{t}\})}{U(\sqrt{t})} \exp\left(-\frac{|x-y|^2}{Ct}\right). \end{aligned}$$

This together with (5.8) implies (5.5) in case (iii). Since $p(x,y,t) = p(y,x,t)$, we also obtain (5.5) in case (iv). Thus Lemma 5.2 follows. □

Next we obtain upper estimates of $p = p(x,y,t)$ in the case where $0 < t \le 1$ and $A^+(\lambda_1) \ge N/2$.

Lemma 5.3 *Assume the same conditions as in Theorem* 1.3 *and* $A^+(\lambda_1) \geq N/2$. *Then there exists a constant* C *such that*

$$p(x,y,t) \leq Ct^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{t}\})U(\min\{|y|,\sqrt{t}\})}{U(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{Ct}\right) \tag{5.9}$$

for all x, $y \in \mathbf{R}^N$ *and* $0 < t < 1$.

For this aim, we prepare the following lemma, which is useful to obtain upper estimates of $p = p(x,y,t)$ inside a parabolic cone. A similar lemma has been used in the study of the behavior of the solutions of the heat equation with a potential (see e.g., [11, 12, 15, 16]).

Lemma 5.4 *Assume the same conditions as in Theorem* 1.1. *Let* $T \geq 0$. *Furthermore, assume that*

$$\zeta(t) := t^{\gamma_1}[\log(c+t)]^{\gamma_2}$$

is monotone decreasing on (T,∞), *where* γ_1, $\gamma_2 \in \mathbf{R}$ *and* $c > 1$. *Let* $\kappa > 0$ *be such that*

$$-s\zeta'(s) \leq \kappa\zeta(s), \qquad s \in (T,\infty). \tag{5.10}$$

Define

$$\begin{aligned} F[U](x) :=& U(|x|)\int_0^{|x|} s^{1-N}[U(s)]^{-2}\left(\int_0^s \tau^{N-1}U(\tau)^2\,d\tau\right)ds, \\ w(x,t) :=& \zeta(s)\left[U(|x|) - \kappa s^{-1}F[U](x)\right]. \end{aligned}$$

Then

$$\partial_t w \geq \Delta w - V(|x|)w \quad \textit{in} \quad \mathbf{R}^N \times (T,\infty).$$

Proof. It follows that $\Delta F - V(|x|)F = U(|x|)$ for $x \in \mathbf{R}^N$. This together with (5.10) implies

$$\partial_t w - \Delta w + V(|x|)w \geq [\zeta'(t) + \kappa t^{-1}\zeta(t)]U(x) \geq 0, \quad x \in \mathbf{R}^N,\ t \in (T,\infty).$$

Thus Lemma 5.4 follows. □

Proof of Lemma 5.3. For any $\sigma > 0$, we define

$$H_\sigma := -\Delta + V_\sigma(|x|), \qquad V_\sigma(|x|) := \frac{V(|x|)}{U(|x|)+\sigma}U(|x|).$$

Let $p_\sigma = p_\sigma(x,y,t)$ be the fundamental solution corresponding to e^{-tH_σ}. It follows from Theorem 1.1 and (1.2) that

$$|V_\sigma(|x|)| \leq |V(|x|)| \leq C|x|^{-2} \text{ in } \mathbf{R}^N, \quad V_\sigma(r) \sim \lambda_1 r^{-2+A^+(\lambda_1)} \quad \text{as} \quad r \to 0. \tag{5.11}$$

In particular, since $A^+(\lambda_1) > 0$, we see that $V_\sigma \in L^q_{\mathrm{loc}}(\mathbf{R}^N)$ for some $q > N/2$. Furthermore, $U_\sigma := U + \sigma$ is a positive harmonic function for H_σ and

$$\int_{\mathbf{R}^N}\left[|\nabla\varphi|^2 + V_\sigma\varphi^2\right]dz = \int_{\mathbf{R}^N}\left|\nabla\frac{\varphi}{U_\sigma}\right|^2 U_\sigma^2\,dz \geq 0$$

for all $\varphi \in C_0^\infty(\mathbf{R}^N)$, which means that H_σ is nonnegative on $L^2(\mathbf{R}^N)$.

In the proof, the letter C_* denotes a generic constant independent of x, y, t and σ. Since H_σ is nonnegative, for any $\epsilon \in (0,1]$, we apply Lemma 5.1 with the aid of (5.11) to obtain

$$p_\sigma(t,x,y) \le C_* t^{-\frac{N}{2}} \exp\left(-\frac{|x-y|^2}{C_* t}\right) \tag{5.12}$$

for all x, $y \in \mathbf{R}^N \setminus B(0,\epsilon\sqrt{t})$ and $t > 0$. On the other hand, since U_σ^2 is an A_2 weight on $B(0,R)$ for any $R > 0$, we apply a similar argument as in the proof of Lemma 5.2 to obtain

$$p_\sigma(x,y,t) \le C_{R,\sigma} t^{-\frac{N}{2}} \frac{U_\sigma(\min\{|x|,\sqrt{t}\})U_\sigma(\min\{|y|,\sqrt{t}\})}{U_\sigma(\sqrt{t})^2} \exp\left(-\frac{|x-y|^2}{C_{R,\sigma} t}\right) \tag{5.13}$$

for all x, $y \in B(0,R)$ and $0 < t \le 1$, where $C_{R,\sigma}$ is a constant depending on R and σ.

Let ϵ be a sufficiently small positive constant to be chosen later. Let x, $y \in \mathbf{R}^N$ and $0 < t \le 1$. In what follows, we divide the proof into the following four cases:

(i) $x, y \in \mathbf{R}^N \setminus B(0,\epsilon\sqrt{t})$; (ii) $x, y \in B(0,\epsilon\sqrt{t})$;

(iii) $x \in \mathbf{R}^N \setminus B(0,\epsilon\sqrt{t})$, $y \in B(0,\epsilon\sqrt{t})$; (iv) $x \in B(0,\epsilon\sqrt{t})$, $y \in \mathbf{R}^N \setminus B(0,\epsilon\sqrt{t})$.

Similarly to Lemma 5.2, by Lemma 5.1 we have (5.9) in case (i).

We consider case (iii). Define

$$\begin{aligned} D_\epsilon(t) &:= \left\{(\xi,s) \in \mathbf{R}^N \times (0,t] \,:\, |\xi| < \epsilon\sqrt{s}\right\}, \\ \partial_p D_\epsilon(t) &:= \left\{(\xi,s) \in \mathbf{R}^N \times [0,t] \,:\, |\xi| = \epsilon\sqrt{s}\right\}. \end{aligned}$$

Let $\kappa := (N + A^+(\lambda_1))/2$ and set

$$\begin{aligned} &v(\xi,s) := p_\sigma(x,\xi,s), \quad w(\xi,s) := s^{-\frac{N+A^+(\lambda_1)}{2}} \left[U_\sigma(|\xi|) - \kappa s^{-1} F[U_\sigma](|\xi|)\right], \\ &z(\xi,s) := v(\xi,s) - \gamma \exp\left(-\frac{|x|^2}{\gamma t}\right) w(\xi,s), \end{aligned} \tag{5.14}$$

where γ is a positive constant. It follows from Lemma 5.4 that

$$\partial_s z \le \Delta z - V_\sigma(|\xi|) z \quad \text{in} \quad \mathbf{R}^N \times (0,\infty). \tag{5.15}$$

Since $U(r) \asymp r^{A^+(\lambda_1)}$ on $(0,1)$ and $A^+(\lambda_1) > 0$, we have

$$\begin{aligned} F[U_\sigma](|\xi|) &= U_\sigma(|\xi|) \int_0^{|\xi|} s^{1-N} [U_\sigma(s)]^{-2} \left(\int_0^s \tau^{N-1} U_\sigma(\tau)^2 \, d\tau\right) ds \\ &\le U_\sigma(|\xi|) \int_0^{|\xi|} s^{1-N} [C_*^{-1} s^{A^+(\lambda_1)} + \sigma]^{-2} \left(\int_0^s \tau^{N-1} (C_* r^{A^+(\lambda_1)} + \sigma)^2 \, d\tau\right) ds \\ &\le U_\sigma(|\xi|) \int_0^{|\xi|} s^{1-N} [C_*^{-1}\sigma^{-1} s^{A^+(\lambda_1)} + 1]^{-2} \cdot \frac{1}{N} s^N (C_* \sigma^{-1} s^{A^+(\lambda_1)} + 1)^2 \, ds \\ &\le \frac{C_*}{2N} |\xi|^2 U_\sigma(|\xi|) \le \frac{C_* \epsilon}{2N} s U_\sigma(|\xi|), \qquad (\xi,s) \in D_\epsilon(t). \end{aligned} \tag{5.16}$$

Taking a sufficiently small $\epsilon > 0$ if necessary, by (5.14) and (5.16) we obtain

$$w(\xi, s) \geq \frac{1}{2} s^{-\frac{N+A^+(\lambda_1)}{2}} U_\sigma(|\xi|) = \frac{1}{2} s^{-\frac{N+A^+(\lambda_1)}{2}} [U(|\xi|) + \sigma] \quad \text{in} \quad D_\epsilon(t).$$

This implies that

$$w(\xi, s) \geq \frac{1}{2} s^{-\frac{N+A^+(\lambda_1)}{2}} \sigma \quad \text{in} \quad D_\epsilon(t), \tag{5.17}$$

$$\begin{aligned} w(\xi, s) &\geq \frac{1}{2} s^{-\frac{N+A^+(\lambda_1)}{2}} U(|\xi|) \geq C_* s^{-\frac{N+A^+(\lambda_1)}{2}} (\epsilon\sqrt{s})^{A^+(\lambda_1)} \\ &\geq C_* \epsilon^{A^+(\lambda_1)} s^{-\frac{N}{2}} \quad \text{on} \quad \partial_p D_\epsilon(t) \setminus \{(0,0)\}. \end{aligned} \tag{5.18}$$

On the other hand, it follows from (5.12) that

$$v(\xi, s) = p_\sigma(x, \xi, s) \leq C_* s^{-\frac{N}{2}} \exp\left(-\frac{|x-\xi|^2}{C_* s}\right) \leq C_* s^{-\frac{N}{2}} \exp\left(-\frac{|x|^2}{C_* t}\right) \tag{5.19}$$

on $\partial_p D_\epsilon(t) \setminus \{(0,0)\}$. Then, by (5.18) and (5.19), taking a sufficiently large constant γ if necessary, we have

$$z(\xi, s) \leq 0 \quad \text{on} \quad \partial_p D_\epsilon(t) \setminus \{(0,0)\}. \tag{5.20}$$

On the other hand, since $|x| \geq \epsilon\sqrt{t}$ and $A^+(\lambda_1) > 0$, by (5.13) we see that

$$\lim_{s \to 0} s^{\frac{N+A^+(\lambda_1)}{2}} v(\xi, s) = 0$$

uniformly for ξ in a neighborhood of the origin. Then, by (5.17) we see that

$$z(\xi, s) \leq 0 \tag{5.21}$$

for $(\xi, s) \in D_\epsilon(t)$ if s is sufficiently small. Therefore, by (5.15), (5.20) and (5.21) we apply the comparison principle to obtain $z \leq 0$ on $D_\epsilon(t)$. This together with (5.14) implies that

$$p_\sigma(x, \xi, s) = v(\xi, s) \leq \gamma \exp\left(-\frac{|x|^2}{\gamma t}\right) w(\xi, s) \leq \gamma s^{-\frac{N+A^+(\lambda_1)}{2}} U_\sigma(|\xi|) \exp\left(-\frac{|x|^2}{\gamma t}\right)$$

for $(\xi, s) \in D_\epsilon(t)$ and $0 < \sigma \leq 1$. Taking $(\xi, s) = (y, t)$, we obtain

$$\begin{aligned} p_\sigma(x, y, t) &\leq \gamma t^{-\frac{N+A^+(\lambda_1)}{2}} U_\sigma(|y|) \exp\left(-\frac{|x|^2}{\gamma t}\right) \\ &\leq C_* t^{-\frac{N+A^+(\lambda_1)}{2}} U_\sigma(|y|) \exp\left(-\frac{|x-y|^2}{C_* t}\right) \\ &\leq C_* t^{-\frac{N}{2}} \frac{U(\min\{|y|, \epsilon\sqrt{t}\}) + \sigma}{U(\sqrt{t})} \exp\left(-\frac{|x-y|^2}{C_* t}\right). \end{aligned} \tag{5.22}$$

Passing to the limit as $\sigma \to 0$, we deduce that

$$\begin{aligned} p(x, y, t) &\leq C_* t^{-\frac{N}{2}} \frac{U(\min\{|y|, \epsilon\sqrt{t}\})}{U(\sqrt{t})} \exp\left(-\frac{|x-y|^2}{C_* t}\right) \\ &\leq C_* t^{-\frac{N}{2}} \frac{U(\min\{|y|, \sqrt{t}\})}{U(\sqrt{t})} \exp\left(-\frac{|x-y|^2}{C_* t}\right), \end{aligned}$$

which means that (5.9) holds in case (iii). Since $p(x,y,t)=p(y,x,t)$, we also obtain (5.9) in case (iv).

It remains to consider case (ii). Let $\tilde{\kappa}:=(N+2A^+(\lambda_1))/2$ and set

$$\begin{aligned}&\tilde{v}(\xi,s):=p_\sigma(\xi,y,s),\quad \tilde{w}(\xi,s):=s^{-\frac{N+2A^+(\lambda_1)}{2}}\left[U_\sigma(|\xi|)-\tilde{\kappa}s^{-1}F[U_\sigma](|\xi|)\right],\\&\tilde{z}(\xi,s):=\tilde{v}(\xi,s)-\gamma'[\gamma' U(\min\{|y|,\epsilon\sqrt{t}\})+\sigma]\exp\left(-\frac{|y|^2}{\gamma' t}\right)\tilde{w}(\xi,s),\end{aligned}\tag{5.23}$$

where γ' is a positive constant. It follows from Lemma 5.4 that

$$\partial_s\tilde{z}\le\Delta_\xi\tilde{z}-V_\sigma(|\xi|)\tilde{z}\quad\text{in}\quad\mathbf{R}^N\times(0,\infty).\tag{5.24}$$

For $(\xi,s)\in\partial_p D_\epsilon(t)\setminus\{(0,0)\}$, we see that $\xi\in\mathbf{R}^N\setminus B(0,\epsilon\sqrt{s})$. Since $U(r)\asymp r^{A^+(\lambda_1)}$ on $(0,1)$ and $A^+(\lambda_1)>0$, we apply (5.9) and (5.22) to obtain

$$\begin{aligned}\tilde{v}(\xi,s)&\le C_* s^{-\frac{N}{2}}\frac{U(\min\{|y|,\epsilon\sqrt{s}\})+\sigma}{U(\sqrt{s})}\exp\left(-\frac{|\xi-y|^2}{C_* s}\right)\\&\le C_* s^{-\frac{N+A^+(\lambda_1)}{2}}[C_* U(\min\{|y|,\epsilon\sqrt{t}\})+\sigma]\exp\left(-\frac{|y|^2}{C_* s}\right)\\&\le C_* s^{-\frac{N+A^+(\lambda_1)}{2}}[C_* U(\min\{|y|,\epsilon\sqrt{t}\})+\sigma]\exp\left(-\frac{|y|^2}{C_* t}\right)\end{aligned}\tag{5.25}$$

for $(\xi,s)\in\partial_p D_\epsilon(t)\setminus\{(0,0)\}$. On the other hand, taking a sufficiently small $\epsilon>0$ if necessary, by (5.16) we have

$$\tilde{w}(\xi,s)\ge\frac{1}{2}s^{-\frac{N+2A^+(\lambda_1)}{2}}U_\sigma(|x|)\quad\text{in}\quad D_\epsilon(t).$$

Then, similarly to (5.17) and (5.18), we see that

$$\tilde{w}(\xi,s)\ge\frac{1}{2}s^{-\frac{N+2A^+(\lambda_1)}{2}}\sigma\quad\text{in}\quad D_\epsilon(t),\tag{5.26}$$

$$\begin{aligned}\tilde{w}(\xi,s)&\ge\frac{1}{2}s^{-\frac{N+2A^+(\lambda_1)}{2}}U(|\xi|)\ge C_* s^{-\frac{N+2A^+(\lambda_1)}{2}}(\epsilon\sqrt{s})^{A^+(\lambda_1)}\\&\ge C_*\epsilon^{A^+(\lambda_1)}s^{-\frac{N+A^+(\lambda_1)}{2}}\quad\text{on}\quad\partial D_\epsilon(t).\end{aligned}\tag{5.27}$$

Taking a sufficiently large constant γ' if necessary, by (5.25) and (5.27) we have

$$\tilde{z}(\xi,s)\le 0\quad\text{on}\quad\partial_p D_\epsilon(t)\setminus\{(0,0)\}.\tag{5.28}$$

Furthermore, by (5.13) we see that

$$\lim_{s\to 0}s^{\frac{N+2A^+(\lambda_1)}{2}}\tilde{v}(\xi,s)=0$$

uniformly for ξ in a neighborhood of the origin. This together with (5.17) implies that

$$\tilde{z}(\xi,s)\le 0\tag{5.29}$$

for $(\xi,s)\in D_\epsilon(t)$ if s is sufficiently small. Therefore, by (5.24), (5.28) and (5.29) we apply the comparison principle to obtain $\tilde z\le 0$ on $D_\epsilon(t)$. This together with (5.23) implies that

$$\begin{aligned} p_\sigma(\xi,y,s)=\tilde v(\xi,s)&\le \gamma'[\gamma' U(\min\{|y|,\epsilon\sqrt{t}\})+\sigma]\exp\left(-\frac{|y|^2}{\gamma' t}\right)\tilde w(\xi,s)\\ &\le C_* s^{-\frac{N+2A^+(\lambda_1)}{2}}[C_* U(\min\{|y|,\epsilon\sqrt{t}\})+\sigma]U_\sigma(|y|)\exp\left(-\frac{|y|^2}{C_* t}\right) \end{aligned}$$

for $(\xi,s)\in D_\epsilon(t)$. Taking $(\xi,s)=(x,t)$ and passing to the limit as $\sigma\to 0$, by (5.4) we obtain

$$\begin{aligned} p(x,y,t)=\lim_{\sigma\to 0}p_\sigma(x,y,t)&\le C_* t^{-\frac{N+2A^+(\lambda_1)}{2}}U(\min\{|y|,\epsilon\sqrt{t}\})U(|x|)\exp\left(-\frac{|y|^2}{C_* t}\right)\\ &\le C_* t^{-\frac{N+2A^+(\lambda_1)}{2}}U(\min\{|y|,\sqrt{t}\})U(|x|)\exp\left(-\frac{|x-y|^2}{C_* t}\right)\\ &\le C_* t^{-\frac{N}{2}}\frac{U(\min\{|y|,\sqrt{t}\})U(\min\{|x|,\sqrt{t}\})}{U(\sqrt{t})^2}\exp\left(-\frac{|x-y|^2}{C_* t}\right). \end{aligned}$$

which means that (5.9) holds in case (ii). Thus Lemma 5.2 follows. □

We complete the proof of Theorem 1.3.

Proof of Theorem 1.3. Let ϵ be a sufficiently small positive constant. Due to Lemmas 5.2 and 5.3, it suffices to prove (1.6) in the case $t>1$.

Let $t>1$. Similarly to Lemma 5.3, the proof is divided into the following four cases:

(i) $x,y\in\mathbf{R}^N\setminus B(0,\epsilon\sqrt{t})$; (ii) $x,y\in B(0,\epsilon\sqrt{t})$;

(iii) $x\in\mathbf{R}^N\setminus B(0,\epsilon\sqrt{t})$, $y\in B(0,\epsilon\sqrt{t})$; (iv) $x\in B(0,\epsilon\sqrt{t})$, $y\in\mathbf{R}^N\setminus B(0,\epsilon\sqrt{t})$.

In case (i), by Lemma 5.1 we have (1.6).

Consider case (iii). Define

$$\begin{aligned} E_\epsilon(t)&:=\left\{(\xi,s)\in\mathbf{R}^N\times(1,t]\,:\,|\xi|<\epsilon\sqrt{s}\right\},\\ \partial_p E_\epsilon(t)&:=\left\{(\xi,s)\in\mathbf{R}^N\times(1,t]\,:\,|\xi|=\epsilon\sqrt{s}\right\}\cup\{(\xi,1)\in\mathbf{R}^N\times\{1\}\,:\,|\xi|\le\epsilon\}. \end{aligned}$$

Let

$$\zeta(s):=\begin{cases} s^{-\frac{N+d}{2}}[\log(2+s)]^{-1} & \text{if } \lambda_2=\lambda_* \text{ and } H \text{ is subcritical},\\ s^{-\frac{N+d}{2}} & \text{otherwise.}\end{cases}$$

It follows from Theorem 1.1 that

$$\zeta(s)\asymp s^{-\frac{N}{2}}U(\sqrt{s})^{-1}\quad\text{in}\quad(1,\infty). \tag{5.30}$$

Since $N+d>0$, we can find $\kappa>0$ such that $-s\zeta'(s)\le\kappa\zeta(s)$ on $(1,\infty)$. Set

$$\begin{aligned} &v(\xi,s):=p(x,\xi,s),\quad w(\xi,s):=\zeta(s)\left[U(|\xi|)-\kappa s^{-1}F[U](|\xi|)\right],\\ &z(\xi,s):=v(\xi,s)-C_1\exp\left(-\frac{|x|^2}{C_1 t}\right)w(\xi,s), \end{aligned} \tag{5.31}$$

where C_1 is a positive constant to be chosen later. It follows from Lemma 5.4 that

$$\partial_s z \le \Delta_\xi z - V(|\xi|)z \quad \text{in} \quad \mathbf{R}^N \times (1,\infty). \tag{5.32}$$

Since (1.6) holds in the case $0 < t \le 1$, we see that

$$\begin{aligned} v(\xi,1) = p(x,\xi,1) &\le C\frac{U(\min\{|x|,1\})U(\min\{|\xi|,1\})}{U(1)^2}\exp\left(-\frac{|x-\xi|^2}{C}\right) \\ &\le CU(|\xi|)\exp\left(-\frac{|x|^2}{Ct}\right) \end{aligned} \tag{5.33}$$

for $\xi \in B(0,1)$. Furthermore, by Lemma 5.1 we have

$$v(\xi,s) \le Cs^{-\frac{N}{2}}\exp\left(-\frac{|x-\xi|^2}{Cs}\right) \le Cs^{-\frac{N}{2}}\exp\left(-\frac{|x|^2}{Ct}\right) \tag{5.34}$$

for $(\xi,s) \in \mathbf{R}^N \times (1,t)$ with $|\xi| = \epsilon\sqrt{s}$. On the other hand, taking a sufficiently small $\epsilon > 0$ if necessary, by (5.16) with $\sigma = 0$ we have

$$w(\xi,s) \ge \frac{1}{2}\zeta(s)U(|\xi|) \quad \text{in} \quad E_\epsilon(t).$$

In particular,

$$w(\xi,1) \ge \frac{1}{2}\zeta(1)U(|\xi|) \tag{5.35}$$

for $\xi \in B(0,\epsilon)$. In addition, by (5.30) we see that

$$w(\xi,s) \ge C^{-1}s^{-\frac{N}{2}} \tag{5.36}$$

for $(\xi,s) \in \mathbf{R}^N \times (1,t)$ with $|\xi| = \epsilon\sqrt{s}$. Taking a sufficiently large C_1 if necessary, by (5.33), (5.34), (5.35) and (5.36) we have

$$z(\xi,s) \le 0 \quad \text{on} \quad \partial_p E_\epsilon(t). \tag{5.37}$$

Therefore, by (5.32) and (5.37) we apply the comparison principle to obtain $z \le 0$ on $E_\epsilon(t)$. This implies that

$$p(x,\xi,s) = v(\xi,s) \le C\exp\left(-\frac{|x|^2}{Ct}\right)w(\xi,t) \le C\zeta(s)U(|\xi|)\exp\left(-\frac{|x|^2}{Ct}\right)$$

on $E_\epsilon(t)$. Taking $(\xi,s) = (y,t)$, by (5.4) and (5.30) we obtain

$$\begin{aligned} p(x,y,t) &\le C\zeta(t)U(|y|)\exp\left(-\frac{|x|^2}{Ct}\right) \le C\zeta(t)U(|y|)\exp\left(-\frac{|x-y|^2}{Ct}\right) \\ &\le Ct^{-\frac{N}{2}}\frac{U(\min\{|y|,\epsilon\sqrt{t}\})}{U(\sqrt{t})}\frac{U(\min\{|x|,\epsilon\sqrt{t}\})}{U(\epsilon\sqrt{t})}\exp\left(-\frac{|x-y|^2}{Ct}\right) \\ &\le Ct^{-\frac{N}{2}}\frac{U(\min\{|x|,\sqrt{t}\})U(\min\{|y|,\sqrt{t}\})}{U(\sqrt{t})^2}\exp\left(-\frac{|x-y|^2}{Ct}\right). \end{aligned}$$

Thus (1.6) holds in case (iii). Since $p(x,y,t)=p(y,x,t)$, (1.6) also holds in case (iv).

It remains to prove (1.6) in case (ii). Set

$$S:=1 \quad \text{if} \quad |x|\le 1, \qquad S:=|x|^2 \quad \text{if} \quad |x|>1.$$

Then it follows that

$$1\le S<t, \qquad U(\min\{|x|,\sqrt{S}\})=U(|x|). \tag{5.38}$$

We show that

$$v(\xi,S)=p(x,\xi,S)\le CS^{-\frac{N}{2}}U(\sqrt{S})^{-2}U(|x|)U(|\xi|)\exp\left(-\frac{|x|^2}{Ct}\right) \tag{5.39}$$

for all $\xi\in B(0,\epsilon\sqrt{S})$. In the case $S=1$, that is $|x|\le 1$, combining Lemmas 5.2 and 5.3 with (5.38), we have (5.39). So we consider the case $S>1$, that is $|x|>1$. Let w and z be as in (5.31). Then z satisfies (5.32) on $\mathbf{R}^N\times(1,S]$. Furthermore, by (1.6) in cases (i) and (iii) we see that

$$\begin{aligned} v(\xi,s)=p(x,\xi,s) &\le Cs^{-\frac{N}{2}}\frac{U(\min\{|x|,\sqrt{s}\})U(\min\{|\xi|,\sqrt{s}\})}{U(\sqrt{s})^2}\exp\left(-\frac{|x-\xi|^2}{Cs}\right)\\ &\le Cs^{-\frac{N}{2}}\exp\left(-\frac{|x|^2}{Ct}\right) \end{aligned} \tag{5.40}$$

for $(\xi,s)\in\mathbf{R}^N\times(1,S]$ with $|\xi|=\epsilon\sqrt{s}$ and that

$$\begin{aligned} v(\xi,1) &\le C\frac{U(\min\{|x|,1\})U(\min\{|\xi|,1\})}{U(1)^2}\exp\left(-\frac{|x-\xi|^2}{C}\right)\\ &\le CU(1)U(|\xi|)\exp\left(-\frac{|x|^2}{Ct}\right) \end{aligned} \tag{5.41}$$

for $\xi\in B(0,\epsilon)$. Then, by (5.35), (5.36), (5.40) and (5.41), taking a sufficiently large C_1 if necessary, we see that

$$z(\xi,s)\le 0 \quad \text{on} \quad \partial_p E_\epsilon(S).$$

Then, by the comparison principle we see that $z(\xi,s)\le 0$ on $E_\epsilon(S)$. This together with (5.30) implies that

$$\begin{aligned} v(\xi,S) &\le C_1S^{-\frac{N}{2}}U(\sqrt{S})^{-1}U(|\xi|)\exp\left(-\frac{|x|^2}{C_1t}\right)\\ &= C_1S^{-\frac{N}{2}}U(\sqrt{S})^{-2}U(|x|)U(|\xi|)\exp\left(-\frac{|x|^2}{C_1t}\right) \end{aligned}$$

for all $\xi\in B(0,\epsilon\sqrt{S})$, which implies (5.39) in the case $S>1$. Therefore inequality (5.39) holds.

We complete the proof of (1.6) in case (ii). Let

$$\tilde{\zeta}(s):=\begin{cases} s^{-\frac{N+2d}{2}}[\log(2+s)]^{-2} & \text{if } \lambda_2=\lambda_* \text{ and } H \text{ is subcritical},\\ s^{-\frac{N+2d}{2}} & \text{otherwise.}\end{cases}$$

It follows from Theorem 1.1 and (5.30) that

$$\tilde{\zeta}(s) \asymp s^{-\frac{N}{2}} U(\sqrt{s})^{-2} \asymp U(\sqrt{s})^{-1}\zeta(s) \quad \text{in} \quad (1,\infty). \tag{5.42}$$

Since $N+2d>0$, we can find $\tilde{\kappa}>0$ such that $-s\tilde{\zeta}'(s) \le \tilde{\kappa}\tilde{\zeta}(s)$ on $(1,\infty)$. Set

$$\begin{aligned}
\tilde{w}(\xi,s) &:= \tilde{\zeta}(s)\left[U(|\xi|) - \tilde{\kappa}s^{-1}F[U](|\xi|)\right], \\
\tilde{z}(\xi,s) &:= v(\xi,s) - C_2 U(|x|)\exp\left(-\frac{|x|^2}{C_2 t}\right)\tilde{w}(\xi,s),
\end{aligned}$$

where C_2 is a positive constant to be chosen later. Then, by Lemma 5.4 we see that

$$\partial_s \tilde{z} \le \Delta_\xi \tilde{z} - V(|\xi|)\tilde{z} \quad \text{in} \quad \mathbf{R}^N \times (1,\infty). \tag{5.43}$$

Since (1.6) holds in case (iv), it follows from (5.30) and (5.38) that

$$\begin{aligned}
v(\xi,s) = p(x,\xi,s) &\le Cs^{-\frac{N}{2}} \frac{U(\min\{|x|,\sqrt{s}\})U(\min\{|\xi|,\sqrt{s}\})}{U(\sqrt{s})^2}\exp\left(-\frac{|x-\xi|^2}{Cs}\right) \\
&\le C\zeta(s)U(|x|)\exp\left(-\frac{|x|^2}{Ct}\right)
\end{aligned} \tag{5.44}$$

for $(\xi,s)\in \mathbf{R}^N\times[S,t]$ with $|\xi|=\epsilon\sqrt{s}$. Furthermore, similarly to (5.35) and (5.36), taking a sufficiently small $\epsilon>0$ if necessary, we deduce from (5.42) that

$$\tilde{w}(\xi,s) \ge \frac{1}{2}\tilde{\zeta}(s)U(|\xi|) \ge C^{-1}\zeta(s) \tag{5.45}$$

for $(\xi,s)\in \mathbf{R}^N\times(S,t]$ with $|x|=\epsilon\sqrt{s}$ and

$$\tilde{w}(\xi,S) \ge \frac{1}{2}\tilde{\zeta}(S)U(|\xi|) \ge C^{-1}S^{-\frac{N}{2}}U(\sqrt{S})^{-2}U(|\xi|) \tag{5.46}$$

for $\xi\in B(0,\epsilon\sqrt{S})$. By (5.39), (5.44), (5.45) and (5.46), taking a sufficiently large C_2 if necessary, we see that

$$\tilde{z} \le 0 \tag{5.47}$$

for all $(\xi,s)\in\mathbf{R}^N\times[S,t]$ with $|\xi|=\epsilon\sqrt{s}$ and all (ξ,S) with $|\xi|<\epsilon\sqrt{S}$. By (5.43) and (5.47) we apply the comparison principle to obtain $\tilde{z}\le 0$ for all $(\xi,s)\in\mathbf{R}^N\times[S,t]$ with $|\xi|\le\epsilon\sqrt{s}$. This implies

$$p(x,\xi,s) = v(\xi,s) \le C_2 U(|x|)\exp\left(-\frac{|x|^2}{C_2 t}\right)\tilde{w}(\xi,s) \le C_2\tilde{\zeta}(s)U(|x|)U(|\xi|)\exp\left(-\frac{|x|^2}{C_2 t}\right)$$

for all $(\xi,s)\in\mathbf{R}^N\times[S,t]$ with $|\xi|\le\epsilon\sqrt{s}$. Taking $(\xi,s)=(y,t)$, by (5.4) and (5.42) we obtain

$$\begin{aligned}
p(x,y,t) &\le C\tilde{\zeta}(t)U(|x|)U(|y|)\exp\left(-\frac{|x|^2}{Ct}\right) \\
&\le Ct^{-\frac{N}{2}}\frac{U(\min\{|x|,\sqrt{t}\})U(\min\{|y|,\sqrt{t}\})}{U(\sqrt{t})^2}\exp\left(-\frac{|x-y|^2}{Ct}\right).
\end{aligned}$$

This means that (1.6) holds in case (ii). Thus Theorem 1.3 follows. □

6 Positive potentials

Proof of Proposition 1.1. We shall use the classical idea that a polynomial decay of a heat kernel is equivalent to a Sobolev inequality. We use this to the kernel $G(x,y,t)$ of the operator $Lv = -\frac{1}{U^2}\mathrm{div}\,(U(x)^2\nabla v)$ used in the proof of Theorem 1.2. The L^p-spaces in consideration here are $L^p(\mathbf{R}^N, U(x)^2dx)$ and since by assumption $U(x) \sim |x|^\alpha$ a Sobolev inequality in this setting is a Caffarelli-Kohn-Nirenberg type inequality. This strategy was already used in [2] to obtain similar bounds for the heat kernel of $-\Delta + \frac{w}{|x|^2}$ for a positive real w.

Let L and $G(x,y,t)$ be as in the proof of Theorem 1.2. Let $\lambda \in \mathbf{R}$ and $\phi \in C^\infty(\mathbf{R}^N)$ and bounded with $|\nabla\phi| \le 1$. Let $L_{\lambda,\phi} := e^{-\lambda\phi}Le^{\lambda\phi}$ and $k_{\lambda,\phi}(x,y,t)$ its associated heat kernel. The bilinear form associated to the operator $L_{\lambda,\phi}$ is given by

$$\begin{aligned}\mathcal{E}_{\lambda,\phi}(u,v) &= \int_{\mathbf{R}^N} (L_{\lambda,\phi}u)vU(x)^2dx \\ &= \int_{\mathbf{R}^N} \nabla(e^{\lambda\phi}u)\nabla(e^{-\lambda\phi}v)U(x)^2dx \\ &= \int_{\mathbf{R}^N} \left[\nabla u\cdot\nabla v + \lambda u\nabla\phi\cdot\nabla v - \lambda v\nabla\phi\cdot\nabla u - \lambda^2 uv\right] U(x)^2dx.\end{aligned}$$

In particular, the quadratic form satisfies

$$\mathcal{E}_{\lambda,\phi}(u,u) = \int_{\mathbf{R}^N} \left[|\nabla u|^2 - \lambda^2|u|^2\right] U(x)^2dx.$$

Recall the weighted Sobolev inequality due to Caffarelli-Korn-Nirenberg [3]

$$\|\nabla u\|^2_{L^2(\mathbf{R}^N,|x|^{2\alpha}dx)} \ge C\|u\|^2_{L^{p_0}(\mathbf{R}^N,|x|^{2\alpha}dx)}, \tag{6.1}$$

where $p_0 := \frac{2(N-2\alpha)}{N-2-2\alpha}$.[1] This together with the fact that $U(x) \sim |x|^\alpha$ implies that

$$\mathcal{E}_{\lambda,\phi}(u,u) + \lambda^2\int_{\mathbf{R}^N} |u|^2U(x)^2dx \ge C\|u\|^2_{L^{p_0}(\mathbf{R}^N,|x|^{2\alpha}dx)}.$$

It is a classical fact that the semigroup $e^{-tL_{\lambda,\phi}}$ is bounded from $L^2(\mathbf{R}^N,U^2dx)$ into $L^{p_0}(\mathbf{R}^N,U^2dx)$ with norm bounded by $Ct^{-1/2}e^{\lambda^2 t}$. The same strategy as in the proof of a Gaussian upper for the heat kernel of uniformly elliptic operator (see, e.g., [8] or [25]) allows to iterate this estimates and see that the semigroup $e^{-tL_{\lambda,\phi}}$ is bounded from $L^2(\mathbf{R}^N,U^2dx)$ into $L^\infty(\mathbf{R}^N,U^2dx)$ with norm bounded by $Ct^{-N/4-\alpha/2}e^{\lambda^2 t}$. Thus,

$$\int_{\mathbf{R}^N} |k_{\lambda,\phi}(x,y,t)|^2U(y)^2dy \le Ct^{-\frac{N}{2}-\alpha}e^{2\lambda^2 t}.$$

Set $R_{\lambda,\phi}(x,y,t) := e^{-\lambda\phi(x)}p(x,y,t)e^{\lambda\phi(y)}$. The latter estimate immediately gives

$$\int_{\mathbf{R}^N} |R_{\lambda,\phi}(x,y,t)|^2dy \le Ct^{-\frac{N}{2}}\left(\frac{|x|}{\sqrt{t}}\right)^{2\alpha}e^{2\lambda^2 t}. \tag{6.2}$$

[1]Here one needs of course $N > 2+2\alpha$. In the case $N \le 2+2\alpha$, we use a Gagliardo-Nirenberg type inequality instead of (6.1). See [3].

On the other hand, since V is non-negative we have the domination property

$$p(x,y,t) \le (4\pi t)^{-\frac{N}{2}} e^{-\frac{|x-y|^2}{4t}}.$$

This and the fact that $|\nabla\phi| \le 1$ imply

$$\int_{\mathbf{R}^N} |R_{\lambda,\phi}(x,y,t)|^2 dy \le Ct^{-\frac{N}{2}} e^{2\lambda^2 t}. \tag{6.3}$$

Combining (6.3) and (6.2) yields

$$\int_{\mathbf{R}^N} |R_{\lambda,\phi}(x,y,t)|^2 dy \le Ct^{-\frac{N}{2}} \left(\min(1, \frac{|x|}{\sqrt{t}})\right)^{2\alpha} e^{2\lambda^2 t}.$$

By the semigroup property and the assumption $U(x) \sim |x|^\alpha$ we have

$$\begin{aligned}
R_{\lambda,\phi}(x,y,t) &= \int_{\mathbf{R}^N} R_{\lambda,\phi}(x,z,t/2) R_{\lambda,\phi}(z,y,t/2) dz \\
&\le \left(\int_{\mathbf{R}^N} |R_{\lambda,\phi}(x,z,t/2)|^2 dz\right)^{1/2} \left(\int_{\mathbf{R}^N} |R_{\lambda,\phi}(z,y,t/2)|^2 dz\right)^{1/2} \\
&\le Ct^{-\frac{N}{2}} \left(\min(1, \frac{|x|}{\sqrt{t}})\right)^{\alpha} \left(\min(1, \frac{|y|}{\sqrt{t}})\right)^{\alpha} e^{\lambda^2 t} \\
&\le Ct^{-\frac{N}{2}} \frac{U(\min\{|x|, \sqrt{t}\}) U(\min\{|y|, \sqrt{t}\})}{U(\sqrt{t})^2} e^{\lambda^2 t}.
\end{aligned}$$

Hence

$$p(x,y,t) \le Ct^{-\frac{N}{2}} \frac{U(\min\{|x|, \sqrt{t}\}) U(\min\{|y|, \sqrt{t}\})}{U(\sqrt{t})^2} e^{\lambda^2 t} e^{\lambda(\phi(x)-\phi(y))}.$$

We change λ into $-\lambda$ and then optimize as usual over λ and ϕ to obtain the upper estimate in Theorem 1.1. □

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