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Integral kernels of Schrödinger semigroups with nonnegative locally bounded potentials

by

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Abstract. We give upper and lower estimates of the heat kernels for Schrödinger operators $H = -\Delta + V$ with nonnegative and locally bounded potentials V in $\mathbb{R}^d$, $d \geq 1$. We observe a factorization: the contribution of the potential is described separately for each spatial variable, and the interplay between the spatial variables is seen only through the Gaussian kernel – optimal in the lower bound and nearly optimal in the upper bound. In some regimes we observe the exponential decay in time with the rate corresponding to the bottom of the spectrum of H. The upper estimate is more local; it applies to general potentials, including confining ones (i.e. $V(x) \to \infty$ as $|x| \to \infty$) and decaying ones (i.e. $V(x) \to 0$ as $|x| \to \infty$), even if they are nonradial, and their mixtures. The lower bound is specialized to the confining case, and the contribution of the potential is described in terms of its radial upper profile. Our results take the sharpest form for confining potentials that are comparable to radial monotone profiles with sufficiently regular growth – in this case they lead to two-sided qualitatively sharp estimates. In particular, we describe the large-time behaviour of *nonintrinsically ultracontractive* Schrödinger semigroups – this has been a long-standing open problem. Our methods combine probabilistic techniques with analytic ideas.

1. Introduction. We consider the Schrödinger operator $H = -\Delta + V$ acting in $L^2(\mathbb{R}^d, dx)$, $d \geq 1$, where the potential $V : \mathbb{R}^d \to [0, \infty)$ is a locally bounded function. The corresponding Schrödinger semigroup $\{e^{-tH} : t \geq 0\}$ consists of integral operators, i.e.

$$e^{-tH} f(x) = \int_{\mathbb{R}^d} u_t(x, y) f(y)\, dy, \qquad f \in L^2(\mathbb{R}^d, dx),\ t > 0.$$

It is known that $(0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d \ni (t, x, y) \mapsto u_t(x, y)$ is a continuous function, symmetric in (x, y). It satisfies the inequality $u_t(x, y) \leq g_t(x, y)$,

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where

$$g_t(x,y) = \frac{1}{(4\pi t)^{d/2}} \exp\left(-\frac{|y-x|^2}{4t}\right)$$

is the Gauss–Weierstrass kernel, the heat kernel of the free kinetic term $-\Delta$. Our standard references for Schrödinger operators and semigroups are the paper by Simon [27] and the monographs by Reed and Simon [23], Demuth and van Casteren [11], and Chung and Zhao [8].

The main goal of the paper is to find upper and lower estimates of the integral kernels $u_t(x,y)$, as uniform and informative as possible. We want to understand the contribution of the potential and the relation between $u_t(x,y)$ and the heat kernel $g_t(x,y)$ of the kinetic term $-\Delta$.

Estimates of Schrödinger heat kernels have been widely studied in the literature. For a class of nonnegative and locally bounded potentials, research concentrated mainly on two extremal situations: when the potential is *confining* (i.e. $V(x) \to \infty$ as $|x| \to \infty$) and *decaying* (i.e. $V(x) \to 0$ as $|x| \to \infty$). Note that confining potentials are locally bounded and *unbounded at infinity*, while decaying ones are always bounded.

Known results for confining potentials include classical *intrinsic ultracontractivity* estimates by Davies and Simon [9, 10], on-diagonal estimates for polynomial potentials obtained by Sikora [26], and short-time bounds by Metafune, Pallara and Rhandi [20], Metafune and Spina [21], and Spina [30]. For the decaying case we refer to the paper by Zhang [32]. See also further references in those papers. It is known to be a challenging problem to identify the actual contribution of the potential in a sharp and clear way. For both cases, the sharpest results were obtained for rather restricted classes of potentials, mainly of polynomial type. Moreover, when the potential is bounded or it grows at infinity not too fast, a connection with the original Gaussian kernel is expected as well. Some estimates include the term $g_{ct}(x,y)$, but the optimality of the constant c for the class of potentials we are interested in this paper is still an open issue. In this connection, we mention the recent papers by Bogdan, Dziubański and Szczypkowski [2] and Jakubowski and Szczypkowski [13] which thoroughly analyze the problem of uniform comparability of the Schrödinger heat kernel with the original heat kernel $g_t(x,y)$ of the kinetic term $-\Delta$, and give sharp conditions for this property. We also refer to these papers for an extensive discussion of the related literature.

Theorems 2.1 and 2.2 – the main results of this paper – give estimates of the kernel $u_t(x,y)$ global in time and space.

The upper estimate in Theorem 2.1 applies to every nonnegative locally bounded potential, i.e. it allows one to analyze in the same framework the functions V of various types, including confining and decaying potentials, functions bounded away from zero or even mixtures of all of these types.

For instance, in the one-dimensional case it covers highly nonsymmetric potentials which are confining on one half-line, and decaying or bounded on the other. This is the first novelty of our paper. Interestingly, Theorem 2.1 easily extends to singular V's. Moreover, this bound matches structurally the lower estimate in Theorem 2.2 which is specialized to confining potentials or potentials with confining components in unbounded subsets of the space. These two theorems lead to qualitatively sharp two-sided estimates for confining potentials that are comparable to radial monotone profiles with sufficiently regular growth – this is the strongest result of the paper; see Examples 6.2 and 6.3 for the statement and illustration. A similar result has also been obtained independently by Chen and Wang in the recent interesting preprint [5], which we discuss in Remark 6.7 below. These estimates clarify the large-time properties of *nonintrinsically ultracontractive* Schrödinger semigroups. This problem has been solved just recently for a large class of nonlocal operators [16], but it remained open for classical Schrödinger semigroups.

We remark that our estimates identify in a fairly informative and uniform way the dependence on the potential and the dimension of the space. Moreover, we find an optimal Gaussian term in the lower bound and show that the Gaussian term in the upper bound can be made nearly optimal. We propose a novel approach which leads to fairly short and direct proofs. It combines probabilistic and analytic ideas, and does not require any further regularity or smoothness assumptions on the potential. To the best of our knowledge, the estimates of this type, global in time and space, have not been available in the literature so far.

The structure of the paper is as follows. In Section 2 we present Theorems 2.1 and 2.2, discuss the structure of estimates, uniform rates and constants, and explain the ideas of proofs. Section 3 contains preliminaries. In Sections 4 and 5 we give the proofs of the upper bound and the lower bound, respectively. Finally, in Section 6, we discuss applications of our estimates and connections to the literature. In particular, Subsection 6.1 is devoted to analysis of confining potentials, and the two-sided estimates we get for this class. In Subsection 6.2 we illustrate the upper bound for decaying potentials. In Subsections 6.3 and 6.4 we analyze the examples of potentials that are bounded away from zero, and some more general cases, including mixtures and nonradial potentials. In Subsection 6.5 we show that Theorem 2.1 extends to singular potentials.

Notation. For $x \in \mathbb{R}^d$ and $r > 0$ we denote $B_r(x) = \{y \in \mathbb{R}^d : |y - x| < r\}$ and $\overline{B}_r(x) = \{y \in \mathbb{R}^d : |y - x| \le r\}$. For $x = 0$ we write B_r, $\overline{B}_r$. Also, $a \wedge b := \min\{a, b\}$, $a \vee b := \max\{a, b\}$.

2. Presentation of results. Our first main result gives an upper estimate in terms of the *lower profile* of the potential,

$$V_*(x) := \inf_{z \in \overline{B}_{|x|/2}(x)} V(z), \qquad x \in \mathbb{R}^d.$$

We use the following notation:

$$H(t,x) := \exp\Big(-\frac{\sqrt{2}}{32}\Big(\Big(V_*(x) + \frac{\mu_0}{4|x|^2}\Big)t \wedge 2|x|\sqrt{V_*(x) + \frac{\mu_0}{4|x|^2}}\Big)\Big),$$

for $x \neq 0$, $H(t,0) := \exp\big(-\frac{\sqrt{2\mu_0}}{32}\big)$, and

$$\gamma_1 := \lambda_0/2.$$

The number $0 \leq \lambda_0 := \inf \sigma(H)$ is the bottom of the spectrum of the Schrödinger operator H, and $\mu_0 > 0$ is the principal eigenvalue of the operator $-\Delta_{B_1}$, the (positive) Dirichlet Laplacian on the ball B_1.

Theorem 2.1. *There exists a constant $c_1 = c_1(d)$ such that for every $0 \leq V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$, $x, y \in \mathbb{R}^d$ and $t > 0$ we have*

$$u_t(x,y) \leq c_1 H(t,x) H(t,y) \big(g_{2t}(x,y) \wedge e^{-\gamma_1 t} g_t(0,0)\big).$$

We note that c_1 can be chosen to be

$$c_1 = 2^{(3d+4)/2} e^{\sqrt{\mu_0}/8} (C_0 \vee C),$$

where the constants C_0 and C (independent of V) come from (3.2) and Lemma 4.3 below.

The upper bound in Theorem 2.1 is *uniform* in $0 \leq V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$ in the sense that the rate $\sqrt{2}/32$ in $H(t,x)$ and the constant c_1 are independent of V. This estimate is a version of a more general result, stated as Theorem 4.1, which allows one to get an upper bound with the Gaussian term $g_{at}(x,y)$ with $a > 1$ arbitrarily close to 1, i.e. the Gaussian term can be made *nearly optimal*. Note, however, that this can be done at the cost of the absolute constant in the exponent of $H(t,x)$. For simplicity, here we just choose $a = 2$. The rate $\sqrt{2}/32$ is not optimal, but we state it here explicitly in order to show the uniform structure of the estimate. For applications of Theorem 2.1, examples and further discussions we refer the reader to Section 6. We remark that the theorem gives qualitatively sharp bounds for a large class of potentials.

Our second main result gives a lower estimate of the kernel $u_t(x,y)$ in terms of the *radial upper profile* of the potential,

$$V^*(r) := \sup_{z \in \overline{B}_{2r}} V(z), \qquad r \geq 0.$$

We use the shorthand notation

$$\begin{aligned}
t_\rho &:= \frac{\rho}{2\sqrt{V^*(\rho)+\frac{\mu_0}{4|x|^2}}}, \qquad \rho \geq 1,\\
K(t,\rho) &:= \exp\left(-\frac{9}{4}\left(\left(V^*(\rho)+\frac{\mu_0}{4\rho^2}\right)t \wedge 2\rho\sqrt{V^*(\rho)+\frac{\mu_0}{4\rho^2}}\right)\right),\\
\rho_x &:= |x| \vee 1,\\
\gamma_2 &:= d + V^*(1) + \mu_0/4.
\end{aligned}$$

THEOREM 2.2. *There exists $c_2 = c_2(d)$ such that for every $0 \leq V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$, $x, y \in \mathbb{R}^d$ and $t > 0$ we have the following estimates:*

(1) *If $4t_{\rho_x \vee \rho_y} \leq t$, then*

$$u_t(x,y) \geq c_2 e^{-\gamma_2 t} g_t(0,0) K(t,\rho_x) K(t,\rho_y).$$

(2) *If $4t_{\rho_x \vee \rho_y} \geq t$, then*

$$u_t(x,y) \geq c_2 K(t, \rho_x \vee \rho_y) g_t(x,y).$$

The constant c_2 in the above theorem can be taken to be

$$c_2 = \frac{(\widetilde{C}/4)^4}{4^d \Gamma(d/2+1)^3},$$

where $\widetilde{C}$ is the constant (independent of V) from the auxiliary estimate (5.1) below.

As before, the estimate in Theorem 2.2 is *uniform* in $0 \leq V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$ – the rate $9/4$ in $K(t,\rho)$ and the constant c_2 are independent of V, and the Gaussian term $g_t(x,y)$ in this bound is optimal. This result is rather specialized to confining potentials for which it leads to a global estimate in terms of the upper profile V^* – this estimate is the most informative for potentials with radial profiles. Together with Theorem 2.1, it also immediately gives two-sided estimates; see Corollary 6.1. These bounds are qualitatively sharp for potentials that are comparable to radial monotone functions with sufficiently regular growth; see Examples 6.2 and 6.3. However, it can still be useful in less regular situations. For example, if V is a potential with confining component in some unbounded subset D of $\mathbb{R}^d$, then our result may give a sharp lower estimate for $x, y \in D$. On the other hand, due to the appearance of the exponential time rate which is always present in our bound, the theorem seems to be useless for decaying potentials. In this case, it just leads to the obvious estimate $u_t(x,y) \geq e^{-Ct} g_t(x,y)$.

Observe that the estimate in Theorem 2.2(1) can be equivalently rewritten as

$$u_t(x,y) \geq c_2 e^{-\gamma_2 t} g_t(0,0) K(t, \rho_x \vee \rho_y) K(t, \rho_x \wedge \rho_y),$$

and the term $K(t, \rho_x \vee \rho_y)$ is already determined by the assumption $4t_{\rho_x \vee \rho_y} \leq t$.

Also, we note that in part (2) we get an estimate with the kernel K in which the rate $9/4$ is replaced by 1. However, for more clarity, in the statement we keep the same rate in both (1) and (2).

Structure of our estimates and the uniform rates and constants. Our estimates show a factorization: the terms H and K are separate for each spatial variable, and if $\lambda_0 > 0$, then additional decay in time is present as well. The interaction between spatial variables is described by the Gaussian kernel.

The structure of H and K is exactly the same; for small spatial variables these functions are less than 1 and bounded away from zero, uniformly in $t > 0$. However, for large z and $t > 0$, they clearly show a competition between the two factors

$$\exp\left(-c\left(V(z) + \frac{\mu_0}{4|z|^2}\right)t\right) \quad \text{and} \quad \exp\left(-2c|z|\sqrt{V(z) + \frac{\mu_0}{4|z|^2}}\right). \tag{2.1}$$

At the technical side, the contribution of the potential is described by the profiles V_* and V^*, and the constant c is equal to $9/4$ in the lower bound and $\sqrt{2}/32$ in the upper bound. Of course, these numerical constants are not optimal, but they are explicit and absolute numbers, independent of the potential V and the dimension d; the dependence on d is expressed through μ_0 only, and our proofs show that the presence of the term $\mu_0/|x|^2$, at least in the first expression in (2.1), is correct and it makes the exponent sharper. This term plays an important role in the proof of the lower estimate. Of course, in the case of confining potentials, the expression $V(z) + \mu_0/(4|z|^2)$ can be replaced by $V(z)$ for large z's, but this is possible only at the cost of the constant depending on V and d – this would destroy the absoluteness of the rate $9/4$ appearing in the lower bound. Also the multiplicative constants c_1, c_2 are independent of V (c_1, c_2 depend on d only). In this sense our results are *uniform* with respect to V. On the other hand, the time rates γ_1, γ_2, giving the estimates of λ_0 (in the confining case, λ_0 is the ground state eigenvalue), are necessarily dependent on the potential and the dimension.

The effect of the competition in (2.1) strongly depends on the type of the potential and the rate of its growth or decay at infinity. Further discussion in Section 6 will be divided into separate parts, including confining and decaying cases.

A few words about the proofs. Our proofs are based on the Feynman –Kac representation of the Schrödinger semigroup $\{e^{-tH} : t \geq 0\}$ with respect to Brownian motion, some general estimates for the exit time of this process from a ball, and the recent sharp estimate for the semigroup of the corresponding killed process. We develop a new approach which allows us to find a rather direct and short argument.

Theorem 2.1 follows from more general Theorem 4.1. The key step in the proof is based on the observation that the Laplace transform of the exit time from a ball mentioned above, evaluated at $\lambda = V(x)$ (formally we see here the lower profile of the potential) takes the form of the second term appearing in (2.1). We use for this the classical result of Wendel [31]. Interestingly, this is exactly the shape of the ground state φ_0 of the Schrödinger operator H [28, 3]. These steps are made in Lemmas 4.5 and 4.3. The proof of Theorem 4.1 is concluded by symmetrizing the estimate obtained in Lemma 4.5, through the Chapman–Kolmogorov (semigroup) property – this leads to the factorization of the estimate in a very natural way.

Proving Theorem 2.2 seems to be a more challenging problem, because we want to find a lower estimate matching the upper bound. More precisely, we want to get a factorization and keep the same structure of the terms appearing in the estimate. First, in Lemma 5.1, we prove a general estimate which covers part (2) of the theorem. The structure of the upper bound and the estimate in this lemma suggest the structure of t_{ρ_x} – the space-dependent threshold time which determines the shape of the estimate. We observe that the correct form of the estimate, matching the upper bound, is determined by the position of the time t with respect to $t_{\rho_x \vee \rho_y}$. The key technical step is made in Lemma 5.2 which allows us to get part (1) of the theorem. The tricky estimates in the proof of this lemma show in a clear way the interplay between the time and the spatial variables. One can say that the key idea used in the proof of the lower bound is to reduce the problem to estimating the semigroup of the process in a ball, without losing too much information. Interestingly, we do not use the joint distribution of the exit position and the exit time of the process from a ball. The only tool we need is the lower estimate for the kernel of the semigroup of the killed process with sharp Gaussian term, recently obtained by Małecki and Serafin [19].

3. Preliminaries. Let $(X_t)_{t\geq 0}$ be the Brownian motion running at twice the speed, with values in $\mathbb{R}^d$, $d \geq 1$, over a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. This is the stochastic process with continuous paths, starting from 0, such that

$$\mathbb{P}(X_t \in dy) = \frac{1}{(4\pi t)^{d/2}} \exp\left(-\frac{|y|^2}{4t}\right) dy, \qquad t > 0,$$

Note that the process $(X_t)_{t\geq 0}$ has the scaling property: X_{at} has the same distribution as $\sqrt{a}X_t$, $a > 0$. We denote by $\mathbb{P}_x$ the probability measure for the process starting from $x \in \mathbb{R}^d$, i.e.

$$\mathbb{P}_x(X_t \in dy) := \mathbb{P}(X_t + x \in dy) = g_t(x, y)\, dy,$$

where

$$g_t(x, y) = \frac{1}{(4\pi t)^{d/2}} \exp\left(-\frac{|y - x|^2}{4t}\right),$$

and by $\mathbb{E}_x$ the expected value with respect to $\mathbb{P}_x$. We use the notation $\mathbb{E}_x[F;\, A] = \int_A F\, d\mathbb{P}_x$.

Let $0 \le V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$ and consider the Schrödinger operator $H = -\Delta + V$. The semigroup operators e^{-tH}, $t > 0$, can be represented via the Feynman–Kac formula:

$$e^{-tH} f(x) = \mathbb{E}_x\Big[\exp\Big(-\int_0^t V(X_s)\, ds\Big) f(X_t)\Big], \qquad f \in L^2(\mathbb{R}^d, dx)$$

(see Simon [29], Demuth and van Casteren [11], or Chung and Zhao [8]). Consequently, the corresponding integral kernels $u_t(x,y)$ can be expressed as

$$u_t(x,y) = \lim_{s \nearrow t} \mathbb{E}_x\big[e^{-\int_0^s V(X_u)\, du} g_{t-s}(X_s, y)\big], \qquad x, y \in \mathbb{R}^d,\ t > 0 \tag{3.1}$$

(see [11, Proposition 2.7]). In particular, $u_t(x,y) \le g_t(x,y)$.

Let $\tau_D := \inf\{t \ge 0 : X_t \notin D\}$ be the first exit time of the process $(X_t)_{t\ge 0}$ from an open and bounded set $D \subset \mathbb{R}^d$. In this paper we mainly consider the case when $D = B_r$, $r > 0$. Recall that the transition semigroup of the Brownian motion killed upon exiting B_r consists of the operators

$$G_t^{B_r} f(x) = \mathbb{E}_x[f(X_t);\, t < \tau_{B_r}] = \int_{B_r} f(y) g_t^{B_r}(x,y)\, dy, \quad f \in L^2(B_r, dy),\ t > 0,$$

with continuous and bounded transition densities $g_t^{B_r}(x,y)$. Due to the scaling property, it is sufficient to analyze the case $r = 1$. All these operators are of Hilbert–Schmidt type; in particular, the spectra of $G_t^{B_1}$, $t > 0$, consist of eigenvalues $e^{-\mu_n t}$, where the numbers $0 < \mu_0 < \mu_1 \le \mu_2 \le \cdots \to \infty$ are eigenvalues of $-\Delta_{B_1}$, the (positive) Dirichlet Laplacian on the ball B_1. The operator Δ_{B_1} is the infinitesimal generator of the semigroup $\{G_t^{B_1} : t \ge 0\}$. The number $\mu_0 := \inf \operatorname{spec}(-\Delta_{B_1})$ is called the *ground state* (or *principal*) *eigenvalue*; the corresponding eigenfunction $\phi_0 \in L^2(B_1, dx)$ is bounded, continuous and strictly positive on B_1.

It is known that due to intrinsic ultracontractivity (see Davies and Simon [10, 9]), there exists a constant $c > 0$ such that

$$g_t^{B_1}(x,y) \le c e^{-\mu_0 t} \phi_0(x)\phi_0(y), \qquad x, y \in B_1,\ t \ge 1.$$

By integrating this inequality over $y \in B_1$, we get

$$\mathbb{P}_x(t < \tau_{B_1}) \le c e^{-\mu_0 t} \phi_0(x) \|\phi_0\|_1, \qquad x \in B_1,\ t \ge 1.$$

Consequently,

$$\mathbb{P}_0(t < \tau_{B_1}) \le C_0 e^{-\mu_0 t}, \qquad t > 0, \tag{3.2}$$

where $C_0 := e^{\mu_0} \vee c\phi_0(0)\|\phi_0\|_1 > 1$.

4. The proof of the upper bound. Throughout this section we use the following constants: for $a > 1$ we define

$$C_1 = C_1(a) := \left(2(C_0 \vee C)^{(a-1)/a} a^{d/2} \left(\frac{a}{a-1}\right)^{\frac{(a-1)d}{2a}}\right)^2$$

(the constant C_0 comes from (3.2) above and C (independent of a and V) is determined in Lemma 4.3 below) and

$$C_2 = C_2(a) := \frac{1}{2a}, \quad C_3 = C_3(a) := \frac{2\mu_0(a-1)}{a^2}, \quad C_4 = C_4(a) := \frac{1}{4}\sqrt{\frac{a-1}{a}}.$$

We first prove the most general Theorem 4.1, and then we come back to Theorem 2.1.

Theorem 4.1. *Let $0 \le V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$ and let $x, y \in \mathbb{R}^d$, $t > 0$, $a > 1$. Then*

$$u_t(x,y) \le C_1 h(t,x) h(t,y) g_{at}(x,y)$$

and

$$u_t(x,y) \le \sqrt{C_1} \frac{1}{(2a\pi t)^{d/2}} \exp\left(-\frac{\lambda_0}{2} t\right) \sqrt{h(t,x)} \sqrt{h(t,y)},$$

where

$$h(t,x) := \exp\left(-\left(\left(C_2 V_*(x) + \frac{C_3}{|x|^2}\right) t \wedge C_4 \sqrt{V_*(x)}\, |x|\right)\right).$$

We use the convention that $1/|x|^2 = +\infty$ for $x = 0$, so that $h(t,0) = 1$. The proof of the theorem will be given after a sequence of lemmas. We start with a remark.

Remark 4.2. The constants appearing in the estimates in Theorem 4.1 are not optimal, but they are explicit. In many cases, it is enough to take e.g. $a = 2$. Nevertheless, depending on applications, one can choose the parameter a to be arbitrarily close to 1, which makes the Gaussian term $g_{at}(x,y)$ nearly optimal. Recall that the lower bound in Theorem 2.2 holds with $g_t(x,y)$. Note, however, that $C_3, C_4 \downarrow 0$ as $a \downarrow 1$.

Lemma 4.3. *There exists a constant $C = C(d) \ge 1$ such that for every $\lambda \ge 0$ and $r > 0$ we have*

$$\mathbb{E}_0[e^{-\lambda \tau_{B_r}}] \le C e^{-\sqrt{\lambda} r/2}.$$

Proof. First note that for $\lambda = 0$ the equality is trivial. Assume that $\lambda > 0$. If $d = 1$, then the assertion simply follows from the classical formula for the Laplace exponent of the first passage time for the one-dimensional Brownian motion (see e.g. [24, Theorem 5.13]). If $d \ge 2$, then we use the result of Wendel [31, (4)], which says that

$$\mathbb{E}_0[e^{-\lambda\tau_{B_r}}] = \frac{1}{2^{(d-2)/2}\Gamma(d/2)} \frac{(\sqrt{\lambda}\, r)^{(d-2)/2}}{I_{(d-2)/2}(\sqrt{\lambda}\, r)}, \tag{4.1}$$

where

$$I_\nu(u) = \sum_{k=0}^{\infty} \frac{(u/2)^{\nu+2k}}{k!\Gamma(\nu+k+1)}, \qquad u, \nu \geq 0, \tag{4.2}$$

is the modified Bessel function of the first kind (see e.g. [12, 10.25.2]). Note that Wendel considered the standard Brownian motion while we work with the Brownian motion running at twice the speed, and τ_{B_r} is the exit time of our process. Therefore the right hand side of (4.1) is the original formula of Wendel with r replaced by $r/\sqrt{2}$ (or equivalently with λ replaced by $\lambda/2$).

It is known (see [12, 10.30.4]) that

$$\lim_{u\to\infty} \frac{I_\nu(u)\sqrt{2\pi u}}{e^u} = 1, \qquad \nu \geq 0.$$

This implies that there exists $u_0 = u_0(d) > 0$ such that

$$\frac{u^{(d-2)/2}}{2^{(d-2)/2}\Gamma(d/2) I_{(d-2)/2}(u)} \leq e^{-u/2}, \qquad u \geq u_0.$$

On the other hand, by keeping only the term for $k = 0$ in the series (4.2), we get

$$\frac{u^{(d-2)/2}}{2^{(d-2)/2}\Gamma(d/2) I_{(d-2)/2}(u)} \leq 1 \leq e^{u_0/2} e^{-u/2}, \qquad u \in (0, u_0].$$

The assertion of the lemma then follows from the representation (4.1) with $C = e^{u_0/2}$. ∎

Remark 4.4. By direct inspection of the last lines of the proof, we can easily obtain the estimate of Lemma 4.3 in this form: for every $\varepsilon \in (0,1)$ there exists a constant $C = C(d,\varepsilon) \geq 1$ such that

$$\mathbb{E}_0[e^{-\lambda\tau_{B_r}}] \leq C e^{-(1-\varepsilon)\sqrt{\lambda} r},$$

i.e. the constant in the exponent can be arbitrarily close to 1 at the cost of the multiplicative constant C. For clarity, we keep the statement and the proof in the present, simpler form.

Lemma 4.5. *Let $0 \leq V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$ and let $x, y \in \mathbb{R}^d$, $t > 0$, $a > 1$. Then*

$$u_t(x,y) \leq \sqrt{C_1} \exp\left(-\left(2\left(C_2 V_*(x) + \frac{C_3}{|x|^2} \right) t \wedge C_4 \sqrt{V_*(x)}\, |x| \right) \right) g_{at}(x,y).$$

Proof. Let $x, y \in \mathbb{R}^d$, $t > 0$ and let $a > 1$. If $x = 0$, then $e^{-C_4\sqrt{V_*(x)}|x|} = 1$. Consequently,

$$u_t(x,y) \le g_t(x,y) \le a^{d/2} g_{at}(x,y) = a^{d/2} e^{-C_4\sqrt{V_*(x)}|x|} g_{at}(x,y)$$

and the estimate trivially holds. Let $x \neq 0$ and denote $b = a/(a-1)$ so that $1/a + 1/b = 1$. We have

$$\begin{aligned}
u_t(x,y) &= \int_{\mathbb{R}^d} u_{t/a}(x,z) u_{t/b}(z,y)\,dz \\
&= \mathbb{E}_x\big[e^{-\int_0^{t/a} V(X_s)ds} u_{t/b}(X_{t/a},y)\big] \\
&= \mathbb{E}_x\big[e^{-\int_0^{t/a} V(X_s)ds} u_{t/b}(X_{t/a},y);\, t/a < \tau_{B_{|x|/2}(x)}\big] \\
&\quad + \mathbb{E}_x\big[e^{-\int_0^{t/a} V(X_s)ds} u_{t/b}(X_{t/a},y);\, t/a \ge \tau_{B_{|x|/2}(x)}\big] \\
&=: \mathrm{I}_1 + \mathrm{I}_2.
\end{aligned}$$

Clearly,

$$\mathrm{I}_1 \le e^{-(t/a)V_*(x)} \mathbb{E}_x[g_{t/b}(X_{t/a},y);\, t/a < \tau_{B_{|x|/2}(x)}]$$

and

$$\mathrm{I}_2 \le \mathbb{E}_x\big[e^{-\int_0^{\tau_{B_{|x|/2}(x)}} V(X_s)ds} g_{t/b}(X_{t/a},y)\big] \le \mathbb{E}_x\big[e^{-V_*(x)\tau_{B_{|x|/2}(x)}} g_{t/b}(X_{t/a},y)\big],$$

and, by Hölder's inequality, we get

$$\mathrm{I}_1 \le e^{-(t/a)V_*(x)} \mathbb{P}_x(t/a < \tau_{B_{|x|/2}(x)})^{1/b} \mathbb{E}_x[(g_{t/b}(X_{t/a},y))^a]^{1/a}, \tag{4.3}$$

$$\mathrm{I}_2 \le \mathbb{E}_x[e^{-bV_*(x)\tau_{B_{|x|/2}(x)}}]^{1/b} \mathbb{E}_x[(g_{t/b}(X_{t/a},y))^a]^{1/a}. \tag{4.4}$$

By space homogeneity and scaling of the Brownian motion, and the estimate (3.2), we obtain

$$\mathbb{P}_x(t/a < \tau_{B_{|x|/2}(x)})^{1/b} = \mathbb{P}_0\left(\frac{4t}{a|x|^2} < \tau_{B_1}\right)^{1/b} \le C_0^{1/b} \exp\left(-\frac{4t}{ab|x|^2}\mu_0\right).$$

Similarly, Lemma 4.3 applied to $\lambda = bV_*(x)$ and $r = |x|/2$ gives the estimate

$$\mathbb{E}_x\big[e^{-bV_*(x)\tau_{B_{|x|/2}(x)}}\big]^{1/b} = \mathbb{E}_0\big[e^{-bV_*(x)\tau_{B_{|x|/2}(0)}}\big]^{1/b} \le C^{1/b} e^{-\frac{\sqrt{V_*(x)}\,|x|}{4\sqrt{b}}}.$$

Moreover,

$$\begin{aligned}
\mathbb{E}_x[(g_{t/b}(X_{t/a},y))^a]^{1/a} &= \Big(\int_{\mathbb{R}^d} g_{t/a}(x,z) g_{t/b}(z,y) (g_{t/b}(z,y))^{a-1}\,dz\Big)^{1/a} \\
&\le \left(\frac{b}{4\pi t}\right)^{\frac{(a-1)d}{2a}} \Big(\int_{\mathbb{R}^d} g_{t/a}(x,z) g_{t/b}(z,y)\,dz\Big)^{1/a} \\
&= \left(\frac{b}{4\pi t}\right)^{\frac{(a-1)d}{2a}} (g_t(x,y))^{1/a} = a^{d/2} b^{\frac{(a-1)d}{2a}} g_{at}(x,y).
\end{aligned}$$

With these estimates we can now come back to (4.3) and (4.4) and write

$$\mathrm{I}_1 \leq C_0^{(a-1)/a} a^{d/2} \Big(\frac{a}{a-1}\Big)^{\frac{(a-1)d}{2a}} \exp\Big(-\frac{t}{a} V_*(x) - \frac{4(a-1)t}{a^2|x|^2}\mu_0\Big) g_{at}(x,y),$$

$$\mathrm{I}_2 \leq C^{(a-1)/a} a^{d/2} \Big(\frac{a}{a-1}\Big)^{\frac{(a-1)d}{2a}} \exp\Big(-\frac{1}{4}\sqrt{\frac{a-1}{a}}\sqrt{V_*(x)}\,|x|\Big) g_{at}(x,y).$$

We conclude the proof by putting together the estimates for the expectations I_1 and I_2. ■

Proof of Theorem 4.1. Let $x, y, z \in \mathbb{R}^d$, $t > 0$ and $a > 1$. First observe that by Lemma 4.5 and the symmetry of the kernel, we have

$$\begin{aligned} &u_{t/2}(x,z) \\ &\quad \leq \sqrt{C_1} \exp\Big(-\Big(\Big(C_2 V_*(x) + \frac{C_3}{|x|^2}\Big)t \wedge C_4\sqrt{V_*(x)}\,|x|\Big)\Big) g_{(a/2)t}(x,z) \end{aligned}$$

and

$$\begin{aligned} &u_{t/2}(z,y) \\ &\quad \leq \sqrt{C_1} \exp\Big(-\Big(\Big(C_2 V_*(y) + \frac{C_3}{|y|^2}\Big)t \wedge C_4\sqrt{V_*(y)}\,|y|\Big)\Big) g_{(a/2)t}(z,y). \end{aligned}$$

The first estimate of the theorem follows directly from these bounds and the Chapman–Kolmogorov identity $u_t(x,y) = \int_{\mathbb{R}^d} u_{t/2}(x,z)u_{t/2}(z,y)\,dz$.

One more use of the Chapman–Kolmogorov property and the symmetry of the kernel, and the Cauchy–Schwarz inequality, give us

$$\begin{aligned} u_t(x,y) &= \int_{\mathbb{R}^d} u_{t/2}(x,z)u_{t/2}(y,z)\,dz \\ &\leq \Big(\int_{\mathbb{R}^d} u_{t/2}^2(x,z)\,dz\Big)^{1/2}\Big(\int_{\mathbb{R}^d} u_{t/2}^2(y,z)\,dz\Big)^{1/2} \\ &= (u_t(x,x))^{1/2}(u_t(y,y))^{1/2} \end{aligned}$$

and

$$\begin{aligned} u_t(x,x) = \int_{\mathbb{R}^d} u_{t/2}^2(x,z)\,dz &= \|e^{-(t/4)H}u_{t/4}(x,\cdot)\|_2^2 \\ &\leq \|e^{-(t/4)H}\|_{2,2}^2\|u_{t/4}(x,\cdot)\|_2^2 = e^{-\frac{\lambda_0}{2}t}u_{t/2}(x,x). \end{aligned}$$

Consequently,

$$u_t(x,y) \leq (u_{t/2}(x,x))^{1/2}(u_{t/2}(y,y))^{1/2}e^{-\frac{\lambda_0}{2}t}. \tag{4.5}$$

Now, from Lemma 4.5 we have

$$
\begin{aligned}
&u_{t/2}(x,x)\\
&\leq \sqrt{C_1}\exp\Big(-\Big(\Big(C_2V_*(x)+\frac{C_3}{|x|^2}\Big)t\wedge C_4\sqrt{V_*(x)}\,|x|\Big)\Big)g_{(a/2)t}(x,x).
\end{aligned}
$$

By applying this estimate to both the diagonal terms on the right hand side of (4.5), we obtain the second claimed bound of the theorem. ∎

Proof of Theorem 2.1. By setting $a=2$ in Theorem 4.1, we have $C_2 = 1/4$, $C_3=\mu_0/2$, $C_4=\sqrt{2}/8$, and consequently

$$
h(t,x)\leq \exp\Big(-\frac{\sqrt{2}}{16}\Big(\Big(V_*(x)+\frac{\mu_0}{4|x|^2}\Big)t\wedge 2|x|\sqrt{V_*(x)}\Big)\Big)
$$

and

$$
\sqrt{h(t,x)}\leq \exp\Big(-\frac{\sqrt{2}}{32}\Big(\Big(V_*(x)+\frac{\mu_0}{4|x|^2}\Big)t\wedge 2|x|\sqrt{V_*(x)}\Big)\Big).
$$

Moreover, recall that

$$
H(t,x)=\exp\Big(-\frac{\sqrt{2}}{32}\Big(\Big(V_*(x)+\frac{\mu_0}{4|x|^2}\Big)t\wedge 2|x|\sqrt{V_*(x)+\frac{\mu_0}{4|x|^2}}\Big)\Big),
$$

for $x\neq 0$, and $H(t,0)=\exp\big(-\frac{\sqrt{2\mu_0}}{32}\big)$. We will prove that

$$
\sqrt{h(t,x)}\leq \exp\Big(\frac{\sqrt{\mu_0}}{16}\Big)H(t,x). \tag{4.6}
$$

Once this is done, the assertion follows from Theorem 4.1 with $a=2$ and the obvious inequality $h(t,x)\leq\sqrt{h(t,x)}$. Since

$$
\sqrt{h(t,0)}=1\leq \exp\Big(\frac{(2-\sqrt{2})\sqrt{\mu_0}}{32}\Big)=\exp\Big(\frac{\sqrt{\mu_0}}{16}\Big)H(t,0),
$$

(4.6) holds for $x=0$. We assume that $x\neq 0$ and consider two cases.

If $V_*(x)\geq \mu_0/(4|x|^2)$, then by the Taylor approximation,

$$
\begin{aligned}
0<|x|\Big(\sqrt{V_*(x)+\frac{\mu_0}{4|x|^2}}-\sqrt{V_*(x)}\Big)&\leq \frac{|x|}{2\sqrt{V_*(x)}}\,\frac{\mu_0}{4|x|^2}\\
&\leq \frac{|x|}{2\sqrt{\frac{\mu_0}{4|x|^2}}}\,\frac{\mu_0}{4|x|^2}=\frac{\sqrt{\mu_0}}{4}.
\end{aligned}
$$

This gives

$$
\exp\Big(-\frac{\sqrt{2}}{16}|x|\sqrt{V_*(x)}\Big)\leq \exp\Big(\frac{\sqrt{\mu_0}}{32}\Big)\exp\Big(-\frac{\sqrt{2}}{16}|x|\sqrt{V_*(x)+\frac{\mu_0}{4|x|^2}}\Big).
$$

On the other hand, if $V_*(x)\leq \mu_0/(4|x|^2)$, then

$$\exp\Big(\frac{\sqrt{2}}{16}|x|\sqrt{V_*(x)+\frac{\mu_0}{4|x|^2}}\Big) \le \exp\Big(\frac{\sqrt{2}}{16}|x|\sqrt{\frac{\mu_0}{2|x|^2}}\Big) = \exp\Big(\frac{\sqrt{\mu_0}}{16}\Big),$$

and consequently

$$\exp\Big(-\frac{\sqrt{2}}{16}|x|\sqrt{V_*(x)}\Big) \le 1 \le \exp\Big(\frac{\sqrt{\mu_0}}{16}\Big)\exp\Big(-\frac{\sqrt{2}}{16}|x|\sqrt{V_*(x)+\frac{\mu_0}{4|x|^2}}\Big).$$

These estimates show that (4.6) holds true. ∎

5. The proof of the lower bound. The proof of Theorem 2.2 consists of several auxiliary results. The only technical tool we use in our reasoning is the lower estimate with sharp Gaussian term of the density of the Brownian motion killed upon exiting a ball. This bound has recently been obtained for small times by Małecki and Serafin [19] (see also the classical result for more general domains by Zhang [33] and the newest paper for convex domains by Serafin [25]). By combining it with the classical intrinsic ultracontractivity estimate (see Davies and Simon [9, 10]) and by using the scaling property, one gets an estimate in the following form which is useful for our purposes: there exists a constant $\widetilde{C} \in (0,1]$ such that

$$g_t^{B_r}(x,y) \ge \widetilde{C}\frac{1 \wedge \frac{(r-|x|)(r-|y|)}{t}}{\big(1 \wedge \frac{r^2}{t}\big)^{(d+2)/2}}\exp\Big(-\mu_0\frac{t}{r^2}\Big)g_t(x,y), \qquad r,t>0,\ x,y \in B_r, \tag{5.1}$$

see [19, Corollary 1].

Lemma 5.1. *Let $0 \le V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$. For all $x,y \in \mathbb{R}^d$ and $\rho > 0$ such that $|x|,|y| \le \rho$, and all $t>0$, we have*

$$u_t(x,y) \ge (\widetilde{C}/4)\exp\Big(-\Big(V^*(\rho)+\frac{\mu_0}{4\rho^2}\Big)t\Big)g_t(x,y). \tag{5.2}$$

Proof. We first observe that by (3.1), for all $r>0$ and $x,y \in B_r$, we have

$$\begin{aligned} u_t(x,y) &\ge \lim_{s \nearrow t}\mathbb{E}_x\big[e^{-\int_0^s V(X_u)\,du}g_{t-s}(X_s,y);\ s<\tau_{B_r}\big] \\ &\ge e^{-t\sup_{z\in B_r}V(z)}\lim_{s\nearrow t}\mathbb{E}_x[g_{t-s}^{B_r}(X_s,y);\ s<\tau_{B_r}] \\ &= e^{-t\sup_{z\in B_r}V(z)}g_t^{B_r}(x,y). \end{aligned}$$

By taking $r=2\rho$, we see from (5.1) that

$$\begin{aligned} g_t^{B_r}(x,y) &\ge \widetilde{C}\frac{1\wedge\frac{\rho^2}{t}}{\big(1\wedge\frac{4\rho^2}{t}\big)^{(d+2)/2}}\exp\Big(-\mu_0\frac{t}{4\rho^2}\Big)g_t(x,y) \\ &\ge (\widetilde{C}/4)\exp\Big(-\mu_0\frac{t}{4\rho^2}\Big)g_t(x,y), \end{aligned} \tag{5.3}$$

and consequently

$$u_t(x,y) \ge (\widetilde{C}/4)\exp\Big(-\Big(V^*(\rho)+\frac{\mu_0}{4\rho^2}\Big)t\Big)g_t(x,y). \ \blacksquare$$

Recall the notation

$$t_\rho = \frac{\rho}{2\sqrt{V^*(\rho)+\frac{\mu_0}{4|x|^2}}}, \quad \rho \ge 1, \quad \text{and} \quad \rho_x = |x| \vee 1.$$

LEMMA 5.2. *Let $0 \le V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$. Then for all $x, y \in \mathbb{R}^d$ and $t > 0$ such that $\rho_y \le \rho_x$ and $t \ge 2t_{\rho_x}$, we have*

$$\begin{aligned} u_t(x,y) \ge{}& \frac{(\widetilde{C}/4)^2}{4^{d/2}\Gamma(d/2+1)(4\pi t)^{d/2}}\exp\Big(-\frac{dt}{2}\Big)\exp\Big(-\Big(V^*(\rho_y)+\frac{\mu_0}{4\rho_y^2}\Big)t\Big) \\ &\times \exp\Big(-\frac{9}{2}\rho_x\sqrt{V^*(\rho_x)+\frac{\mu_0}{4\rho_x^2}}\Big). \end{aligned}$$

Proof. Since $t > t_{\rho_x}$, we can write

$$\begin{aligned} u_t(x,y) &= \mathbb{E}_x\big[e^{-\int_0^{t_{\rho_x}} V(X_s)ds}u_{t-t_{\rho_x}}(X_{t_{\rho_x}},y)\big] \\ &\ge \mathbb{E}_x\big[e^{-\int_0^{t_{\rho_x}} V(X_s)ds}u_{t-t_{\rho_x}}(X_{t_{\rho_x}},y) : t_{\rho_x} < \tau_{B_{2\rho_x}}\big] \\ &\ge e^{-t_{\rho_x}V^*(\rho_x)}\mathbb{E}_x[u_{t-t_{\rho_x}}(X_{t_{\rho_x}},y) : t_{\rho_x} < \tau_{B_{2\rho_x}},\ X_{t_{\rho_x}} \in B_{\rho_y}]. \end{aligned} \tag{5.4}$$

By Lemma 5.1, on the set $\{X_{t_{\rho_x}} \in B_{\rho_y}\}$ we have

$$\begin{aligned} u_{t-t_{\rho_x}}(X_{t_{\rho_x}},y) &\ge (\widetilde{C}/4)\exp\Big(-\Big(V^*(\rho_y)+\frac{\mu_0}{4\rho_y^2}\Big)t\Big)g_{t-t_{\rho_x}}(X_{t_{\rho_x}},y) \\ &= \frac{\widetilde{C}/4}{(4\pi(t-t_{\rho_x}))^{d/2}}\exp\Big(-\Big(V^*(\rho_y)+\frac{\mu_0}{4\rho_y^2}\Big)t\Big)\exp\Big(-\frac{|y-X_{t_{\rho_x}}|^2}{4(t-t_{\rho_x})}\Big), \end{aligned}$$

and because $t_{\rho_x} \le t - t_{\rho_x} \le t$ and $\rho_y \le \rho_x$, this estimate can be continued as follows:

$$\begin{aligned} &\ge \frac{\widetilde{C}/4}{(4\pi t)^{d/2}}\exp\Big(-\Big(V^*(\rho_y)+\frac{\mu_0}{4\rho_y^2}\Big)t\Big)\exp\Big(-\frac{4\rho_y^2}{4t_{\rho_x}}\Big) \\ &\ge \frac{\widetilde{C}/4}{(4\pi t)^{d/2}}\exp\Big(-\Big(V^*(\rho_y)+\frac{\mu_0}{4\rho_y^2}\Big)t\Big)\exp\Big(-\frac{\rho_x^2}{t_{\rho_x}}\Big) \\ &= \frac{\widetilde{C}/4}{(4\pi t)^{d/2}}\exp\Big(-\Big(V^*(\rho_y)+\frac{\mu_0}{4\rho_y^2}\Big)t\Big)\exp\Big(-2\rho_x\sqrt{V^*(\rho_x)+\frac{\mu_0}{4\rho_x^2}}\Big). \end{aligned}$$

With this bound we can come back to (5.4) and write

$$u_t(x,y) \geq \frac{\widetilde{C}/4}{(4\pi t)^{d/2}} \exp\left(-\left(V^*(\rho_y) + \frac{\mu_0}{4\rho_y^2}\right)t\right) \exp\left(-2\rho_x\sqrt{V^*(\rho_x) + \frac{\mu_0}{4\rho_x^2}}\right)$$
$$\times \exp\left(-\frac{\rho_x V^*(\rho_x)}{2\sqrt{V^*(\rho_x) + \frac{\mu_0}{4|x|^2}}}\right)\mathbb{P}_x[t_{\rho_x} < \tau_{B_{2\rho_x}}, X_{t_{\rho_x}} \in B_{\rho_y}].$$

We only need to estimate the last probability. By using (5.3) and $t_{\rho_x} < t$, we get

$$\begin{aligned}
\mathbb{P}_x[t_{\rho_x} < \tau_{B_{2\rho_x}}, X_{t_{\rho_x}} \in B_{\rho_y}] &\geq \int_{B_1} g_{t_{\rho_x}}^{B_{2\rho_x}}(x,z)\,dz \\
&\geq \frac{\widetilde{C}|B_1|}{4(4\pi t_{\rho_x})^{d/2}} \exp\left(-\mu_0\frac{t_{\rho_x}}{4\rho_x^2}\right)\exp\left(-\frac{4\rho_x^2}{4t_{\rho_x}}\right) \\
&\geq \frac{\widetilde{C}\pi^{d/2}}{4\Gamma(d/2+1)(4\pi t)^{d/2}} \exp\left(-\mu_0\frac{t_{\rho_x}}{4\rho_x^2}\right)\exp\left(-\frac{\rho_x^2}{t_{\rho_x}}\right) \\
&\geq \frac{\widetilde{C}}{4^{1+d/2}\Gamma(d/2+1)} \exp\left(-\frac{dt}{2} - \mu_0\frac{t_{\rho_x}}{4\rho_x^2}\right)\exp\left(-2\rho_x\sqrt{V^*(\rho_x) + \frac{\mu_0}{4\rho_x^2}}\right),
\end{aligned}$$

where in the last line we have used the inequality $t^{-d/2} \geq e^{-(d/2)t}$. This leads to

$$u_t(x,y) \geq \frac{\widetilde{C}^2}{4^{2+d/2}\Gamma(d/2+1)(4\pi t)^{d/2}} \exp\left(-\frac{dt}{2}\right)\exp\left(-\left(V^*(\rho_y) + \frac{\mu_0}{4\rho_y^2}\right)t\right)$$
$$\times \exp\left(-\frac{9}{2}\rho_x\sqrt{V^*(\rho_x) + \frac{\mu_0}{4\rho_x^2}}\right).$$

In the last line we have used the equality

$$\exp\left(-\frac{\rho_x V^*(\rho_x)}{2\sqrt{V^*(\rho_x)+\frac{\mu_0}{4|x|^2}}}\right)\exp\left(-\mu_0\frac{t_{\rho_x}}{4\rho_x^2}\right) = \exp\left(-\frac{1}{2}\rho_x\sqrt{V^*(\rho_x)+\frac{\mu_0}{4\rho_x^2}}\right). \ \blacksquare$$

We are now ready to prove the main result of this section.

Proof of Theorem 2.2. Let $x, y \in \mathbb{R}^d$ and $t > 0$. Part (2) follows directly from Lemma 5.1 with $\rho = \rho_x \vee \rho_y$ and the inequality $\widetilde{C}/4 \geq c_2$. We only need to establish (1).

Assume that $4t_{\rho_x\vee\rho_y} \leq t$ and $\rho_x \geq \rho_y$. In particular, $t_{\rho_x\vee\rho_y} = t_{\rho_x}$. Observe that

$$4t_{\rho_z} \leq t \iff 2\rho_z\sqrt{V^*(\rho_z) + \frac{\mu_0}{4\rho_z^2}} \leq \left(V^*(\rho_z) + \frac{\mu_0}{4\rho_z^2}\right)t.$$

In particular,

$$4t_{\rho_z} \leq t \implies K(t,\rho_z) = \exp\left(-\frac{9}{2}\rho_z\sqrt{V^*(\rho_z) + \frac{\mu_0}{4\rho_z^2}}\right)$$

and

$$4t_{\rho_z} \geq t \implies K(t,\rho_z) = \exp\left(-\frac{9}{4}\left(V^*(\rho_z) + \frac{\mu_0}{4\rho_z^2}\right)t\right).$$

In order to complete the proof, we need to consider two cases and use the above observations.

Let first $4t_{\rho_y} \leq t$. Since $2t_{\rho_x} \leq t/2$ and $2t_{\rho_y} \leq t/2$, we can use Lemma 5.2 and symmetry to get

$$\begin{aligned} u_{t/2}(x,z) \geq{}& \frac{(\widetilde{C}/4)^2}{4^{d/2}\Gamma(d/2+1)}\,\frac{1}{(2\pi t)^{d/2}}\exp\left(-\left(\frac{d}{2} + V^*(1) + \frac{\mu_0}{4}\right)\frac{t}{2}\right) \\ &\times \exp\left(-\frac{9}{2}\rho_x\sqrt{V^*(\rho_x) + \frac{\mu_0}{4\rho_x^2}}\right) \end{aligned}$$

and

$$\begin{aligned} u_{t/2}(z,y) \geq{}& \frac{(\widetilde{C}/4)^2}{4^{d/2}\Gamma(d/2+1)}\,\frac{1}{(2\pi t)^{d/2}}\exp\left(-\left(\frac{d}{2} + V^*(1) + \frac{\mu_0}{4}\right)\frac{t}{2}\right) \\ &\times \exp\left(-\frac{9}{2}\rho_y\sqrt{V^*(\rho_y) + \frac{\mu_0}{4\rho_y^2}}\right) \end{aligned}$$

whenever $|z| \leq 1$. By the Chapman–Kolmogorov property and the inequality $t^{-d/2} \geq e^{-(d/2)t}$, we then obtain the estimate

$$\begin{aligned} u_t(x,y) &\geq \int_{B_1} u_{t/2}(x,z)u_{t/2}(z,y)\,dz \\ &\geq \left(\frac{(\widetilde{C}/4)^2}{4^{d/2}\Gamma(d/2+1)}\right)^2 \frac{|B_1|}{\pi^{d/2}(4\pi t)^{d/2}} e^{-\lambda_2 t} K(t,\rho_x)K(t,\rho_y) \\ &= c_2 e^{-\lambda_2 t} g_t(0,0)K(t,\rho_x)K(t,\rho_y). \end{aligned}$$

This is exactly what we wanted to prove.

Suppose now that $4t_{\rho_y} \geq t$. Recall that $2t_{\rho_x} \leq t$ and $\rho_x \geq \rho_y$. Then, by Lemma 5.2,

$$\begin{aligned} u_t(x,y) &\geq \frac{\sqrt{c_2}}{(4\pi t)^{d/2}} \exp\left(-\frac{dt}{2}\right)\exp\left(-\frac{9}{4}\left(V^*(\rho_y) + \frac{\mu_0}{4\rho_y^2}\right)t\right) \\ &\qquad \times \exp\left(-\frac{9}{2}\rho_x\sqrt{V^*(\rho_x) + \frac{\mu_0}{4\rho_x^2}}\right) \\ &\geq c_2 \exp(-\lambda_2 t) g_t(0,0)K(t,\rho_y)K(t,\rho_x). \end{aligned}$$

This completes the proof. ■

6. Applications, previous results, discussion and examples

6.1. Qualitatively sharp two-sided bounds for confining potentials. Recall that the Schrödinger operator with confining potential has compact resolvent and purely discrete spectrum, $0 < \lambda_0 = \inf \sigma(H)$ is a simple eigenvalue, and the corresponding eigenfunction $\varphi_0 \in L^2(\mathbb{R}^d, dx)$ is continuous, bounded and strictly positive on $\mathbb{R}^d$. We refer to λ_0 and φ_0 as the *ground state* eigenvalue and eigenfunction.

The framework of confining potentials provides important examples of intrinsically ultracontractive Schrödinger semigroups (see Davies and Simon [10], Davies [9] and Bañuelos [1]). One of the equivalent definitions says that the semigroup $\{e^{-tH} : t \geq 0\}$ is *intrinsically ultracontractive* (IUC for short) if for every $t > 0$ there exists $c = c(t)$ such that for every $x, y \in \mathbb{R}^d$ we have $u_t(x,y) \leq c\varphi_0(x)\varphi_0(y)$. This implies the following two-sided estimates: for every $t_0 > 0$ there exists $\widetilde{c} = \widetilde{c}(t_0) \geq 1$ such that

$$\frac{1}{\widetilde{c}} e^{-\lambda_0 t}\varphi_0(x)\varphi_0(y) \leq u_t(x,y) \leq \widetilde{c} e^{-\lambda_0 t}\varphi_0(x)\varphi_0(y), \qquad x, y \in \mathbb{R}^d,\ t \geq t_0$$

(the lower bound for every fixed $t_0 > 0$ follows from [10, Theorem 3.2, (iv)⇒(vi)]; the two-sided bound extends to $t \geq t_0$ by the eigenequation $U_t\varphi_0 = e^{-\lambda_0 t}\varphi_0$). For many examples of potentials it is known that φ_0 is comparable to $\exp(-c|x|\sqrt{V(x)}\,)$, typically with different constant c from above and from below (see Simon [28] and Carmona [3], and references in those papers). Clearly, this leads to qualitatively sharp two-sided estimates for large times. On the other hand, estimates for non-IUC semigroups have been an open problem for a long time. For example, if

$$V(x) = |x|^\alpha, \qquad \alpha > 0, \tag{6.1}$$

then IUC holds if and only if $\alpha > 2$. More recently, this example has been studied by Sikora [26] who proved upper bounds for the full range of $\alpha > 0$ and $t > 0$, and a two-sided on-diagonal estimate. Short time upper estimates of a similar type for more general potentials were obtained by Metafune and Spina [21] and Spina [30]. Metafune, Pallara and Rhandi [20] analyzed the constant in the intrinsic ultracontractivity estimate for small t's. We also refer the reader to the paper by Ouhabaz and Rhandi [22] for upper estimates for uniformly elliptic operators.

Our Theorems 2.1 and 2.2 immediately give the following, global in time and space, two-sided estimates for general nonnegative locally bounded confining potentials, in both IUC and non-IUC settings. Recall that the functions H and K and the constants $\gamma_1, \gamma_2, c_1, c_2$ come from the statements of these theorems.

Corollary 6.1. *For every confining potential $0 \leq V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$ and $x, y \in \mathbb{R}^d$, $t > 0$ we have the following estimates:*

(1) *If $4t_{\rho_x \vee \rho_y} \leq t$, then*

$$c_2 e^{-\gamma_2 t} K(t, \rho_x) K(t, \rho_y) g_t(0,0) \leq u_t(x,y) \leq c_1 e^{-\gamma_1 t} H(t,x) H(t,y) g_t(0,0).$$

(2) *If* $4t_{\rho_x \vee \rho_y} \geq t$, *then*

$$c_2 K(t,\rho_x) K(t,\rho_y) g_t(x,y) \leq u_t(x,y) \leq c_1 H(t,x) H(t,y) g_{2t}(x,y).$$

These estimates take the sharpest form for potentials comparable to radial monotone functions that grow at infinity sufficiently regularly. The estimates are fully uniform if the growth of the potential is not too fast. We give an illustration with the following two examples. Example 6.2 is general, and Example 6.3 gives applications to some specific classes of potentials.

Example 6.2 (Potentials with radial monotone profiles). Let $0 \leq V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$ be a confining potential such that there exists a constant $m \geq 1$ satisfying

$$V^*(|x|) \leq m V_*(x), \qquad |x| \geq 1. \tag{6.2}$$

Define $W(r) := V^*(r)$. Then W is referred to as the *radial monotone profile* of the potential V.

It is convenient to introduce the following rate functions:

$$\widetilde{K}(t,x) := \exp\left(-\frac{9}{4}\left(\left(W(\rho_x) + \frac{\mu_0}{4\rho_x^2}\right)t \wedge 2\rho_x \sqrt{W(\rho_x) + \frac{\mu_0}{4\rho_x^2}}\right)\right)$$

with $\rho_x = |x| \vee 1$,

$$\widetilde{H}(t,x) := \exp\left(-\frac{\sqrt{2}}{32m}\left(\left(W(|x|) + \frac{\mu_0}{4|x|^2}\right)t \wedge 2|x|\sqrt{W(|x|) + \frac{\mu_0}{4|x|^2}}\right)\right)$$

for $|x| \geq 1$, and $\widetilde{H}(t,x) = 1$ for $|x| < 1$. Moreover, let

$$\gamma_1 = \lambda_0/2, \qquad \gamma_2 = d + W(1) + \mu_0/4.$$

Observe that $\widetilde{K}(t,x)$ and $\widetilde{H}(t,x)$ take exactly the same form

$$\exp\left(-c\left(\left(W(|x|) + \frac{\mu_0}{4|x|^2}\right)t \wedge 2|x|\sqrt{W(|x|) + \frac{\mu_0}{4|x|^2}}\right)\right)$$

for $|x| \geq 1$ and $t > 0$, and they differ only in the value of the constant c in the exponent. Moreover, we always have

$$0 < \exp\left(-\frac{9}{2}\sqrt{W(1) + \frac{\mu_0}{4}}\right) \leq \widetilde{K}(t,x) \leq \widetilde{H}(t,x) = 1, \qquad |x| < 1,\ t > 0.$$

From Corollary 6.1 we obtain the following qualitatively sharp uniform two-sided estimates:

(1) If

$$\frac{2(\rho_x \vee \rho_y)}{\sqrt{W(\rho_x \vee \rho_y) + \frac{\mu_0}{4(\rho_x \vee \rho_y)^2}}} \leq t,$$

then

$$c_2 e^{-\gamma_2 t} \widetilde{K}(t,x) \widetilde{K}(t,y) g_t(0,0) \leq u_t(x,y) \leq c_1 e^{-\gamma_1 t} \widetilde{H}(t,x) \widetilde{H}(t,y) g_t(0,0).$$

(2) If

$$\frac{2(\rho_x \vee \rho_y)}{\sqrt{W(\rho_x \vee \rho_y) + \frac{\mu_0}{4(\rho_x \vee \rho_y)^2}}} \geq t,$$

then

$$c_2 \widetilde{K}(t,x) \widetilde{K}(t,y) g_t(x,y) \leq u_t(x,y) \leq c_1 \widetilde{H}(t,x) \widetilde{H}(t,y) g_{2t}(x,y).$$

We now apply Example 6.2 to specific potentials.

Example 6.3 (Polynomial and logarithmic potentials). Consider the following classes of potentials.

(1) *Polynomial potentials*: Let

$$V(x) = k|x|^\alpha, \qquad \alpha, k > 0.$$

Clearly, we have

$$V_*(x) = k(|x|/2)^\alpha \quad \text{and} \quad V^*(r) = k(2r)^\alpha.$$

Moreover, $\gamma_2 = d + k \cdot 2^\alpha + \mu_0/4$. Observe that (6.2) is true for $m = 4^\alpha$, uniformly in $k > 0$. Consequently, the estimates from Example 6.2 hold with

$$W(r) = k(2r)^\alpha \quad \text{and} \quad m = 4^\alpha.$$

Moreover, the rate $9/4$ in the function $\widetilde{K}(t,x)$ (the lower bound) is uniform in $\alpha > 0$ and $k > 0$, and the rate $\sqrt{2}/(32m)$ in $\widetilde{H}(t,x)$ (the upper bound) is uniform in $k > 0$ and $\alpha \in (0, \alpha_0]$, for every fixed $\alpha_0 > 0$ – it can be chosen to be $\sqrt{2}/(32 \cdot 4^{\alpha_0})$.

Our result applies to both IUC ($\alpha > 2$) and non-IUC ($\alpha \in (0,2]$) cases. In the non-IUC setting, the estimates are fully uniform in $k > 0$ and $\alpha \in (0,2]$.

(2) *Logarithmic potentials*: Let

$$V(x) = \log^\alpha(2 + k|x|), \qquad \alpha, k > 0.$$

One has

$$V_*(x) = \log^\alpha(2 + k(|x|/2)), \qquad V^*(r) = \log^\alpha(2 + k(2r)),$$

and $\gamma_2 = d + \log^\alpha(2 + 2k) + \mu_0/4$. Moreover, one checks directly that (6.2) holds with $m = 3^\alpha$, uniformly in $k > 0$. Consequently, we obtain estimates as in Example 6.2 with

$$W(r) = \log^\alpha(2 + k(2r)) \quad \text{and} \quad m = 3^\alpha.$$

In particular, the rate $9/4$ in the function $\widetilde{K}(t,x)$ (the lower bound) is uniform in $\alpha > 0$ and $k > 0$, and the rate $\sqrt{2}/(32m)$ in $\widetilde{H}(t,x)$ (the upper bound) is uniform in $k > 0$ and $\alpha \in (0, \alpha_0]$, for every fixed $\alpha_0 > 0$ – it can be chosen to be $\sqrt{2}/(32 \cdot 3^{\alpha_0})$.

Note that such potentials lead to non-IUC semigroups for every $\alpha > 0$. Our estimates are fully uniform in $k > 0$ and $\alpha \in (0, \alpha_0]$, for every fixed $\alpha_0 > 0$.

We remark that one of our primary motivations was to understand the large time properties of the Schrödinger semigroups with confining potentials which are not IUC. This is related to the recent progress in the field of nonlocal Schrödinger operators. First note that in order to describe the large time regularity of the semigroup, it is enough to study the *asymptotic* version of IUC (aIUC for short), which is more general; see [15] for more details. For sharp necessary and sufficient conditions for aIUC in the nonlocal case we refer the reader to Kulczycki and Siudeja [17], Kaleta and Kulczycki [14], Kaleta and Lőrinczi [15], and Chen and Wang [6, 7] (see also the related important paper by Kwaśnicki [18] for stable semigroups on unbounded sets).

In [16], Kaleta and Schilling observed in the nonlocal setting that the Schrödinger semigroup with confining potential which is not aIUC (no matter how slow the growth of V at infinity is!) still manifests a weaker version of regularity, which can be described as follows: there exist an increasing function ρ (determined by the kinetic term and the potential) such that $\rho(t) \uparrow \infty$ as $t \uparrow \infty$, and a constant $c \geq 1$, such that

$$\frac{1}{c} e^{-\lambda_0 t} \varphi_0(x)\varphi_0(y) \leq u_t(x,y) \leq c e^{-\lambda_0 t} \varphi_0(x)\varphi_0(y), \qquad |x| \wedge |y| \leq \rho(t),\ t \geq t_0 \tag{6.3}$$

(c is uniform in t and x, y). This is called *progressive* IUC (pIUC for short).

Our estimates show that such a property does not hold for classical Schrödinger semigroups. However, we can observe a weaker version of this two-sided bound which is qualitatively sharp. Suppose we are in the setting of Example 6.2. Moreover, assume that the potential V is a continuous function such that the map

$$\rho \mapsto \tau(\rho) := \frac{2\rho}{\sqrt{W(\rho) + \frac{\mu_0}{4\rho^2}}}$$

is increasing and $\tau(\rho) \to \infty$ as $\rho \to \infty$. It then follows from the estimates in Example 6.2 that there are constants $c_1, \ldots, c_6 > 0$ such that

$$\begin{aligned} c_1 e^{-c_2 t} &\exp\Big(-c_3\big(|x|\sqrt{W(|x|)} + |y|\sqrt{W(|y|)}\big)\Big) \\ &\leq u_t(x,y) \leq c_4 e^{-c_5 t} \exp\Big(-c_6\big(|x|\sqrt{W(|x|)} + |y|\sqrt{W(|y|)}\big)\Big) \end{aligned}$$

whenever

$$\tau(\rho_x \vee \rho_y) \leq t \quad \text{and} \quad t \geq t_0 > 0. \tag{6.4}$$

Clearly, $t \mapsto \rho(t) := \tau^{-1}(t)$ is an increasing function such that $\rho(t) \to \infty$ as $t \to \infty$, and the first inequality in (6.4) can be rephrased as $\rho_x \vee \rho_y \leq \rho(t)$. Moreover, there are constants $c_7, \ldots, c_{10} > 0$ such that

$$c_7 \exp\big(-c_8|x|\sqrt{W(|x|)}\big) \leq \varphi_0(x) \leq c_9 \exp\big(-c_{10}|x|\sqrt{W(|x|)}\big), \qquad x \in \mathbb{R}^d$$

(see Carmona and Simon [3, 4]). This leads to a weaker, qualitative version of (6.3). On the other hand, the time-space domain $\rho_x \vee \rho_y \le \rho(t)$ cannot be replaced with $\rho_x \wedge \rho_y \le \rho(t)$ as in the original pIUC property (6.3). Indeed, take an arbitrary function $\rho(t)$ as above and suppose that there are constants $c_1, c_2, c_3 > 0$ and $t_0 > 0$ such that

$$c_1 e^{-c_2 t} \exp\Big(-c_3\big(|x|\sqrt{W(|x|)} + |y|\sqrt{W(|y|)}\big)\Big) \le u_t(x,y) \tag{6.5}$$

for $|x| \le \rho(t) < |y|$ and $t \ge t_0$. If the profile W is strictly subquadratic (e.g. $W(r) = r^\beta$, $\beta \in (0,2)$), then this cannot hold as we always have

$$u_t(x,y) \le g_t(x,y) = (4\pi t)^{-d/2} \exp\left(\frac{|y-x|^2}{4t}\right), \qquad x, y \in \mathbb{R}^d,\ t > 0.$$

Indeed, (6.5) does not hold, which can be easily seen by fixing $t > t_0$ and letting $|y| \to \infty$.

A similar qualitative property can also be derived from the estimates obtained by Chen and Wang [5].

6.2. Upper estimate for decaying potentials. Our result immediately gives an upper estimate for *decaying* potentials, i.e. when $V(x) \to 0$ as $|x| \to \infty$. For clarity, we illustrate this with the potential

$$V(x) = k(1 \vee |x|)^{-\alpha}, \qquad \alpha, k > 0 \tag{6.6}$$

(we remark that for the upper bound it is enough to assume that V is bounded from below by the expression on the right hand side of (6.6)). The estimates for potentials of this type were obtained in a more general setting of manifolds by Zhang [32]. We compare these results with our upper estimate.

We have

$$V_*(x) = k \cdot \begin{cases} 1 & \text{for } |x| \le 2/3, \\ \big(\frac{3}{2}|x|\big)^{-\alpha} & \text{for } |x| \ge 2/3. \end{cases}$$

The following estimate can be easily derived from Theorem 2.1.

Example 6.4. Let V be as in (6.6). For all $x, y \in \mathbb{R}^d$ and $t > 0$ we have the following upper bound:

$$u_t(x,y) \le c_1 \widetilde{H}(t,x) \widetilde{H}(t,y) g_{2t}(x,y),$$

where $\widetilde{H}(t,x) = 1$ for $|x| < 1$ and

$$\widetilde{H}(t,x) := \begin{cases} \exp\big(-\frac{\sqrt{2}}{32} \cdot \big(\frac{2}{3}\big)^\alpha \big(\frac{kt}{|x|^\alpha} \wedge 2\sqrt{k}|x|^{1-\alpha/2}\big)\big) & \text{if } \alpha \in (0,2), \\ 1 & \text{if } \alpha \ge 2, \end{cases}$$

for $|x| \ge 1$. The rate in the exponent is an explicit constant which is uniform in the coupling parameter $k > 0$ and $\alpha \in (0, \alpha_0]$, for every fixed $\alpha_0 > 0$.

As explained in Section 2, our Theorem 2.2 is not sharp enough to give a similar lower bound for decaying potentials. This is a much more difficult problem that requires a subtle argument. On the other hand, this example shows that at least for potentials as in (6.6) with $\alpha \in (0,2)$, the function $\widetilde{H}(t,x)$ resulting from Theorem 2.1 is sharp in one of the time-space regions. For small t's the kernel $u_t(x,y)$ is just comparable to $g_t(x,y)$, so we only look at large times. Indeed, if $t \le (2/\sqrt{k})|x|^{1+\alpha/2}$, then $\widetilde{H}(t,x) = \exp(-ckt/|x|^{\alpha})$, which is qualitatively the same as the function $w_2(x,t)$ in the lower estimate of [32, Theorem 1.2]; this means that we improve the power in the exponent of the function $w_1(x,t)$ in [32, Theorem 1.1] for this time-space region (see the comments in [32, Remark 1.2]). In fact, the exponent in our function $\widetilde{H}(t,x)$ is qualitatively better in the larger time-space region which is roughly described by $\sqrt{t} \le |x|^{1+\alpha/2}$. We also remark that due to Theorem 4.1 the Gaussian term in the estimate above can be made nearly optimal at the cost of the rate in $\widetilde{H}$, and we have uniform control with respect to parameter $k > 0$ and $\alpha \in (0, \alpha_0]$. On the other hand, if $\sqrt{t} \ge |x|^{1+\alpha/2}$, then the estimate in [32, Theorem 1.1] is sharper than ours. For $\alpha > 2$ the estimate above is trivial, but it is also sharp.

6.3. Upper estimate for potentials bounded away from zero. We can also give a nontrivial upper estimate for potentials that are *bounded away from zero outside a bounded set*, i.e. the functions V for which

(6.7) there exist $\kappa > 0$ and $r_0 \ge 0$ such that $V(x) \ge \kappa$ for $|x| \ge r_0$.

Theorem 2.1 immediately gives the following estimate.

Example 6.5. Let V be as in (6.7). For all $x, y \in \mathbb{R}^d$ and $t > 0$ we have

$$u_t(x,y) \le c_1 \widetilde{H}(t,x)\widetilde{H}(t,y) g_{2t}(x,y),$$

where $\widetilde{H}(t,x) = 1$ for $|x| < 2r_0$ and

$$\widetilde{H}(t,x) = \exp\big(-(\sqrt{2}/32)(\kappa t \wedge 2\sqrt{\kappa}|x|)\big) \quad \text{for } |x| \ge 2r_0.$$

Moreover, if $r_0 = 0$ or just $\lambda_0 > 0$, then $g_{2t}(x,y)$ can be replaced with $e^{-(\lambda_0/2)t} g_t(0,0)$.

6.4. Upper estimate for more general, nonradial potentials. Observe that by using Theorem 2.1 we can also get an upper estimate of the same type for highly nonradial potentials, including confining, decaying, bounded-away-from-zero ones, and mixtures. This follows from the fact that $H(t,x)$ depends only on the values of the potential V in the ball $\overline{B}_{|x|/2}(x)$. It seems to be a novelty even if $d = 1$. Let $\alpha_1, \alpha_2, c > 0$. For a quick overview, we just list some examples of potentials on $\mathbb{R}$:

(1) (nonsymmetric confining potential):

$$V(x) = \begin{cases} x^{\alpha_1}, & x \ge 0, \\ (-x)^{\alpha_2}, & x \le 0, \end{cases} \quad \text{with} \quad \alpha_1 \ne \alpha_2.$$

(2) (nonsymmetric decaying potential):

$$V(x) = \begin{cases} (1 \vee x)^{-\alpha_1}, & x \geq 0, \\ (1 \vee -x)^{-\alpha_2}, & x \leq 0, \end{cases} \quad \text{with} \quad \alpha_1 \neq \alpha_2.$$

(3) (mixture of confining and decaying potentials):

$$V(x) = \begin{cases} (1 \vee x)^{-\alpha_1}, & x \geq 0, \\ (-x)^{\alpha_2}, & x \leq 0, \end{cases} \quad \text{or} \quad V(x) = \begin{cases} x^{\alpha_1}, & x \geq 0, \\ (1 \vee -x)^{-\alpha_2}, & x < 0. \end{cases}$$

(4) (mixture of confining/decaying and constant potentials):

$$V(x) = \begin{cases} c, & x \geq 0, \\ (-x)^{\alpha_1}, & x < 0, \end{cases} \quad \text{or} \quad V(x) = \begin{cases} (1 \vee x)^{-\alpha_1}, & x > 0, \\ c, & x \leq 0. \end{cases}$$

For all of the examples of this type we obtain an upper bound similar to those in Examples 6.3–6.5 above, but with $\widetilde{H}$ which takes a different form for $x > 0$ and $x < 0$.

6.5. Upper estimate for singular potentials. We now show that applications of our Theorem 2.1 go beyond the scope of locally bounded potentials. Suppose we are given $V \geq 0$ such that $V \in K_{\mathrm{loc}}(\mathbb{R}^d) \setminus L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$, where $K_{\mathrm{loc}}(\mathbb{R}^d)$ denotes the *local Kato class* corresponding to the Laplacian (or the Brownian motion). Recall that a Borel function V belongs to $K_{\mathrm{loc}}(\mathbb{R}^d)$ if for every compact set $C \subset \mathbb{R}^d$ we have

$$\lim_{t \to 0} \sup_{x \in \mathbb{R}^d} \int_0^t \int_{\mathbb{R}^d} g_s(x,y) |V \mathbb{1}_C|(y) \, dy \, ds = 0.$$

It is known that the Schrödinger operator $H = -\Delta + V$ can be defined in the sense of quadratic forms as a positive selfadjoint operator on $L^2(\mathbb{R}^d)$ (see e.g. Simon [27] and Demuth and van Casteren [11]). The semigroup operators e^{-tH}, $t > 0$, are integral operators; due to the Feynman–Kac formula the corresponding integral kernels $u_t(x,y)$ are given by (3.1). For a number $m > 0$ we define $V^m := V \wedge m$ and consider $H_m = -\Delta + V^m$. Clearly, $V^m \in L^\infty(\mathbb{R}^d)$, and e^{-tH_m}, $t > 0$, are integral operators with kernels $u_t^m(x,y)$. Since $V^m \leq V$ for $m > 0$, by (3.1) we get $u_t(x,y) \leq u_t^m(x,y)$ for all $t > 0$ and $x, y \in \mathbb{R}^d$. Then, by applying Theorem 2.1 to the kernel $u_t^m(x,y)$, we obtain

$$u_t(x,y) \leq c_1 H^m(t,x) H^m(t,y) g_{2t}(x,y), \qquad x, y \in \mathbb{R}^d, \, t > 0,$$

where $H^m(t,x)$ is $H(t,x)$ with V_* replaced with $V_*^m := \inf_{z \in \overline{B}_{|x|/2}(x)} V^m(z)$. It is now enough to observe that $V_*^m \nearrow V_*$ as $m \nearrow \infty$, which leads to $H^m \to H$ (all the constants appearing in these shape functions are uniform with respect to the potential!). Consequently, we get the following upper bound:

Corollary 6.6. *Let* $0 \le V \in K_{\mathrm{loc}}(\mathbb{R}^d)$. *Then*

$$u_t(x,y) \le c_1 H(t,x)H(t,y)g_{2t}(x,y), \qquad x,y \in \mathbb{R}^d,\ t>0,$$

where H *is defined with* V_* *in place of the original* V.

Depending on applications, one can also apply the estimate in Theorem 4.1 to get $g_{at}(x,y)$ for any $a>1$ instead of $g_{2t}(x,y)$ in this bound.

If $d \ge 3$, then typical examples of potentials covered by the above corollary include

$$V(x) = \frac{c}{|x|^{\alpha}} \quad \text{or} \quad V(x) = \sum_{k=1}^{N} \frac{c_k}{|z_k - x|^{\alpha_k}},$$

where $\alpha, \alpha_k \in (0,2)$, $c, c_k > 0$, $z_k \in \mathbb{R}^d$, $N \in \mathbb{N}$, or the sums of such functions and some nonnegative locally bounded confining potentials (cf. [27, Section A.2]). We remark that Corollary 6.6 extends to more singular potentials $V(x) = c|x|^{-\alpha}$, where $\alpha \ge 2$ and $c>0$; $\alpha = 2$ is *critical* in the sense that it is the smallest parameter for which $V \notin K_{\mathrm{loc}}(\mathbb{R}^d)$. However, for such potentials the classical Feynman–Kac formula with respect to the Brownian motion in the whole $\mathbb{R}^d$ does not hold. In order to overcome this obstacle, one can first consider the process with the restricted state space to represent the kernel u and then show that $u \le u^m$.

Remark 6.7. While the present manuscript was being completed, J. Wang informed us about his recent preprint [5] with X. Chen, where the authors provide the two-sided qualitatively sharp estimates for the heat kernels of Schrödinger operators with nonnegative, locally bounded, confining potentials V, which are comparable to radial and monotone profiles g. This result is related to our Examples 6.3 and 6.2 which apply to the same class of potentials.

Our work was performed simultaneously with, and independently of, [5] (our preprint appeared on the arXiv in February 2023). The estimates in [5] have a completely different structure from ours, which seems to be related to the fact that the argument in [5] requires the assumption that $s \mapsto (1+s)/\sqrt{g(s)}$ is an almost monotone function. Note that our Theorem 2.1 covers a larger class of potentials, as it applies to general nonnegative locally bounded potentials or even singular ones. The arguments in [5] and in our paper are based on completely different ideas. The key step in our proof of the upper estimate is based on the fact that the Laplace transform of the exit time from a ball with radius proportional to the norm of x and evaluated at $\lambda = V(x)$ takes the shape of the ground state $\varphi_0(x)$ of the Schrödinger operator H. Here we apply the classical result of Wendel [31]. In the proof of the lower estimate, we use directly the estimate (with optimal Gaussian term) for the semigroup of a Brownian motion in a ball, which was recently discovered by Małecki and Serafin [19], and combine this bound with the direct estimates in Lemma 5.2. This is described in more detail at the end of Section 2. Our proof does not use any information on the joint distribution of the exit position and the exit time of Brownian motion from a ball, which is the main tool in [5]. Our approach leads to qualitatively sharp estimates with explicit numerical rates, uniform in V, with clear dependence on the dimension d, and optimal or nearly optimal Gaussian terms, which are obtained by rather short and direct proofs. The constants in the estimates of [5] are not explicit; they seem to depend on V and d in an implicit fashion.

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References

[1] R. Bañuelos, *Intrinsic ultracontractivity and eigenfunction estimates for Schrödinger operators* J. Funct. Anal. 100 (1991), 181–206.

[2] K. Bogdan, J. Dziubański, and K. Szczypkowski, *Sharp Gaussian estimates for heat kernels of Schrödinger operators*, Integral Equations Operator Theory 91 (2019), art. 3, 20 pp.

[3] R. Carmona, *Pointwise bounds for Schrödinger eigenstates*, Comm. Math. Phys. 62 (1978), 97–106.

[4] R. Carmona and B. Simon, *Pointwise bounds on eigenfunctions and wave packets in N-body quantum systems. V. Lower bounds and path integrals*, Comm. Math. Phys. 1 (1981), 59–98.

[5] X. Chen and J. Wang, *Two-sided heat kernel estimates for Schrödinger operators with unbounded potentials*, arXiv:2301.06744 (2023).

[6] X. Chen and J. Wang, *Intrinsic contractivity properties of Feynman–Kac semigroups for symmetric jump processes with infinite range jumps*, Front. Math. China 10 (2015), 753–776.

[7] X. Chen and J. Wang, *Intrinsic ultracontractivity of Feynman–Kac semigroups for symmetric jump processes*, J. Funct. Anal. 270 (2016), 4152–4195.

[8] K. L. Chung and Z. X. Zhao, *From Brownian Motion to Schrödinger's Equation*, Grundlehren Math. Wiss. 312, Springer, Berlin, 1995.

[9] E. B. Davies, *Heat Kernels and Spectral Theory*, Cambridge Tracts in Math. 92, Cambridge Univ. Press, Cambridge, 1990.

[10] E. B. Davies and B. Simon, *Ultracontractivity and the heat kernel for Schrödinger operators and Dirichlet laplacians*, J. Funct. Anal. 59 (1984), 335–395.

[11] M. Demuth and J. A. van Casteren, *Stochastic Spectral Theory for Selfadjoint Feller Operators: A Functional Integration Approach*, Springer, 2000.

[12] *NIST Digital Library of Mathematical Functions.* http://dlmf.nist.gov/, Release 1.1.2 of 2021-06-15.

[13] T. Jakubowski and K. Szczypkowski, *Sharp and plain estimates for Schrödinger perturbation of Gaussian kernel*, J. Anal. Math. (online, 2023).

[14] K. Kaleta and T. Kulczycki, *Intrinsic ultracontractivity for Schrödinger operators based on fractional Laplacians*, Potential Anal. 33 (2010), 313–339.

[15] K. Kaleta and J. Lőrinczi, *Pointwise eigenfunction estimates and intrinsic ultracontractivity-type properties of Feynman–Kac semigroups for a class of Lévy processes*, Ann. Probab. 43 (2015), 1350–1398.

[16] K. Kaleta and R. L. Schilling, *Progressive intrinsic ultracontractivity and heat kernel estimates for non-local Schrödinger operators*, J. Funct. Anal. 279 (2020), art. 108606, 69 pp.

[17] T. Kulczycki and B. Siudeja, *Intrinsic ultracontractivity of the Feynman–Kac semigroup for relativistic stable processes*, Trans. Amer. Math. Soc. 358 (2006), 5025–5057.

[18] M. Kwaśnicki, *Intrinsic ultracontractivity for stable semigroups on unbounded open sets*, Potential Anal. 31 (2009), 57–77.

[19] J. Małecki and G. Serafin, *Dirichlet heat kernel for the Laplacian in a ball*, Potential Anal. 52 (2020), 545–563.

[20] G. Metafune, D. Pallara, and A. Rhandi, *Kernel estimates for Schrödinger operators*, J. Evol. Equations 6 (2006), 433–457.

[21] G. Metafune and C. Spina, *Kernel estimates for a class of Schrödinger semigroups*, J. Evol. Equations 7 (2007), 719–742.

[22] E. M. Ouhabaz and A. Rhandi, *Kernel and eigenfunction estimates for some second order elliptic operators*, J. Math. Anal. Appl. 387 (2012), 799–806.

[23] M. Reed and B. Simon, *Methods of Modern Mathematical Physics. IV. Analysis of Operators*, Academic Press, New York, 1978.

[24] R. L. Schilling and L. Partzsch, *Brownian Motion*, De Gruyter, Berlin, 2012.

[25] G. Serafin, *Laplace Dirichlet heat kernels in convex domains*, J. Differential Equations 314 (2021), 700–732.

[26] A. Sikora, *On-diagonal estimates on Schrödinger semigroup kernels and reduced heat kernels*, Comm. Math. Phys. 188 (1997), 233–249.

[27] B. Simon, *Schrödinger semigroups.* Bull. Amer. Math. Soc. 7 (1982), 447–526.

[28] B. Simon, *Pointwise bounds on eigenfunctions and wave packets in N-body quantum systems. III*, Trans. Amer. Math. Soc. 208 (1975), 317–329.

[29] B. Simon, *Functional Integration and Quantum Physics*, Pure Appl. Math. 86, Academic Press, New York, 1979.

[30] C. Spina, *Kernel estimates for a class of Kolmogorov semigroups*, Arch. Math. (Basel) 91 (2008), 265–279.

[31] J. G. Wendel, *Hitting spheres with Brownian motion*, Ann. Probab. 8 (1980), 164–169.

[32] Q. S. Zhang, *Large time behavior of Schrödinger heat kernels and applications*, Comm. Math. Phys. 210 (2000), 371–398.

[33] Q. S. Zhang, *The boundary behavior of heat kernels of Dirichlet laplacians*, J. Differential Equations 182 (2002), 416–430.

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