Abstract. With \((X,d,m)\) an RCD\((K,N)\) space for some \(K \in \mathbb{R}, N \in [1,\infty)\), let \(H\) be the self-adjoint Laplacian induced by the underlying Cheeger form. Given \(\alpha \in [0,1]\) we introduce the \(\alpha\)-Kato class of potentials on \((X,d,m)\), and given a potential \(V : X \to \mathbb{R}\) in this class, with \(H_V\) the natural self-adjoint realization of the Schrödinger operator \(H + V\) in \(L^2(X,m)\), we use Brownian coupling methods and perturbation theory to prove that for all \(t > 0\) there exists an explicitly given constant \(A(V,K,\alpha,t) < \infty\), such that for all \(\Psi \in L^\infty(X,m), x, y \in X\) one has
\[
\left|e^{-tH_V}\Psi(x) - e^{-tH_V}\Psi(y)\right| \leq A(V,K,\alpha,t)\|
\Psi\|_\infty d(x,y)^\alpha.
\]
In particular, all \(L^\infty\)-eigenfunctions of \(H_V\) are globally \(\alpha\)-Hölder continuous. This result applies to multi-particle Schrödinger semigroups and, by the explicitness of the Hölder constants, sheds some light into the geometry of such operators.

Dedicated to the memory of Kazumasa Kuwada.

1. Introduction
Among several other fundamental results, T. Kato has proved the following result in 1957 in his seminal paper on mathematical quantum mechanics [20]: consider the multi-particle Schrödinger operator \(H_V = -\Delta + V\) in \(L^2(\mathbb{R}^3^m)\) with a potential \(V : \mathbb{R}^{3m} \to \mathbb{R}\) of the form
\[
V(x) = \sum_{1 \leq j \leq m} V_j(x_j) + \sum_{1 \leq j < k \leq m} V_{jk}(x_j - x_k) \quad \text{with } V_j, V_{jk} \in L^q(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)
\]
for some \(q \geq 2\). Then all eigenfunctions (or more generally, elements of \(\cap_n \text{Dom}(H^n_V)\)) of \(H_V\) are globally \(\alpha\)-Hölder continuous for all \(0 < \alpha < 2 - 3/q\). In particular, applying this result with
\[
V_j(x) := -\sum_{i=1}^l Z_i/|x - R_i|, \quad V_{jk}(x) := 1/|x|
\]
one finds that the eigenfunctions of any molecular Schrödinger operator having \(m\) electrons, \(l\) nuclei and having its \(i\)-th nucleus sitting \(R_i\) with \(\sim Z_i\) protons is globally \(\alpha\)-Hölder continuous for all \(0 < \alpha < 1\). The fact that the above class of potentials depend on the linear surjective maps
\[
\pi_{ij} : \mathbb{R}^{3m} \to \mathbb{R}^3, \quad \pi_{ij}(x_1, \ldots, x_m) := x_i - x_j,
\]
and the fact that Kato’s proof heavily relies on the Fourier transform, raises the following natural question:

What is the geometry behind Kato’s global regularity result?

Rather than studying regularity properties of eigenfunctions, we take the approach of studying $L^\infty \to C^{0,\alpha}$ mapping properties of the underlying Schrödinger semigroup $e^{-tH_V}$, $t > 0$, following B. Simon’s seminal paper [31]. This procedure relies on the spectral theorem, showing that $H_V \Psi = \lambda \Psi$ implies $\Psi = e^{t\lambda}e^{-tH_V} \Psi$ for all $t \geq 0$.

The global mapping property $L^\infty \to C^{0,\alpha}$ of a Schrödinger semigroup $e^{-tH_V}$ is well-known to be delicate even for $V = 0$ in Riemannian geometry: indeed, the heat semigroup on an arbitrary noncompact Riemannian manifold $M$ need not be globally Lipschitz smoothing, while it is, if $M$ is complete with a Ricci curvature bounded from below.

Being motivated by this fact, we pick RCD($K$, $N$) spaces as our state spaces in this paper. These are metric measure spaces having a Ricci curvature bounded from below by the constant $K$ and having a dimension $\leq N$ in the sense of Sturm [36], Lott/Villani [24] (see also [40, 27, 10]), and which have the additional property that the underlying heat flow is linear. Originally, RCD($K$, $N$) spaces have been introduced for $N = \infty$ by Ambrosi/Gigli/Savaré [4], and they have been studied systematically for the special case $N < \infty$ by Erbar/Kuwada/Sturm [12] and more recently by Cavalletti/Milman [8]. An essential feature of these spaces is that they have a canonically given Laplacian whose heat semigroup is globally Lipschitz smoothing [4, 3]. We refer the reader to Remark 3.3 below and the references therein for examples and some of the essential stability properties of these spaces.

Given an RCD($K$, $N$) space $X \equiv (X, d, m)$ and $0 \leq \alpha \leq 1$ we introduce a new class $K^\alpha(X)$ of potentials $V : X \to \mathbb{R}$ which we call the $\alpha$-Kato class of $(X, d, m)$ (cf. Definition 3.7), and which refines the usual Kato class $K(X)$ in the sense that $K(X) = K^0(X)$. For any $V \in K^\alpha(X)$, $\alpha \in (0, 1]$ it turns out that one can naturally define a Schrödinger semigroup $e^{-tH_V}$ in $L^2(X)$. Our main result (cf. Theorem 3.9 below) states that this Schrödinger semigroup has the smoothing property

$$e^{-tH_V} : L^\infty(X) \to C^{0,\alpha}(X) \quad \text{for all } t > 0,$$

with Hölder constants depending explicitly on $K$, $\alpha$, $t$ and $V$.

Theorem 3.9 is fundamentally new even for the RCD($0$, $N$) space induced by the Euclidean $\mathbb{R}^N$, in the sense that it can deal with more general potentials than in Kato’s paper and that it provides explicit constants. To the best of our knowledge, Theorem 3.9 can only be compared with Theorem B.3.5 in [31], where B. Simon has proved a local $\alpha$-Hölder smoothing result for Schrödinger semigroups in $\mathbb{R}^N$ under an $\alpha$-dependent Kato type assumption on the potential.

As an application of our main result, we prove a Hölder smoothing result for multi-particle Schrödinger semigroups with $L^q$-potentials on Riemannian manifolds having a Ricci curvature bounded from below by a constant, where the above maps $\pi_{ij}$ are replaced by very general surjective Riemannian submersions. This yields a natural generalization of Kato’s
result to the Riemannian setting (cf. Corollary 3.10) and ultimately explains the geometry behind Kato’s Euclidean result.

Finally, we apply our results to produce explicit $L^r(\mathbb{R}^{3m}) \to C^{0,\alpha}(\mathbb{R}^{3m})$ bounds for the Schrödinger semigroup $e^{-tH_{R,Z}}$ corresponding to a molecule (here, as above, $R$ is the location vector of the nuclei and $Z$ the corresponding charge vector), where $r \in [1, \infty]$, $\alpha \in (0, 1)$. Our methods produce explicit Hölder constants that have an $\alpha$-dependence of the form

$$C_{m,Z} \left( t^{-\alpha - \frac{3m}{2\nu}} e^{C_{R,Z}t} + \frac{t^{-\alpha + \frac{3m}{2\nu}} e^{C_{R,Z}t}}{1/2 - \alpha/2} \right),$$

where $C_{m,Z}, C_{R,Z} > 0$, which shows that one cannot take $\alpha \not\in [0, 1]$ in order to obtain $L^r(\mathbb{R}^{3m}) \to C^{0,1}(\mathbb{R}^{3m})$ (=Lipschitz) estimates. This fact is consistent with Kato’s result and the fact that in this case $V_{R,Z} \in \bigcap_{\alpha \in (0,1)} \mathcal{K}^\alpha(\mathbb{R}^{3m}) \setminus \mathcal{K}^1(\mathbb{R}^{3m})$.

On the other hand, Kato proves ‘by hand’ that molecular Schrödinger semigroups map $L^r(\mathbb{R}^{3m}) \to C^{0,1}(\mathbb{R}^{3m})$, a fact which becomes rather mysterious from the point of view of our probabilistic methods and which raises the following open question:

**Is there a ‘probabilistic’ proof of the smoothing property $e^{-tH_{R,Z}} : L^r(\mathbb{R}^{3m}) \to C^{0,1}(\mathbb{R}^{3m})$ with $V_{R,Z}$ the potential of a molecule as above?**

We close the introduction with some remarks concerning our proof of Theorem 3.9, which comes in two steps: without making use of Fukushima’s [14] or Ma/Röckner’s [25] abstract theory for (quasi-) regular Dirichlet forms we first show that for all initial points $x \in X$ there is a natural Wiener measure or Brownian motion measure $\mathbb{P}^x$ on the space of continuous paths $[0, \infty) \to X$, which allows us to obtain maximal Brownian couplings for all pairs of initial points $x, y$ [3]. In particular, the coupling time of such a coupling can be estimated by $\mathfrak{d}(x, y)$ times the constant from the afore mentioned $L^\infty(X) \to C^{0,1}(X)$ smoothing property of the heat semigroup on $X$, and this fact allows us to deduce that the heat semigroup on $X$ is $L^\infty(X) \to C^{0,\alpha}(X)$ smoothing for all $0 < \alpha \leq 1$. Being equipped with this self-improvement property, we use perturbation theory to show that

$$e^{-tH_{V}} : L^\infty(X) \to C^{0,\alpha}(X) \quad \text{for } V’s \text{ in } \mathcal{K}^\alpha(X)$$

to complete the proof.

**Acknowledgements:** The author would like to thank L. Ambrosio, Z.-Q. Chen, K. Kuwae and N. Savaré for very helpful discussions.

2. **Couplings of diffusions**

In the sequel, given probability measures $\mu_1$ and $\mu_2$ on a measurable space $(\Omega, \mathcal{F})$, we denote with $\mathcal{C}(\mu_1, \mu_2)$ the set of all couplings of $\mu_1$ and $\mu_2$, that is, the set of all probability

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1 which yield the existence of the Wiener measure for quasi-almost every initial point
2 We refer the reader to Section 2 below for the basics of couplings of diffusions.
measures on \((\Omega \times \Omega, \mathcal{F} \otimes \mathcal{F})\) such that \((\pi_j)_*\mu = \mu_j\) for \(j = 1, 2\), where \(\pi_j : \Omega \times \Omega \to \Omega\) denotes the projection onto the \(j\)-th slot. Furthermore, we denote with
\[
\delta(\mu_1, \mu_2) := \sup_{B \in \mathcal{F}} |\mu_1(B) - \mu_2(B)|
\]
the total variation distance.

Let \(X \equiv (X, \mathcal{A})\) be a complete separable locally compact metric space. The space \(C([0, \infty), X)\) of continuous paths \(\omega : [0, \infty) \to X\) is always equipped with its topology of locally uniform convergence. By a diffusion on \(X\) we will simply understand a family of Borel probability measures \(\mathcal{P} = (\mathcal{P}^x)_{x \in X}\) on \(C([0, \infty), X)\) such that

- \(\mathcal{P}^x\{\omega : \omega(0) = z\} = 1\) for all \(z \in X\),
- the map \(z \mapsto \mathcal{P}^x(A)\) is Borel measurable, for all Borel sets \(A \subset C([0, \infty), X)\),
- \(\mathcal{P}\) has the strong Markov property with respect to the natural filtration of \(C([0, \infty), X)\).

In the above situation, given \(x, y \in X\), a continuous \(X \times X\)-valued process
\[
(X, Y) : (\Omega, \mathcal{F}, P) \to C([0, \infty), X \times X)
\]
is called a coupling from \(x\) to \(y\) of \(\mathcal{P}\), if \((X, Y)_*P \in \mathcal{G}(\mathcal{P}^x, \mathcal{P}^y)\), and then the coupling is called successful, if with the coupling time
\[
\tau(X, Y) := \inf\{s > 0 : X_s = Y_s', \text{ for all } s' \geq s\} : \Omega \to [0, \infty],
\]
one has \(P\{\tau(X, Y) = \infty\} = 0\), and maximal, if one has
\[
P\{\tau(X, Y) > t\} = \frac{1}{2}\delta((X_t)_*P, (Y_t)_*P) \text{ for all } t > 0.
\]

An abstract result by Sverchkov/Smirnov [38] for couplings of c.d.l.g Markov processes states that for all \(x, y \in X\) there exists a maximal coupling of \(\mathcal{P}\) from \(x\) to \(y\). The following result, which should be well-known to the experts (cf. [18] for a special case of part a)), will allow us to switch from global Lipschitz-smoothing to global Hölder-smoothing results later on, a rather subtle business on noncompact spaces:

**Proposition 2.1.** a) Assume
\[
(X, Y) : (\Omega, \mathcal{F}, P) \to C([0, \infty), X \times X)
\]
is a coupling of \(\mathcal{P}\) from \(x \in X\) to \(y \in X\). Then for all \(t > 0\) one has
\[
P\{\tau(X, Y) > t\} \geq \frac{1}{2}\delta((X_t)_*P, (Y_t)_*P).
\]

b) For every function \(F : (0, \infty) \to (0, \infty)\) the following statements are equivalent:

i) For all \(x, y \in X\) there exists a coupling
\[
(X, Y) : (\Omega, \mathcal{F}, P) \to C([0, \infty), X \times X)
\]
of \(\mathcal{P}\) from \(x\) to \(y\) with
\[
P\{\tau(X, Y) > t\} \leq \frac{1}{2}F(t)\vartheta(x, y) \text{ for all } t > 0.
\]
Proof. a) Let \( B \subset X \) be an arbitrary Borel set. Assuming w.l.o.g. that \( P\{X_t \in B\} \geq P\{Y_t \in B\} \), we have

\[
P\{\tau(X, Y) > t\} \geq P\{X_t \neq Y_t\} \geq P\{X_t \in B, Y_t \neq B\} \geq |P\{X_t \in B\} - P\{Y_t \in B\}|.
\]

b) ii) \( \Rightarrow \) i): Given \( x, y \in X \) we pick a maximal coupling (3) of \( \mathcal{P} \) from \( x \) to \( y \). Then we have

\[
P\{\tau(X, Y) > t\} = \frac{1}{2} \sup_{B \subset X, B \text{ Borel}} \left| \int 1_B(\omega(t)) \mathcal{P}^x(d\omega) - \int 1_B(\omega(t)) \mathcal{P}^y(d\omega) \right| \leq \frac{1}{2} F(t) \mathfrak{d}(x, y).
\]

i) \( \Rightarrow \) ii): One can estimate as follows:

\[
\left| \int f(\omega(t)) \mathcal{P}^x(d\omega) - \int f(\omega(t)) \mathcal{P}^y(d\omega) \right|
\]

\[
= \left| \int (f(X_t) - f(Y_t)) dP \right|
\]

\[
= \left| \int_{\{\tau(X, Y) > t\}} (f(X_t) - f(Y_t)) dP \right|
\]

\[
\leq P\{\tau(X, Y) > t\} 2 \|f\|_\infty
\]

\[
\leq F(t) \mathfrak{d}(x, y) \|f\|_\infty.
\]

iii) \( \Rightarrow \) ii): Trivial.

ii) \( \Rightarrow \) iii): this follows from (3), \( P(\cdot) \leq 1 \) and ii) \( \Rightarrow \) i),

\[
\left| \int f(\omega(t)) \mathcal{P}^x(d\omega) - \int f(\omega(t)) \mathcal{P}^y(d\omega) \right|
\]

\[
\leq P\{\tau(X, Y) > t\} \alpha 2 \|f\|_\infty
\]

\[
\leq F(t)^\alpha 2^{1/\alpha} \mathfrak{d}(x, y)^\alpha \|f\|_\infty,
\]

completing the proof.

\[\Box\]

3. Schrödinger semigroups on RCD(K, N) spaces

Assume now \( X \equiv (X, \mathfrak{d}, m) \) is a metric measure measure, that is, \( (X, \mathfrak{d}) \) is a complete separable metric space, \( m \) is a \( \sigma \)-finite Borel measure which is finite on all open balls \( B(x, r) \). In particular, \( m \) has a full support. In the sequel, as we have applications in quantum mechanics in mind, we understand the spaces \( L^q(X) = L^q(X, m) \) to be over \( \mathbb{C} \), and we consider sesquilinear maps to be antilinear in the first slot. The \( L^q(X) \)-norms will
simply be denoted with \( \| \cdot \|_{L^2} \).

The Cheeger form

\[
\text{Ch} : L^2(X) \longrightarrow [0, \infty]
\]
on \( X \) is defined to be the \( L^2 \)-lower semicontinuous relaxation of the functional

\[
\tilde{\text{Ch}} : L^2(X) \cap \text{Lip}(X) \longrightarrow [0, \infty], \quad \tilde{\text{Ch}}(f) := \int_X \left( \limsup_{y \to x} \frac{|f(x) - f(y)|}{\mathfrak{d}(x, y)} \right)^2 m(dx),
\]

where \( \limsup_{y \to x} |f(x) - f(y)|/\mathfrak{d}(x, y)^{-1} \) is set 0 if \( x \) is isolated. In other words, for all \( f \in L^2(X) \) one sets

\[
\text{Ch}(f) := \liminf_{n \to \infty} \left\{ \tilde{\text{Ch}}(f_n) : (f_n)_{n \in \mathbb{N}} \subset L^2(X) \cap \text{Lip}(X), \|f_n - f\|_{L^2} \text{ as } n \to \infty \right\}
\]

One gets a functional \( \mathcal{E} \) on \( L^2(X) \) with domain of definition

\[
\text{Dom}(\mathcal{E}) := \{ f : \text{Ch}(f) < \infty \}
\]

by setting

\[
\mathcal{E}(f) := \text{Ch}(f) \quad \text{for all } f \in \text{Dom}(\mathcal{E}).
\]

**Definition 3.1.** The metric measure space \( X \) is called **infinitesimally Hilbertian**, if \( \mathcal{E} \) is a quadratic form.

Then, as shown by Savaré [30], \( \mathcal{E} \) is a strongly local quasi-regular Dirichlet form in the sense of Ma/Röckner [25]. With \( H \) the nonnegative self-adjoint operator in \( L^2(X) \) corresponding to \( \mathcal{E} \), the Laplacian on \( X \), the heat semigroup

\[
(e^{-tH})_{t \geq 0} \subset \mathcal{L}(L^2(X))
\]
on \( X \) is defined via functional calculus. Moreover, \( \mathcal{E} \) admits a carré du champ operator, that is, there exists a uniquely determined symmetric and positive sesquilinear map

\[
\Gamma(\cdot, \cdot) : \text{Dom}(\mathcal{E}) \times \text{Dom}(\mathcal{E}) \longrightarrow L^1(X),
\]
such that for all \( f_1, f_2, f_3 \in \text{Dom}(\mathcal{E}) \cap L^\infty(X) \) one has

\[
\mathcal{E}(f_1 f_3, f_2) + \mathcal{E}(f_2 f_3, f_1) - \mathcal{E}(f_3, f_1 f_2) = \int_X f_3 \Gamma(f_1, f_2) dm.
\]

One sets \( \Gamma(f) := \Gamma(f, f) \in L^1_{\geq 0}(X) \).

**Definition 3.2.** Given \( K \in \mathbb{R}, \ N \in [1, \infty] \), the metric measure space \( X \) is called an \( \text{RCD}(K, N) \) space, if

- \( X \) is infinitesimally Hilbertian,
- there exist \( x_0 \in X, \ a, b > 0 \), such that for all \( r > 0 \) one has \( m(B(x_0, r)) \leq ae^{br^2} \),
- all real-valued \( f \in \text{Dom}(\mathcal{E}) \) with \( |\Gamma(f)| \leq 1 \) a.e. admit a Lipschitz-continuous representative,
- one has the following abstract Bochner inequality: for all real-valued \( f_1 \in \text{Dom}(H) \) with \( Hf_1 \in \text{Dom}(\mathcal{E}) \), and all \( f_2 \in \text{Dom}(H) \cap L^\infty(X) \) with \( Hf_2 \in L^\infty(X) \) one has

\[
\int_X \Gamma(f_1, Hf_1) f_1 dm - \frac{1}{2} \int_X \Gamma(f_1) Hf_2 dm \geq K \int_X \Gamma(f_1) f_2 dm + \frac{1}{N} \int_X (Hf_1)^2 f_2 dm.
\]
Remark 3.3. 1. Several equivalent characterizations of the RCD($K, N$) property have been obtained by Erbar/Kuwada/Sturm [12] and by Cavalletti/Milman [8]. In particular, it is shown in [8] that the RCD$^*$($K, N$) condition (which is defined for $N < \infty$ and based on the CD$^*$($K, N$) condition defined in [6]), is equivalent to the RCD($K, N$) condition. Moreover, RCD($K, N$) spaces are stable under tensorization and satisfy natural stability and local-to-global results [12, 3].

2. On a smooth geodesically complete Riemannian manifold $M$ equipped with its geodesic distance and its Riemannian volume measure one has $\text{Dom}(\mathcal{E}) = W^{1,2}(M)$ and
\[
\mathcal{E}(f_1, f_2) = \int_M (\nabla f_1, \nabla f_2) dm.
\]
Moreover, $M$ is RCD($K, N$), if and only if $\text{Ric} \geq K$ and $\text{dim}(M) \leq N$ [33]. In particular, in this case one has $H = -\Delta$, the (unique self-adjoint realization of the) Laplace-Beltrami operator.

3. A new interesting class of possibly very singular RCD($K, N$) spaces has been established by Bertrand/Ketterer/Mondello/Richard in [7]: there the authors show that every compact smoothly stratified space $X$ with an iterated edge metric on its regular part (which is a smooth open Riemannian manifold) canonically induces an infinitesimally Hilbertian metric measure space, which is RCD($K, N$) if and only if $\text{dim}(X) \leq N$ and $X$ has a singular Ricci curvature bounded from below by $K$ in the sense of [7].

We assume from here on that $X$ is an RCD($K, N$) space for some $K \in \mathbb{R}$ and some $N \in [1, \infty)$.

As pointed out by Kuwada/Kuwae [21], then $X$ is locally compact (see also the proof of Lemma 3.4 below) and in fact $\mathcal{E}$ becomes a regular strongly local Dirichlet form in $L^2(X)$. Moreover, one has the mapping property
\[
e^{-tH} : L^2(X) \rightarrow C(X) \quad \text{for all } t > 0,
\]
and there exists a uniquely determined continuous map
\[
(0, \infty) \times X \times X \ni (t, x, y) \mapsto p(t, x, y) \in [0, \infty),
\]
the heat kernel of $H$, with the following property: for all $f \in L^2(X)$, $t > 0$, $x \in X$, one has
\[
e^{-tH} f(x) = \int_X p(t, x, y) f(y) m(dy).
\]
In addition, the heat kernel has the following properties $s, t > 0, x, y \in X$:
- symmetry: $p(t, y, x) = p(t, x, y),$
- Chapman-Kolmogorov: $p(t+s, x, y) = \int_X p(t, x, y) p(s, y, z) m(dz),$
- conservativeness: $\int_X p(t, x, z) m(dz) = 1.$

The asserted regularity facts on the heat kernel follow from abstract results on Dirichlet spaces obtained by Sturm in [33, 34], in combination with the validity of appropriate local Poincaré inequalities finite dimensional RCD spaces. The latter have been established by
Lemma 3.4. There exists a unique diffusion $\mathfrak{P}$ on $X$ such that for all $x_0 \in X$, $n \in \mathbb{N}$, $0 < t_1 < \cdots < t_n$, and all Borel sets $A_1, \ldots, A_n \subset M$ one has

$$\mathfrak{P}^{x_0}\{\omega : \omega(t_1) \in A_1, \ldots, \omega(t_n) \in A_n\}$$

(6)

$$= \int \cdots \int 1_{A_1}(x_1)p(\delta_0, x_0, x_1) \cdots 1_{A_n}(x_n)p(\delta_{n-1}, x_{n-1}, x_n)m(dx_1) \cdots m(dx_n),$$

where $\delta_j := t_{j+1} - t_j$, $t_0 := 0$. Moreover, for every $x \in X$, $\alpha < 1/2$, the measure $\mathfrak{P}^x$ is concentrated on locally $\alpha$-Hölder continuous paths and is called Brownian motion measure or Wiener measure with initial point $x$.

Remark 3.5. As $\mathcal{E}$ is a regular local Dirichlet form, it follows immediately from Fukushima’s theory [14] that we can pick a diffusion $\mathfrak{P}$ on $X$ which satisfies (6) for $\mathcal{E}$-quasi every $x_0 \in X$. However, from the author’s point of view, this approach would make the formulation of Proposition 3.1 b) and of our main result Theorem 3.9 below somewhat artificial. Such a ‘quasi-sure’ formulation could even be carried out for $\text{RCD}(K, \infty)$ spaces using the Ma-Röckner correspondence [25] between local quasi-regular Dirichlet forms and diffusions, as the main ingredient of our machinery (which is Corollary 3.6 below) is an $L^\infty$-to-Lipschitz smoothing result for the heat semigroup by Ambrosio/Gigli/Savaré [3], which is valid in the infinite dimensional case $N = \infty$, too (and also for the fractional metric measure spaces considered in [2]). Instead we establish the correspondence of $\mathcal{E}$ with a pointwise uniquely determined diffusion by hand, using classical methods from Markov processes in combination with a Li-Yau heat kernel estimate for $\text{RCD}(K, N)$ spaces, which has been obtained by Jiang/Zhang [19], and which to the best of the author’s knowledge really needs $N < \infty$.

Proof of Lemma 3.4. The existence of a unique probability measure $\mathfrak{P}^{x_0}$ on $C([0, \infty), X)$ satisfying (6) and giving full measure on $\alpha$-Hölder continuous paths follows from Kolmogorov’s theorems on consistency and the existence of a (Hölder)-continuous modification, if we can show that for all $T > 0$ there exists $C_T > 0$, such that for all $0 < s < t \leq T$ one has

$$\int_X p(t_1, z, x_1, x_0) \int_X \mathcal{D}(x_1, x_2)^2 p(t_2 - t_1, x_1, x_2)m(dx_2)m(dx_1) \leq C_T(t_2 - t_1)^2. \quad (7)$$

In order to show (7), we are going to prove that there exists $C_T > 0$ such that for all $x \in X$, $0 < t \leq T$ one has

$$\int_X \mathcal{D}(x, y)^2 p(t, x, y)m(dy) \leq C_T t^2.$$

The Li-Yau upper heat kernel estimate [19] implies the existence of $C'_T > 0$ (which only depends on $T$, $N$ and $K$) and $C > 0$ (which only depends on $N$ and $K$) such that for all $x, y \in X$, $0 < t < T$ one has

$$p(t, x, y) \leq C'_T m(x, \sqrt{t})^{-1}e^{-\frac{N(x,y)^2}{C't}}, \quad \text{with } m(x, \sqrt{t}) := m(B(x, \sqrt{t})).$$
Moreover, one has the following local volume doubling property: there exists a constant $C''_T > 0$ (which only depends on $T$, $K$, $N$) such that for all $0 < t < T$, $x \in X$, one has $m(x, 2t) \leq C''_T m(x, t)$. As pointed out in [21], local volume doubling follows from the Bishop-Gromov volume inequality, which also implies that $X$ is locally compact, and which holds under the measure contraction property assumption [36], which is satisfied RCD spaces [12, 9]. By a standard argument (cf. Lemma 5.27 in [29]), local volume doubling implies the existence of constants $\nu_T \geq 1$, $C'''_T, C''''_T > 0$ (which only depend on $C''_T$), such that for all $s, t > 0$, $x \in X$ one has

$$\frac{m(x, t)}{m(x, s)} \leq C''''_T \left( \frac{t}{s} \right)^{\nu_T} e^{C'''_T \frac{t}{s}}, \quad (8)$$

Now fix arbitrary $0 < t \leq T$, $x \in X$. Then Li-Yau implies

$$\int_X \mathfrak{d}(x, y)^2 p(t, x, y) m(dy) \leq C'_T m(x, \sqrt{t})^{-1} \int_{B(x,t)} \mathfrak{d}(x, y)^2 e^{-\frac{\mathfrak{d}(x, y)^2}{ct}} m(dy)$$

$$+ C'_T m(x, \sqrt{t})^{-1} \int_{X \setminus B(x,t)} \mathfrak{d}(x, y)^2 e^{-\frac{\mathfrak{d}(x, y)^2}{ct}} m(dy).$$

Using (8) we find

$$m(x, \sqrt{t})^{-1} \int_{B(x,t)} \mathfrak{d}(x, y)^2 e^{-\frac{\mathfrak{d}(x, y)^2}{ct}} m(dy) \leq t^2 \frac{m(x, t)}{m(x, \sqrt{t})} \leq C''''_T t^{2\nu_T/2} e^{C'''_T \frac{t}{s}},$$

which has the desired form.

For the second integral we have

$$m(x, \sqrt{t})^{-1} \int_{X \setminus B(x,t)} \mathfrak{d}(x, y)^2 e^{-\frac{\mathfrak{d}(x, y)^2}{ct}} m(dy)$$

$$\leq m(x, \sqrt{t})^{-1} \int_{\{y \in X : kt \leq \mathfrak{d}(x, y) \leq (k+1)t\}} \mathfrak{d}(x, y)^2 e^{-\frac{\mathfrak{d}(x, y)^2}{ct}} m(dy)$$

$$\leq t^2 \sum_{k=1}^{\infty} \frac{m(x, (k+1)t)}{m(x, \sqrt{t})} (k+1)^2 e^{-\frac{C''''_T}{2}} \leq C''''_T t^{2(\nu_T + 1)} \sum_{k=1}^{\infty} (k+1)^2 e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} (k+1)}$$

$$\leq C''''_T \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr$$

$$= C''''_T \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr$$

$$= C''''_T \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr$$

$$= C''''_T \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr$$

$$= C''''_T \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr$$

$$= C''''_T \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr$$

$$= C''''_T \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr \int_{\mathbb{R}} e^{-\nu_T \frac{C''''_T}{2} + \frac{C''''_T}{2} r} dr$$

which in view of $\nu_T \geq 1$ again has the desired form. Above we have used (8) and the trivial inequality $(1 + a)^\nu \leq e^{\nu a}, a \in \mathbb{R}, \nu > 0$.

Having established the existence of a unique family of probability measures $\mathfrak{P} = (\mathfrak{P}^z)_{z \in X}$ on $C([0, \infty), X)$ satisfying (8) for all $x_0 \in X$, note that by a montone class argument one
has
\[
\int f(\omega(t))\mathcal{P}^x(d\omega) = \int_X p(t, x, y)f(y)m(dy) \quad \text{for all bounded } f : X \to \mathbb{R}, \ t > 0, \ x \in X.
\]

Then
\[
\lim_{t \to 0^+} \int f(\omega(t))\mathcal{P}^x(d\omega) = f(x) \quad \text{for all bounded continuous } f : X \to \mathbb{R}
\]
follows from Proposition 3.2 in [3], showing that that \(\mathcal{P}^x\) is concentrated on paths starting from \(x\), and the Chapman-Kolmogorov equation immediately imply that \(\mathcal{P}\) has the Markov property. The strong Markov property then follows from the continuity of \(x \mapsto \int f(\omega(t))\mathcal{P}^x(d\omega)\) for all \(t \geq 0\) and all bounded continuous \(f : X \to \mathbb{R}\), which is a consequence of (9) and Proposition 3.2 in [3].

Note that by construction we have absolute continuity property
\[
m(A) = 0 \Rightarrow \int_0^t P^x(\omega : \omega(s) \in A)ds = 0 \quad \text{for all Borel } A \subset X, \ t \geq 0.
\]

For obvious reasons, any coupling of \(\mathcal{P}\) is called a coupling of Brownian motions on \(X\).

**Proposition 3.6.** For all \(x, y \in X\) there exists a coupling
\[
(\Xi, \Upsilon) : (\Omega, \mathcal{F}, P) \to C([0, \infty), X \times X)
\]
of Brownian motions \((X, \mathfrak{d}, m)\) from \(x\) to \(y\) with
\[
P(\tau(\Xi, \Upsilon) > t) \leq F_K(t)\mathfrak{d}(x, y) \quad \text{for all } t > 0,
\]
where
\[
F_K(t) := \begin{cases} \sqrt{\frac{2}{t}}, & \text{if } K = 0 \\ \frac{2\sqrt{k}}{e^{2t} - 1}, & \text{if } K \neq 0 \end{cases}
\]
in particular, every such coupling is successful if \(K \leq 0\), and one has the following global Hölder estimate: for all \(\alpha \in [0, 1)\), all real-valued \(f \in L^\infty(X, m)\), \(t > 0\),
\[
|e^{-tH}f(x) - e^{-tH}f(y)| \leq 2^{1-\alpha} F_K(t)\mathfrak{d}(x, y)^\alpha \|f\|_{L^\infty}.
\]

**Proof.** In view of Proposition 2.1 and (9), the claim follows immediately from the following Lipschitz smoothing result (cf. Theorem 3.17 in combination with Theorem 4.17 in [3]): one has
\[
|e^{-tH}f(x) - e^{-tH}f(y)| \leq F_K(t)\mathfrak{d}(x, y) \|f\|_{L^\infty}.
\]

The following class of potentials will be the perturbations of \(H\) that will be considered in the sequel:
Definition 3.7. Given \( \alpha \in [0, 1] \), a Borel function \( V : X \to \mathbb{R} \) is said to be in the \( \alpha \)-Kato class \( \mathcal{K}^\alpha(X) \) of \( X \), if

\[
\lim_{t \to 0^+} \sup_{x \in X} \int_0^t s^{-\alpha/2} \int_X p(s, x, y)|V(y)|m(dy)ds = 0.
\]

Note that the Kato property only depends on the \( m \)-equivalence induced by \( V \), and that

\[
\int_0^t s^{-\alpha/2} \int_X p(s, x, y)|V(y)|m(dy)ds = \int_0^t s^{-\alpha/2} \int |V(\omega(s))| \mathfrak{P}^\alpha(d\omega)ds.
\]

Each \( \mathcal{K}^\alpha(X) \) is a linear space and \( \mathcal{K}(X) := \mathcal{K}^0(X) \) is the usual Kato class. One has

\[
\mathcal{K}^\alpha(X) \subset \mathcal{K}^\beta(X), \quad \text{if } \alpha \geq \beta,
\]

\[
L^\infty(X) \subset \mathcal{K}^\alpha(X).
\]

The following lemma allows to test the Kato assumption in typical applications:

Lemma 3.8. a) Let \( \alpha \in [0, 1] \) and \( q \in [1, \infty) \) with \( q > N/(2 - \alpha) \) one has

\[
L^q_{1/m}(X) + L^\infty(X) \subset \mathcal{K}^\alpha(X),
\]

where

\[
L^q_{1/m}(X) := \left\{ W : \int_X \frac{|W(x)|^q}{m(B(x, 1))} m(dx) < \infty \right\}.
\]

b) Assume \( M, \widetilde{M} \) are geodesically complete smooth Riemannian manifolds with Ricci curvature \( \geq K \) and let \( \pi : \widetilde{M} \to M \) be a smooth surjective Riemannian submersion such that fibers \( \pi^{-1}(y) \subset \widetilde{M} \) are minimal submanifolds for all \( y \in M \). Then for all Borel functions \( \phi : C([0, \infty), M) \to [0, \infty], x \in \widetilde{M} \), using an obvious notation, one has

\[
\int \phi(\pi(\omega)) \mathfrak{P}^\alpha(d\omega) \leq \int \phi(\omega) \mathfrak{P}^\pi(\omega).
\]

In particular, for all \( \alpha \in [0, 1] \) one has \( \pi^* \mathcal{K}^\alpha(\widetilde{M}) \subset \mathcal{K}^\alpha(M) \).

Proof. a) It suffices to show that \( V \in \mathcal{K}^\alpha(X) \) for all \( V \in L^q_{1/m}(X) \). This can be seen follows: for all \( 0 < s < 1, x \in M \) one has,

\[
\int_X p(s, x, y)|V(y)|m(dy) = \int_X p(s, x, y)^{1 - \frac{1}{q}} p(s, x, y)^{\frac{1}{q}} |V(y)|\mu(dy)
\]

\[
\leq \left( \int_X p(s, x, y)\mu(dy) \right)^{\frac{1}{q}} \left( \int_X |V(y)|^q p(s, x, y)\mu(dy) \right)^{\frac{1}{q}}
\]

\[
\leq C(K, N, q) \left( 1 + s^{-\frac{N}{2q}} \right) \left( \int_X |V(y)|^q m(B(x, 1))^{-1} m(dy) \right)^{\frac{1}{q}},
\]

where the second estimate follows from

\[
\int_X p(s, x, y)\mu(dy) \leq 1.
\]
and the Li-Yau heat kernel bound in combination with Bishop-Gromov’s volume estimate (cf. Example IV.18 in [16] for a detailed argument).

b) The asserted estimate has been shown in [17], and the asserted inclusion is a trivial consequence of the estimate.

Note that $L^q_1(X) \subseteq L^q(X)$ by the Bishop-Gromov inequality, while the other inclusion typically requires $\inf_{x \in X} m(B(x, 1)) > 0$. It is certainly an interesting problem to check how possible further properties of the Kato classes (for example, uniformly local $L^q$-conditions for the Kato classes, or Green’s function characterizations of these spaces) depend on the geometry of $X$. Here, the methods developed by Kuwae and Takahashi in [23] should be applicable in principle (see also [11, 16]).

The Kato condition is linked to operator theory through the following fact: for all $\epsilon > 0$ there exists $C_\epsilon < \infty$, which depends on $\epsilon$ (and $V$), such that [16, 37]

$$
\int_X V(x)|f(x)|^2 m(dx) \leq C_\epsilon \mathcal{E}(f) + \epsilon \|f\|^2_{L^2} \quad \text{for all } f \in \text{Dom}(\mathcal{E}).
$$

In the language of perturbation theory this estimate means that the symmetric sesquilinear form in $L^2(X)$ induced by $V$ is infinitesimally $\mathcal{E}$-bounded, and so the KLMN-theorem [39] implies that the symmetric sesquilinear form

$$
\text{Dom}(\mathcal{E}) \times \text{Dom}(\mathcal{E}) \ni (f_1, f_2) \longmapsto \mathcal{E}(f_1, f_2) := \mathcal{E}(f, g) + \int_X \overline{V(x)} f_1(x) f_2(x) m(dx) \in \mathbb{C}
$$

is semibounded from below and closed (it is densely defined as $\mathcal{E}$ is so). Thus $\mathcal{E}_V$ canonically induces a self-adjoint semibounded from below operator $H_V$ in $L^2(X)$.

Let

$$(e^{-tH_V})_{t \geq 0} \subseteq \mathcal{L}(L^2(X))$$

denote the Schrödinger semigroup induced by $V$. For all $V \in \mathcal{K}(X)$ one has the Feynman-Kac formula, which states that for all $\Psi \in L^2(X)$, $t > 0$ and $m$-a.e. $x \in X$ one has

$$
e^{-tH_V} \Psi(x) = \int e^{-\int_0^t V(\omega(s))ds} \Psi(\omega(t)) \mathcal{P}_x^t (d\omega).$$

The latter formula can be proved precisely as in the Riemannian case [16]. If $\Psi \in L^q(X)$, $q \in [1, \infty]$, then we take the RHS of the Feynman-Kac formula as a pointwise well-defined representative of $e^{-tH_V} \Psi(x)$, which as a function of $x$ defined an element on $L^q(X)$.

Here comes our main result:

**Theorem 3.9.** Let $\alpha \in (0, 1]$, $V \in \mathcal{K}^\alpha(X)$, $t > 0$.

a) For all $x, y \in X$, $\Phi \in L^\infty(X)$ one has

$$
|e^{-tH_V} \Phi(x) - e^{-tH_V} \Phi(y)| \leq \left(2^{1-\alpha} F_K(t)^\alpha + A(V, K, \alpha, t) \right) \|\Phi\|_{L^\infty} d(x, y)^\alpha,
$$

where

$$
A(V, K, \alpha, t) := 2^{2-\alpha} \sup_{x \in X} \int e^{-\int_0^t V(\omega(s))ds} \mathcal{P}_x^t (d\omega) \cdot \int_0^t F_K(s)^\alpha \int_X p(s, x, y)|V(y)| m(dy) ds < \infty.
$$
b) For all \( x, y \in X, \lambda \in \mathbb{R} \) and all \( \Psi \in \text{Dom}(H_V) \cap L^\infty(X) \) with \( H_V \Psi = \lambda \Psi \) one has
\[
|\Psi(x) - \Psi(y)| \leq e^{\lambda t} \left( 2^{1-\alpha} F_K(t)^\alpha + 2^{2-\alpha} C(V, K, \alpha, t/2) C_{\text{exp}}(V,t) \right) \|\Psi\|_{L^\infty} \|q(x,y)^\alpha.}
\]

Proof. a) Given \( r > 0 \) set
\[
C_{\text{exp}}(V, r) := \sup_{x \in X} \int e^{-\int_0^r V(\omega(s))ds} \mathfrak{P}^x (d\omega),
\]
\[
C(V, K, \alpha, r) := \sup_{x \in X} \int_0^r F_K(s)^\alpha \int_X p(s, x, y)|V(y)|m(dy)ds,
\]
so that
\[
A(V, K, \alpha, r) = 2^{2-\alpha} C(V, K, \alpha, r/2) C_{\text{exp}}(V, r).
\]
We have
\[
C_{\text{exp}}(V, r) \leq 2e^{C_V r} < \infty
\]
by the so called Khashminkii’s lemma, which can be proved precisely as in the Riemannian case \[1, 10\]. In order to show \( C(V, K, \alpha, r) < \infty \), as \( F_K \) is bounded on each compact subset of \([0, \infty)\) and as \( F_K^\alpha \) behaves like \( s^{-\alpha/2} \) near \( s = 0 \), it suffices to show
\[
\sup_{x \in X} \int_0^t s^{-\alpha/2} \int_X p(s, x, y)|V(y)|m(dy)ds < \infty.
\]
We can follow the argument from \[22\]: pick a \( t' > 0 \) with
\[
\sup_{x \in X} \int_0^{t'} s^{-\alpha/2} \int_X p(s, x, y)|V(y)|m(dy)ds < \infty
\]
and an \( l \in \mathbb{N} \) with \( t < lt' \). Then we can estimate
\[
\sup_{x \in X} \int_0^{t'} s^{-\alpha/2} \int_X p(s, x, y)|V(y)|m(dy) ds \leq \sup_{x \in X} \int_0^{lt'} s^{-\alpha/2} p(s, x, y)|V(y)|m(dy) ds
\]
\[
= \sup_{x \in X} \int_0^{lt'} \sum_{k=1}^{l} \int_0^{(k-1)t'+s} ((k-1)t'+s)^{-\alpha/2} p((k-1)t'+s, x, y)|V(y)|ds m(dy)
\]
\[
\leq \sum_{k=1}^{l} \sup_{x \in X} \int_0^{lt'} s^{-\alpha/2} p((k-1)t'+s, x, y)|V(y)|ds m(dy)
\]
\[
= \sum_{k=1}^{l} \sup_{x \in X} \int_X p((k-1)t', x, z) \int_0^{t'} s^{-\alpha/2} \int_X p(s, z, y)|V(y)|m(dy) ds m(dz)
\]
\[
\leq \sup_{x \in X} \int_0^{t'} s^{-\alpha/2} \int_X p(s, z, y)|V(y)|m(dy) ds \left( \sum_{k=1}^{l} \sup_{x \in X} \int_X p((k-1)t', x, z)m(dz) \right)
\]
where we have used the Chapman-Kolmogorov identity and \( \int_X p((k-1)t', x, z) m(dz) \leq 1 \).

In order to prove the asserted Hölder estimate, we denote the seminorm on the space \( C^{0, \alpha}(X) \) of \( \alpha \)-Hölder continuous functions \( f : X \to \mathbb{C} \) by

\[
\|f\|_{0, \alpha} = \sup_{x \neq y} |f(x) - f(y)| d(x, y)^{-\alpha}.
\]

Let \( \Phi \in L^\infty(X) \) and define \( V_n := \max(V, n) \), \( V_{n,m} := \min(m, V_n) \) for \( m, n \in \mathbb{N} \).

Du-Hamel’s formula states that

\[
e^{-tH} \Phi = e^{-tH} \Phi + \int_0^t e^{-\frac{s}{2}H} e^{-\frac{s}{2}H} V_{n,m} e^{-(t-s)H} V_{n,m} \Phi \, ds,
\]

a fact which can proved using the Markov property of \( \mathfrak{P} \). Thus we have

(16) \[
\|e^{-tH} \Phi\|_{C^{0, \alpha}} \leq \|e^{-tH} \Phi\|_{C^{0, \alpha}} + \int_0^t \|e^{-\frac{s}{2}H}\|_{L^\infty \to C^{0, \alpha}} \|e^{-\frac{s}{2}H} V_{n,m}\|_{L^\infty \to L^\infty} \|e^{-(t-s)H} V_{n,m} \Phi\|_{L^\infty} \, ds.
\]

Proposition 3.6 implies

(18) \[
\|e^{-tH} \Phi\|_{C^{0, \alpha}} \leq 2^{1-\alpha} F_K(t)^\alpha \|\Phi\|_{L^\infty},
\]

and

(19) \[
\|e^{-\frac{s}{2}H}\|_{L^\infty \to C^{0, \alpha}} \leq 2^{1-\alpha} F_K(s/2)^\alpha.
\]

By the Feynman-Kac formula we have

(20) \[
\|e^{-(t-s)H} V_{n,m} \Phi\|_{L^\infty} \leq C_{\exp}(V, t) \|\Phi\|_{L^\infty}.
\]

Finally, given \( f \in L^\infty(X) \) one has

\[
\int_0^t \|e^{-\frac{s}{2}H}\|_{L^\infty \to C^{0, \alpha}} \|e^{-\frac{s}{2}H} V_{n,m} f\|_{L^\infty} \, ds
\]
\[
\leq 2^{1-\alpha} \int_0^t F_K(s/2)^\alpha \sup_x \int_X p(s/2, x, y) |V_{n,m}(y)| m(dy) ds \|f\|_{L^\infty}
\]
\[
\leq 2^{2-\alpha} \sup_x \int_0^{t/2} F_K(s)^\alpha \int_X p(s, x, y) |V_{n,m}(y)| m(dy) ds \|f\|_{L^\infty}
\]
\[
\leq 2^{2-\alpha} C(V, K, \alpha, t/2) \|f\|_{L^\infty},
\]
where we the second inequality can be seen as follows: pick a sequence \( x_l \) in \( X \) such that
\[
F_K(s/2)^\alpha \int_X p(s/2, x_l, y)\vert V_{n,m}(y)\vert \text{m}(dy) \leq F_K(s/2)^\alpha \int_X p(s/2, x_{l+1}, y)\vert V_{n,m}(y)\vert \text{m}(dy),
\]
and so
\[
\begin{align*}
\sup_x F_K(s/2)^\alpha \int_X p(s/2, x, y)\vert V_{n,m}(y)\vert \text{m}(dy) &= \lim_l F_K(s/2)^\alpha \int_X p(s/2, x_l, y)\vert V_{n,m}(y)\vert \text{m}(dy),
\end{align*}
\]
and so
\[
\begin{align*}
\int_0^t F_K(s/2)^\alpha \sup_x \int_X p(s/2, x, y)\vert V_{n,m}(y)\vert \text{m}(dy)ds &= \int_0^t \lim_l F_K(s/2)^\alpha \int_X p(s/2, x_l, y)\vert V_{n,m}(y)\vert \text{m}(dy)ds \\
&= \lim_l \int_0^t F_K(s/2)^\alpha \int_X p(s/2, x, y)\vert V_{n,m}(y)\vert \text{m}(dy)ds \\
&\leq \sup_x \int_0^t F_K(s/2)^\alpha \int_X p(s/2, x, y)\vert V_{n,m}(y)\vert \text{m}(dy)ds \\
&= 2 \sup_x \int_0^{t/2} F_K(s)^\alpha \int_X p(s, x, y)\vert V_{n,m}(y)\vert \text{m}(dy)ds,
\end{align*}
\]
by monotone convergence. Thus we have
\[
(21) \quad \int_0^t \| e^{-\frac{t}{2}H} \|_{L^\infty \to C^{0,\alpha}} \| e^{-\frac{t}{2}H} V_{n,m} \|_{L^\infty \to L^\infty} ds \leq 2^{2-\alpha} C(V, K, \alpha, t/2).
\]
Putting together (13)-(21) we arrive at the following inequality: for all \( x, y \in X, \Phi \in L^\infty(X) \) one has
\[
\begin{align*}
|e^{-tH_{n,m}} \Phi(x) - e^{-tH_{n,m}} \Phi(y)| &\leq \left(2^{1-\alpha} F_K(t)^\alpha + 2^{2-\alpha} C(V, K, \alpha, t/2) C_{\text{exp}}(V, t) \right) \| \Phi \|_{L^\infty} \delta(x, y)^\alpha.
\end{align*}
\]
It remains to prove
\[
\lim_n \lim_m \left| e^{-tH_{n,m}} \Phi(x) - e^{-tH_{n,m}} \Phi(y) \right| = \left| e^{-tH_V} \Phi(x) - e^{-tH_V} \Phi(y) \right|.
\]
Here, by linearity, we can assume \( \Phi \geq 0 \). Then
\[
\lim_n \left| e^{-tH_{n,m}} \Phi(x) - e^{-tH_{n,m}} \Phi(y) \right| = \left| e^{-tH_V} \Phi(x) - e^{-tH_V} \Phi(y) \right|
\]
follows from the Feynman-Kac formula and monotone convergence, and
\[
\lim_n \left| e^{-tH_{n}} \Phi(x) - e^{-tH_{n}} \Phi(y) \right| = \left| e^{-tH_V} \Phi(x) - e^{-tH_V} \Phi(y) \right|
\]
follows from the Feynman-Kac formula and dominated convergence (using Khashminskii’s lemma), completing the proof of part a).
b) This follows from part a) using \( e^{-tH_V} \Psi = e^{-t\lambda} \Psi \) by the spectral calculus.
Combining this result with Lemma 3.8 we immediately get:
Corollary 3.10. Let $M, \tilde{M}$ be smooth geodesically complete Riemannian manifolds with Ricci curvature $\geq K$ and let $\alpha \in (0, 1]$. Let $\pi_j, \pi_{ij} : \tilde{M} \to M$ be a finite collection of smooth surjective Riemannian submersions such that fibers $\pi_j^{-1}(y), \pi_{ij}^{-1}(y) \subset \tilde{M}$ are minimal submanifolds for all $y \in M$, and let

$$V_j \in L^q_{1/m}(M) + L^\infty(M) \text{ for some } q_j > \dim(M)/(2 - \alpha),$$

$$V_{ij} \in L^q_{1/m}(M) + L^\infty(M) \text{ for some } q_{ij} > \dim(M)/(2 - \alpha).$$

Then one has

$$V := \sum_j V_j \circ \pi_j + \sum_{ij} V_{ij} \circ \pi_{ij} \in K^\alpha(\tilde{X}),$$

and for all $x, y \in \tilde{X}$, $\Phi \in L^\infty(\tilde{M})$ it holds that

$$|e^{-tH_V}\Phi(x) - e^{-tH_{Vs}}\Phi(y)| \leq \left(2^{1 - \alpha} F_K(t)^\alpha + B(V, K, \alpha, t)\right) \|\Phi\|_{L^\infty(\mathcal{D}(x, y)^\alpha)},$$

where

$$B(V, K, \alpha, t) := 2^{2 - \alpha} \sup_{x \in M} \int e^{-\sum_j \int_0^t V_j(s)ds - \sum_{ij} \int_0^t V_{ij}(s)ds} \mathbb{P}^x(d\omega) \times \left(\sum_j \int_0^t F_K(s)^\alpha \int_M p(s, x, y)|V_j(y)|m(dy)ds + \sum_{ij} \int_0^t F_K(s)^\alpha \int_M p(s, x, y)|V_{ij}(y)|m(dy)ds\right) < \infty.$$ 

Note that in the above situation $H_V$ is the unique self-adjoint realization of $-\Delta + V$ (cf. [16] for the asserted essential self-adjointness).

4. Application to molecular Schrödinger operators

Assume $M = \mathbb{R}^3$, $\tilde{M} = \mathbb{R}^{3m}$. Pick $l \in \mathbb{N}$, $R \in \mathbb{R}^{3l}$ and $Z \in [0, \infty)^l$ consider the potential

$$V_{R, Z} : \mathbb{R}^{3m} \to \mathbb{R}, \quad V_{R, Z}(x_1, \ldots, x_m) := -\sum_{j=1}^m \sum_{i=1}^l \frac{Z_i}{|x_j - R_i|} + \sum_{1 \leq i < j \leq m} \frac{1}{|x_i - x_j|}$$

of a molecule having $l$ nuclei and $m$ electrons, where the $j$-th nucleus carries $Z_j$ protons is considered to be fixed in $R_j$ (infinite mass limit). The elementary charge has been set equal to $1$. Then with

$$\pi_j : \mathbb{R}^{3m} \to \mathbb{R}^3, \quad (x_1, \ldots, x_m) \mapsto x_j,$$

$$\pi_{ij} : \mathbb{R}^{3m} \to \mathbb{R}^3, \quad (x_1, \ldots, x_m) \mapsto x_i - x_j,$$

$$V_j(x) := \sum_{i=1}^l Z_i/|x - R_i|,$$

$$V_{ij}(x) := 1/|x|,$$
one finds that the assumptions of the Corollary 3.10 are satisfied, for all \( \alpha \in (0, 1) \), since

\[ V_j, V_{ij} \in L^q(\mathbb{R}^{3m}) + L^\infty(\mathbb{R}^{3m}) \quad \text{for all } q \in [1, 3). \]

In fact, one has \( V_{R,Z} \in K^\alpha(\mathbb{R}^{3m}) \), if and only if \( \alpha < 1 \). In the sequel, \( C_{a,b,\ldots} > 0 \) denotes a constant which only depends on the parameters \( a, b, \ldots \), and which may change from line to line. Since

\[ e^{-\frac{i}{2} H_{V_{R,Z}} : L^r(\mathbb{R}^{3m}) \rightarrow L^\infty(\mathbb{R}^{3m})}, \]

with

\[ \left\| e^{-\frac{i}{2} H_{V_{R,Z}}} \right\|_{L^r(\mathbb{R}^{3m}) \rightarrow L^\infty(\mathbb{R}^{3m})} \leq C t^{-\frac{3m}{2r}} e^{C_{R,Z} t}, \]

we obtain from

\[ e^{-t H_{V_{R,Z}} = e^{-\frac{i}{2} H_{V_{R,Z}}} e^{-\frac{i}{2} H_{V_{R,Z}}}} \]

and Corollary 3.10 the following smoothing property,

\[ e^{-t H_{V_{R,Z}} : L^r(\mathbb{R}^{3m}) \rightarrow C^0,\alpha(\mathbb{R}^{3m})} \quad \text{for all} \quad t > 0, \quad r \in [1, \infty], \quad \alpha \in (0, 1), \]

with

\[ \left\| e^{-t H_{V_{R,Z}}} \right\|_{L^r(\mathbb{R}^{3m}) \rightarrow C^0,\alpha(\mathbb{R}^{3m})} \leq \left\| e^{-\frac{i}{2} H_{V_{R,Z}}} \right\|_{L^r(\mathbb{R}^{3m}) \rightarrow L^\infty(\mathbb{R}^{3m})} \left\| e^{-\frac{i}{2} H_{V_{R,Z}}} \right\|_{L^r(\mathbb{R}^{3m}) \rightarrow L^\infty(\mathbb{R}^{3m})} \]

\[ \leq C \left( 2^{1-\alpha} t^{-\alpha/2} + B(V_{R,Z}, K, \alpha, t) \right) t^{-\frac{3m}{2r}} e^{C_{R,Z} t}. \]

Using

\[ 4\pi \int_0^\infty p(r, y, R) dr = |y - R|^{-1}, \]

Fubini, Chapman-Kolmogorov and

\[ p(u, a, b) \leq C u^{-\frac{3}{2}}, \]

we get

\[ \int_{\mathbb{R}^3} p(s, x, y) |y - R|^{-1} d\mathbf{y} = 4\pi \int_0^\infty \int_{\mathbb{R}^3} p(s, x, y) p(r, y, R) d\mathbf{y} dr \]

\[ = 4\pi \int_0^\infty p(s + r, x, R) dr \]

\[ \leq C \int_0^\infty (s + r)^{-3/2} dr \leq C s^{-1/2}, \]

\[ ^3 \text{This mapping properties relies in the fact that the Euclidean space is ultracontractive.} \]
and so using $F_K|_{K=0}(s) \leq Cs^{-1/2}$,
\[
\sum_{j=1}^{m} \int_0^t F_K|_{K=0}(s)^\alpha \int_{\mathbb{R}^3} p(s, x, y)|V_j(y)|dyds \\
\leq C_{m, Z} \int_0^t s^{-\alpha/2-1/2} ds \\
= C_{m, Z} \frac{t^{-\alpha/2+1/2}}{1/2 - \alpha/2},
\]
and likewise
\[
\sum_{1 \leq i < j \leq m} \int_0^t F_K|_{K=0}(s)^\alpha \int_{\mathbb{R}^3} p(s, x, y)|V_{ij}(y)|dyds \\
\leq C_m \frac{t^{-\alpha/2+1/2}}{1/2 - \alpha/2},
\]
and so
\[
B(V_{R, Z}, K, \alpha, t)|_{K=0} \leq C_{m, Z} \frac{t^{-\alpha/2+1/2}}{1/2 - \alpha/2} e^{C_{R, Z} t},
\]
we arrive at the estimate
\[
\left\| e^{-tH_{V_{R, Z}}} \right\|_{L^r(\mathbb{R}^{3m}) \to C^{0, \alpha}(\mathbb{R}^{3m})} \leq C_{m, Z} \left( t^{-\alpha/2} \frac{3m}{2r} e^{C_{R, Z} t} + \frac{t^{-\alpha/2} + \frac{3m}{2r} e^{C_{R, Z} t}}{1/2 - \alpha/2} \right).
\]

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