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Exponential product approximation to the integral kernel of the Schrödinger semigroup and to the heat kernel of the Dirichlet Laplacian

By *Takashi Ichinose* at Kanazawa and *Hideo Tamura* at Okayama

Abstract. We know by the studies for the last decade that the norm convergence of the exponential product formula holds true even for a class of unbounded operators. As a natural development of this recent research, we study how the product formula approximates integral kernels of Schrödinger semigroups. Our emphasis is placed on the case of singular potentials. The Dirichlet Laplacian is regarded as a special case of Schrödinger operators with singular potentials. We also discuss the approximation to the heat kernel generated by the Dirichlet Laplacian through the product formula.

1. Introduction

It is known as the Trotter-Kato product formula [13], [19] that the semigroup $\exp(-tZ)$, $t \geqq 0$, generated by the sum $Z = X + Y$ of two operators X and Y acting on a Hilbert space is approximated by the exponential product formula

$$\exp(-tZ) = s - \lim_{N\to\infty} \big(\exp\big(-(t/N)Y\big)\exp\big(-(t/N)X\big)\big)^N$$

in the strong sense under suitable conditions on the pair (X, Y). If X and Y are bounded, the norm convergence follows from the Baker-Campbell-Hausdorff formula. Then we know that

$$\|e^{-tZ} - (e^{-(t/N)Y}e^{-(t/N)X})^N\| = O(N^{-1}) \tag{1.1}$$

for the approximation of the nonsymmetric form and that

$$\|e^{-tZ} - (e^{-(t/2N)X}e^{-(t/N)Y}e^{-(t/2N)X})^N\| = O(N^{-2}) \tag{1.2}$$

for the approximation of the symmetric form, where $\| \ \|$ denotes the operator norm of bounded operators. We note that the error bounds $O(N^{-1})$ and $O(N^{-2})$ on the right-hand sides are optimal (see [12] for details). The norm convergence has been extended to a wide class of pairs of self-adjoint operators not necessarily bounded since it was first established by Helffer [7] and Rogava [15] independently. After the works, various kinds of improvements have been done by many authors (see [8], [9], [10], [20] for extensive references and related subjects). Among a lot of literatures, the work [12] together with [10] has established that the convergence holds true with error bound $O(N^{-1})$ for both the symmetric and nonsymmetric approximations under the general assumption that $Z = X + Y$ is self-adjoint with domain $\mathscr{D}(Z) = \mathscr{D}(X) \cap \mathscr{D}(Y)$ for two self-adjoint operators X and Y bounded from below. In particular, $O(N^{-1})$ is the optimal error bound even for the symmetric approximation, which is different from the case of bounded operators. This has been shown by constructing an example of pair (X, Y) for which (1.2) is estimated by $c_t N^{-1}$, $c_t > 0$, from below for $t > 0$. The original idea of construction is due to [18].

As stated at the beginning, our aim is to analyze how the exponential product formula approximates the kernel $E(x, y; t)$ of the semigroup $\exp(-tH)$ generated by the Schrödinger operator $H = H_0 + V$, $H_0 = -\Delta$, acting on $L^2(\mathbb{R}^n)$. The present work is a continuation to our recent work [11] where the same problem has been studied for a class of smooth potentials. A special emphasis here is placed on the case that potentials admit singularities. The Dirichlet Laplacian is regarded as a special case of Schrödinger operators with singular potentials. We also discuss the approximation to the heat kernel generated by the Dirichlet Laplacian through the product formula.

We begin by summarizing the results obtained in [11] which show how sharp the kernel of the Schrödinger semigroup is approximated through the product formula. We there have assumed that $V(x) \in C^\infty(\mathbb{R}^n)$ is a nonnegative smooth function and satisfies

$$V(x) \geqq C\langle x\rangle^\rho, \quad |\partial_x^\alpha V(x)| \leqq C_\alpha \langle x\rangle^{\rho-\delta|\alpha|} \tag{1.3}$$

for some constants $C > 0$, $\rho \geqq 0$ and δ, $0 < \delta \leqq 1$ ($\delta = 0$ is allowed if $\rho = 0$), where $\langle x\rangle = (1 + |x|^2)^{1/2}$. We define the symmetric approximation $K_N(t)$ by

$$K_N(t) = \big(\exp\big(-(t/2N)H_0\big)\exp\big(-(t/N)V\big)\exp\big(-(t/2N)H_0\big)\big)^N \tag{1.4}$$

and the nonsymmetric approximation $G_N(t)$ by

$$G_N(t) = \big(\exp\big(-(t/N)V\big)\exp\big(-(t/N)H_0\big)\big)^N. \tag{1.5}$$

We also denote by $K_N(x, y; t)$ and $G_N(x, y; t)$ the kernels of operators $K_N(t)$ and $G_N(t)$ respectively. Then we have proved that $|K_N(x, y; t) - E(x, y; t)| = O(N^{-2})$ and that

$$|G_N(x, y; t) - E(x, y; t) - (t/2N)E_1(x, y; t)| = O(N^{-2})$$

and $\big|\big(G_N(x, y; t) + G_N(y, x; t)\big)/2 - E(x, y; t)\big| = O(N^{-2})$ as $N \to \infty$, where

$$E_1(x, y; t) = E(x, y; t)V(y) - V(x)E(x, y; t)$$

is the kernel of the commutator $[H_0, \exp(-tH)] = [\exp(-tH), V]$ and all the error bounds are uniform in $(x, y) \in \mathbb{R}^n \times \mathbb{R}^n$ and locally in $t > 0$ ($t \in [1/c, c], c > 1$). The convergence is still true for all derivatives in x and y. We note that $G_N(y, x; t)$ is the kernel of the adjoint operator

$$G_N(t)^* = \big(\exp\big(-(t/N)H_0\big)\exp\big(-(t/N)V\big)\big)^N.$$

The proof is based on the pseudodifferential calculus, and it relies on the regularity assumption of potentials in an essential way.

The above results have an important application to the theory on the finite dimensional approximation to path integrals. Let $dW_{x,y}^t$ be the conditional Wiener measure over the set

$$W_{x,y}^t = \{r(s) \in C([0,t] \to \mathbb{R}^n) : r(0) = x, r(t) = y\}$$

of continuous paths which take the values x and y at their endpoints 0 and t respectively. According to the Feynman-Kac formula ([6], [14]), $E(x, y; t)$ has the representation

$$E(x, y; t) = \int \exp\left(-\int_0^t V\big(r(s)\big)\, ds\right) dW_{x,y}^t,$$

while $K_N(x, y; t)$, $G_N(x, y; t)$ and $G_N(y, x; t)$ are represented as follows:

$$K_N(x, y; t) = \int \exp\left(-(t/N)\sum_{k=0}^{N-1} V\big(r(s_k)\big)\right) dW_{x,y}^t$$

with $s_k = (k + 1/2)t/N$, and

$$G_N(x, y; t) = \int \exp\left(-(t/N)\sum_{k=0}^{N-1} V\big(r(t_k)\big)\right) dW_{x,y}^t,$$

$$G_N(y, x; t) = \int \exp\left(-(t/N)\sum_{k=0}^{N-1} V\big(r(t_{k+1})\big)\right) dW_{x,y}^t$$

with $t_k = kt/N$. Thus we obtain the error bound of a time-sliced approximation to the kernel of $\exp(-tH)$. The work [17] has also studied the convergence of time-sliced approximation by estimating directly the difference between two kernels represented by the Feynman-Kac formula to show that the error bound is of order $O(N^{-\kappa})$ for a class of C^2 smooth potentials satisfying (1.3) for $|\alpha| \leqq 2$, where $\kappa = 1$ for $0 \leqq \rho \leqq 2\delta$ and $\kappa = 2\delta/\rho$ for $\rho > 2\delta$. The proof is based on a probabilistic idea and still requires regularity assumption (although not necessarily C^∞ smoothness) of potentials.

The main results obtained in this work are formulated as the two theorems below. As stated above, a special attention is paid to the case when $V(x)$ has singularities. Let

$$H_0 = -\Delta, \quad A = H_0 + 1, \tag{1.6}$$

be self-adjoint operators on $L^2 = L^2(\mathbb{R}^n)$ with domain $H^2(\mathbb{R}^n)$, where $H^s(\mathbb{R}^n)$ denotes the Sobolev space of order s. We make the following assumption on the potential $V(x)$: (V) $V(x) \geqq 0$ is nonnegative and

$$VA^{-\alpha} : L^2 \to L^2 \tag{1.7}$$

is bounded for some α, $0 < \alpha < 1$, as the multiplication operator by $V(x)$. The assumption $V \geqq 0$ is only for notational brevity. We have only to assume that $V(x) > -c$, $c > 0$, is bounded from below. Under assumption (V), we have that $\|V(H_0 + \lambda)^{-1}\| \to 0$ as $\lambda \to \infty$, and hence it follows from Kato-Rellich theorem that $H = H_0 + V$ becomes self-adjoint with the same domain $H^2(\mathbb{R}^n)$ as H_0. We also have that $A(H+1)^{-1}$ as well as $(H+1)A^{-1}$ is bounded as an operator acting on L^2. If, for example, $n = 3$, then (1.7) is easily seen to be fulfilled for $V(x)$ admitting the decomposition $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. The positive Coulomb potential $V(x) = c/|x|$, $c > 0$, is a typical example. The first theorem is formulated as follows.

Theorem 1.1. *Suppose that $V(x)$ fulfills (V). Denote by $E(x, y; t)$ the kernel of $\exp(-tH)$ and by $K_N(x, y; t)$ and $G_N(x, y; t)$ the kernels of $K_N(t)$ and $G_N(t)$ defined by (1.4) and (1.5) respectively. Let $(p, q) \in \mathbb{R}^n \times \mathbb{R}^n$ be fixed. If $V(x)$ is C^∞ smooth around both points p and q, then*

$$|K_N(p, q; t) - E(p, q; t)| = O(N^{-1}), \quad |G_N(p, q; t) - E(p, q; t)| = O(N^{-1})$$

as $N \to \infty$, and the convergence is true in the sense of C^∞ topology in a neighborhood of $(p, q) \in \mathbb{R}^n \times \mathbb{R}^n$, where the order estimate is locally uniform in $t > 0$ $(t \in [1/c, c], c > 1)$.

We make an important comment on the convergence at singular points where $V(x)$ is divergent. This seems to be a subtle problem. For example, we consider the positive Coulomb potential $V(x) = c/|x|$, $c > 0$, in three dimensions. We know the convergence $\|G_N(t) - \exp(-tH)\| = O(N^{-1})$ in the operator norm. However, the convergence of the kernel $G_N(x, y; t)$ at the origin is not true. In fact, $G_N(x, y; t)$ takes the value $G_N(0, y; t) = 0$ at $x = 0$ for all N, because $V(0) = +\infty$. On the other hand, we can explicitly calculate the value

$$E(0, 0; t) = (c/4\pi) \int_0^\infty e^{-t\lambda} (e^{c\pi/\sqrt{\lambda}} - 1)^{-1} \, d\lambda > 0 \tag{1.8}$$

for $V(x) = c/|x|$, $c > 0$. Thus the convergence at singular points is not expected in general. The relation (1.8) itself is interesting. We prove it in the appendix at the end of the paper.

We move to the problem on the approximation for the heat kernel generated by the Dirichlet Laplacian. Let $\exp(-tH_D)$ be the semigroup generated by the Dirichlet Laplacian $H_D = -\Delta$ over a domain Ω in $\mathbb{R}^n$. If we define the potential $V(x)$ as $V(x) = 0$ on Ω and $V(x) = +\infty$ on the complement Ω^c of Ω, then we have

$$\exp(-tH_D) \sim \exp\big(-t(H_0 + V)\big)$$

in a formal way. The operator $\exp(-tV)$, $t > 0$, acts as the multiplication by the characteristic function χ_Ω of Ω, and the exponential product formula takes the form

$$\begin{aligned} \exp(-tH_D) &\sim \lim_{N\to\infty} \big(\exp\big(-(t/N)V\big)\exp\big(-(t/N)H_0\big)\big)^N \chi_\Omega \\ &= \lim_{N\to\infty} \big(\chi_\Omega \exp\big(-(t/N)H_0\big)\chi_\Omega\big)^N. \end{aligned} \tag{1.9}$$

The strong convergence follows from the abstract theory due to Kato [13] (see Friedman [5], Theorem 2, also). The product

$$(1.10)\qquad \left(\chi_\Omega \exp\left(-i(t/N)H_0\right)\chi_\Omega\right)^N$$

with $t > 0$ replaced by it is often called the Zeno product formula. This kind of product appears in the problem on the position measurement in quantum systems (Zeno quantum effect). In fact, the product (1.10) describes the frequent measurement to check whether a particle localized in Ω at $t = 0$ is still in Ω. If (1.10) is strongly convergent to the propagator $\exp(-itH_D)$ as $N \to \infty$, this means that continuous observations hinder transitions to states different from the initial one and that a quantum particle can not move to where it is not. It corresponds to Zeno's paradox denying the possibility of motion to a flying arrow. This is the reason why (1.10) is called the Zeno product formula. The strong convergence of the Zeno product formula has been discussed in the physical literatures (for example see [4] and references there). However the rigorous proof does not seem to have been done, and it remains as an interesting mathematical problem.

We shall formulate the second main theorem. Let

$$H_D = -\Delta, \quad \mathscr{D}(H_D) = H^2(\Omega) \cap H_0^1(\Omega),$$

be the Dirichlet Laplacian over a bounded domain $\Omega \subset \mathbb{R}^n$ with smooth boundary $\partial\Omega$. The operator H_D is self-adjoint in $L^2(\Omega)$. We denote by $\exp(-tH_D)$, $t \geqq 0$, the semigroup generated by H_D and by $E_D(x, y; t)$ the integral kernel of $\exp(-tH_D)$. We also denote by $G_{ND}(x, y; t)$ the integral kernel of the operator

$$(1.11)\qquad G_{ND}(t) = \left(J \exp\left(-(t/N)H_0\right)J^*\right)^N : L^2(\Omega) \to L^2(\Omega),$$

where $J : L^2(\mathbb{R}^n) \to L^2(\Omega)$ denotes the restriction. The kernel $G_{ND}(x, y; t)$ takes a simple form

$$G_{ND}(x, y; t) = \int_\Omega \cdots \int_\Omega \left(\prod_{j=0}^{N-1} E_0(z_j, z_{j+1}; t/N)\right) dz$$

for $(x, y) = (z_0, z_N) \in \Omega \times \Omega$, where $z = (z_1, \ldots, z_{N-1})$ and

$$E_0(x, y; t) = (4\pi t)^{-n/2} \exp(-|x - y|^2/4t)$$

is the heat kernel of $\exp(-tH_0)$. Then the second theorem is stated as follows.

Theorem 1.2. *Let the notation be as above. Then*

$$|G_{ND}(x, y; t) - E_D(x, y; t)| = O(N^{-\sigma}), \quad N \to \infty,$$

for any σ, $0 < \sigma < 1/6$, *and the error bound is locally uniform in* $(x, y) \in \Omega \times \Omega$ *and in* $t > 0$.

We add two comments to the above theorem. (1) We note that the theorem implies the strong convergence in (1.9). In fact, the weak convergence follows from the theorem at once, and the semigroup property yields

$$\|G_{ND}(t)f\|^2 = \big(G_{ND}(t)G_{ND}(t)f, f\big) \to \big(\exp(-2tH_D)f, f\big) = \|\exp(-tH_D)f\|^2$$

for $f \in L^2(\Omega)$, where $(\ ,\ )$ denotes the L^2 scalar product in $L^2(\Omega)$. This proves the strong convergence. (2) The error bound $O(N^{-\sigma})$ with $0 < \sigma < 1/6$ is not sharp. The proof of the theorem is based on the large coupling approximation to the Dirichlet Laplacian, where an essential role is played by Theorem 3.3 due to Demuth, Kirsch and McGillivray [3]. According to their theorem, it is anticipated that the optimal error bound is $O(N^{-\sigma})$ with $0 < \sigma < 1/2$ (see Proposition 5.1 also).

The proof of both the theorems is based on the convergence of exponential product formula in the operator norm on the Sobolev spaces. We denote by $\|\ \|_m$ the norm of bounded operators when considered as an operator from L^2 into $H^m(\mathbb{R}^n)$ for $m \geqq 0$ (not necessarily integer). If, in particular, $m = 0$, then we simply write $\|\ \|$ for $\|\ \|_0$. For example, the following proposition plays an essential role in proving Theorem 1.1.

Proposition 1.1. *Assume the same assumptions and keep the same notation as in Theorem* 1.1. *Let $\psi_p, \psi_q \in C_0^\infty(\mathbb{R}^n \to \mathbb{R})$ be smooth real functions with support around p and q respectively. Assume that $V(x)$ is C^∞ smooth on the support of ψ_p and ψ_q. Then*

$$\big\|\psi_p\big(\exp(-tH) - K_N(t)\big)\psi_q\big\|_m = O(N^{-1})$$

and

$$\big\|\psi_p\big(\exp(-tH) - G_N(t)\big)\psi_q\big\|_m + \big\|\psi_p\big(\exp(-tH) - G_N(t)^*\big)\psi_q\big\|_m = O(N^{-1})$$

as $N \to \infty$ for any $m \geqq 0$, where the order estimate is locally uniform in $t > 0$.

Theorem 1.1 is obtained as a consequence of the celebrated kernel theorem due to Agmon [1], Theorem 3.1.

Lemma 1.1. *Let $T : L^2 \to L^2$ be a bounded operator. Assume that the range of T is contained in $H^m(\mathbb{R}^n)$ for some $m > n$ and that the range of the adjoint operator T^* is also contained in $H^m(\mathbb{R}^n)$. Then T is an integral operator with a continuous and bounded kernel $T(x, y)$, $(x, y) \in \mathbb{R}^n \times \mathbb{R}^n$, and the kernel obeys the bound*

$$|T(x, y)| \leqq c(\|T\|_m + \|T^*\|_m)^{n/m}\|T\|^{1-n/m}$$

for some $c > 0$ independent of T.

We end the section by proving Theorem 1.1, accepting Proposition 1.1 as proved. This proposition is proved in sections 2, 3 and 4, and Theorem 1.2 is proved in sections 5 and 6.

Proof of Theorem 1.1. Let A be as in (1.6). We apply Lemma 1.1 to

$$T = \psi_p\big(\exp(-tH) - K_N(t)\big)\psi_q,$$

where $\psi_p(x) = 1$ and $\psi_q(x) = 1$ around p and q respectively. Then it follows from Proposition 1.1 that $\|A^m T\| + \|A^m T^*\| = O(N^{-1})$ for any $m \geqq 0$. Hence we have $\|TA^m\| + \|T^*A^m\| = O(N^{-1})$ by adjoint, and

$$\|A^{m/2}TA^{m/2}\| + \|A^{m/2}T^*A^{m/2}\| = O(N^{-1})$$

by interpolation. This yields the desired bound $O(N^{-1})$ on the difference between $K_N(p,q;t)$ and $E(p,q;t)$ in the sense of C^∞ topology. Similarly the bound on the difference between $G_N(p,q;t)$ and $E(p,q;t)$ is obtained by making use of Lemma 1.1 for $T = \psi_p\big(\exp(-tH) - G_N(t)\big)\psi_q$. $\square$

2. Approximation to kernels of Schrödinger semigroups

In this section we complete the proof of Theorem 1.1 by proving Proposition 1.1. For two smooth functions $\psi, \eta \in C_0^\infty(\mathbb{R}^n \to \mathbb{R})$ with compact support, we use the notation

$$\psi \prec \eta, \tag{2.1}$$

provided that both ψV and ηV are C^∞ smooth and that

$$\psi\eta = \psi, \quad \operatorname{dist}(\operatorname{supp}\psi, \operatorname{supp}\chi) > 0$$

for $\chi(x) = 1 - \eta(x)$, where $\operatorname{dist}(\Sigma_1, \Sigma_2)$ denotes the distance between two sets Σ_1 and Σ_2. For brevity, we prove Proposition 1.1 for the case $t = 1$ only. We set

$$T_0(s) = \exp(-sH_0), \quad T(s) = \exp(-sH)$$

and we define

$$K(\tau) = T_0(\tau/2)\exp(-\tau V)T_0(\tau/2), \quad \tau = 1/N. \tag{2.2}$$

Then $K_N(1) = K(\tau)^N$ for $K_N(t)$ defined by (1.4) with $t = 1$.

We accept three preliminary lemmas below as proved to prove the proposition. Throughout the statements of these lemmas, $m \geqq 0$ is nonnegative (not necessarily integer), and two real smooth functions $\psi \in C_0^\infty(\mathbb{R}^n)$ and $\omega \in C^\infty(\mathbb{R}^n)$ are assumed to satisfy the relation

$$\psi \prec \theta, \quad \omega = 1 - \theta. \tag{2.3}$$

Lemma 2.1. *The operator $T(s) = \exp(-sH)$ has the following properties*:

(1) *$A^m\psi T(s)\omega A$, $A^m\psi T(s)\psi A^{-m} : L^2 \to L^2$ are bounded uniformly in $s \in [0,1]$.*

(2) *$\|A^m\psi T(s)\| = O(s^{-m})$ and $\|A^m\psi T(s)A\| = O(s^{-m-1})$.*

Lemma 2.2. *The operator $D(\tau)$ defined by*

$$D(\tau) = T(\tau) - K(\tau) \tag{2.4}$$

has the following properties:

(1) $\|A^{-1}D(\tau)A^{-1}\| = O(\tau^2)$, $\tau \to 0$.

(2) $\|A^m \psi D(\tau)\omega\| = O(\tau^2)$.

(3) $\|A^m \psi D(\tau)A^{-m}\| = O(\tau^2)$, *and in particular*, $\|\psi D(\tau)\| = O(\tau^2)$.

Lemma 2.3. *The operator* $K(\tau)$ *defined by* (2.2) *has the following properties*:

(1) $A\omega K(\tau)^k \psi : L^2 \to L^2$ *is bounded uniformly in* τ *and* k, $0 \leqq k \leqq N$.

(2) $\|A^m \psi K(\tau)^k\| = k^{-m} O(\tau^{-m})$ *uniformly in* k, $1 \leqq k \leqq N$.

Lemma 2.1 is proved at the end of this section, and Lemmas 2.2 and 2.3 are proved in sections 3 and 4 respectively. We note that the statements of the lemmas remain true for the adjoint operators. Throughout the entire discussion, we use such a simple consequence without further references, and also we often use the notation $O_p(\tau^\nu)$ to denote the class of bounded operators of which the norm obeys the bound $O(\tau^\nu)$ as $\tau \to 0$. In particular, $O_p(1)$ denotes the class of operators bounded uniformly in τ, and $O_p(\tau^\infty)$ the class of operators with bound $O(\tau^L)$ for any $L \gg 1$. We sometimes denote by $O_p(1)$ a class of bounded operators independent of parameter τ also.

Proof of Proposition 1.1. The proof is rather long and is divided into four steps.

(1) According to notation (2.1), we take $\{\eta_j\}$, $0 \leqq j \leqq 1$, in such a way that

$$\psi_p \prec \eta_0 \prec \eta_1, \quad \psi_q \prec \eta_0 \prec \eta_1 \tag{2.5}$$

and we set $\chi_j = 1 - \eta_j$. The first three steps are devoted to proving that

$$\left\|A^m \psi_p \left(T(1) - K(\tau)^N\right)\psi_q\right\| = O(\tau), \tag{2.6}$$

which implies the statement for the symmetric product $K_N(1)$ in the proposition. To prove (2.6), we represent the difference $T(1) - K(\tau)^N$ as

$$T(1) - K(\tau)^N = T(\tau)^N - K(\tau)^N = \sum_{k=1}^{N} T\big((k-1)\tau\big)D(\tau)K(\tau)^{N-k}.$$

We evaluate the norm of the operator

$$X_k(\tau) = A^m \psi_p T\big((k-1)\tau\big)D(\tau)K(\tau)^{N-k}\psi_q, \quad 1 \leqq k \leqq N,$$

to show that $\sum_{k=1}^{N} \|X_k(\tau)\| = O(\tau)$. This yields (2.6).

(2) We decompose $X_k(\tau)$ into the sum

$$X_k(\tau) = A^m \psi_p T\big((k-1)\tau\big)(\eta_0 + \chi_0)D(\tau)K(\tau)^{N-k}\psi_q = Y_k(\tau) + Z_k(\tau).$$

We first consider $Y_k(\tau)$. We further decompose $Y_k(\tau)$ into the sum

$$Y_k(\tau) = A^m\psi_p T\big((k-1)\tau\big)\eta_0 D(\tau)(\eta_1+\chi_1)K(\tau)^{N-k}\psi_q = Y_{k1}(\tau)+Y_{k2}(\tau).$$

By Lemma 2.1 (1) with $\psi = \eta_1$,

$$A^m\psi_p T\big((k-1)\tau\big)\eta_1 A^{-m} = A^m\psi_p A^{-m}\big(A^m\eta_1 T\big((k-1)\tau\big)\eta_1 A^{-m}\big) : L^2 \to L^2$$

is uniformly bounded, and also by Lemma 2.2 (2), $A^m\eta_0 D(\tau)\chi_1 = O_p(\tau^2)$. Hence we have

$$Y_{k2}(\tau) = \big(A^m\psi_p T\big((k-1)\tau\big)\eta_1 A^{-m}\big)\big(A^m\eta_0 D(\tau)\chi_1\big)K(\tau)^{N-k}\psi_q = O_p(\tau^2),$$

and $\sum_{k=1}^{N}\|Y_{k2}(\tau)\| = O(\tau)$. We write $Y_{k1}(\tau)$ as

$$Y_{k1}(\tau) = \big(A^m\psi_p T\big((k-1)\tau\big)\eta_1 A^{-m}\big)\big(A^m\eta_0 D(\tau)A^{-m}\big)A^m\eta_1 K(\tau)^{N-k}\psi_q$$

for k with $1 \leqq k < [N/2]$, and $Y_{k1}(\tau)$ as

$$Y_{k1}(\tau) = \big(A^m\psi_p T\big((k-1)\tau\big)\big)\big(\eta_0 D(\tau)\big)\eta_1 K(\tau)^{N-k}\psi_q$$

for k with $[N/2] \leqq k \leqq N$, where $[N/2]$ denotes the greatest integer not exceeding $N/2$. Note that $N/2 \leqq N-k \leqq N$, provided that $1 \leqq k < [N/2]$. We apply Lemmas 2.1 (1), 2.2 (3) and 2.3 (2) to $Y_{k1}(\tau)$ with k, $1 \leqq k < [N/2]$, and Lemmas 2.1 (2) and 2.2 (3) to $Y_{k1}(\tau)$ with k, $[N/2] \leqq k \leqq N$. Then we get $\sum_{k=1}^{N}\|Y_{k1}(\tau)\| = O(\tau)$.

(3) We proceed to operator $Z_k(\tau)$. We decompose $Z_k(\tau)$ into the sum

$$Z_k(\tau) = A^m\psi_p T\big((k-1)\tau\big)\chi_0 D(\tau)(\eta_1+\chi_1)K(\tau)^{N-k}\psi_q = Z_{k1}(\tau)+Z_{k2}(\tau).$$

If we write $Z_{k1}(\tau)$ as

$$Z_{k1}(\tau) = \big(A^m\psi_p T\big((k-1)\tau\big)\chi_0\big)\big(D(\tau)\eta_1\big)K(\tau)^{N-k}\psi_q,$$

then it follows from Lemmas 2.1 (1) and 2.2 (3) that $Z_{k1}(\tau) = O_p(\tau^2)$, and if we write $Z_{k2}(\tau)$ as

$$Z_{k2}(\tau) = \big(A^m\psi_p T\big((k-1)\tau\big)\chi_0 A\big)\big(A^{-1}D(\tau)A^{-1}\big)A\chi_1 K(\tau)^{N-k}\psi_q,$$

then it follows from Lemmas 2.1 (1), 2.2 (1) and 2.3 (1) that $Z_{k2}(\tau) = O_p(\tau^2)$. This yields $\sum_{k=1}^{N}\|Z_k(\tau)\| = O(\tau)$, and hence (2.6) is obtained.

(4) We here introduce the new notation $F \sim G$. This means that two bounded operators F and G obey $\|F-G\| = O(\tau)$. We set

$$G(\tau) = e^{-\tau V}T_0(\tau) = e^{-\tau V}\exp(-\tau H_0), \quad J(\tau) = G(\tau)^* = T_0(\tau)e^{-\tau V},$$

and $J_N(1) = G_N(1)^*$ for $G_N(1)$ defined by (1.5) with $t = 1$. Then $G_N(1) = G(\tau)^N$ and $J_N(1) = J(\tau)^N$. According to the above notation, the aim in the final step is to show that

(2.7) $$\Gamma_N(\tau) = A^m\psi_p G_N(1)\psi_q = A^m\psi_p G(\tau)^N\psi_q \sim A^m\psi_p K(\tau)^N\psi_q,$$

(2.8) $$\Lambda_N(\tau) = A^m\psi_p J_N(1)\psi_q = A^m\psi_p J(\tau)^N\psi_q \sim A^m\psi_p K(\tau)^N\psi_q,$$

which, together with (2.6), imply the statement for the nonsymmetric products $G_N(1)$ and $G_N(1)^*$ in the proposition. The proof of two relations (2.7) and (2.8) requires the following lemma which is proved after completing the proof of the proposition.

Lemma 2.4. *One has the following statements*:

(1) $A^m\psi T_0(\tau)\omega = O_p(\tau^\infty)$.

(2) $A^m[g, T_0(\tau)]A^{-m-1/2} = O_p(\tau)$ *for* $g \in C_0^\infty(\mathbb{R}^n)$, *where* $[X, Y]$ *denotes the commutator* $[X, Y] = XY - YX$ *between two operators* X *and* Y.

(3) $[A^m\psi T(s), T_0(\tau)] = O_p(\tau)$ *uniformly in* $s \in [\delta, 1]$, $\delta > 0$.

We now start by proving (2.7). Let $\{\eta_j\}$, $0 \leqq j \leqq 1$, be as in (2.5) and we set $\chi_j = 1 - \eta_j$ again. Then we obtain

(2.9) $$A^m\eta_j T\big((N-1)\tau\big)\eta_j \sim A^m\eta_j K(\tau)^{N-1}\eta_j$$

by (2.6). We write $\Gamma_N(\tau)$ as

$$\begin{aligned}\Gamma_N(\tau) &= A^m\psi_p e^{-\tau V}T_0(\tau/2)K(\tau)^{N-1}T_0(\tau/2)\psi_q\\ &= A^m\psi_p e^{-\tau V}T_0(\tau/2)(\chi_0+\eta_0)K(\tau)^{N-1}T_0(\tau/2)\psi_q.\end{aligned}$$

Since $A^m\psi_p e^{-\tau V}T_0(\tau/2)\chi_0 = O_p(\tau^\infty)$ by Lemma 2.4 (1), it follows that

$$\Gamma_N(\tau) \sim A^m\psi_p e^{-\tau V}T_0(\tau/2)\eta_0 K(\tau)^{N-1}T_0(\tau/2)\psi_q.$$

The operator $A^m\eta_0 K(\tau)^{N-1}$ is bounded uniformly in τ by Lemma 2.3 (2), and also $\chi_0 T_0(\tau/2)\psi_q$ is of class $O_p(\tau^\infty)$. Hence

$$\begin{aligned}\Gamma_N(\tau) &\sim \big(A^m\psi_p e^{-\tau V}T_0(\tau/2)A^{-m}\big)\big(A^m\eta_0 K(\tau)^{N-1}\big)\eta_0 T_0(\tau/2)\psi_q\\ &\sim \big(A^m\psi_p e^{-\tau V}T_0(\tau/2)A^{-m}\big)\big(A^m\eta_0 T\big((N-1)\tau\big)\eta_0\big)T_0(\tau/2)\psi_q\end{aligned}$$

by (2.9). Note that $\psi_p\eta_0 = \psi_p$ and $\eta_0\eta_1 = \eta_0$. Since $A^m\eta_0 T\big((N-1)\tau\big)$ is uniformly bounded by Lemma 2.1 (2), we further have

$$\Gamma_N(\tau) \sim \big(A^m\psi_p\eta_1 e^{-\tau V}T_0(\tau/2)A^{-m-1/2}\big)\big(A^{m+1/2}\eta_0 T\big((N-1)\tau\big)\big)T_0(\tau/2)\psi_q.$$

We here use Lemma 2.4 (2) with $g = \eta_1 e^{-\tau V} \in C_0^\infty(\mathbb{R}^n)$ to obtain that

$$\begin{aligned}\Gamma_N(\tau) &\sim A^m\psi_p T_0(\tau/2)\eta_1 e^{-\tau V}\eta_0 T\big((N-1)\tau\big)T_0(\tau/2)\psi_q\\ &= \big(A^m\psi_p T_0(\tau/2)e^{-\tau V}\eta_0 A^{-m}\big)\big(A^m\eta_1 T\big((N-1)\tau\big)T_0(\tau/2)\big)\psi_q.\end{aligned}$$

Hence Lemma 2.4 (3) and (2.9) yield that

$$\begin{aligned}\Gamma_N(\tau) &\sim \big(A^m\psi_p T_0(\tau/2)e^{-\tau V}\eta_0 A^{-m}\big)T_0(\tau/2)\big(A^m\eta_1 T\big((N-1)\tau\big)\big)\psi_q\\ &\sim \big(A^m\psi_p T_0(\tau/2)e^{-\tau V}\eta_0 A^{-m}T_0(\tau/2)\big)A^m\eta_1 K(\tau)^{N-1}\psi_q.\end{aligned}$$

We further have

$$\begin{aligned}\Gamma_N(\tau) &\sim \big(A^m\psi_p T_0(\tau/2)e^{-\tau V}\eta_1 A^{-m}\big)\big(A^m\eta_0 T_0(\tau/2)\eta_1\big)K(\tau)^{N-1}\psi_q\\ &\sim \big(A^m\psi_p T_0(\tau/2)\eta_0\big)e^{-\tau V}T_0(\tau/2)K(\tau)^{N-1}\psi_q\\ &\sim A^m\psi_p T_0(\tau/2)e^{-\tau V}T_0(\tau/2)K(\tau)^{N-1}\psi_q = A^m\psi_p K(\tau)^N\psi_q,\end{aligned}$$

because $A^m\eta_0 T_0(\tau/2)\chi_1$ and $A^m\psi_p T_0(\tau/2)\chi_0$ are both of class $O_p(\tau^\infty)$. This proves (2.7).

We proceed to proving (2.8). This is verified in almost the same way as (2.7). We have

$$\begin{aligned}\Lambda_N(\tau) &\sim A^m\psi_p T_0(\tau/2)\eta_0 K(\tau)^{N-1}\eta_0 T_0(\tau/2)e^{-\tau V}\psi_q\\ &\sim A^m\psi_p T_0(\tau/2)\eta_0 T\big((N-1)\tau\big)\eta_0 T_0(\tau/2)e^{-\tau V}\psi_q\\ &\sim A^m\psi_p T_0(\tau/2)\eta_0 T\big((N-1)\tau\big)T_0(\tau/2)\eta_0 e^{-\tau V}\psi_q.\end{aligned}$$

The operator $A^m\eta_0 T\big((N-1)\tau\big)A$ is uniformly bounded by Lemma 2.1 (2) and

$$\|A^{-1}[T_0(\tau/2),\eta_0 e^{-\tau V}]\psi_q\| = O(\tau)$$

by Lemma 2.4 (2) with $g = \eta_0 e^{-\tau V} \in C_0^\infty(\mathbb{R}^n)$. Thus we have

$$\Lambda_N(\tau) \sim (A^m\psi_p A^{-m})\big(T_0(\tau/2)A^m\eta_0 T\big((N-1)\tau\big)\big)\eta_0 e^{-\tau V}T_0(\tau/2)\psi_q.$$

We further use Lemmas 2.3 (2), 2.4 (3) and (2.9) to obtain that

$$\begin{aligned}\Lambda_N(\tau) &\sim A^m\psi_p T\big((N-1)\tau\big)T_0(\tau/2)\eta_0 e^{-\tau V}T_0(\tau/2)\psi_q\\ &\sim A^m\psi_p T\big((N-1)\tau\big)\eta_1 T_0(\tau/2)\eta_0 e^{-\tau V}T_0(\tau/2)\psi_q\\ &\sim A^m\psi_p K(\tau)^{N-1}\eta_1 T_0(\tau/2)\eta_0 e^{-\tau V}T_0(\tau/2)\psi_q\\ &\sim A^m\psi_p K(\tau)^{N-1}T_0(\tau/2)e^{-\tau V}\eta_0 T_0(\tau/2)\psi_q\\ &\sim A^m\psi_p K(\tau)^{N-1}T_0(\tau/2)e^{-\tau V}T_0(\tau/2)\psi_q = A^m\psi_p K(\tau)^N\psi_q.\end{aligned}$$

This yields (2.8) and completes the proof of the proposition. □

We end the section by proving Lemmas 2.1 and 2.4.

Proof of Lemma 2.1. Throughout the proof, we often use the relation

$$[e^{-sX}, Y] = e^{-sX}Y - Ye^{-sX} = \int_0^s e^{-tX}[Y,X]e^{-(s-t)X}\,dt. \tag{2.10}$$

(1) We first deal with the operator $\Phi_m(s) = A^m \psi T(s) \omega A : L^2 \to L^2$ with $s \in [0,1]$. The uniform boundedness is shown by induction on $m \geqq 0$. We may assume that there exists $\eta \in C_0^\infty(\mathbb{R}^n)$ such that

$$\psi \prec \theta \prec \eta \tag{2.11}$$

for $\theta = 1 - \omega \in C_0^\infty(\mathbb{R}^n)$, and we set $\chi = 1 - \eta$. By assumption, $\psi\omega = 0$. Hence $\Phi(s)$ is represented in the integral form

$$\Phi_m(s) = \int_0^s T(s-t)[H, A^m\psi]T(t)\omega A\,dt$$

by making use of relation (2.10). The commutator in the integrand is calculated as

$$[H, A^m\psi] = A^m[H_0, \psi]\eta + [\eta V, A^m\psi]\eta + \chi V A^m \psi,$$

because $\psi\chi = 0$. We note that the third operator on the right-hand side takes the form

$$\chi V A^m \psi = V A^{-1}(A\chi A^m \psi A^L)A^{-L} = O_p(1)A^{-L}$$

for any $L \gg 1$. This follows by assumption (V) and by pseudodifferential calculus. In fact, the standard calculus of symbols shows that $A\chi A^m\psi A^L$ is a pseudodifferential operator with symbol of Hörmander class $S_{1,0}^{-N}$ for any $N \gg 1$, and hence $A\chi A^m \psi A^L = O_p(1)$. If we fix γ as $1/2 < \gamma < 1$ and set $d = \gamma - 1/2 > 0$, then we have

$$[H, A^m\psi] = A^\gamma O_p(1) A^{m-d}\eta + O_p(1)A^{-L}, \tag{2.12}$$

because $A^m[H_0, \psi]$ and $[\eta V, A^m\psi]$ are pseudodifferential operators with symbol class $S_{1,0}^{2m-1}$. As already stated in the previous section,

$$(H+1)^{-1}A, \quad A^{-1}(H+1) : L^2 \to L^2 \tag{2.13}$$

are bounded. We have

$$O_p(1)A^{-L}T(t)\omega A = O_p(1)\big(A^{-1}(H+1)\big)T(t)\big((H+1)^{-1}A\big)(A^{-1}\omega A) = O_p(1)$$

for the second operator $O_p(1)A^{-L}$ on the right-hand side of (2.12). We use the inductive assumption for the first operator $A^\gamma O_p(1)A^{m-d}\eta$ to get

$$\int_0^s \|T(s-t)A^\gamma O_p(1)A^{m-d}\eta T(t)\omega A\|\,dt = O(1)\int_0^s (s-t)^{-\gamma}\,dt = O(1).$$

It remains to check the case $m = 0$ in order that the induction goes well. To this end, we have only to show that

$$\|\Phi(s)\| = \left\| \int_0^s T(s-t)[H_0, \psi]\eta T(t)\omega A\,dt \right\| = O(1)$$

uniformly in s. By (2.11), $\operatorname{supp}\eta \cap \operatorname{supp}\omega = \emptyset$. We take the commutator between η and $T(t)$ to obtain that

$$\Phi(s) = \int_0^s \int_0^t T(s-t)[H_0, \psi]T(t-\sigma)[H_0, \eta]T(\sigma)\omega A \, d\sigma \, dt.$$

Since $[H_0, \psi] = A^{1/2}O_p(1)$ and $[H_0, \eta] = A^{3/4}O_p(1)A^{-1/4}$, $\Phi(s)$ obeys

$$\|\Phi(s)\| = O(1)\int_0^s \int_0^t (s-t)^{-1/2}(t-\sigma)^{-3/4}\sigma^{-3/4} \, d\sigma \, dt = O(1).$$

This enables us to push forward an inductive argument and we obtain the uniform boundedness of $\Phi_m(s) = A^m \psi T(s)\omega A$.

We proceed to the other operator $A^m \psi T(s)\psi A^{-m}$. By assumption, $V(x)$ is smooth on the support of ψ. Hence it follows by elliptic regularity and by interpolation that

$$A^m \psi (H+1)^{-m}, \quad (H+1)^m \psi A^{-m} : L^2 \to L^2$$

are bounded. This implies that

$$A^m \psi T(s)\psi A = \left(A^m \psi (H+1)^{-m}\right)T(s)\left((H+1)^m \psi A^{-m}\right)$$

is also bounded uniformly in $s \in [0, 1]$. Thus the proof of (1) is complete.

(2) As already seen, $A^m \psi (H+1)^{-m} : L^2 \to L^2$ is bounded and hence

$$\|A^m \psi T(s)\| = O(1)\|(H+1)^m \exp(-sH)\| = O(s^{-m}).$$

A similar argument applies to the second operator

$$A^m \psi T(s)A = A^m \psi (H+1)^{-m}\left((H+1)^{m+1}T(s)\right)(H+1)^{-1}A$$

and (2) is proved. □

Proof of Lemma 2.4. (1) Since ψ vanishes on the support of ω, (1) is shown as an immediate consequence of pseudodifferential calculus. This is also obtained by making repeated use of relation (2.10).

(2) The operator in (2) is represented as

$$A^m[g, T_0(\tau)]A^{-m-1/2} = \int_0^\tau T_0(s)(A^m[H_0, g]A^{-m-1/2})T_0(\tau - s) \, ds$$

by use of (2.10), and a pseudodifferential calculus shows that the integrand is uniformly bounded. This proves (2).

(3) We represent the commutator as

$$[A^m \psi T(s), T_0(\tau)] = \int_0^\tau T_0(t)[H_0, A^m \psi T(s)] T_0(\tau - t)\, dt.$$

The commutator in the integrand is further calculated as

$$[H_0, A^m \psi T(s)] = A^m [H_0, \psi] T(s) + A^m \psi H_0 T(s) - A^m \psi T(s) H_0.$$

If $s \geqq \delta > 0$, then it follows from Lemma 2.1 (2) that the first and second operators on the right-hand side are bounded, and the boundedness of the third operator also follows from the relation

$$A^m \psi T(s) H_0 = A^m \psi (H+1) T(s) \big((H+1)^{-1} H_0\big).$$

Thus (3) is proved. □

3. Properties of difference operator $D(\tau)$: Proof of Lemma 2.2

In this section we show some properties of operator $D(\tau)$ defined by (2.4) through a series of lemmas. Then Lemma 2.2 is obtained as a result of these lemmas. We use the constant α, $0 < \alpha < 1$, with the meaning ascribed in (1.7) in the statement of the lemmas.

Lemma 3.1. *The operator $D(\tau)$ has the following properties*:

(1) $D(\tau) A^{-\alpha} = O_p(\tau)$.

(2) $A^{-1} D(\tau) A^{-1} = O_p(\tau^2)$.

(3) $A D(\tau) A^{-\alpha} = O_p(1)$.

Proof. (1) We write $D(\tau)$ as

$$D(\tau) = \big(T(\tau) - T_0(\tau)\big) + \big(T_0(\tau) - K(\tau)\big) = F_1(\tau) + F_2(\tau) \tag{3.1}$$

and we represent $F_1(\tau)$ and $F_2(\tau)$ in the integral form

$$F_1(\tau) = -\int_0^\tau T(t) V T_0(\tau - t)\, dt, \quad F_2(\tau) = \int_0^\tau T_0(\tau/2) \exp(-tV) V T_0(\tau/2)\, dt.$$

Then it follows from (1.7) that $F_1(\tau) A^{-\alpha}$ and $F_2(\tau) A^{-\alpha}$ are both of class $O_p(\tau)$.

(2) If we decompose $A^{-1} T(\tau) A^{-1}$ into the product of three operators

$$A^{-1} T(\tau) A^{-1} = \big(A^{-1}(H+1)\big)\big((H+1)^{-1} T(\tau) (H+1)^{-1}\big)\big((H+1) A^{-1}\big),$$

then it follows from (2.13) that

$$A^{-1}T(\tau)A^{-1} = A^{-1}(1-\tau H)A^{-1} + O_p(\tau^2)$$

and also we have

$$\begin{aligned} A^{-1}K(\tau)A^{-1} &= A^{-1}T_0(\tau/2)(1-\tau V)T_0(\tau/2)A^{-1} + O_p(\tau^2) \\ &= A^{-1}(1-\tau H_0 - \tau V)A^{-1} + O_p(\tau^2) \end{aligned}$$

by (1.7). The two relations above yield (2).

(3) Let $F_1(\tau)$ and $F_2(\tau)$ be as in (3.1). Since $AT_0(\tau/2) = O_p(\tau^{-1})$, it is easy to see that $AF_2(\tau)A^{-\alpha} = O_p(1)$. We decompose $F_1(\tau)$ into the sum

$$F_1(\tau) = -\left(\int_0^{\tau/2} + \int_{\tau/2}^{\tau}\right) T(t)VT_0(\tau - t)\,dt = F_{11}(\tau) + F_{12}(\tau).$$

For the same reason as above, we see that $AF_{12}(\tau)A^{-\alpha} = O_p(1)$. On the other hand, $AF_{11}(\tau)A^{-\alpha}$ takes the form

$$\begin{aligned} AF_{11}(\tau)A^{-\alpha} &= \left(A(H+1)^{-1}\right)\int_0^{\tau/2} T'(t)VA^{-\alpha}T_0(\tau - t)\,dt + O_p(\tau) \\ &= O_p(1)\int_0^{\tau/2} T(t)VA^{-\alpha}H_0T_0(\tau - t)\,dt + O_p(1) \end{aligned}$$

by partial integration. Since $H_0T_0(\tau - t) = O_p(\tau^{-1})$ for t, $0 < t < \tau/2$, it follows that $AF_{11}(\tau)A^{-\alpha} = O_p(1)$. This proves (3). □

We here introduce some auxiliary operators. Let ψ, θ and η be as in (2.11). We define

$$H_1 = H_0 + W, \quad W = \eta V, \tag{3.2}$$

where $W = \eta V \in C_0^\infty(\mathbb{R}^n \to \mathbb{R})$. We further set

$$T_1(s) = \exp(-sH_1), \quad K_1(\tau) = T_0(\tau/2)\exp(-\tau W)T_0(\tau/2). \tag{3.3}$$

The semigroup $T_1(t)$ enjoys the same properties as in Lemma 2.1, and $D(\tau)$ is decomposed into the sum

$$D(\tau) = D_1(\tau) + D_2(\tau) + D_3(\tau), \tag{3.4}$$

where

$$D_1(\tau) = T(\tau) - T_1(\tau), \quad D_2(\tau) = T_1(\tau) - K_1(\tau), \quad D_3(\tau) = K_1(\tau) - K(\tau).$$

Lemma 3.2.

$$A^m\psi D_1(\tau) = O_p(\tau^\infty), \quad A^m\psi D_3(\tau) = O_p(\tau^\infty).$$

Proof. Let $\eta \in C_0^\infty(\mathbb{R}^n)$ be as in (3.2). We set $\chi = 1 - \eta$ for η as above. Then $\psi\chi = 0$. We represent $D_1(\tau)$ in the integral form

$$D_1(\tau) = -\int_0^\tau T_1(s)\chi V T(\tau - s)\, ds. \tag{3.5}$$

Since $A^m \psi T_1(s)\chi A = O_p(\tau^\infty)$ for s, $0 \leqq s \leqq \tau$, by pseudodifferential calculus, it follows from (1.7) that $A^m \psi D_1(\tau)$ is also of class $O_p(\tau^\infty)$. The operator $D_3(\tau)$ is represented in the integral form

$$\begin{aligned} D_3(\tau) &= T_0(\tau/2)(e^{-\tau W} - e^{-\tau V})T_0(\tau/2) \\ &= \int_0^\tau T_0(\tau/2)e^{-sW}\chi V e^{-(\tau-s)V} T_0(\tau/2)\, ds. \end{aligned} \tag{3.6}$$

Since $A^m \psi T_0(\tau/2)e^{-sW}\chi A = O_p(\tau^\infty)$, we have $A^m \psi D_3(\tau) = O_p(\tau^\infty)$. This completes the proof. □

Lemma 3.3. *Let $D_2(\tau)$ be as in* (3.4). *Then one has*:

(1) $A^m \psi D_2(\tau)\omega A = O_p(\tau^3)$.

(2) $A^m D_2(\tau) A^{-m+\kappa} = O_p(\tau^{2-\kappa})$ *for* κ, $0 \leqq \kappa \leqq 1$, *and if, in particular*, $m = 0$ *and* $\kappa = 0$, *then* $D_2(\tau) = O_p(\tau^2)$.

Proof. We first recall that $W = \eta V \in C_0^\infty(\mathbb{R}^n)$. The proof makes repeated use of relation (2.10). We calculate $K_1'(s) = (d/ds)K_1(s)$ as

$$K_1'(s) = -H_1 K_1(s) + R_1(s) + R_2(s),$$

where

$$R_1(s) = -[T_0(s/2), W]e^{-sW} T_0(s/2), \quad R_2(s) = -T_0(s/2)[e^{-sW}, H_0/2]T_0(s/2).$$

We can further calculate the remainder terms as follows:

$$R_1(s) = R_0(s) + R_{10}(s), \quad R_2(s) = -R_0(s) + R_{20}(s),$$

where $R_0(s) = sT_0(s/2)[H_0/2, W]e^{-sW}T_0(s/2)$, and

$$R_{10}(s) = \int_0^s \int_0^t T_0\big((s-\sigma)/2\big)[H_0/2, [H_0/2, W]]T_0(\sigma/2)e^{-sW}T_0(s/2)\, d\sigma\, dt,$$

$$R_{20}(s) = -\int_0^s \int_0^t T_0(s/2)e^{-\sigma W}[W, [W, H_0/2]]e^{-(s-\sigma)W}T_0(s/2)\, d\sigma\, dt.$$

Hence the Duhamel principle yields

$$D_2(\tau) = -\int_0^\tau T_1(\tau - s)\big(R_{10}(s) + R_{20}(s)\big)\, ds. \tag{3.7}$$

(1) Note that $\psi \in C_0^\infty(\mathbb{R}^n)$ vanishes on the support of ω. We see by pseudodifferential calculus that the two operators

$$A^m \psi T_1(\tau - s) T_0\big((s-\sigma)/2\big)[H_0/2, [H_0/2, W]] T_0(\sigma/2) e^{-sW} T_0(s/2)\omega A : L^2 \to L^2$$

and

$$A^m \psi T_1(\tau - s) T_0(s/2) e^{-\sigma W}[W, [W, H_0/2]] e^{-(s-\sigma)W} T_0(s/2)\omega A : L^2 \to L^2$$

are bounded uniformly in σ, t and s. This yields the desired relation.

(2) The two double commutators in the integrand satisfy

$$[H_0, [H_0, W]] = A^{-m+1/2} O_p(1) A^{m+1/2}, \quad [W, [W, H_0]] = A^{-m} O_p(1) A^m$$

by pseudodifferential calculus, and also it is easy to see that $A^m T_1(s) A^{-m}$ and $A^m e^{-sW} A^{-m}$ are bounded uniformly in $s \in [0, \tau]$. Hence we have

$$\begin{aligned} \|A^m D_2(\tau) A^{-m+\kappa}\| &= O(1) \int_0^\tau \int_0^s \int_0^t (\tau - s)^{-1/2} s^{-(1/2+\kappa)}\, d\sigma\, dt\, ds \\ &= O(1) \int_0^\tau (\tau - s)^{-1/2} s^{3/2-\kappa}\, ds = O(\tau^{2-\kappa}). \end{aligned}$$

This proves (2). □

Lemma 2.2 is obtained as an immediate consequence of Lemmas 3.1, 3.2 and 3.3.

Proof of Lemma 2.2. (1) is nothing but Lemma 3.1 (2), and (2) and (3) follow from Lemmas 3.2 and 3.3 at once. □

The lemma below is used for proving Lemma 2.3 in section 4.

Lemma 3.4. *Let $\theta = 1 - \omega \in C_0^\infty(\mathbb{R}^n)$. Then $A\omega D(\tau)\theta = O_p(\tau)$.*

Proof. We decompose $D(\tau)$ into the sum (3.4). The integral representation (3.5) of $D_1(\tau)$ admits the decomposition

$$D_1(\tau) = -\left\{ \int_0^{\tau/2} + \int_{\tau/2}^{\tau} \right\} T(s) V \chi T_1(\tau - s)\, ds = D_{11}(\tau) + D_{12}(\tau).$$

We note that θ vanishes on the support of $\chi = 1 - \eta$. Since $A\omega T(s) = O_p(\tau^{-1})$ for s, $\tau/2 < s < \tau$, and since $A^\alpha \chi T_1(\tau - s)\theta = O_p(\tau^\infty)$, it follows that

$$A\omega D_{12}(\tau)\theta = O_p(\tau^\infty). \tag{3.8}$$

By partial integration, $A\omega D_{11}(\tau)\theta$ takes the form

$$A\omega D_{11}(\tau)\theta = \big(A\omega(H+1)^{-1}\big)\int_0^{\tau/2}\big(T'(s)-T(s)\big)V\chi T_1(\tau-s)\theta\,ds$$

$$= O_p(1)\int_0^{\tau/2} T(s)V\chi H_1 T_1(\tau-s)\theta\,ds + O_p(\tau^\infty),$$

and hence $A\omega D_{11}(\tau)\theta = O_p(\tau^\infty)$. This, together with (3.8), implies that $A\omega D_1(\tau)\theta$ is of class $O_p(\tau^\infty)$. We use Lemma 3.3 (2) with $m=\kappa=1$ to obtain that

$$A\omega D_2(\tau)\theta = (A\omega A^{-1})AD_2(\tau)\theta = O_p(\tau).$$

We consider $A\omega D_3(\tau)\theta$. By (3.6), this is represented as

$$A\omega D_3(\tau)\theta = \big(A\omega T_0(\tau/2)\big)\int_0^{\tau} e^{-(\tau-s)V}(VA^{-\alpha})\big(A^\alpha\chi e^{-sW}T_0(\tau/2)\theta\big)\,ds.$$

We have $A\omega T_0(\tau/2) = O_p(\tau^{-1})$ and $A^\alpha\chi e^{-sW}T_0(\tau/2)\theta = O_p(\tau^\infty)$, so that $A\omega D_3(\tau)\theta$ is of class $O_p(\tau^\infty)$. Thus the proof is complete. □

4. Proof of Lemma 2.3

The section is devoted to proving Lemma 2.3.

Proof of Lemma 2.3. (1) We prove by induction on k, $0 \leqq k \leqq N$, that

$$\|A\omega K(\tau)^k\psi\| \leqq M$$

for some constant $M>0$ independent of τ and k. The case $k=0$ is obvious. We assume as an inductive assumption that

$$\|A\omega K(\tau)^l\psi\| \leqq M, \quad 0 \leqq l \leqq k-1, \tag{4.1}$$

for some $M>0$. We may also assume that $k \gg 1$ large enough. In fact, it can be seen from the argument below that $\|A\omega K(\tau)^l\psi\| \leqq M_0$ for $0 \leqq l \leqq k_0$, M_0 being independent of τ, provided that k_0 is fixed. We now write $A\omega K(\tau)^k\psi$ as

$$A\omega K(\tau)^k\psi = A\omega T(k\tau)\psi - \sum_{j=1}^{k}\Lambda_{jk}(\tau),$$

where

$$\Lambda_{jk}(\tau) = A\omega T\big((j-1)\tau\big)D(\tau)K(\tau)^{k-j}\psi, \quad 1 \leqq j \leqq k.$$

By Lemma 2.1 (1), we have

$$\|A\omega T(k\tau)\psi\| = O(1) \tag{4.2}$$

uniformly in k. We evaluate each operator $\Lambda_{jk}(\tau)$, and we show that there exists ρ, $0 < \rho < 1$, such that

$$\sum_{j=1}^{k} \|\Lambda_{jk}\| \leqq C + cM^{\alpha} + \rho M \tag{4.3}$$

for some constants c, $C > 0$ independent of k, M being as in (4.1). This, together with (4.2), implies that

$$\|A\omega K(\tau)^{k}\psi\| \leqq C + cM^{\alpha} + \rho M$$

for another $C > 0$. Hence we can take $M > 0$ so large that (4.1) is still true for $j = k$, and hence the desired uniform boundedness is obtained.

We start with

$$\Lambda_{1k}(\tau) = A\omega D(\tau)(\theta + \omega)K(\tau)^{k-1}\psi.$$

By Lemmas 3.1 and 3.4, we have $\|AD(\tau)A^{-\alpha}\| = O(1)$ and $\|A\omega D(\tau)\theta\| = O(1)$. Hence, by interpolation, it follows from (4.1) that

$$\|\Lambda_{1k}(\tau)\| = O(1) + O(1)\|A^{\alpha}\omega K(\tau)^{k-1}\psi\| = O(1) + O(1)M^{\alpha}. \tag{4.4}$$

Next we evaluate $\Lambda_{jk}(\tau)$ with $2 \leqq j < L < k$, where $L \gg 1$ is determined later. We decompose it into the sum

$$\Lambda_{jk}(\tau) = A\omega T\big((j-1)\tau\big)D(\tau)(\omega + \theta)K(\tau)^{k-j}\psi = \Lambda_{jk1}(\tau) + \Lambda_{jk2}(\tau).$$

Note that $L\tau \leqq N\tau = 1$. Since $A\omega T\big((j-1)\tau\big)$ is bounded by

$$\|A\omega(H+1)^{-1}\| \times \big\|(H+1)T\big((j-1)\tau\big)\big\| = (j-1)^{-1}O(\tau^{-1}) \tag{4.5}$$

and since $D(\tau)\omega = \big(D(\tau)A^{-\alpha}\big)A^{\alpha}\omega = O_p(\tau)A^{\alpha}\omega$ by Lemma 3.1, we have

$$\sum_{j=2}^{L-1} \|\Lambda_{jk1}(\tau)\| = O(1)\left(\sum_{j=2}^{L-1}(j-1)^{-1}\right)M^{\alpha} = O(1)\log L \times M^{\alpha}$$

by interpolation again. On the other hand, the sum

$$\sum_{j=2}^{L-1} \|\Lambda_{jk2}(\tau)\| = O(1)$$

is uniformly bounded, because $D(\tau)\theta = O_p(\tau^2)$ by Lemma 2.2. This, together with (4.4), implies that

$$\sum_{j=1}^{L-1} \|\Lambda_{jk}(\tau)\| = O(1) + O(1)\log L \times M^{\alpha}. \tag{4.6}$$

We consider $\Lambda_{jk}(\tau)$ with $L \leqq j \leqq k$. We decompose it into the sum

$$\Lambda_{jk}(\tau) = \Lambda_{jk3}(\tau) + \Lambda_{jk4}(\tau) + \Lambda_{jk5}(\tau),$$

where

$$\Lambda_{jk3}(\tau) = A\omega T\big((j-1)\tau\big)\omega D(\tau)\omega K(\tau)^{k-j}\psi,$$
$$\Lambda_{jk4}(\tau) = A\omega T\big((j-1)\tau\big)\omega D(\tau)\theta K(\tau)^{k-j}\psi,$$
$$\Lambda_{jk5}(\tau) = A\omega T\big((j-1)\tau\big)\theta D(\tau)K(\tau)^{k-j}\psi.$$

Now let ρ be fixed as $0 < \rho < 1$. We use the inductive assumption (4.1) for

$$\Lambda_{jk3}(\tau) = \big(A\omega T\big((j-1)\tau\big)\omega A\big)\big(A^{-1}D(\tau)A^{-1}\big)\big(A\omega K(\tau)^{k-j}\psi\big).$$

Since $A\omega T\big((j-1)\tau\big)\omega A$ obeys

$$\big\|A\omega T\big((j-1)\tau/2\big)T\big((j-1)\tau/2\big)\omega A\big\| = (j-1)^{-2}O(\tau^{-2})$$

by (4.5) and since $A^{-1}D(\tau)A^{-1} = O_p(\tau^2)$ by Lemma 2.2, we can take $L \gg 1$ so large that

$$\sum_{j=L}^{k}\|\Lambda_{jk3}(\tau)\| = O(1)\left(\sum_{j=L}^{k}(j-1)^{-2}\right)M \leqq \rho M, \tag{4.7}$$

because $\sum_{j=L}^{\infty} j^{-2} \to 0$ as $L \to \infty$. Since $D(\tau)\theta = O_p(\tau^2)$ by Lemma 2.2, we have

$$\sum_{j=L}^{k}\big(\|\Lambda_{jk4}(\tau)\| + \|\Lambda_{jk5}(\tau)\|\big) = \left(\sum_{j=L}^{k}(j-1)^{-1}\right)O(\tau) = O(1). \tag{4.8}$$

Thus we combine (4.6)~(4.8) to obtain (4.3) and the proof of (1) is complete.

(2) This is verified by induction on $m \geqq 0$. The case $m = 0$ is obvious. We write $A^m\psi K(\tau)^k$ as

$$A^m\psi K(\tau)^k = A^m\psi T(k\tau) - \sum_{j=1}^{k}\Gamma_{jk}(\tau),$$

where

$$\Gamma_{jk}(\tau) = A^m\psi T\big((j-1)\tau\big)D(\tau)K(\tau)^{k-j}, \quad 1 \leqq j \leqq k.$$

By Lemma 2.1, the first operator on the right-hand side obeys

$$\|A^m\psi T(k\tau)\| = k^{-m}O(\tau^{-m}).$$

We assert that

$$\sum_{j=1}^{k} \|\Gamma_{jk}(\tau)\| = k^{-m} O(\tau^{-m}) \tag{4.9}$$

uniformly in k, $1 \leqq k \leqq N$, which implies (2). We may assume that $k \gg 1$. By Lemma 3.1, $\|A^{-1}D(\tau)\| = O(\tau)$. If $[k/2] < j \leqq k$, then

$$\big\|A^m \psi T\big((j-1)\tau\big)A\big\| = k^{-m-1} O(\tau^{-m-1})$$

by Lemma 2.1. This implies that $\|\Gamma_{jk}(\tau)\| = k^{-m-1}O(\tau^{-m})$, and hence

$$\sum_{j=[k/2]+1}^{k} \|\Gamma_{jk}(\tau)\| = k^{-m} O(\tau^{-m}). \tag{4.10}$$

Next we assume that $1 \leqq j \leqq [k/2]$. Let $\eta \in C_0^\infty(\mathbb{R}^n)$ be as in (2.11) and let $D_j(\tau)$, $1 \leqq j \leqq 3$, be as in (3.4). Recall that $\theta \prec \eta$, $\theta + \omega = 1$ and $\eta + \chi = 1$. We decompose $\Gamma_{jk}(\tau)$ into the sum

$$\Gamma_{jk}(\tau) = \Gamma_{jk1}(\tau) + \Gamma_{jk2}(\tau) + \Gamma_{jk3}(\tau) + \Gamma_{jk4}(\tau),$$

where

$$\Gamma_{jk1}(\tau) = A^m \psi T\big((j-1)\tau\big) D_1(\tau) K(\tau)^{k-j},$$

$$\Gamma_{jk2}(\tau) = A^m \psi T\big((j-1)\tau\big) D_2(\tau) \chi K(\tau)^{k-j},$$

$$\Gamma_{jk3}(\tau) = A^m \psi T\big((j-1)\tau\big) D_2(\tau) \eta K(\tau)^{k-j},$$

$$\Gamma_{jk4}(\tau) = A^m \psi T\big((j-1)\tau\big) D_3(\tau) K(\tau)^{k-j}.$$

The two operators $D_1(\tau)$ and $D_3(\tau)$ are easily seen from the integral representation (3.5) and (3.6) to obey $A^{-1}D_1(\tau) = O_p(\tau)$ and $A^{-1}D_3(\tau) = O_p(\tau)$. If we write $\Gamma_{jk1}(\tau)$ as

$$\Gamma_{jk1}(\tau) = \Big(\big(B_j(\tau)\omega A\big)A^{-1}D_1(\tau) + \big(B_j(\tau)A^{-m}\big)\big(A^m \theta D_1(\tau)\big)\Big)K(\tau)^{k-j}$$

with $B_j(\tau) = A^m \psi T\big((j-1)\tau\big)$, it follows by Lemmas 2.1 and 3.2 that $\Gamma_{jk1}(\tau) = O_p(\tau)$, and hence

$$\sum_{j=1}^{[k/2]} \|\Gamma_{jk1}(\tau)\| = O(1) = k^{-m} O(\tau^{-m}), \tag{4.11}$$

because $k \leqq N = 1/\tau$. A similar argument applies to $\Gamma_{jk4}(\tau)$, and we get

$$\sum_{j=1}^{[k/2]} \|\Gamma_{jk4}(\tau)\| = k^{-m} O(\tau^{-m}). \tag{4.12}$$

We can also show in a similar way that

$$\sum_{j=1}^{[k/2]} \|\Gamma_{jk2}(\tau)\| = k^{-m} O(\tau^{-m}). \tag{4.13}$$

In fact, we write $\Gamma_{jk2}(\tau) = B_j(\tau) D_2(\tau) \chi K(\tau)^{k-j}$ and decompose $B_j(\tau) D_2(\tau) \chi$ into the sum

$$B_j(\tau) D_2(\tau) \chi = \big(B_j(\tau)\omega\big) D_2(\tau)\chi + \big(B_j(\tau) A^{-m}\big) A^m \theta D_2(\tau)\chi.$$

Then it follows from Lemmas 2.1 and 3.3 that $\Gamma_{jk2}(\tau) = O_p(\tau^2)$, and hence (4.13) is obtained. The inductive assumption is used for

$$\Gamma_{jk3}(\tau) = \big(B_j(\tau) A^{-m}\big)\big(A^m D_2(\tau) A^{-m+1/2}\big) A^{m-1/2} \eta K(\tau)^{k-j}.$$

Then the third factor obeys

$$\|A^{m-1/2} \eta K(\tau)^{k-j}\| = k^{-m+1/2} O(\tau^{-m+1/2}), \quad 1 \leqq j \leqq [k/2],$$

by inductive assumption. By Lemma 3.3 (2) with $\kappa = 1/2$, $A^m D_2(\tau) A^{-m+1/2} = O_p(\tau^{3/2})$, and hence we have

$$\sum_{j=1}^{[k/2]} \|\Gamma_{jk3}(\tau)\| = k^{-m+1/2} O(\tau^{-m+1}) = k^{-m} O(\tau^{-m}) \tag{4.14}$$

by Lemma 2.1. We combine (4.10) and (4.11)$\sim$(4.14) to get (4.9), and the proof of (2) is complete. $\square$

5. Approximation to heat kernel generated by Dirichlet Laplacian

This section is devoted to proving Theorem 1.2. Recall that $E_D(x, y; t)$ is the kernel of the semigroup $T_D(t) = \exp(-tH_D) : L^2(\Omega) \to L^2(\Omega)$ generated by the Dirichlet Laplacian H_D and that $G_{ND}(x, y; t)$ is the integral kernel of the operator $G_{ND}(t)$ defined by (1.11), where Ω is assumed to be a bounded domain with smooth boundary. It seems to be difficult to evaluate directly the difference between two kernels $E_D(x, y; t)$ and $G_{ND}(x, y; t)$. The strategy is to introduce the Schrödinger operator with confining potential with large coupling constant as an auxiliary operator. We set $\tau = t/N \ll 1$ for $t > 0$ fixed and we write U for the multiplication by the characteristic function of the complement Ω^c of domain Ω. Then we define

$$H_\tau = H_0 + U_\tau = H_0 + \tau^{-\nu} U, \quad T_\tau(s) = \exp(-sH_\tau)$$

and

$$\Pi(\tau) = \exp(-\tau U_\tau) T_0(\tau) = \exp(-\tau^{1-\nu} U) \exp(-\tau H_0)$$

with constant ν, $0 < \nu < 1/2$. These operators act on $L^2(\mathbb{R}^n)$ and the constant ν is determined as $\nu = 1/3$ in the course of the proof of Theorem 1.2. For two real smooth functions

$\psi, \eta \in C_0^\infty(\Omega)$ with support in Ω, we use the notation $\psi \prec \eta$ with the meaning $\psi\eta = \psi$ ascribed in (2.1) and we often regard a function with support in Ω as a function over the whole space $\mathbb{R}^n$ in a natural way. The proof of Theorem 1.2 is based on the following two propositions.

Proposition 5.1. *Let $\psi \in C_0^\infty(\Omega)$. Then*

$$\left\| \psi\big(T_D(s) - T_\tau(s)\big)\psi \right\|_m = O(\tau^\sigma), \quad \tau \to 0,$$

for any $m \geqq 0$, where σ satisfies $0 < \sigma < \nu/2$ and the error bound is locally uniform in $s > 0$ $(s \in [1/c, c], c > 1)$.

Proposition 5.2. *Let $\psi \in C_0^\infty(\Omega)$ and set $\Pi_{N\tau}(t) = \Pi(\tau)^N$. Then*

$$\left\| \psi\big(T_\tau(t) - \Pi_{N\tau}(t)\big)\psi \right\| = O(\tau^{1/2-\nu}|\log \tau|)$$

and

$$\left\| \psi\big(T_\tau(t) - \Pi_{N\tau}(t)\big)\psi \right\|_m + \left\| \psi\big(T_\tau(t) - \Pi_{N\tau}(t)^*\big)\psi \right\|_m = O(\tau^{-1-\nu})$$

locally uniformly in $t > 0$.

We complete the proof of Theorem 1.2 before proving these propositions. Propositions 5.1 and 5.2 are proved at the end of this section and in the next section respectively.

Proof of Theorem 1.2. We denote by $E_\tau(x, y; t)$ and $\Pi_{N\tau}(x, y; t)$ the integral kernels of operators $\exp(-tH_\tau)$ and $\Pi_{N\tau}(t)$ respectively. By the maximum principle, we know that $0 \leqq E_D(x, y; s) \leqq E_0(x, y; s)$, where $E_0(x, y; s)$ is the heat kernel of $T_0(s) = \exp(-sH_0)$. Hence it follows that

$$0 \leqq E_D(x, y; t) \leqq G_{ND}(x, y; t) \leqq \Pi_{N\tau}(x, y; t)$$

over $\Omega \times \Omega$. We estimate the difference $E_D(x, y; t) - G_{ND}(x, y; t)$ in question as

$$\begin{aligned} (5.1) \qquad & |E_D(x, y; t) - G_{ND}(x, y; t)| \\ & \leqq \Pi_{N\tau}(x, y; t) - E_D(x, y; t) \\ & = \big(\Pi_{N\tau}(x, y; t) - E_\tau(x, y; t)\big) + \big(E_\tau(x, y; t) - E_D(x, y; t)\big). \end{aligned}$$

Let $\psi \in C_0^\infty(\Omega)$. By Proposition 5.1 and Lemma 1.1, we see that the second term on the right-hand side of (5.1) obeys

$$\left| \psi\big(E_\tau(x, y; t) - E_D(x, y; t)\big)\psi \right| = O(\tau^\sigma)$$

for any σ, $0 < \sigma < \nu/2$, and Proposition 5.2 enables us to take $m \gg 1$ so large that the first term satisfies

$$\left| \psi\big(\Pi_{N\tau}(x, y; t) - E_\tau(x, y; t)\big)\psi \right| = O(\tau^\mu)$$

for any μ, $0 < \mu < 1/2 - \nu$. We now choose $\nu = 1/3$. Then $\nu/2 = 1/2 - \nu = 1/6$ and we obtain that $E_D(x, y; t) - G_{ND}(x, y; t)$ obeys the desired bound $O(\tau^\sigma)$, $0 < \sigma < 1/6$. □

Remark 5.1. We note that the convergence in Theorem 1.2 is still valid in the C^∞ sense. Roughly speaking, this is verified in the following way. By Theorem 1.2, it follows that $\|\psi(T_D(t) - G_{ND}(t))\psi\| = O(\tau^\sigma)$ for any σ, $0 < \sigma < 1/6$. We can also show that

$$\|H_D^m \psi(T_D(t) - G_{ND}(t))\psi\| = O(\tau^{-1})$$

for any $m \gg 1$ as an operator acting on $L^2(\Omega)$. This, together with Lemma 1.1, yields the desired result. We are going to discuss the detailed matter elsewhere.

We end the section by proving Proposition 5.1.

Proof of Proposition 5.1. Recall that $J : L^2 = L^2(\mathbb{R}^n) \to L^2(\Omega)$ is the restriction defined by $(Jf)(x) = f(x)$ for $x \in \Omega$. The proof relies on [3], Theorem 3.3 (see [2], Theorem 8.31 also). According to the theorem, $JT_\tau(s) - T_D(s)J$ satisfies

$$\|JT_\tau(s) - T_D(s)J\| \leqq g_\sigma(s)\tau^\sigma, \quad s > 0, \tag{5.2}$$

as a bounded operator from L^2 to $L^2(\Omega)$, where $\sigma > 0$ is as in the proposition, and $g_\sigma(s)$ is locally integrable over $[0, \infty)$. It should be noted that $g_\sigma(s)$ is integrable near $s = 0$. Let $\varphi, \eta \in C_0^\infty(\Omega)$ with $0 \leqq \varphi, \eta \leqq 1$. Then it follows from (5.2) that

$$\|\eta(T_\tau(s) - T_D(s))\varphi\| \leqq g_\sigma(s)\tau^\sigma. \tag{5.3}$$

We set $w(t) = \varphi(u(t) - v(t))$, where $u(t) = T_D(t)\varphi f$ and $v(t) = T_\tau(t)\varphi f$ with $f \in L^2$. Then w solves

$$\partial_t w + H_0 w = [\varphi, H_0](v - u), \quad w(0) = 0.$$

The solution $w(t)$ is given by the Duhamel principle

$$w(t) = \int_0^t T_0(t - s)[\varphi, H_0](v(s) - u(s))\, ds.$$

We may assume that $\psi \prec \varphi \prec \eta$. Then ψ vanishes and $\eta = 1$ on the support of $\nabla\varphi$. Hence $A^m \psi T_0(s)[\varphi, H_0] : L^2 \to L^2$ is bounded uniformly in $s \geqq 0$, and we obtain

$$\|A^m \psi(T_D(t) - T_\tau(t))\psi\| = O(\tau^\sigma)$$

by (5.3). This proves the proposition. □

6. Proof of Proposition 5.2

The proof of Proposition 5.2 is based on the idea from Rogava [15]. We begin by stating a series of lemmas used in proving the proposition. Let $A = H_0 + 1$ be as in (1.6). We define

$$A_\tau = A + U_\tau = A + \tau^{-\nu} U, \quad S_\tau(s) = \exp(-sA_\tau)$$

and

$$\Lambda(\tau) = \exp(-\tau U_\tau) S_0(\tau) = \exp(-\tau^{1-\nu} U) S_0(\tau),$$

where $S_0(s) = \exp(-sA)$. According to the above notation, the difference $T_\tau(t) - \Pi(\tau)^N$ in Proposition 5.2 is represented as

$$T_\tau(t) - \Pi(\tau)^N = e^t \big(S_\tau(t) - \Lambda(\tau)^N \big)$$

and hence it suffices to prove the proposition for $S_\tau(t) - \Lambda(\tau)^N$.

Lemma 6.1. *The operators A and A_τ satisfy the following relations*:

(1) $A_\tau^{-1/2} A^{1/2} = O_p(1)$.

(2) $A_\tau^{-1} A = O_p(\tau^{-\nu/2})$.

(3) $A_\tau^{1/2} A^{-1/2} = O_p(\tau^{-\nu/2})$.

Lemma 6.2. *Let $m \geqq 0$. Suppose that $\psi \prec \theta$, and set $\omega = 1 - \theta$. Then $S_\tau(s)$ obeys the following bounds uniformly in $s \in [0, t]$, $t > 0$ being fixed*:

(1) $A^m \psi S_\tau(s) \psi A^{-m} = O_p(1)$.

(2) $A^m \psi S_\tau(s) \omega = O_p(\tau^{-\nu})$.

Lemma 6.3. *Let $\Gamma(\tau)$ be defined by*

$$\Gamma(\tau) = S_0(\tau/2) \exp(-\tau U_\tau) S_0(\tau/2) = S_0(\tau/2) \exp(-\tau^{1-\nu} U) S_0(\tau/2),$$

and let $E_A(\lambda)$, $\lambda > 0$, be the spectral resolution associated with $A = H_0 + 1$. Set $P_\tau = E_A\big((0, 1/\tau)\big)$ and $Q_\tau = \mathrm{Id} - P_\tau$. Then $\Gamma(\tau)^j$ takes the form

$$\Gamma(\tau)^j = (\tau^{-1/2} A^{-1/2} P_\tau + Q_\tau) B_j(\tau), \quad 1 \leqq j \leqq N,$$

where $B_j(\tau) : L^2 \to L^2$ obeys the bound $\|B_j(\tau)\| = O(j^{-1/2})$ uniformly in τ.

Lemma 6.4. *Let $\psi \in C_0^\infty(\Omega)$. Define*

$$R(\tau) = S_\tau(\tau) - \Gamma(\tau), \quad \tilde{R}(\tau) = S_\tau(\tau) - \Lambda(\tau). \tag{6.1}$$

Then these two operators have the following properties:

(1) $A^m \psi R(\tau) = O_p(\tau^\infty)$ *and similarly for* $\tilde{R}(\tau)$.

(2) $A_\tau^{-1} R(\tau) A^{-1/2} = O_p(\tau^{3/2-\nu})$.

(3) $A_\tau^{-1} R(\tau) = O_p(\tau^{1-\nu})$.

We prove these lemmas after completing the proof of Proposition 5.2. For brevity, we prove the proposition and lemmas for the case $t = 1$ only, so that $\tau = 1/N$.

Proof of Proposition 5.2. Let $\Gamma(\tau)$ be as in Lemma 6.3. We first prove that

$$\|\psi(S_\tau(1) - \Gamma(\tau)^N)\psi\| = O(\tau^{1/2-\nu}|\log\tau|). \tag{6.2}$$

The difference is represented as

$$\psi(S_\tau(1) - \Gamma(\tau)^N)\psi = \psi(S_\tau(\tau)^N - \Gamma(\tau)^N)\psi = \sum_{k=1}^{N} X_k(\tau),$$

where $X_k(\tau) = \psi S_\tau((k-1)\tau)R(\tau)\Gamma(\tau)^{N-k}\psi$ and $R(\tau)$ is defined by (6.1). If $k = 1$ or N, then it follows from Lemma 6.4 that $X_1(\tau) = O_p(\tau^\infty)$ and $X_N(\tau) = O_p(\tau^\infty)$. When $2 \leqq k \leqq N-1$, we decompose $X_k(\tau)$ into the product

$$X_k(\tau) = (\psi S_\tau((k-1)\tau)A_\tau)(A_\tau^{-1}R(\tau))(\tau^{-1/2}A^{-1/2}P_\tau + Q_\tau)B_{N-k}(\tau)\psi$$

by Lemma 6.3. Hence $X_k(\tau)$ obeys

$$\|X_k(\tau)\| = (k-1)^{-1}(N-k)^{-1/2}O(\tau^{-\nu})$$

by Lemmas 6.3 and 6.4. This implies (6.2). Once (6.2) is established, we can show in almost the same way as in the proof of Proposition 1.1 that

$$\|\psi(S_\tau(1) - \Lambda(\tau)^N)\psi\| = O(\tau^{1/2-\nu}|\log\tau|).$$

We skip the details.

Next we shall show that

$$\|A^m\psi(S_\tau(1) - \Lambda(\tau)^N)\psi\| = O(\tau^{-1-\nu}) \tag{6.3}$$

for any $m > 0$. To prove this, we write

$$A^m\psi(S_\tau(1) - \Lambda(\tau)^N)\psi = \sum_{k=1}^{N} Y_k(\tau),$$

where $Y_k(\tau) = A^m\psi S_\tau((k-1)\tau)\tilde{R}(\tau)\Lambda(\tau)^{N-k}\psi$ and $\tilde{R}(\tau)$ is as in Lemma 6.4. Let $\psi \prec \theta \prec \eta$ and set $\omega = 1 - \theta$. Then $Y_k(\tau)$ admits the decomposition

$$\begin{aligned} Y_k(\tau) = {} & (A^m\psi S_\tau((k-1)\tau)\omega)\tilde{R}(\tau)\Lambda(\tau)^{N-k}\psi \\ & + (A^m\psi S_\tau((k-1)\tau)\theta A^{-m})(A^m\eta\tilde{R}(\tau))\Lambda(\tau)^{N-k}\psi. \end{aligned}$$

By Lemma 6.2, the first operator on the right-hand side obeys the bound $O(\tau^{-\nu})$, and by Lemmas 6.2 and 6.4, the second one obeys $O(\tau^\infty)$. Hence (6.3) is obtained. We can show in a similar way that

$$\left\|A^m\psi\left(S_\tau(1)-\left(\Lambda(\tau)^*\right)^N\right)\psi\right\| = O(\tau^{-1-\nu})$$

for any $m > 0$. Thus the proof of the proposition is complete. □

It remains to prove Lemmas 6.1∼6.4.

Proof of Lemma 6.1. (1) Since $A_\tau \geqq A$ and $A_\tau \geqq \tau^{-\nu}U$ in the form sense, (1) follows at once.

(2) Similarly we have

$$UA_\tau^{-1/2} = O_p(\tau^{\nu/2}). \tag{6.4}$$

If we write $A_\tau^{-1}A = 1 - \tau^{-\nu}A_\tau^{-1}U$, then (2) follows from (6.4).

(3) We calculate

$$A_\tau A^{-1} = 1 + \tau^{-\nu}UA^{-1} = O_p(\tau^{-\nu}).$$

Hence (3) is obtained by interpolation. □

Proof of Lemma 6.2. (1) Since ψ has support in Ω, it follows by elliptic regularity and by interpolation that

$$A^m\psi S_\tau(s)\psi A^{-m} = (A^m\psi A_\tau^{-m})S_\tau(s)(A_\tau^m\psi A^{-m}) = O_p(1)$$

uniformly in s.

(2) We represent $S_\tau(s)$ as

$$S_\tau(s) = S_0(s) - \tau^{-\nu}\int_0^s S_0(t)US_\tau(s-t)\,dt.$$

As is easily seen, $A^m\psi S_0(s)\omega = O_p(1)$ and $A^m\psi S_0(s)U = O_p(1)$. Hence we have $A^m\psi S_\tau(s)\omega = O_p(\tau^{-\nu})$. □

Proof of Lemma 6.3. We first note that

$$0 \leqq \Gamma(\tau) \leqq S_0(\tau) \leqq 1 \tag{6.5}$$

in the form sense. We decompose $\Gamma(\tau)^j$ into the product

$$\Gamma(\tau)^j = E_j(\tau)(\tau^{-1/2}A^{-1/2}P_\tau + Q_\tau),$$

where $E_j(\tau) = F_j(\tau)L(\tau)L_0(\tau)$ with $F_j(\tau) = \Gamma(\tau)^j\left(1-\Gamma(\tau)\right)^{1/2}$, and

$$L(\tau) = \left(1-\Gamma(\tau)\right)^{-1/2}\left(1-S_0(\tau)\right)^{1/2},$$

$$L_0(\tau) = \left(1-S_0(\tau)\right)^{-1/2}(\tau^{1/2}A^{1/2}P_\tau + Q_\tau).$$

It is easy to see that $\|F_j(\tau)\| = O(j^{-1/2})$ uniformly in τ, and also it follows from (6.5) that $\|L(\tau)\| \leqq 1$. There exists $c > 0$ such that $(1 - e^{-\lambda})^{-1/2}\lambda^{1/2} \leqq c$ for $0 < \lambda \leqq 1$ and $(1 - e^{-\lambda})^{-1/2} \leqq c$ for $\lambda \geqq 1$. This implies that $\|L_0(\tau)\| \leqq c$. If we put $B_j(\tau) = E_j(\tau)^*$, then we combine these estimates to obtain the lemma. □

Proof of Lemma 6.4. (1) We decompose $R(\tau)$ into the sum

$$R(\tau) = \big(S_\tau(\tau) - S_0(\tau)\big) + \big(S_0(\tau) - \Gamma(\tau)\big) = R_1(\tau) + R_2(\tau).$$

The first operator $R_1(\tau)$ is represented in the integral form

$$R_1(\tau) = -\tau^{-\nu} \int_0^\tau S_0(s)US_\tau(\tau - s)\,ds.$$

As is easily seen, $A^m\psi S_0(s)U = O_p(\tau^\infty)$ uniformly in $s \in [0, \tau]$, and hence $A^m\psi R_1(\tau)$ is of class $O_p(\tau^\infty)$. The second operator $R_2(\tau)$ equals

$$R_2(\tau) = S_0(\tau/2)\big(1 - \exp(-\tau^{1-\nu}U)\big)S_0(\tau/2).$$

Since $1 - \exp(-\tau^{1-\nu}U)$ vanishes over Ω, we can easily see that $A^m\psi R_2(\tau) = O_p(\tau^\infty)$. Thus $A^m\psi R(\tau) = O_p(\tau^\infty)$. A similar argument applies to $\tilde{R}(\tau)$.

(2) By definition, we have

$$A_\tau^{-1}R(\tau)A^{-1/2} = A_\tau^{-1}\big(S_\tau(\tau) - \Gamma(\tau)\big)A^{-1/2}.$$

If we write $A_\tau^{-1}S_\tau(\tau)A^{-1/2}$ as

$$A_\tau^{-1}S_\tau(\tau)A^{-1/2} = \big(A_\tau^{-1}\exp(-\tau A_\tau)A_\tau^{-1/2}\big)A_\tau^{1/2}A^{-1/2},$$

then it follows from Lemma 6.1 (3) that

$$A_\tau^{-1}S_\tau(\tau)A^{-1/2} = A_\tau^{-1}(1 - \tau A_\tau)A^{-1/2} + O_p(\tau^{3/2-\nu/2}). \tag{6.6}$$

On the other hand, $A_\tau^{-1}\Gamma(\tau)A^{-1/2}$ takes the form

$$\begin{aligned} A_\tau^{-1}\Gamma(\tau)A^{-1/2} &= A_\tau^{-1}S_0(\tau/2)\big(1 - \tau^{1-\nu}U + O_p(\tau^{2(1-\nu)})\big)S_0(\tau/2)A^{-1/2} \\ &= A_\tau^{-1}\big(S_0(\tau) - \tau^{1-\nu}S_0(\tau/2)US_0(\tau/2)\big)A^{-1/2} + O_p(\tau^{2(1-\nu)}). \end{aligned}$$

We obtain

$$A_\tau^{-1}S_0(\tau)A^{-1/2} = A_\tau^{-1}A\big(A^{-1}S_0(\tau)A^{-1/2}\big) = A_\tau^{-1}(1 - \tau A)A^{-1/2} + O_p(\tau^{3/2-\nu})$$

by Lemma 6.1 and we decompose $A_\tau^{-1}S_0(\tau/2)US_0(\tau/2)A^{-1/2}$ into the product

$$A_\tau^{-1/2}(A_\tau^{-1/2}A^{1/2})\big(A^{-1/2}S_0(\tau/2)\big)U\big(S_0(\tau/2)A^{-1/2}\big)$$

to obtain that

$$\tau^{1-\nu}A_\tau^{-1}S_0(\tau/2)US_0(\tau/2)A^{-1/2} = \tau A_\tau^{-1}U_\tau A^{-1/2} + O_p(\tau^{3/2-\nu}).$$

Thus it follows that

$$A_\tau^{-1}\Gamma(\tau)A^{-1/2} = A_\tau^{-1}(1-\tau A_\tau)A^{-1/2} + O_p(\tau^{3/2-\nu}),$$

which, together with (6.6), yields the desired bound.

(3) This is shown in almost the same way as (2). We have $A_\tau^{-1}S_\tau(\tau) = A_\tau^{-1} + O_p(\tau)$ and

$$A_\tau^{-1}\Gamma(\tau) = A_\tau^{-1}S_0(\tau/2)\big(1 + O_p(\tau^{1-\nu})\big)S_0(\tau/2) = A_\tau^{-1} + O_p(\tau^{1-\nu}).$$

This proves (3). □

7. Appendix

We conclude the paper by proving (1.8). The Whittaker functions $M_{\kappa,\mu}(z)$ and $W_{\kappa,\mu}(z)$, $z \in \mathbb{C}$, satisfy the equation

$$W'' + \big(-1/4 + \kappa/z + \big(\mu^2 - (1/4)\big)/z^2\big)W = 0$$

as a pair of linearly independent solutions. The proof uses the functions with $\mu = 1/2$ only. We set $M_\kappa(z) = M_{\kappa,1/2}(z)$ and $W_\kappa(z) = W_{\kappa,1/2}(z)$, which solve

$$W'' + (-1/4 + \kappa/z)W = 0. \tag{7.1}$$

These functions are known to have the following asymptotic properties ([16]):

$$M_\kappa(z) = z + O(|z|^2), \quad |z| \to 0, \tag{7.2}$$

$$W_\kappa(z) \sim e^{-z/2}z^\kappa, \quad |z| \to \infty,\ -\pi < \arg z < \pi, \tag{7.3}$$

$$M_\kappa(z) \sim -\big(e^{-i\kappa\pi}/\Gamma(1+\kappa)\big)e^{-z/2}z^\kappa + \big(1/\Gamma(1-\kappa)\big)e^{z/2}z^{-\kappa}, \quad |z| \to \infty, \tag{7.4}$$

along $-\pi/2 < \arg z < 3\pi/2$, where $\Gamma(p)$ is the gamma function. The Wronskian is calculated as

$$W(M_\kappa, W_\kappa) = -1/\Gamma(1-\kappa) \tag{7.5}$$

by (7.3) and (7.4), provided that κ is not a positive integer.

We now consider the Schrödinger operator $H = H_0 + V$ with the positive Coulomb potential $V(x) = c/|x|$, $c > 0$, in three dimensions. We work in the polar coordinate system. Let U be the unitary operator defined by

$$(Uv)(r,\theta) = rv(r\theta) : L^2(\mathbb{R}^3) \to L^2(0,\infty) \otimes L^2(S^2),$$

where $r = |x| \in (0, \infty)$ and $\theta = x/|x| \in S^2$. Then the adjoint operator U^* is defined by $(U^*u)(x) = |x|^{-1}u(|x|, x/|x|)$, and we have

$$UHU^* = -d^2/dr^2 + c/r + \Delta_S/r^2,$$

where Δ_S denotes the Laplace-Beltrami operator acting on $L^2(S^2)$. As is well known, Δ_S has eigenvalues $l(l+1)$ with multiplicity $2l+1$, $l \geqq 0$ being a nonnegative integer, and the normalized eigenfunction associated with zero eigenvalue is the constant function $(4\pi)^{-1/2}$. The value $E(0,0;t)$ in (1.8) is determined only by a contribution from $l = 0$. We denote by $h_0 = -d^2/dr^2 + c/r$ the self-adjoint operator in $L^2(0,\infty)$ with the vanishing boundary condition at $r = 0$ and by $g_0(r,\rho;\zeta)$, $\operatorname{Im}\zeta \neq 0$, the Green function of the resolvent $(h_0 - \zeta)^{-1}$. Then the spectral function $e_0(r,\rho;\lambda)$, $\lambda > 0$, is defined by

$$e_0(r,\rho;\lambda) = (2\pi i)^{-1}\big(g_0(r,\rho;\lambda + i0) - g_0(r,\rho;\lambda - i0)\big)$$

and the value $E(0,0;t)$ is given by

$$E(0,0;t) = \int_0^\infty e^{-t\lambda}s_0(\lambda)\,d\lambda,$$

where $s_0(\lambda) = (4\pi)^{-1}\lim_{\rho\to 0}\lim_{r\to 0} r^{-1}e_0(r,\rho;\lambda)\rho^{-1}$. We assert that

$$s_0(\lambda) = (c/4\pi)(e^{c\pi/\sqrt{\lambda}} - 1)^{-1}. \tag{7.6}$$

To show this, we calculate $g_0(r,\rho;\lambda \pm i\varepsilon)$. If we take account of (7.1)~(7.5), then the standard way yields

$$g_0(r,\rho;\lambda \pm i\varepsilon) = \big(\Gamma(1-\kappa_\pm)/\sigma_\pm\big)M_{\kappa_\pm}\big(\sigma_\pm(r\wedge\rho)\big)\,W_{\kappa_\pm}\big(\sigma_\pm(r\vee\rho)\big)$$

after making a change of variables, where $r\wedge\rho = \min(r,\rho)$, $r\vee\rho = \max(r,\rho)$, and

$$\sigma_\pm = \sigma_\pm(\varepsilon) = \mp 2i(\lambda \pm i\varepsilon)^{1/2}, \quad \kappa_\pm = \kappa_\pm(\varepsilon) = \mp i(c/2)(\lambda \pm i\varepsilon)^{-1/2}$$

with $\pm\operatorname{Im}(\lambda \pm i\varepsilon)^{1/2} > 0$. If we further set $\sigma = 2i\lambda^{1/2}$ and $\kappa = (ic/2)\lambda^{-1/2}$, then $\sigma_\pm(\varepsilon) \to \mp\sigma$ and $\kappa_\pm(\varepsilon) \to \mp\kappa$ as $\varepsilon \to 0$. Thus

$$g_0(r,\rho;\lambda \pm i0) = \mp\big(\Gamma(1\pm\kappa)/\sigma\big)M_{\mp\kappa}\big(\mp\sigma(r\wedge\rho)\big)\,W_{\mp\kappa}\big(\mp\sigma(r\vee\rho)\big).$$

By (7.2), $\lim_{r\to 0} r^{-1}M_{\mp\kappa}(\mp\sigma r) = \mp\sigma$, and hence we have

$$\lim_{r\to 0} r^{-1}e_0(r,\rho;\lambda) = (2\pi i)^{-1}\Gamma(1+\kappa)\Gamma(1-\kappa)\,Y(\rho;\lambda),$$

where

$$Y(\rho;\lambda) = \big(1/\Gamma(1-\kappa)\big)W_{-\kappa}(-\sigma\rho) - \big(1/\Gamma(1+\kappa)\big)W_\kappa(\sigma\rho).$$

By (7.3), $Y(\rho;\lambda)$ behaves like

$$Y(\rho;\lambda) \sim \big(1/\Gamma(1-\kappa)\big)e^{\sigma\rho/2}(-\sigma\rho)^{-\kappa} - \big(1/\Gamma(1+\kappa)\big)e^{-\sigma\rho/2}(\sigma\rho)^{\kappa}$$

as $\rho \to \infty$, and $\arg(-\sigma\rho) = \arg(-i2\lambda^{1/2}\rho)$ must equal $-\pi/2$. Hence $(-\sigma\rho)^{-\kappa} = e^{i\kappa\pi}(\sigma\rho)^{-\kappa}$, and it follows from (7.4) that $Y(\rho;\lambda) = e^{i\kappa\pi}M_\kappa(\sigma\rho)$. This yields

$$\lim_{r\to 0} r^{-1}e_0(r,\rho;\lambda) = (2\pi i)^{-1}\kappa\big(\pi/\sin\kappa\pi\big)e^{i\kappa\pi}M_\kappa(\sigma\rho)$$

by the formula $\Gamma(1+\kappa)\Gamma(1-\kappa) = \kappa\Gamma(\kappa)\Gamma(1-\kappa) = \kappa(\pi/\sin\kappa\pi)$. Thus

$$s_0(\lambda) = (4\pi)^{-1}(2\pi i)^{-1}\kappa\sigma(\pi/\sin\kappa\pi)e^{i\kappa\pi} = (c/4\pi)(e^{c\pi/\sqrt{\lambda}} - 1)^{-1}$$

by (7.2). We can get the desired relation (7.6). If we let $c \to 0$, then

$$E(0,0;t) \to (4\pi)^{-1}\int_0^\infty e^{-t\lambda}\lambda^{1/2}\,d\lambda = (4\pi t)^{-3/2}.$$

The limit just coincides with the value corresponding to the free Hamiltonian H_0.

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Department of Mathematics, Kanazawa University, Kanazawa, 920-1192, Japan
e-mail: ichinose@kenroku.kanazawa-u.ac.jp

Department of Mathematics, Okayama University, Okayama, 700-8530, Japan
e-mail: tamura@math.okayama-u.ac.jp

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