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Error bounds on exponential product formulas for Schrödinger operators

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1. Introduction.

We study an error bound in the operator norm for the Trotter-Kato product formula of Schrödinger semigroups with potentials growing at infinity. Let

$$H = -\Delta + V = H_0 + V$$

be the Schrödinger operator acting on the space $L^2 = L^2(R^n)$. Then the Trotter-Kato product formula ([**1**, **7**, **10**]) says that

$$s - \lim_{N \to \infty} K(t/N)^N = \exp(-tH)$$

strongly in L^2, where $K(t) : L^2 \to L^2$ is defined as

$$K(t) = \exp(-tV/2)\exp(-tH_0)\exp(-tV/2), \quad t \geq 0, \tag{1.1}$$

which is often called the Kac operator or the transfer operator in statistical mechanics. The aim here is to evaluate the error bound in the operator norm as $N \to \infty$ for the exponential product formula above.

We first state the obtained results somewhat loosely. The error bound seems to depend heavily on growth order and smooth property of potentials. Assume that $V(x)$ behaves like

$$V(x) \sim |x|^\rho, \quad |x| \to \infty,$$

for some $\rho \geq 0$. Let

$$e(N) = \|\exp(-tH) - K(t/N)^N\|$$

be the error term in question, $t > 0$ being fixed, where $\|\cdot\|$ denotes the operator norm as a bounded operator from L^2 into itself. Then

$$e(N) = O(N^{-1}) \quad \text{for } 0 \leq \rho < 2, \quad e(N) = O(N^{-2/\rho}) \quad \text{for } \rho \geq 2$$

for a class of C^2-smooth potentials and

$$e(N) = O(N^{-1/2}) \quad \text{for } 0 \leq \rho < 2, \quad e(N) = O(N^{-1/\rho}) \quad \text{for } \rho \geq 2$$

for a class of C^1-smooth potentials. We can further prove the error bound $e(N) = O(N^{-2/3})$ for bounded potentials without assuming smoothness conditions. The same error bounds can be also shown to remain true in trace norm, provided that $\rho > 0$.

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We shall explain the recent related results. It is Helffer ([**4**]) who first proved the error bound $O(N^{-1})$, when $V(x)$ is a C^∞-smooth potential with growth order $\rho = 2$. The proof uses the pseudodifferential calculus and the obtained bound was applied to the study on the spectral properties of Kac operators. A similar bound has been extended by Dia-Schatzman [**2**] to a class of C^4-smooth potentials. In the recent work [**6**], one of the authors (T. Ichinose) together with Takanobu has studied the error bound problem for a wide class of potentials under some assumption on the relation between growth order and smooth property of potentials. The L^p error bound has been also discussed there, including the case of magnetic Schrödinger operators. Most of the results obtained here overlap with those in [**6**] but include several new results (for example, error bound in trace norm, error bound for C^1-smooth potentials growing rapidly at infinity, error bound for bounded potentials, etc). The method employed in [**6**] is based on the Feynman-Kac formula and is of probabilistic character, while the proof here is purely analytical and is done by repeated use of simple commutator computations. Thus the idea, in principle, is similar to that in [**2**] but the technical details are quite different. We further note that the present method also applies to magnetic Schrödinger operators under a slight modification. The matter will be briefly discussed in the last section.

Finally we must refer to Rogava's work [**9**], where a rather abstract result is announced with only a sketch of proof. Roughly speaking, the result is that the semigroup $\exp(-t(A+B))$ obeys the error bound $O(N^{-1/2}\log N)$, if both the operators A and B are non-negative self-adjoint and B is relatively bounded with respect to A. This result does not apply to Schrödinger operators with potentials growing at infinity. In section 5, we consider the error bound for bounded potentials and make a further comment on the Rogava bound (see Remark after Theorem 5.1).

We conclude the section by stating a formal commutator relation

$$[\exp(-tA), B] = \int_0^t \exp(-sA)[B, A]\exp(-(t-s)A)\,ds.$$

This relation can be easily verified, if the domain problem is neglected, and it is repeatedly used without further references throughout the entire discussion. The domain problem is easily justified in later applications.

2. Error bound for C^2-smooth potentials.

We first consider the error bound for Schrödinger operators with C^2-smooth potentials. Throughout this section, the potential $V(x)$ is assumed to fulfill the following assumption:

$(V)_2$ $V(x)$ is a C^2-smooth real function such that for some $\rho \geq 0$

$$V(x) \geq c\langle x\rangle^\rho, \quad c > 0,$$

$$|\partial_x^\alpha V(x)| \leq C_\alpha \langle x\rangle^{(\rho-|\alpha|)_+}, \quad 0 \leq |\alpha| \leq 2,$$

where $\langle x\rangle = (1+|x|^2)^{1/2}$ and $(s)_+ = \max(s,0)$. The strict positivity of potential does not matter to the discussion below. It is enough to assume that $V(x) \geq c\langle x\rangle^\rho$ only for $|x| > R$, $R \gg 1$. In fact, we have only to consider $V(x) + M$, $M \gg 1$, as a potential in place of $V(x)$ in such a case.

Under this assumption, the operator H admits a unique positive self-adjoint realization in L^2. We denote this self-adjoint realization as the same notation H and define the Kac operator $K(t)$ associated with H by (1.1). Then the main result in the present section is formulated as follows.

Theorem 2.1. *Assume that* $(V)_2$ *is fulfilled. Then one has*

$$\|\exp(-tH) - K(t/N)^N\| = \begin{cases} O(N^{-1}), & 0 \leq \rho < 2, \\ O(N^{-2/\rho}), & \rho \geq 2, \end{cases}$$

as $N \to \infty$, *where the order relations are locally uniform in* $t \geq 0$ $(t \in [0,a], 0 < a < \infty)$.

Throughout the whole exposition, we use the terminology *locally uniform* in $t \geq 0$ and in $t > 0$ with the meaning that $t \in [0,a]$ and $t \in [a,b], 0 < a < b < \infty$, respectively. The above theorem follows as an immediate consequence of the basic lemma below. This lemma plays a central role in proving all the other theorems as well as Theorem 2.1.

Lemma 2.2.

$$\|\exp(-tH) - K(t)\| = \begin{cases} O(t^2), & 0 \leq \rho < 2, \\ O(t^{1+2/\rho}), & \rho \geq 2, \end{cases}$$

as $t \to 0$.

We prepare one lemma to prove Lemma 2.2.

Lemma 2.3. *Let* Q_m *be the multiplication operator with* $\langle x\rangle^m$ *and let* D_j *be the differential operator* $-i\partial/\partial x_j$. *Assume that* $m \geq 0$. *Then one has*:

(1) $\|Q_{-m}\exp(-tH_0)Q_m\| = O(1), \quad t \to 0.$

(2) $\|Q_{-m}\exp(-tH_0)D_jQ_m\| = O(t^{-1/2}), \quad t \to 0.$

We proceed with the argument, accepted this lemma as proved.

Proof of Lemma 2.2. The proof is divided into three steps.

(1) We first calculate $K'(t) = (d/dt)K(t)$ as

$$K'(t) = -HK(t) + R(t),$$

where $R(t) = R_1(t) + R_2(t)$ and

$$R_1(t) = [H_0, \exp(-tV/2)]\exp(-tH_0)\exp(-tV/2)$$

$$R_2(t) = \exp(-tV/2)[V/2, \exp(-tH_0)]\exp(-tV/2).$$

We assert that

$$\|R(t)\| = \begin{cases} O(t), & 0 \le \rho < 2, \\ O(t^{2/\rho}), & \rho \ge 2. \end{cases} \tag{2.1}$$

If this is verified, then the lemma immediately follows by the Duhamel principle.

(2) We prove the assertion (2.1) only for the case $\rho \ge 2$. We often use the trivial estimate

$$\|Q_m \exp(-tV)\| = O(t^{-m/\rho}), \quad m \ge 0,$$

without further references in the argument below. We now write $H_0 = D_j D_j$ by use of the summation convention and calculate the commutator

$$\begin{aligned}[H_0, \exp(-tV/2)] = & - t[D_j, V]D_j \exp(-tV/2) \\ & - (t/2)[D_j, [D_j, V]] \exp(-tV/2) \\ & - (t^2/4)[D_j, V][D_j, V] \exp(-tV/2).\end{aligned}$$

By assumption $(V)_2$ (recall that $V(x)$ is C^2-smooth), the last two operators on the right side obey the bound $O(t^{2/\rho})$ and hence

$$R_1(t) = -tAK(t) + O_b(t^{2/\rho}) \tag{2.2}$$

with $A = [D_j, V]D_j$, where $O_b(t^\nu)$ denotes an operator the norm of which obeys the bound $O(t^\nu)$ as $t \to 0$.

(3) Next we deal with the operator $R_2(t)$. We calculate the commutator

$$[H_0, V/2] = [D_j, V]D_j + [D_j, [D_j, V/2]] = A + B,$$

so that

$$[V/2, \exp(-tH_0)] = \int_0^t \exp(-\tau H_0)(A + B) \exp(-(t - \tau)H_0)\, d\tau.$$

Decompose B as $B = Q_m(Q_{-m} B Q_{-m})Q_m$ with $m = (\rho - 2)/2$ and use assumption $(V)_2$ and Lemma 2.3 (1). Then we obtain that

$$\left\| \exp(-tV/2) \int_0^t \exp(-\tau H_0) B \exp(-(t - \tau)H_0)\, d\tau \exp(-tV/2) \right\| = O(t^{2/\rho}).$$

Thus

$$R_2(t) = tAK(t) + R_{21}(t) + R_{22}(t) + O_b(t^{2/\rho}),$$

where

$$R_{21}(t) = t[\exp(-tV/2), A] \exp(-tH_0) \exp(-tV/2),$$

$$R_{22}(t) = \exp(-tV/2) \int_0^t [\exp(-\tau H_0), A] \exp(-(t - \tau)H_0)\, d\tau \exp(-tV/2).$$

It is easy to see that

$$\|R_{21}(t)\| = O(t^{2/\rho}).$$

We shall prove that $R_{22}(t)$ also obeys the same bound as above. To see this, we rewrite $R_{22}(t)$ as

$$R_{22}(t) = \exp(-tV/2)\int_0^t F(\tau)\exp(-(t-\tau)H_0)\,d\tau\exp(-tV/2),$$

where

$$F(\tau) = -\int_0^\tau \exp(-sH_0)[H_0, A]\exp(-(\tau-s)H_0)\,ds.$$

We calculate the commutator

$$[H_0, A] = [H_0, [D_j, V]D_j] = D_k V_{kj} D_j + V_{kj} D_k D_j$$

by use of the summation convention again, where $V_{kj} = [D_k, [D_j, V]]$. Decompose V_{kj} as $V_{kj} = Q_m(Q_{-m}V_{kj}Q_{-m})Q_m, m = (\rho-2)/2$, or as $V_{kj} = Q_l(Q_{-l}V_{kj})$, $l = \rho - 2$, and use Lemma 2.3. Since $D_j H_0^{-1/2} : L^2 \to L^2$ is bounded, the operator $F(\tau)$ takes the form

$$\begin{aligned}F(\tau) &= Q_m \int_0^\tau O_b(s^{-1/2})O_b((\tau-s)^{-1/2})\,ds\,Q_m \\ &\quad + Q_l\int_0^\tau O_b(1)O_b((\tau-s)^{-1/2})\,ds\,H_0^{1/2} \\ &= Q_m O_b(1) Q_m + Q_l O_b(\tau^{1/2})H_0^{1/2}.\end{aligned}$$

Hence we make use of Lemma 2.3 again to obtain that

$$\|R_{22}(t)\| = O(t^{2/\rho}) + O(t^{-1+2/\rho})\int_0^t O(\tau^{1/2})O((t-\tau)^{-1/2})\,d\tau = O(t^{2/\rho}).$$

Summing up, we have

$$R_2(t) = tAK(t) + O_b(t^{2/\rho}),$$

which, together with (2.2), implies (2.1) and hence the proof of the lemma is complete. □

PROOF OF LEMMA 2.3. The lemma is easy to prove. The proof is done by induction. By interpolation, it suffices to prove the lemma only for integer $m \geq 0$. The case $m = 0$ is trivial for both (1) and (2). Assume the case $0 \leq m \leq k$ for (1) and (2). To prove (1) for the case $m = k+1$, it is enough to show that

$$\|Q_{-k-1}[\exp(-tH_0), Q_{k+1}]\| = O(1), \quad t \to 0. \tag{2.3}$$

We represent the above commutator as

$$[\exp(-tH_0), Q_{k+1}] = -\int_0^t \exp(-sH_0)[H_0, Q_{k+1}]\exp(-(t-s)H_0)\,ds.$$

The commutator in the integrand takes the form

$$[H_0, Q_{k+1}] = b_j(x)D_j + b_0(x),$$

where $b_j(x) = O(|x|^k)$ and $b_0(x) = O(|x|^{k-1})$ as $|x| \to \infty$. Hence (2.3) can be easily obtained by inductive assumption. A similar argument applies to (2). The commutator $[H_0, D_jQ_{k+1}]$ takes the form

$$[H_0, D_jQ_{k+1}] = D_lb_{lm}(x)D_m + b_l(x)D_l + b_0(x),$$

where $b_{lm}(x) = O(|x|^k)$, $b_l(x) = O(|x|^{k-1})$ and $b_0(x) = O(|x|^{k-2})$. Hence (2) is again obtained by inductive assumption. Thus the proof is complete. □

We end the section by making a brief comment on the basic lemma above.

REMARK 2.4. If $V(x)$ satisfies

$$|\partial_x^\alpha V(x)| \le C_\alpha \langle x\rangle^{(\rho-\delta|\alpha|)_+}, \quad 0 \le |\alpha| \le 2,$$

for some $0 \le \delta \le 1$, then we can show by a slight modification of the argument in the proof of Lemma 2.2 that

$$\|\exp(-tH) - K(t)\| = \begin{cases} O(t^2), & 0 \le \rho < 2\delta, \\ O(t^{1+2\delta/\rho}), & \rho \ge 2\delta. \end{cases}$$

3. Error bound in trace norm.

We here prove that the same error bound as in Theorem 2.1 remains true in trace norm. Let $\mathscr{C}_p, p \ge 1$, be the Neumann-Schatten class of compact operators and denote by $\|\cdot\|_p$ the norm in $\mathscr{C}_p$. We still assume $(V)_2$ with $\rho > 0$. Then the j-th eigenvalue λ_j of H is well known to behave like $\lambda_j \sim j^\nu, \nu = (2/n)\rho/(2+\rho)$, as $j \to \infty$. Hence the operator $\exp(-tH)$, $t > 0$, is of class $\mathscr{C}_p$ for any $p \ge 1$ and is continuous as a function of $t > 0$ with values in $\mathscr{C}_1$. Such a semigroup is often called a Gibbs semigroup. The trace $\mathrm{Tr}(\exp(-\beta H)), \beta > 0$ being an inverse temperature, is called the partition function of the system governed by Hamiltonian H and is one of the most important quantities to be investigated in quantum statistical mechanics.

THEOREM 3.1. *Assume $(V)_2$ for some $\rho > 0$ strictly positive. Then one has*

$$\|\exp(-tH) - K(t/N)^N\|_1 = \begin{cases} O(N^{-1}), & 0 \le \rho < 2, \\ O(N^{-2/\rho}), & \rho > 2, \end{cases}$$

as $N \to \infty$ and hence the trace $\mathrm{Tr}(\exp(-tH) - K(t/N)^N)$ of difference between both operators also obeys the same bound as above, where the order relations are locally uniform in $t > 0$ $(t \in [a,b], 0 < a < b < \infty)$.

REMARK. The convergence in trace norm of exponential product formula has been proved by [**5**, **8**] in the abstract setting. The result there requires the assumption that

$\exp(-tH_0), t > 0$, is of trace class for the unperturbed operator H_0. Thus it does not seem to apply to the present case directly.

The proof is done through a series of lemmas. We again consider only the case $\rho \geq 2$. We now fix δ as $0 < \delta < 1/\rho$. Then there exists $\gamma = \gamma(\delta) \gg 1$ such that

$$Z_\delta = (H_0 + 1)^{-\delta}(V + 1)^{-\delta} \in \mathscr{C}_\gamma.$$

LEMMA 3.2. *Let δ and γ be as above. Then*

$$\|K(t/N)\|_\gamma = O(N^{2\delta}), \quad N \to \infty,$$

locally uniformly in $t > 0$.

PROOF. The lemma is easy to prove. We write $K(t/N)$ as

$$K(t/N) = \exp(-tV/2N)\exp(-tH_0/N)(H_0 + 1)^\delta Z_\delta (V + 1)^\delta \exp(-tV/2N).$$

Then the lemma follows at once. □

LEMMA 3.3.

$$\|K(t/N)^N\|_\gamma = O(1), \quad N \to \infty,$$

locally uniformly in $t > 0$.

PROOF. We write $T(t)$ for $\exp(-tH)$. Then

$$\exp(-tH) - K(t/N)^N = T(t/N)^N - K(t/N)^N = \sum_{j=1}^{N} X_j(t/N),$$

where

$$X_j(t) = K(t)^{j-1}(T(t) - K(t))T(t)^{N-j}.$$

If $1 \leq j \leq [N/2], [\cdot]$ being the Gauss notation, then

$$\|T(t/N)^{N-j}\|_\gamma = \|\exp(-(1 - j/N)tH)\|_\gamma = O(1), \quad N \to \infty,$$

and hence

$$\|X_j(t/N)\|_\gamma = O(N^{-1-2/\rho})$$

by Lemma 2.2. On the other hand, if $[N/2] < j \leq N$, then Lemma 2.2 again, together with Lemma 3.2, implies that

$$\|X_j(t/N)\|_\gamma = O(N^{-1-2/\rho+2\delta}).$$

Thus it follows that

$$\|\exp(-tH) - K(t/N)^N\|_\gamma = O(N^{2(\delta-1/\rho)}).$$

Since $\delta - 1/\rho < 0$ by choice, the lemma is obtained immediately. □

LEMMA 3.4.

$$\|K(t/N)^N\|_{\gamma/2} = O(1), \quad N \to \infty,$$

locally uniformly in $t > 0$.

PROOF. Let $X_j(t/N), 1 \le j \le N$, be as in the proof of Lemma 3.3. First it is easy to see that

$$\|X_j(t/N)\|_{\gamma/2} = O(N^{-1-2/\rho}), \quad 1 \le j \le [N/2],$$

by Lemma 2.2. Next we consider the case $[N/2] < j \le N$. As is well known (for example, see the book [**3**]), the Hölder inequality

$$\|AB\|_r \le \|A\|_p \|B\|_q, \quad 1/p + 1/q = 1/r, \tag{3.1}$$

holds for $p, q \ge 1$. We use this inequality with pair $(p,q) = (\gamma,\gamma)$. Then we have

$$\|X_j(t/N)\|_{\gamma/2} = O(N^{-1-2/\rho+2\delta}), \quad [N/2] < j \le N,$$

by Lemmas 2.2, 3.2 and 3.3. Thus the lemma is proved in the same way as in the proof of Lemma 3.3. □

COMPLETION OF PROOF OF THEOREM 3.1. We repeat the same argument as in the proof of Lemma 3.4 to obtain that

$$\|K(t/N)^N\|_{\gamma/L} = O(1), \quad N \to \infty, \tag{3.2}$$

for any $L \gg 1$ with $\gamma/L \ge 1$ and, in particular,

$$\|K(t/N)^N\|_1 = O(1), \quad N \to \infty,$$

locally uniformly in $t > 0$. For example, we use (3.1) with pair $(p,q) = (\gamma/2, \gamma)$ to prove (3.2) for $L = 3$. Thus the proof of the theorem is complete. □

4. Error bound for C^1-smooth potentials.

We here consider the error bound for Schrödinger operators with C^1-smooth potentials. Throughout this section, we assume the potential $V(x)$ to satisfy that:

$(V)_1$ $V(x)$ is a C^1-smooth real function such that for some $\rho \ge 0$

$$V(x) \ge c\langle x\rangle^\rho, \quad c > 0,$$

$$|\partial_x^\alpha V(x)| \le C_\alpha \langle x\rangle^{(\rho-|\alpha|)_+}, \quad 0 \le |\alpha| \le 1.$$

The main result here is stated as follows.

THEOREM 4.1. *Let the notations be the same as in Theorem* 2.1. *Assume that* $(V)_1$ *is fulfilled. Then one has*

$$\|\exp(-tH) - K(t/N)^N\| = \begin{cases} O(N^{-1/2}), & 0 \le \rho < 2, \\ O(N^{-1/\rho}), & \rho \ge 2, \end{cases}$$

as $N \to \infty$, *where the order relations are locally uniform in* $t > 0$.

REMARK. The order relations above may be improved to be locally uniform in $t \geq 0$, if we look at the t-dependence more carefully in the proof. A similar comment applies to Theorem 5.1 also.

The proof uses an approximation by smooth potentials. Let $\psi(x)$ be a smooth non-negative function such that

$$\operatorname{supp}\psi \subset \{x \in R^n : |x| < 1\} \quad \text{and} \quad \int \psi(x)\,dx = 1.$$

We set

$$\nu = 0 \quad \text{if} \quad 0 \leq \rho < 1, \quad \nu = \rho - 1 \quad \text{if} \quad 1 \leq \rho < 2, \quad \nu = 1 \quad \text{if} \quad \rho \geq 2,$$

and $\delta = (1+\nu)/2$. We approximate the potential $V(x)$ under consideration by mollifier

$$V_\varepsilon(x) = (\varepsilon\langle x\rangle^\nu)^{-n} \int \psi((x-y)/\varepsilon\langle x\rangle^\nu)\,V(y)\,dy, \quad 0 < \varepsilon \ll 1.$$

Then the lemma below follows from $(V)_1$ and it can be easily verified by a simple calculation. We skip its proof.

LEMMA 4.2. *Let $V_\varepsilon(x)$ be as above. Then one has:*

(1) $V_\varepsilon(x) \geq c\langle x\rangle^\rho, c > 0.$

(2) $|\partial_x^\alpha V_\varepsilon(x)| \leq C_\alpha \langle x\rangle^{(\rho-|\alpha|)_+} \leq C_\alpha \langle x\rangle^{(\rho-\delta|\alpha|)_+}, \quad 0 \leq |\alpha| \leq 1.$

(3) $|\partial_x^\alpha V_\varepsilon(x)| \leq C_\alpha \varepsilon^{-1} \langle x\rangle^{(\rho-\delta|\alpha|)_+}, \quad |\alpha| = 2.$

(4) $|V_\varepsilon(x) - V(x)| \leq C\varepsilon\langle x\rangle^{(\rho-1)_+ + \nu}.$

Here the constants are all independent of ε.

We now define the Hamiltonian H_ε as $H_\varepsilon = H_0 + V_\varepsilon$ with potential $V_\varepsilon(x)$ approximated above and the associated Kac operator $K_\varepsilon(t)$ as

$$K_\varepsilon(t) = \exp(-tV_\varepsilon/2)\exp(-tH_0)\exp(-tV_\varepsilon/2), \quad t \geq 0.$$

The proof of the above theorem requires several simple lemmas.

LEMMA 4.3.

$$\|\exp(-tH) - \exp(-tH_\varepsilon)\| = O(\varepsilon), \quad \varepsilon \to 0,$$

locally uniformly in $t \geq 0$.

PROOF. We again denote by Q_m the multiplication operator with $\langle x\rangle^m$. The difference in the lemma is written in the integral form

$$\int_0^t \exp(-sH)(V_\varepsilon - V)\exp(-(t-s)H_\varepsilon)\,ds.$$

By assumption and Lemma 4.2 (1), both the operators

$$(H+1)^{-1/2}Q_{\rho/2}, \quad (H_\varepsilon+1)^{-1/2}Q_{\rho/2} : L^2 \to L^2$$

are bounded and, in particular, the second one is bounded uniformly in ε. Hence we have

$$\|\exp(-tH)Q_{\rho/2}\| = O(t^{-1/2}), \quad \|\exp(-tH_\varepsilon)Q_{\rho/2}\| = O(t^{-1/2}).$$

This, again together with Lemma 4.2 (4), proves the lemma. □

Lemma 4.4. *Let $\mu = (\rho - 1)_+ + \nu, 0 \leq \mu \leq \rho$, be as in Lemma 4.2 and let $\{\theta, \sigma\}$ be a pair such that $\theta \geq 0, \sigma \geq 0$ and $\theta + \sigma = \mu$. Then one has*

$$\|K_\varepsilon(t) - K(t)\| = O(\varepsilon) \quad \text{and} \quad \|Q_{-\theta}(K_\varepsilon(t) - K(t))Q_{-\sigma}\| = tO(\varepsilon)$$

as $\varepsilon \to 0$ uniformly in $t \geq 0$ and, in particular,

$$\|Q_{-\theta}(K_\varepsilon(t/N) - K(t/N))Q_{-\sigma}\| = \varepsilon O(N^{-1}), \quad N \to \infty,$$

locally uniformly in $t \geq 0$.

Proof. The lemma can be easily proved by use of Lemma 4.2 (4) and of Lemma 2.3. □

Lemma 4.5.

$$\|Q_{-m}(\exp(-tH_\varepsilon) - K_\varepsilon(t))Q_m\| = \begin{cases} \varepsilon^{-1}O(t^2), & 0 \leq \rho < 2, \\ \varepsilon^{-1}O(t^{1+2/\rho}), & \rho \geq 2, \end{cases} \tag{4.1}$$

as $t \to 0$ uniformly in ε and hence

$$\|\exp(-tH_\varepsilon) - K_\varepsilon(t/N)^N\| = \begin{cases} \varepsilon^{-1}O(N^{-1}), & 0 \leq \rho < 2, \\ \varepsilon^{-1}O(N^{-2/\rho}), & \rho \geq 2, \end{cases} \tag{4.2}$$

as $N \to \infty$ uniformly in ε and locally uniformly in $t \geq 0$.

Proof. Let $\delta = (1 + \nu)/2$ be as in Lemma 4.2, so that $\delta = 1$ for $\rho \geq 2$, $\delta = \rho/2$ for $1 \leq \rho < 2$ and $\delta = 1/2$ for $0 \leq \rho < 1$. We note that $0 \leq \rho < 1$ and $\rho \geq 1$ imply $0 \leq \rho < 2\delta$ and $\rho \geq 2\delta$, respectively (see Remark 2.4). Thus, if we take account of Lemma 4.2 (2) and (3), (4.1) with $m = 0$ is proved in exactly the same way as in the proof of Lemma 2.2 and hence (4.2) follows at once. The general case with non-zero $m \neq 0$ can be also proved by a slight modification of the argument used in the proof of Lemma 2.2. In fact, we can easily show by repeated use of Lemma 2.3 that the remainder terms $Q_{-m}R_j(t)Q_m, 1 \leq j \leq 2$, obey the same bound as in the case $m = 0$. □

Lemma 4.6. *Let $0 \leq \gamma \leq \rho$. Then $Q_\gamma(H_\varepsilon + 1)^{-\gamma/\rho} : L^2 \to L^2$ is bounded from L^2 into itself uniformly in ε and hence*

$$\|Q_\gamma \exp(-tH_\varepsilon)\| = O(t^{-\gamma/\rho}), \quad t \to 0.$$

Proof. As is easily seen,

$$Q_{\rho/2}(H_\varepsilon + 1)^{-1}Q_{\rho/2}, \quad Q_{\rho/2}(H_\varepsilon + 1)^{-1}D_j : L^2 \to L^2$$

are bounded. Hence $Q_\rho(H_\varepsilon+1)^{-1}$ is also bounded by use of the relation

$$Q_\rho(H_\varepsilon+1)^{-1} = Q_{\rho/2}(H_\varepsilon+1)^{-1}Q_{\rho/2} + Q_{\rho/2}(H_\varepsilon+1)^{-1}[H_0, Q_{\rho/2}](H_\varepsilon+1)^{-1}.$$

Thus the lemma follows by interpolation at once. □

We are now in a position to prove Theorem 4.1 in question.

PROOF OF THEOREM 4.1. For brevity, we again consider only the case $\rho \geq 2$, so that $\nu = \delta = 1$ and $\mu = \rho$. Almost the same argument applies to the other case also. The proof is divided into three steps.

(1) We start by showing the following

LEMMA 4.7. *Let $2 \leq k \leq N$. Then one has*

$$\|Q_\rho(K_\varepsilon(t/N)^k - \exp(-k(t/N)H_\varepsilon))\| = \varepsilon^{-1}O(N^{-2/\rho}\log N)$$

locally uniformly in $t > 0$.

PROOF. We write $T_\varepsilon(t)$ for $\exp(-tH_\varepsilon)$. Then we have

$$Q_\rho(K_\varepsilon(t/N)^k - T_\varepsilon(t/N)^k) = \sum_{j=1}^{K} Q_\rho Y_{j\varepsilon,k}(t/N),$$

where

$$Y_{j\varepsilon,k}(t) = T_\varepsilon(t)^{j-1}(K_\varepsilon(t) - T_\varepsilon(t))K_\varepsilon(t)^{k-j}.$$

Note that $\|Q_\rho K_\varepsilon(t/N)\| = O(N)$. If $j = 1$, then it follows from Lemma 4.5 with $m = \rho$ that

$$\|Q_\rho Y_{1\varepsilon,k}(t/N)\| = \varepsilon^{-1}O(N^{-2/\rho}).$$

If $2 \leq j \leq k$, then

$$\|Q_\rho T_\varepsilon(t/N)^{j-1}\| = j^{-1}O(N)$$

by Lemma 4.6 and hence it follows again from Lemma 4.5 with $m = 0$ that

$$\|Q_\rho Y_{j\varepsilon,k}(t/N)\| = \varepsilon^{-1}j^{-1}O(N^{-2/\rho}).$$

This yields the lemma at once. □

By Lemma 4.5, we obtain

$$\|K_\varepsilon(t/N)^k - \exp(-k(t/N)H_\varepsilon)\| = \varepsilon^{-1}O(N^{-2/\rho}), \quad 2 \leq k \leq N,$$

and hence it follows by interpolation that

$$\|Q_\gamma(K_\varepsilon(t/N)^k - \exp(-k(t/N)H_\varepsilon))\| = \varepsilon^{-1}O(N^{-2/\rho}\log N), \quad 0 \leq \gamma \leq \rho.$$

Thus we have by Lemma 4.6 that

$$\|Q_\gamma K_\varepsilon(t/N)^k\| = \varepsilon^{-1}O(N^{-2/\rho}\log N) + k^{-\gamma/\rho}O(N^{\gamma/\rho}) \tag{4.3}$$

for k and γ as above.

(2) The second step toward the proof is to show the following

LEMMA 4.8. *Let $3 \le k \le N$. Then one has*

$$\|K(t/N)^k - \exp(-k(t/N)H)\| = O(N^{-1/\rho}\log N)$$

locally uniformly in $t > 0$.

PROOF. We again write $T(t)$ for $\exp(-tH)$ and decompose the difference in question into the sum of three operators;

$$K(t/N)^k - \exp(-k(t/N)H) = K(t/N)^k - T(t/N)^k = \sum_{p=1}^{3} I_{p\varepsilon,k}(t/N),$$

where

$$I_{1\varepsilon,k}(t) = K(t)^k - K_\varepsilon(t)^k, \quad I_{2\varepsilon,k}(t) = K_\varepsilon(t)^k - T_\varepsilon(t)^k, \quad I_{3\varepsilon,k}(t) = T_\varepsilon(t)^k - T(t)^k.$$

By Lemmas 4.3 and 4.5, the second and third operators on the right side obey the bounds

$$\|I_{2\varepsilon,k}(t/N)\| = \varepsilon^{-1}O(N^{-2/\rho}), \quad \|I_{3\varepsilon,k}(t/N)\| = \varepsilon O(1).$$

Thus we now take ε as

$$\varepsilon = N^{-1/\rho}.$$

The first operator is represented as

$$I_{1\varepsilon,k}(t/N) = \sum_{j=1}^{k} Z_{j\varepsilon,k}(t/N),$$

where

$$Z_{j\varepsilon,k}(t) = K_\varepsilon(t)^{j-1}(K(t) - K_\varepsilon(t))K(t)^{k-j}.$$

If $j = 1$ or 2, then it follows from Lemma 4.4 that

$$\|Z_{j\varepsilon,k}(t/N)\| = \varepsilon O(1) = O(N^{-1/\rho})$$

and also if $3 \le j \le k \le N$, then it follows from Lemma 4.4 and bound (4.3) with $\gamma = \rho$ that

$$\|Z_{j\varepsilon,k}(t/N)\| = O(N^{-1-2/\rho}\log N) + j^{-1}O(N^{-1/\rho})$$

for $\varepsilon = N^{-1/\rho}$. Thus we have

$$\|I_{1\varepsilon,k}(t/N)\| = O(N^{-1/\rho}\log N)$$

with ε as above. This completes the proof. □

As is easily seen,

$$\|Q_\rho K(t/N)^k\| + \|Q_\rho \exp(-k(t/N)H)\| = O(N)$$

and hence Lemma 4.8 implies that

$$\|Q_\gamma(K(t/N)^k - \exp(-k(t/N)H))\| = O(N^{-(1-\gamma/\rho)/\rho+\gamma/\rho}\log N)$$

for $3 \le k \le N$ and $0 \le \gamma \le \rho$. Thus we have by Lemma 4.6 that

$$\|Q_\gamma K(t/N)^k\| = O(N^{-(1-\gamma/\rho)/\rho+\gamma/\rho}\log N) + k^{-\gamma/\rho}O(N^{\gamma/\rho}) \tag{4.4}$$

for k and γ as above.

(3) The proof is completed in this step. We repeat the same argument as in the proof of Lemma 4.8 to obtain that

$$K(t/N)^N - T(t/N)^N = \sum_{j=1}^{N} Z_{j\varepsilon,N}(t/N) + O_b(N^{-1/\rho}).$$

If $j = 1, 2$ or $N-3 \le j \le N-1$, then

$$\|Z_{j\varepsilon,N}(t/N)\| = \varepsilon O(1) = O(N^{-1/\rho})$$

by Lemma 4.4. Next we evaluate $Z_{j\varepsilon,N}(t/N)$ with $3 \le j \le N-4$. Let the pair $\{\theta, \sigma\}, \theta + \sigma = \mu = \rho$, be as in Lemma 4.4. We choose $\sigma > 0$ small enough and decompose $Z_{j\varepsilon,N}(t)$ into the product of three operators

$$Z_{j\varepsilon,N}(t) = [K_\varepsilon(t)^{j-1}Q_\theta][Q_{-\theta}(K(t) - K_\varepsilon(t))Q_{-\sigma}][Q_\sigma K(t)^{N-j}].$$

By Lemma 4.4, it follows from bounds (4.3) and (4.4) that

$$\sum_{j=3}^{N-4}\|Z_{j\varepsilon,N}(t/N)\| = O(N^{-1/\rho}) + O(N^{-1/\rho})\left[\sum_{j=3}^{N-4} j^{-\theta/\rho}(N-j)^{-\sigma/\rho}\right]$$

with $\varepsilon = N^{-1/\rho}$. This proves the theorem. □

5. Error bound for bounded potentials.

In this section, we study the error estimate for a class of bounded potentials without assuming any smoothness conditions. We use the notations $H_0, H = H_0 + V$ and $K(t)$ with the meanings ascribed in the previous sections. The main result obtained here is formulated as follows.

THEOREM 5.1. *Assume that $V(x) \ge 0$ is a non-negative bounded function. Then one has*

$$\|\exp(-tH) - K(t/N)^N\| = O(N^{-2/3}), \quad N \to \infty,$$

locally uniformly in $t > 0$.

REMARK. The bound in the theorem is sharper than the bound $O(N^{-1/2}\log N)$ obtained by Rogava [**9**], when applied to the Schrödinger operator $H = H_0 + V$ with bounded potential $V(x)$. The idea developed in the proof of the theorem seems to extend to a certain class of singular potentials. The details will be discussed elsewhere ([**11**]).

The proof is again done by approximation. Let $\varphi_0(s), s \in [0,\infty)$, be a smooth cut-off function such that $0 \le \varphi_0(s) \le 1, \varphi_0 = 1$ for $0 \le s \le 1$ and $\varphi_0 = 0$ for $s \ge 2$. Then we define

$$V_\varepsilon = \varphi_0(\varepsilon H_0) V \varphi_0(\varepsilon H_0)$$

for $0 < \varepsilon \ll 1$ small enough and set $H_\varepsilon = H_0 + V_\varepsilon$. We also denote by $K_\varepsilon(t)$, $t \ge 0$, the Kac operator associated with H_ε.

The proof of the theorem above is done through a series of lemmas.

LEMMA 5.2. *Let* $\varphi_\infty(s) = 1 - \varphi_0(s)$. *Then one has*:

$$\|(\exp(-tH) - \exp(-tH_0))\varphi_\infty(\varepsilon H_0)\| = O(\varepsilon),$$

$$\|(\exp(-tH_\varepsilon) - \exp(-tH_0))\varphi_\infty(\varepsilon H_0)\| = O(\varepsilon)$$

locally uniformly in $t \ge 0$.

PROOF. We prove only the first relation. A similar argument applies to the second one. We write the difference in the integral form and use the estimate

$$\|\exp(-tH_0)\varphi_\infty(\varepsilon H_0)\| \le e^{-t/\varepsilon}.$$

Then the first relation can be easily obtained. □

LEMMA 5.3.

$$\|\exp(-tH) - \exp(-tH_\varepsilon)\| = O(\varepsilon)$$

locally uniformly in $t \ge 0$.

PROOF. We again write the difference in the integral form. By Lemma 5.2, we have

$$\|\exp(-tH)\varphi_\infty(\varepsilon H_0)\| \le e^{-t/\varepsilon} + O(\varepsilon).$$

A similar estimate is also true for $\exp(-tH_\varepsilon)$. This proves the lemma. □

The lemma below can be also easily proved.

LEMMA 5.4.

$$\|\exp(-tH) - \exp(-tH_\varepsilon)\| = O(t), \quad t \to 0,$$

uniformly in ε *and, in particular,*

$$\|\exp(-(t/N)H) - \exp(-(t/N)H_\varepsilon)\| = O(N^{-1}), \quad N \to \infty,$$

locally uniformly in $t \ge 0$.

LEMMA 5.5.

$$\|\exp(-tH_\varepsilon) - K_\varepsilon(t)\| = \varepsilon^{-2}O(t^3), \quad t \to 0,$$

and hence

$$\|\exp(-tH_\varepsilon) - K_\varepsilon(t/N)^N\| = \varepsilon^{-2}O(N^{-2}), \quad N \to \infty.$$

PROOF. We use almost the same argument as in the proof of Lemma 2.2. We calculate

$$K_\varepsilon'(t) = -H_\varepsilon K_\varepsilon(t) + R_\varepsilon(t).$$

Since $\|[H_0, V_\varepsilon]\| = O(\varepsilon^{-1})$ and

$$\|[V_\varepsilon, [H_0, V_\varepsilon]]\| = O(\varepsilon^{-1}), \quad \|[H_0, [H_0, V_\varepsilon]]\| = O(\varepsilon^{-2}),$$

we see that the remainder operator $R_\varepsilon(t)$ obeys the bound

$$\|R_\varepsilon(t)\| = \varepsilon^{-2}O(t^2), \quad t \to 0.$$

This proves the lemma. □

LEMMA 5.6. *The difference $K_\varepsilon(t/N) - K(t/N)$ takes the form*

$$K_\varepsilon(t/N) - K(t/N) = \varphi_\infty(\varepsilon H_0)O_b(N^{-1}) + O_b(N^{-1})\varphi_\infty(\varepsilon H_0) + O_b(N^{-2}),$$

where all the order relations are uniform in ε and locally uniform in $t \geq 0$.

PROOF. The lemma can be easily proved, if we take account of the fact that the commutators

$$[\exp(-tV/N), \varphi_\infty(\varepsilon H_0)], \quad [\exp(-tV_\varepsilon/N), \varphi_\infty(\varepsilon H_0)]$$

are both of class $O_b(N^{-1})$, which is verified by use of a simple commutator calculus. □

We now prove Theorem 5.1.

PROOF OF THEOREM 5.1. (1) Let $T(t) = \exp(-tH)$ and $T_\varepsilon(t) = \exp(-tH_\varepsilon)$ again. Then

$$K(t/N)^N - \exp(-tH) = K(t/N)^N - T(t/N)^N = \sum_{p=1}^{3} J_{p\varepsilon}(t/N),$$

where

$$J_{1\varepsilon}(t) = K(t)^N - K_\varepsilon(t)^N, \quad J_{2\varepsilon}(t) = K_\varepsilon(t)^N - T_\varepsilon(t)^N, \quad J_{3\varepsilon}(t) = T_\varepsilon(t)^N - T(t)^N.$$

By Lemmas 5.3 and 5.5, the second and third operators on the right side obey the bounds

$$\|J_{2\varepsilon}(t/N)\| = \varepsilon^{-2}O(N^{-2}), \quad \|J_{3\varepsilon}(t/N)\| = \varepsilon O(1).$$

Thus we now take ε as

$$\varepsilon = N^{-2/3}.$$

Then it follows that

$$K(t/N)^N - \exp(-tH) = J_{1\varepsilon}(t/N) + O_b(N^{-2/3}).$$

(2) The first operator $J_{1\varepsilon}(t/N)$ is represented as

$$J_{1\varepsilon}(t/N) = \sum_{j=1}^{N} A_{j\varepsilon}(t/N),$$

where

$$A_{j\varepsilon}(t) = K_\varepsilon(t)^{j-1}(K(t) - K_\varepsilon(t))K(t)^{N-j}.$$

Hence, by Lemma 5.6, it obeys the bound

$$\|J_{1\varepsilon}(t/N)\| = O(N^{-1})\sum_{j=3}^{N-2} \|K_\varepsilon(t/N)^{j-1}\varphi_\infty(\varepsilon H_0)\|$$
$$+ O(N^{-1})\sum_{j=3}^{N-2} \|\varphi_\infty(\varepsilon H_0)K(t/N)^{N-j}\| + O(N^{-1}).$$

Lemma 5.7. *Let $\varepsilon = N^{-2/3}$ be as above. Then one has*

$$\|K_\varepsilon(t/N)^k\varphi_\infty(\varepsilon H_0)\| = O(N^{-2/3}) + O(e^{-ck/\varepsilon N}), \quad 2 \le k \le N,$$

with some $c > 0$, where the order relations are locally uniform in $t > 0$.

Lemma 5.8. *Let $\varepsilon = N^{-2/3}$ be again as above. Then one has*

$$\|K(t/N)^k\varphi_\infty(\varepsilon H_0)\| = O(N^{-2/3}) + O(e^{-ck/\varepsilon N}), \quad 2 \le k \le N,$$

with the same $c > 0$ as in Lemma 5.7, where the order relations are locally uniform in $t > 0$.

These two lemmas complete the proof. In fact, it follows that

$$\|J_{1\varepsilon}(t/N)\| = O(N^{-2/3}) + O(N^{-1})\sum_{j=3}^{N-2} e^{-cj/\varepsilon N}$$
$$= O(N^{-2/3}) + \varepsilon O(1) = O(N^{-2/3}).$$

Thus the proof is complete.

(3) The last step is devoted to proving the two lemmas above.

Proof of Lemma 5.7. We first note that

$$\|T_\varepsilon(t/N) - K_\varepsilon(t/N)\| = O(N^{-5/3}) \le O(N^{-1}) \tag{6.1}$$

for $\varepsilon = N^{-2/3}$. This follows immediately from Lemma 5.5. We now consider the operator

$$T_\varepsilon(t/N)^k - K_\varepsilon(t/N)^k = \sum_{j=1}^{k} W_{j\varepsilon,k}(t/N),$$

where

$$W_{j\varepsilon,k}(t) = K_\varepsilon(t)^{j-1}(T_\varepsilon(t) - K_\varepsilon(t))T_\varepsilon(t)^{k-j}.$$

If $j = k$, then it follows from (6.1) that

$$\|W_{k\varepsilon,k}(t/N)\| = O(N^{-1})$$

and also if $1 \le j \le k-1$, then

$$\|W_{j\varepsilon,k}(t/N)\varphi_\infty(\varepsilon H_0)\| = O(N^{-1})\{\varepsilon + e^{-c(k-j)/\varepsilon N}\}$$

locally uniformly in $t > 0$, because

$$\|T_\varepsilon(t/N)^{k-j}\varphi_\infty(\varepsilon H_0)\| = O(\varepsilon) + O(e^{-c(k-j)/\varepsilon N})$$

by Lemma 5.2. This yields that

$$\|(T_\varepsilon(t/N)^k - K_\varepsilon(t/N)^k)\varphi_\infty(\varepsilon H_0)\| = \varepsilon O(1) + O(N^{-1}) = O(N^{-2/3})$$

and hence the lemma follows again from Lemma 5.2 at once. □

Proof of Lemma 5.8. The proof is exactly the same as that of the previous lemma. By Lemmas 5.4, 5.5 and 5.6, we have

$$\|T(t/N) - K(t/N)\| = O(N^{-1}).$$

This enables us to repeat the same argument as in the proof of Lemma 5.7 and the proof is complete. □

We can combine Lemma 2.2 and Theorem 5.1 to establish the error bound for a little wider class of potentials. For example, consider $V(x) = |x|^\rho, 0 < \rho < 1$, which is not C^1-smooth. We decompose $V(x)$ into $V(x) = V_0(x) + V_1(x)$, where $V_0(x)$ is a bounded function with compact support and $V_1(x)$ is a smooth function vanishing in a neighborhood of the origin. Set $H_1 = H_0 + V_1$. As is easily seen, the argument used in the proof of Theorem 5.1 applies to $H = H_1 + V_0$ and we obtain

$$\|\exp(-tH) - K_1(t/N)^N\| = O(N^{-2/3}),$$

where $K_1(t) = \exp(-tV_0/2)\exp(-tH_1)\exp(-tV_0/2)$. On the other hand, it follows from Lemma 2.2 that

$$\|\exp(-tH_1) - \exp(-tV_1/2)\exp(-tH_0)\exp(-tV_1/2)\| = O(t^2), \quad t \to 0.$$

Thus we have

$$\|\exp(-tH) - K(t/N)^N\| = O(N^{-2/3}).$$

This improves the bound $O(N^{-\rho/2})$ obtained in [6] (Theorem 2.2) for the above type of potentials.

6. Error bound for magnetic Schrödinger operators.

The argument developed here applies to magnetic Schrödinger operators

$$H = \Pi_j\Pi_j + V = H_0 + V,$$

where $\Pi_j = D_j - a_j(x), a_j(x)$ (magnetic potential) being a real function, and $V(x)$ fulfills the assumption $(V)_2$ or $(V)_1$. Since Π_j and $\Pi_k, j \neq k$, do not necessarily commute with each other

$$[\Pi_j, \Pi_k] = ib_{jk}, \quad b_{jk}(x) = \partial_j a_k - \partial_k a_j,$$

the argument requires a slight modification. We assume that the magnetic field b_{jk} is a bounded function, so that $\Pi_j\Pi_k(H_0 + 1)^{-1} : L^2 \to L^2$ is bounded. If we take account of the relation $[\Pi_j, V] = [D_j, V]$, all the results obtained here can be shown to remain true for magnetic Schrödinger operators. We omit the detailed statements. In the special case that $a_j(x)$ is a polynomial, it is known (Guibourg [12]) that the operator $\Pi_j\Pi_k(H_0 + 1)^{-1}$ is bounded, even if b_{jk} is not necessarily assumed to be bounded. We do not know whether or not the results obtained here extend to such a class of magnetic potentials.

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