THE SEMICLASSICAL ESTIMATE OF THE EIGENVALUE SPLITTING FOR THE KAC OPERATOR

By

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Abstract. We estimate for small $h > 0$ the eigenvalue splitting of the two largest eigenvalues $\mu_1(h)$ and $\mu_2(h)$ of the Kac operator

$$K(h) = \exp(-V(x)/2) \exp(h^2\Delta) \exp(-V(x)/2)$$

with potentials $V(x)$ not necessarily uniformly strictly convex, by comparing it with the eigenvalue gap of the Schrödinger operator. The method is based on Helffer’s idea. If $V(x) = |x|^\rho$, $0 < \rho < \infty$, then we have

$$\frac{\mu_2(h)}{\mu_1(h)} = 1 - (e_2 - e_1)h^{2\rho/(\rho+2)} + O(h^{\rho+2}), \quad h \downarrow 0,$$

where $e_1$ and $e_2$ are the two smallest eigenvalues of the Schrödinger operator $-\Delta + |x|^\rho$.

1. Introduction and the Main Result

The Kac operator

$$K(h) = \exp(-V(x)/2) \exp(h^2\Delta) \exp(-V(x)/2),$$

is a transfer operator for a Kac model [6] in statistical mechanics, where $0 < h \leq 1$ is the Planck constant, $\Delta$ is the Laplacian and $V(x)$ is a real-valued function on $\mathbb{R}^d$.

This model has been recently visited by Helffer [2], [3], [4] to consider the large dimensional behavior of the correlation function which involves the quotient of the two largest eigenvalues $\mu_1(h)$ and $\mu_2(h)$ of the Kac operator $K(h)$. He has assumed in [2] that $V(x)$ is uniformly strictly convex in the sense that $V(x)$ is a $C^\infty$ function satisfying

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Received April 21, 1997
Revised October 2, 1997
\[ \sigma = \inf_{x \in \mathbb{R}^d} (\text{Hess } V)(x) > 0, \]

and

\begin{equation}
|\partial^a V(x)| \leq C_2 \langle x \rangle^{2-|a|}, \quad 0 \leq |x| < \infty, \quad V(x) \geq C|x|^2 - 1/C, \quad C > 0,
\end{equation}

where \((s)_+ = s \vee 0\) and \(\langle x \rangle = (1 + |x|^2)^{1/2}\). Then he has obtained the estimate of the eigenvalue splitting of the Kac operator for \(h > 0\)

\begin{equation}
\mu_2(h) / \mu_1(h) \leq \exp(-\cosh^{-1}(h^2 \sigma + 1)).
\end{equation}

On the other hand, though (1.3) already implies a semiclassical eigenvalue splitting for the Kac operator, he has given in [3, Remark 2.3]

\begin{equation}
\mu_2(h) / \mu_1(h) = \exp(-(E_2(h) - E_1(h))) + O(h^2), \quad h \to 0,
\end{equation}

which semiclassically relates the quotient of the two largest eigenvalues \(\mu_1(h)\) and \(\mu_2(h)\) of the Kac operator \(K(h)\) to the quotient of the two smallest eigenvalues \(E_1(h)\) and \(E_2(h)\) of the Schrödinger operator

\begin{equation}
H(h) = H_0(h) + V = -h^2 \Delta + V(x).
\end{equation}

Moreover, if we know a semiclassical asymptotic expansion of \(E_2(h) - E_1(h)\), we can get with (1.4) a semiclassical estimate of the eigenvalue splitting for the Kac operator \(K(h)\). The class of uniformly strictly convex potentials contains the harmonic oscillator potential but not other important potentials like \(|x|^4\), etc.

The aim of this paper is to extend his result (1.4) to the case for some more general potentials which may not be uniformly strictly convex, to obtain a semiclassical eigenvalue splitting for the Kac operator \(K(h)\) with the aid of a semiclassical asymptotic expansion of \(E_2(h) - E_1(h)\).

To get our result corresponding to (1.4) we assume that \(V(x)\) satisfies with constants \(c > 0, \rho > 0, 0 \leq m < \infty\) and \(0 < \kappa \leq 1\),

\begin{enumerate}
\item \(V(x) = V_0(x) + V_1(x), \quad V_j(x) \geq 0, \quad j = 0, 1,\)
\item \(V_0(x) \in C^{m,\kappa}_0(\mathbb{R}^d),\)
\item \(V_1(x) \in C^{\infty}(\mathbb{R}^d), \quad V_1(x) \geq c \langle x \rangle^\rho\) on \(|x| > R \quad (R \gg 1),\)
\item \(|\partial^a V_1(x)| \leq C_{\alpha} \langle x \rangle^{|\alpha| - 1}, \quad 0 \leq |x| \leq 2,\)
\end{enumerate}

where \(C^{m,\kappa}_0(\mathbb{R}^d)\) is the family of the \(m\)-times continuously differentiable functions \(f(x)\) in \(\mathbb{R}^d\) with compact support whose derivatives \(\partial^a f, |\alpha| = m\), are \(\kappa\)-Hölder
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continuous. Under the condition (1.6), the Kac operator $K(h)$ is a trace class operator and has a simple largest eigenvalue. On the other hand, under the condition (1.6), $H(h)$ admits a unique nonnegative selfadjoint extension in $L^2(\mathbb{R}^d)$ (e.g. [9, Theorem X. 28]). We denote this extension by the same notation $H(h)$ in (1.5). Then $H(h)$ has only purely discrete spectrum and has a simple first eigenvalue $E_1(h)$ (e.g. [10, Theorem XIII. 47]). Therefore it has the eigenvalue gap $E_2(h) - E_1(h)$, where $E_2(h)$ is the second eigenvalue of $H(h)$.

To obtain a semiclassical asymptotic expansion of $E_2(h) - E_1(h)$, we assume further that

(1) $V(x) = 0$ if and only if $x = 0$,

(2) $V_1(x) \equiv 0$ on $|x| \leq 1/2$,

(3) $V_0(x) \in C^\infty(\mathbb{R}^d \setminus \{0\})$, $\text{supp } V_0 \subset \{x \in \mathbb{R}^d | |x| \leq 1\}$,

$$V_0(x) \sim w(x) \sum_{|x|=0}^\infty a_x x^x, \text{ near } x = 0,$$

with $a_0 \neq 0$, where $w(x)$ is a positively homogeneous function in $C^\infty(\mathbb{R}^d \setminus \{0\})$ with $\omega(\lambda x) = \lambda^{\kappa+m}w(x)$ for $\lambda > 0$. The condition (1) in (1.7) is essential in our case because it assures $V(x)$ is a one well potential. If we exclude this condition we encounter the double well potential. The double well potential case is a future problem for us, although Helffer has already treated it in [4]. The potential $V(x) = |x|^p$, $0 < p < \infty$, is one of the typical examples which satisfy these conditions. In fact, putting $V_0(x) = \chi(x)V(x)$, $V_1(x) = (1 - \chi(x))V(x)$, where $\chi(x)$ is a $C^\infty$ cut-off function with $0 \leq \chi(x) \leq 1$ in $\mathbb{R}^d$ and $\text{supp } \chi(x) \subset \{x \in \mathbb{R}^d | |x| \leq 1\}$, we see $V$ satisfies (1.6) and (1.7) by taking $m = [p] - 1$ and $\kappa = p - m$. Here $[p]$ is the largest integer that is not greater than $p$.

With $w(x)$ in (3) of (1.7), we put

(1.8) $$H_\kappa = -\Delta + a_0 w(x).$$

Then $H_\kappa$ also admits a unique nonnegative selfadjoint extension in $L^2(\mathbb{R}^d)$, which is also denoted by the same notation $H_\kappa$ as in (1.8). It also has only purely discrete spectrum and has a simple first eigenvalue.

The main result of this paper is the following theorem.

**Theorem 1.1.** Let $V(x)$ satisfy the conditions (1.6) and (1.7) and let $\mu_1(h)$ and $\mu_2(h)$ be the two largest eigenvalues of the Kac operator $K(h)$. Let $e_1$ and $e_2$ be the two smallest eigenvalues of the Schrödinger operator $H_\kappa$. Then one has
\begin{equation}
\mu_2(\hbar)/\mu_1(\hbar) = \begin{cases} 
1 - (e_2 - e_1)\hbar^2 + O(\hbar^{\kappa+m}), & \kappa + m < \sqrt{2}, \\
1 - (e_2 - e_1)\hbar^2 - \Xi\hbar^{\kappa+\beta} + O(\hbar^{\kappa+m+2}), & \kappa + m \geq \sqrt{2},
\end{cases}
\end{equation}

as \( \hbar \to 0 \), with \( \alpha = 2(\kappa + m)/(\kappa + m + 2) \) and \( \beta = 2/(\kappa + m + 2) \), where the constant \( \Xi \) depends on \( (a_2)^0_{|x|} \) in (3) in (1.7) and \( \Xi = 0 \) if \( V(x) = a_0w(x) \).

In Section 2, to get a formula like (1.4), we shall estimate the operator norm of the difference between the Kac operator and the exponential of the Schrödinger operator. There we use simple commutator method. In Section 3 we prove semiclassical asymptotic expansions of the eigenvalues of the Schrödinger operator with the conditions (1.6) and (1.7). In Section 4 we prove Theorem 1.1 by using the theorems proved in Section 2 and Section 3 and give a non-trivial example.

2. Semiclassical Error Estimate for the Kac Operator

In this section we shall observe the difference between the Kac operator \( K(h) \) and the exponential \( \exp(-H(h)) \) of the Schrödinger operator \( H(h) \) in \( L^2 \) operator norm. The problem has been recently studied first by Helffer [3] for potential \( V(x) \) satisfying \( |\partial^a V(x)| \leq C_2<x>^{(2-a)}_+ \) and then by Ichinose-Takanobii [5] and Doumeki-Ichinose-Tamura [1] for some more general potentials.

This result can be used to relate the two largest eigenvalues \( \mu_1(\hbar) \) and \( \mu_2(\hbar) \) of the Kac operator \( K(h) \) to the two smallest ones \( E_1(h) \) and \( E_2(h) \) of the Schrödinger operator \( H(h) \) such as in (1.4). Though the method of this section is very similar to the paper [1], we include it to make the paper self-contained.

As a semiclassical error bound between the Kac operator and the exponential of the Schrödinger operator we have the following theorem.

**THEOREM 2.1.** Let \( V(x) \) satisfy the condition (1.6). Let \( H(h) \) be the Schrödinger operator with potential \( V(x) \) and let \( K(h) \) be the associated Kac operator. Then one has

\[ \| \exp(-H(h)) - K(h) \| = O(h^{\kappa+m+2}), \]

as \( h \to 0 \).

To prove Theorem 2.1 we shall show the following proposition.

**PROPOSITION 2.1.** Let \( V(x) \) and \( H(h) \) be the same as in Theorem 2.1. Then one has the estimate for \( a > 0 \) and for small \( t > 0 \)
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\[
\left\| \exp \left( -\frac{t}{\hbar} H(\hbar) \right) - K(t; \hbar) \right\| = \hbar^{-1} O(t^{1+a(\kappa+m) \wedge 2}) \\
+ O(t^{2-a(2-\kappa-m)_+}) + \hbar^{-1+\rho/2} O(t^{3-a(1-\kappa-m)_+ - (\rho-1)_+ / \rho}) \\
+ \hbar^{-1} O(t^{3-2a(1-\kappa-m)_+}) + \hbar^{-1+2(\rho-1)_+ / \rho} O(t^{3-2(\rho-1)_+ / \rho}) \\
+ \hbar^{(\rho-2)_+ / \rho} O(t^{2-(\rho-2)_+ / \rho}),
\]

uniformly in \( \hbar \in (0,1] \), where

\[
K(t; \hbar) = \exp \left( -\frac{t}{\hbar} V/2 \right) \exp \left( -\frac{t}{\hbar} H_0(\hbar) \right) \exp \left( -\frac{t}{\hbar} V/2 \right).
\]

In the beginning we prove Theorem 2.1, accepting that Proposition 2.1 has been established.

**Proof of Theorem 2.1.** From Proposition 2.1 we determine the asymptotic order in \( \hbar \) by putting \( t = \hbar \). We have the following constraint among the parameters \( a, \kappa \) and \( m \)

\[
a((\kappa + m) \wedge 2) \geq 0, \quad -a(2 - \kappa - m)_+ + 2 \geq 0,
\]

\[
-2a(1 - \kappa - m)_+ + 2 \geq 0, \quad -a(1 - \kappa - m)_+ + 2 \geq 0.
\]

Here we want to take the order in \( \hbar \) as large as possible. Then this constraint determines \( a = 1 \). Thus we have proved Theorem 2.1.

In the rest of this section we shall prove Proposition 2.1, which follows from some successive lemmas.

Let \( \phi(x) \) be a normalized smooth non-negative even function compactly supported in the unit ball. We define for \( 0 < \epsilon \ll 1 \)

\[
V_{0,\epsilon}(x) = \epsilon^{-d} \int \phi \left( \frac{x - y}{\epsilon} \right) V_0(y) \, dy,
\]

and put \( V_\epsilon(x) = V_{0,\epsilon}(x) + V_1(x) \). Note the following identity

\[
\exp \left( -\frac{t}{\hbar} H(\hbar) \right) - K(t; \hbar) = \left( \exp \left( -\frac{t}{\hbar} H(\hbar) \right) - \exp \left( -\frac{t}{\hbar} H_\epsilon(\hbar) \right) \right) \\
\quad + \left( \exp \left( -\frac{t}{\hbar} H_\epsilon(\hbar) \right) - K_\epsilon(t; \hbar) \right) \\
\quad + (K_\epsilon(t; \hbar) - K(t; \hbar)) \\
\equiv D_1(t; \hbar) + D_2(t; \hbar) + D_3(t; \hbar),
\]

In the beginning we prove Theorem 2.1, accepting that Proposition 2.1 has been established.
where
\[ H_\varepsilon(h) = H_0(h) + V_\varepsilon = -\hbar^2 \Delta + V_\varepsilon(x), \]
\[ K_\varepsilon(t; h) = \exp \left( -\frac{t}{\hbar} V_\varepsilon/2 \right) \exp \left( -\frac{t}{\hbar} H_0(h) \right) \exp \left( -\frac{t}{\hbar} V_\varepsilon/2 \right). \]

To prove Proposition 2.1 it is enough to estimate the asymptotic orders of the norms of \( D_1(t; h), \) \( D_2(t; h) \) and \( D_3(t; h). \) To do so we should study some properties of \( V_{0, \varepsilon}. \)

**Lemma 2.1.** \( V_{0, \varepsilon} \) defined as above satisfies the following inequalities

1. \[ |V_{0, \varepsilon}(x) - V_0(x)| \leq C\varepsilon^{(\kappa+m)^2}, \]
2. \[ |\partial^a V_{0, \varepsilon}(x)| \leq C \varepsilon^{-|\alpha|} (\kappa-m)^m, \quad 1 \leq |\alpha| \leq 2, \]

where the constant \( C \) is independent of \( \varepsilon. \)

**Proof.**

(1) By the Hölder continuity of \( V_0, \) the case \( m = 0 \) is trivial. We can prove the case \( m \geq 1 \) by using Taylor's theorem

\[ V_0(x + z) - V_0(x) = \sum_{k=1}^{m-1} \frac{1}{k!} (z \partial)^k V_0(x) + \frac{1}{(m-1)!} \int_0^1 d\tau (1 - \tau)^{m-1} (z \partial)^m V_0(x + \tau z) \]

and noting the fact that

\[ \int \phi \left( \frac{x-y}{\varepsilon} \right) (x_i - y_i) dy = 0. \]

(2) We can obtain (2), noting

\[ \int (\partial^a \phi) \left( \frac{x-y}{\varepsilon} \right) V_0(x) dy = 0, \quad |\alpha| > 0. \quad \square \]

First we shall evaluate the norm of \( D_1(t; h). \)

**Lemma 2.2.** One has
\[ \|D_1(t; h)\| = \varepsilon^{(\kappa+m)^2} h^{-1} O(t), \]
uniformly in \( h \in (0, 1]. \)
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Proof. We have
\[
\exp\left(-\frac{t}{\hbar} H_\epsilon(h)\right) - \exp\left(-\frac{t}{\hbar} H(h)\right)
\]
\[
= \int_0^t \exp\left(-\frac{s}{\hbar} H_\epsilon(h)\right) (H(h) - H_\epsilon(h)) \exp\left(-\frac{(t-s)}{\hbar} H(h)\right) ds
\]
\[
= \int_0^t \exp\left(-\frac{s}{\hbar} H_\epsilon(h)\right) (V_0(x) - V_{0,\epsilon}(x)) \exp\left(-\frac{(t-s)}{\hbar} H(h)\right) ds.
\]
Use Lemma 2.1 (1), then we get the desired estimate for $D_1(t; h)$.

Next we evaluate the norm of $D_3(t; h)$.

Lemma 2.3. One has
\[
\|D_3(t; h)\| = e^{(\kappa + \eta^2) h^{-1} O(t)},
\]
uniformly in $h \in (0, 1]$.

Proof. This evaluation can be done immediately by considering the identity
\[
K_\epsilon(t; h) - K(t; h)
\]
\[
= \exp\left(-\frac{t}{\hbar} V_\epsilon/2\right) \exp\left(-\frac{t}{\hbar} H_0(h)\right) \exp\left(-\frac{t}{\hbar} V_\epsilon/2\right)
\]
\[
- \exp\left(-\frac{t}{\hbar} V_\epsilon/2\right) \exp\left(-\frac{t}{\hbar} H_0(h)\right) \exp\left(-\frac{t}{\hbar} V/2\right)
\]
\[
+ \exp\left(-\frac{t}{\hbar} V_\epsilon/2\right) \exp\left(-\frac{t}{\hbar} H_0(h)\right) \exp\left(-\frac{t}{\hbar} V/2\right)
\]
\[
- \exp\left(-\frac{t}{\hbar} V/2\right) \exp\left(-\frac{t}{\hbar} H_0(h)\right) \exp\left(-\frac{t}{\hbar} V/2\right)
\]
\[
= (\exp\left(-\frac{t}{\hbar} V_\epsilon/2\right) - \exp\left(-\frac{t}{\hbar} V/2\right)) \exp\left(-\frac{t}{\hbar} H_0(h)\right) \exp\left(-\frac{t}{\hbar} V/2\right)
\]
\[
+ \exp\left(-\frac{t}{\hbar} V_\epsilon/2\right) \exp\left(-\frac{t}{\hbar} H_0(h)\right) (\exp\left(-\frac{t}{\hbar} V_\epsilon/2\right) - \exp\left(-\frac{t}{\hbar} V/2\right)).
\]
Here we note the formula
\[
\exp\left(-\frac{t}{\hbar} V_{\varepsilon}/2\right) - \exp\left(-\frac{t}{\hbar} V/2\right)
= \frac{1}{2\hbar} \int_0^t \exp\left(-\frac{s}{\hbar} V_{\varepsilon}/2\right) (V_0(x) - V_{0,\varepsilon}(x)) \exp\left(-\frac{(t-s)}{\hbar} V/2\right) ds.
\]

Then we have Lemma 2.3

Finally we make a semiclassical estimate of the norm of \(D_2(t;\hbar)\).

**Lemma 2.4.** One has

\[
\|D_2(t;\hbar)\| = e^{-\left(2-\kappa-m\right)\hbar} O(t^2) + e^{-\left(1-\kappa-m\right)\hbar^{-1} + \hbar^{-1} + \hbar^{-2}\rho} O(t^2 - \hbar^{-1} + \hbar^{-2}\rho)
+ \hbar^{-2}\rho} O(t^2 - \hbar^{-1} + \hbar^{-2}\rho)
+ \hbar^{-2}\rho} O(t^2 - \hbar^{-1} + \hbar^{-2}\rho),
\]

as \(t \to 0\), uniformly in \(\hbar \in (0,1]\).

**Proof.** Since \(K_\varepsilon(t;\hbar)\) is strongly continuous in \(t\), elementary calculation yields

\[
\frac{d}{dt} K_\varepsilon(t;\hbar) = -\frac{1}{\hbar} H_\varepsilon(\hbar) K_\varepsilon(t;\hbar) - R_\varepsilon(t;\hbar).
\]

Solving this differential equation, we get

\[
(2.3) \quad D_2(t;\hbar) = \exp\left(-\frac{t}{\hbar} H_\varepsilon(\hbar)\right) - K_\varepsilon(t;\hbar) = \int_0^t \exp\left(-\frac{(t-s)}{\hbar} H_\varepsilon(\hbar)\right) R_\varepsilon(s;\hbar) ds,
\]

where

\[
R_\varepsilon(t;\hbar) = R_{1,\varepsilon}(t;\hbar) + R_{2,\varepsilon}(t;\hbar),
\]

\[
R_{1,\varepsilon}(t;\hbar) = \left[\exp\left(-\frac{t}{\hbar} V_{\varepsilon}/2\right), H_0(\hbar)/\hbar\right] \exp\left(-\frac{t}{\hbar} H_0(\hbar)\right) \exp\left(-\frac{t}{\hbar} V_{\varepsilon}/2\right),
\]

\[
R_{2,\varepsilon}(t;\hbar) = \exp\left(-\frac{t}{\hbar} V_{\varepsilon}/2\right) \left[\exp\left(-\frac{t}{\hbar} H_0(\hbar)\right), V_{\varepsilon}/(2\hbar)\right] \exp\left(-\frac{t}{\hbar} V_{\varepsilon}/2\right).
\]

Then to prove Lemma 2.4 it is enough to show
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(2.4) \[ \| R(t; \hbar) \| = e^{-(2-\kappa-m)} O(t) + e^{-(1-\kappa-m)} \hbar^{-1+\rho(1-\rho)/\rho} O(t^{2-(\rho-1)}/\rho) \]
\[ + e^{-(1-\kappa-m)} \hbar^{-1} O(t^2) + \hbar^{(\rho-2)/\rho} O(t^{1-(\rho-2)}/\rho) \]
\[ + \hbar^{-1+2(\rho-1)/\rho} O(t^{2-2(\rho-1)/\rho}), \quad t \to 0, \]
uniformly in \( \hbar \in (0, 1) \).

First we study \( R_{i,i}(t; \hbar) \). Writing \( H_0(\hbar) = \hbar^2 D_j^2 \) by use of the summation convention, where \( D_j = -i\partial/\partial x_j \), we have by a simple commutator calculus

(2.5) \[ \left[ D_j^2, \exp \left( -\frac{t}{\hbar} V_{e/2} \right) \right] \]
\[ = -\frac{t}{\hbar} [D_j, [D_j, V_{e/2}]] \exp \left( -\frac{t}{\hbar} V_{e/2} \right) \]
\[ - \frac{t^2}{\hbar^2} [D_j, V_{e/2}] [D_j, V_{e/2}] \exp \left( -\frac{t}{\hbar} V_{e/2} \right) \]
\[ - 2 \frac{t}{\hbar} [D_j, V_{e/2}] D_j \exp \left( -\frac{t}{\hbar} V_{e/2} \right) \]
\[ = -\frac{t}{\hbar} [D_j, [D_j, V_{0,e/2}]] \exp \left( -\frac{t}{\hbar} V_{e/2} \right) - \frac{t}{\hbar} [D_j, [D_j, V_{1/2}]] \exp \left( -\frac{t}{\hbar} V_{e/2} \right) \]
\[ - \frac{t^2}{\hbar^2} [D_j, V_{0,e/2}] [D_j, V_{0,e/2}] \exp \left( -\frac{t}{\hbar} V_{e/2} \right) \]
\[ - \frac{t^2}{\hbar^2} [D_j, V_{1/2}] [D_j, V_{1/2}] \exp \left( -\frac{t}{\hbar} V_{e/2} \right) \]
\[ - 2 \frac{t}{\hbar} [D_j, V_{0,e/2}] D_j \exp \left( -\frac{t}{\hbar} V_{e/2} \right) \]
\[ - 2 \frac{t}{\hbar} [D_j, V_{e/2}] D_j \exp \left( -\frac{t}{\hbar} V_{e/2} \right). \]

By Lemma 2.1 (2) we can obtain the inequalities

(2.6) \[ \| [D_j, [D_j, V_{0,e}]] \| \leq C e^{-(2-\kappa-m)}/\hbar, \]
\[ \| [D_j, V_{0,e}] \| \leq C e^{-(1-\kappa-m)}/\hbar. \]

From (1.6) we have

(2.7) \[ \| [D_j, V_1] \| \leq C_1 \langle x \rangle^{(\rho-1)}/\hbar, \]
\[ \| [D_j, [D_j, V_1]] \| \leq C_2 \langle x \rangle^{(\rho-2)}/\hbar. \]
We note for $0 < a < \rho$,

\[
\exp\left(-\frac{t}{\hbar} V_{e}\right) \langle x \rangle^a \leq C\left(\frac{\hbar}{t}\right)^{a/\rho}, \quad t \to 0. \tag{2.8}
\]

Then as an immediate consequence from (2.5) \~ (2.8) we get

\[
R_{1,\epsilon}(t; \hbar) = t[D_{f}, V_{e}]K_{e}(t; \hbar) + e^{-\frac{2(1-\kappa-m)}{\epsilon} \hbar^{-1} O_{b}(t^2)}
\]
\[
+ \frac{e^{-\frac{1-\kappa-m}{\epsilon} \hbar^{1+(\rho-1)_{\rho}}}}{\hbar^{(\rho-2)_{\rho}/\rho}} O_{b}(t^{2-(\rho-1)_{\rho}/\rho}) + \frac{e^{-\frac{\hbar^{1-(\rho-2)_{\rho}/\rho}}{\rho}}}{\hbar^{(\rho-2)_{\rho}/\rho}} O_{b}(t^{2-(\rho-1)_{\rho}/\rho}), \quad t \to 0,
\]

uniformly in $\hbar \in (0, 1]$, where $O_{b}(t^{a})$ is a bounded operator whose order in $t$ is $a$.

Second we evaluate $R_{2,\epsilon}(t; \hbar)$. To this end we express the commutator factor in $R_{2,\epsilon}(t; \hbar)$ by the following integral formula

\[
\left[\exp\left(-\frac{t}{\hbar} H_{0}(\hbar)\right), V_{e}/2\right]
\]
\[
= \frac{1}{\hbar^2} \int_{0}^{t} \exp\left(-\frac{s}{\hbar} H_{0}(\hbar)\right)[H_{0}(\hbar), V_{e}/2] \exp\left(-\frac{(t-s)}{\hbar} H_{0}(\hbar)\right) ds
\]
\[
= \int_{0}^{t} \exp\left(-\frac{s}{\hbar} H_{0}(\hbar)\right)[D_{f}^2, V_{e}/2] \exp\left(-\frac{(t-s)}{\hbar} H_{0}(\hbar)\right) ds.
\]

Then easy calculation yields

\[
[D_{f}^2, V_{e}/2] = [D_{f}, V_{e}]D_{f} + [D_{f}, [D_{f}, V_{e}/2]] \equiv A + B. \tag{2.11}
\]

Substituting (2.11) into (2.10) and taking commutator, we get

\[
R_{2,\epsilon}(t; \hbar) = -tAK_{e}(t; \hbar) - R_{21}(t; \hbar) - R_{22}(t; \hbar) - R_{23}(t; \hbar), \tag{2.12}
\]

where

\[
R_{21}(t; \hbar) = t \left[\exp\left(-\frac{t}{\hbar} V_{e}/2\right), A\right] \exp\left(-\frac{t}{\hbar} H_{0}(\hbar)\right) \exp\left(-\frac{t}{\hbar} V_{e}/2\right),
\]
\[
R_{22}(t; \hbar) = \exp\left(-\frac{t}{\hbar} V_{e}/2\right) \int_{0}^{t} \exp\left(-\frac{\hbar}{\hbar} H_{0}(\hbar)\right) B \exp\left(-\frac{(t-s)}{\hbar} H_{0}(\hbar)\right)
\]
\[
\times \exp\left(-\frac{t}{\hbar} V_{e}/2\right) ds,
\]
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\[ R_{23}(t; \hbar) = \exp \left( -\frac{t}{\hbar} V_\varepsilon/2 \right) \int_0^t \left[ \exp \left( -\frac{s}{\hbar} H_0(\hbar) \right), A \right] \]

\[ \times \exp \left( -\frac{(t-s)}{\hbar} H_0(\hbar) \right) \exp \left( -\frac{t}{\hbar} V_\varepsilon/2 \right) ds. \]

The commutator factor in \( R_{21}(t; \hbar) \) is calculated as

\[ \left[ \exp \left( -\frac{t}{\hbar} V_\varepsilon/2 \right), A \right] = -[D_j, V_\varepsilon] \left[ D_j, \exp \left( -\frac{t}{\hbar} V_\varepsilon/2 \right) \right] \]

\[ = \frac{t}{\hbar} [D_j, V_\varepsilon][D_j, V_\varepsilon/2] \exp \left( -\frac{t}{\hbar} V_\varepsilon/2 \right) \]

\[ = \frac{t}{\hbar} [D_j, V_\varepsilon][D_j, V_\varepsilon/2] \exp \left( -\frac{t}{\hbar} V_\varepsilon/2 \right) \]

\[ + \frac{t}{\hbar} [D_j, V_\varepsilon][D_j, V_1] \exp \left( -\frac{t}{\hbar} V_\varepsilon/2 \right) \]

\[ + \frac{t}{\hbar} [D_j, V_1][D_j, V_1/2] \exp \left( -\frac{t}{\hbar} V_\varepsilon/2 \right). \]

Then from (2.6) \( \sim \) (2.8) we can evaluate \( R_{21}(t; \hbar) \) as

\[ (2.13) \quad \| R_{21}(t; \hbar) \| = e^{-2\left(1-\kappa-m\right)+} \hbar^{-1} O(t^2) + O\left(t^{2-\rho} \right) \]

\[ + \hbar^{-1+2(\rho-1)/\rho} O\left(t^{2-(\rho-1)/\rho}\right), \quad t \to 0, \]

uniformly in \( \hbar \in (0, 1] \). By Lemma 2.1 and (1.6) we have

\[ |B| \leq C e^{-\left(2-m-\kappa\right)\hbar} + C_2 \langle x \rangle^{\rho-2}. \]

To evaluate \( R_{22}(t; \hbar) \) we use this fact and the next lemma, which we shall show later.

**Lemma 2.5.** For every nonnegative number \( l \), one has

1. \[ \| \langle x \rangle^{-l} \exp \left( -\frac{t}{\hbar} H_0(\hbar) \right) \langle x \rangle^l \| = O(1), \quad t \to 0, \]

2. \[ \| \langle x \rangle^{-l} \exp \left( -\frac{t}{\hbar} H_0(\hbar) \right) D_j \langle x \rangle^l \| = \hbar^{-1/2} O(t^{-1/2}), \quad t \to 0, \]

uniformly in \( \hbar \in (0, 1] \).

Decompose \( B \) as \( B = \langle x \rangle^{\rho-2} / 2 \langle x \rangle^{-(\rho-2)} B \langle x \rangle^{-(\rho-2)} / 2 \langle x \rangle^{\rho-2} / 2 \) and use Lemma 2.1 and Lemma 2.5 (1). Then \( R_{22}(t; \hbar) \) takes the form
\[
\exp\left(-\frac{t}{\hbar} V_e/2\right) \langle x \rangle^{(p-2)/2} \int_0^t O_b(s) \langle x \rangle^{(p-2)/2} \exp\left(-\frac{t}{\hbar} V_e/2\right) \\
+ e^{-(2-K-m)} \int_0^t O_b(s) ds,
\]

where \( O_b(1) \) is some bounded operator whose order in \( t \) is 0. From the condition (1.6) we obtain

\[(2.14) \quad \| R_{22}(t; \hbar) \| = e^{-2(K-m)} O(t) + \hbar^{(p-2)/2} O(t^{1-(p-2)/2}), \quad t \to 0,
\]

uniformly in \( \hbar \in (0,1) \).

We shall prove that \( R_{23}(t; \hbar) \) obeys almost the same bound as (2.13) and (2.14). To this end we rewrite \( R_{23}(t; \hbar) \) as an integral expression

\[(2.15) \quad R_{23}(t; \hbar) = \exp\left(-\frac{t}{\hbar} V_e/2\right) \int_0^t F(s; \hbar) \exp\left(-\frac{(t-s)}{\hbar} H_0(\hbar)\right) ds \exp\left(-\frac{t}{\hbar} V_e/2\right),
\]

where

\[(2.16) \quad F(s; \hbar) = -\int_0^s \exp\left(-\frac{\tau}{\hbar} H_0(\hbar)\right) [H_0(\hbar)/\hbar, A] \exp\left(-\frac{(s-\tau)}{\hbar} H_0(\hbar)\right) d\tau.
\]

We can calculate the commutators

\[(2.17) \quad [H_0(\hbar), A] = \hbar^2 [D_k^2, A],
\]

\[ [D_k^2, A] = [D_k, [D_j, V_e]] D_j D_k + D_k [D_k, [D_j, V_e]] D_j,
\]

\[ [D_k, [D_j, V_e]] = [D_k, [D_j, V_{0,e}]] + [D_k, [D_j, V_1]].
\]

By Lemma 2.5 (2) and Lemma 2.1 we rewrite \( F(s; \hbar) \) as

\[ F(s; \hbar) = e^{-2(K-m)} \hbar \int_0^s \hbar^{-1/2} O_b((s-\tau)^{-1/2}) \hbar^{-1/2} O_b((s-\tau)^{-1/2}) d\tau \\
+ e^{-2(K-m)} \hbar \int_0^s \hbar^{-1/2} O_b((s-\tau)^{-1/2}) H_0^{1/2} d\tau \\
+ \langle x \rangle^{(p-2)/2} \hbar \int_0^s \hbar^{-1/2} O_b((s-\tau)^{-1/2}) H_0^{1/2} \langle x \rangle^{(p-2)/2} d\tau \\
= e^{-2(K-m)} O_b(1) + e^{-2(K-m)} \hbar^{1/2} O_b(s^{1/2}) H_0^{1/2} \\
+ \langle x \rangle^{(p-2)/2} O_b(1) \langle x \rangle^{(p-2)/2} + \langle x \rangle^{(p-2)/2} \hbar^{1/2} O_b(s^{1/2}) H_0^{1/2},
\]
The Semiclassical Estimate of the Eigenvalue

where \( H_0 = -\Delta \) and \( O_b(t^a) \) is a bounded operator whose order in \( t \) is \( a \). From (2.8) we get the estimate

\[
\tag{2.18} \| R_{23}(t; h) \| = e^{-(2-k-m) + O(t) + h^{(p-2)/\rho} O(t^{1-(p-2)/\rho})}, \quad t \to 0,
\]

uniformly in \( h \in (0, 1] \).

From (2.13), (2.14) and (2.18) we have with (2.12)

\[
\tag{2.19} R_{2,3}(t; h) = -t[D_j, V_\epsilon]D_j K_\epsilon(t; h) + e^{-(1-k-m) + h^{-1} O_b(t^2)}
\]

\[
+ e^{-(2-k-m) + h^{(p-2)/\rho} O_b(t^{1-(p-2)/\rho})}
\]

\[
+ e^{-(2-k-m) + h^{(p-2)/\rho} O_b(t^{1-(p-2)/\rho})}
\]

\[
+ h^{1+2(p-1)/\rho} O_b(t^{2-(p-1)/\rho}), \quad t \to 0,
\]

uniformly in \( h \in (0, 1] \). Summing up (2.9) and (2.19) we have the estimate (2.4). In view of (2.3) we have thus proved Lemma 2.4.

**Proof of Proposition 2.1.** From Lemma 2.2 ~ 2.4 we have Proposition 2.1 by putting \( \epsilon = t^a \) with \( a > 0 \).

Finally we give the proof of Lemma 2.5, which we have used in the proof of Lemma 2.4.

**Proof of Lemma 2.5.** By interpolation, it suffices to prove (1) and (2) only for every integer \( k \geq 0 \).

(1) The proof is done by induction. The case \( k = 0 \) is trivial. We assume the case \( 0 \leq k \leq k \). If it is shown that

\[
\tag{2.20} \left\| \langle x \rangle^{-(k+1)} \left[ \exp \left( \frac{-t}{h} H_0(h) \right), \langle x \rangle^{k+1} \right] \right\| = O(1), \quad t \to 0,
\]

then the case \( k = k + 1 \) follows at once and the proof is complete. To prove (2.20), we represent the commutator as

\[
\left[ \exp \left( \frac{-t}{h} H_0(h) \right), \langle x \rangle^{k+1} \right]
\]

\[
= - \int_0^t \exp \left( \frac{-s}{h} H_0(h) \right) [H_0(h)/h, \langle x \rangle^{k+1}] \exp \left( \frac{(t-s)}{h} H_0(h) \right) ds.
\]
The commutator in the integrand takes the form

\[ [H_0, \langle x \rangle^{k+1}] \sim b_j(x) D_j + b_0(x), \]

where \( b_j(x) = O(|x|^k) \) and \( b_0(x) = O(|x|^{k-1}) \) as \( |x| \to \infty \). Noting \( D_j (H_0 + 1)^{-1/2} \) is bounded, we have (2.20). This ends the proof of Lemma 2.5 (1).

(2) Noting that \( \| D_j (H_0 + 1)^{-1/2} \| = O(1/h) \) and

\[
\| H_0(h)^{1/2} \exp \left( -\frac{t}{h} H_0(h) \right) \| = h^{1/2} O(r^{-1/2}), \quad t \to 0,
\]

uniformly in \( h \in (0,1] \), the case \( l = 0 \) follows at once. We assume the case \( 0 \leq l \leq k \). Then by Lemma 2.5 (1) we have

\[
(2.21) \quad \langle x \rangle^{-(k+1)} \exp \left( -\frac{t}{h} H_0(h) \right) D_j \langle x \rangle^{k+1}
\]

\[ = O_b(1) + \langle x \rangle^{-(k+1)} \exp \left( -\frac{t}{h} H_0(h) \right) \langle x \rangle^{k+1} D_j. \]

We take the commutator between \( \exp \left( -(t/h)H_0(h) \right) \) and \( \langle x \rangle^{k+1} \) in (2.21). Then

\[
(2.22) \quad \langle x \rangle^{-(k+1)} \exp \left( -\frac{t}{h} H_0(h) \right) \langle x \rangle^{k+1} D_j
\]

\[ = \langle x \rangle^{-(k+1)} \langle x \rangle^{k+1} \exp \left( -\frac{t}{h} H_0(h) \right) D_j
\]

\[ - \langle x \rangle^{-(k+1)} \int_0^t \exp \left( -\frac{s}{h} H_0(h) \right) [H_0(h)/h, \langle x \rangle^{k+1}] \exp \left( -\frac{(t-s)}{h} H_0(h) \right) ds D_j. \]

The second term in (2.22) takes the form

\[-\langle x \rangle^{-(k+1)} h \int_0^t \exp \left( -\frac{s}{h} H_0(h) \right) (D_j b_j(x) + b_0(x)) \exp \left( -\frac{(t-s)}{h} H_0(h) \right) D_j ds. \]

where \( b_j(x) = O(|x|^k) \) and \( b_0(x) = O(|x|^{k-1}) \) as \( |x| \to \infty \). Therefore by the assumption of the induction

\[
\langle x \rangle^{-(k+1)} \exp \left( -\frac{t}{h} H_0(h) \right) \langle x \rangle^{k+1} D_j
\]

\[ = h^{-1/2} O_b(t^{-1/2}) + h \int_0^t h^{-1/2} O_b(s^{-1/2}) h^{-1/2} O_b((t-s)^{-1/2}) = h^{-1/2} O_b(t^{-1/2}). \]

This ends the proof of Lemma 2.5 (2). \( \square \)
Remark 2.1. From Proposition 2.1, one can also obtain an error bound of the operator norm for the Trotter-Kato product formula such as in [3], [5] or [1]

\[
\|\exp(-tH(1)) - (K(t/N; 1))^N\| = \begin{cases} O(N^{-(\epsilon + m)/2})^{(1/2)}, & m = 0, 1, \\ O(N^{-2/p \wedge 1}), & m \geq 2, \end{cases}
\]

as \( N \to \infty \). This estimate corresponds to the result of the paper [5] but the paper [1] did not include the case \( m = 0, 1 \). In fact, set \( \hbar = 1 \) in Proposition 2.1. Then we have

\[
\|\exp(-tH(1)) - K(t; 1)\| = O(t^{1+a((\kappa + m) \wedge 2)}) + O(t^{2-a(2-\kappa - m)_+}) + O(t^{3-a(1-\kappa - m)_+}) \\
+ O(t^{3-a(1-\kappa - m)_+ - (\rho-1)_+ / \rho}) + O(t^{2-(\rho-1)_+ / \rho}) + O(t^{-2(\rho-1)_+ / \rho}), \quad t \to 0.
\]

Then we have the constraint conditions in \( a \) such as

\[
a((\kappa + m) \wedge 2) + 1 \geq 0, \quad -a(2-\kappa - m)_+ + 2 \geq 0,
\]

\[
-2a(1-\kappa - m)_+ + 3 \geq 0, \quad 3 - a(1-\kappa - m)_+ - (\rho-1)_+ / \rho \geq 0.
\]

We should take the order in \( t \) as large as possible. Therefore we choose \( a = 1/2 \). Then we have

\[
\|\exp(-tH(1)) - K(t; 1)\| = \begin{cases} O(t^{1+(\kappa + m)/2})^{(1+2/\rho)}, & m = 0, 1, \\ O(t^{1+2/\rho} \wedge 2), & m \geq 2, \end{cases}
\]

at \( t \to 0 \). This estimate and standard telescope argument yield the desired error bound (2.23) of the operator norm for the Trotter-Kato product formula. \( \square \)

3. Semiclassical Asymptotic Expansions of Eigenvalues for the Schrödinger Operator

In this section we see semiclassical asymptotic expansions of the eigenvalues for the Schrödinger operator with one well potential. For this purpose we have assumed the asymptotic expansion (3) in (1.7) for the potential \( V_0(x) \). Under the assumptions (1.6) and (1.7), \( H(\hbar) \) has only discrete spectrum. We label these eigenvalues by \( E_j(\hbar) \), where we list the eigenvalues in increasing size, including multiplicity,

\[
E_1(\hbar) < E_2(\hbar) \leq E_3(\hbar) \leq \cdots.
\]
Under the condition (1.7) $H_\kappa$ in (1.8) also has only discrete spectrum. Let $(e_j)_{j=1}^\infty$ be the eigenvalues of $H_\kappa$ listed in increasing size, including multiplicity,

$$e_1 < e_2 \leq e_3 \leq \cdots,$$

and let $(\tilde{e}_j)_{j=1}^\infty$ be the set of distinct values $\tilde{e}_j$, ordered by size, with multiplicity $m_j$, so that $\tilde{e}_1 = e_1$ and $\tilde{e}_2 = e_2$. Then we can determine explicitly the first asymptotic coefficient of $E_j(h)$.

**Theorem 3.1.** Let $V(x)$ satisfy the conditions (1.6) and (1.7). Then there exist $m_j$ not necessarily distinct eigenvalues $E_{k(j)}(h)$ of the Schrödinger operator $H(h)$ satisfying

$$\lim_{h \to 0} \frac{E_{k(j)}(h)}{h^\alpha} = \tilde{e}_j$$

with

$$\alpha = \frac{2(\kappa + m)}{\kappa + m + 2}, \quad \beta = \frac{2}{\kappa + m + 2}.$$

Moreover we have

**Theorem 3.2.** Let $V(x)$ satisfy (1.6) and (1.7). For each $\tilde{e}_j$ there are $m_j$ not necessarily distinct eigenvalues $E_{k(j)}(h)$ of $H(h)$ satisfying

$$E_{k(j)}(h) \sim h^\alpha \left( \tilde{e}_j + \sum_{l=1}^{\infty} \tilde{c}_l^{k(j)} h^{\beta l} \right),$$

as $h \to 0$, with the same $\alpha$ and $\beta$ as in Theorem 3.1, where the $\tilde{c}_l^{k(j)}$ are some constants depending on $(a_s)_{|s|=0}^\infty$ in (3) in (1.7) and $\tilde{c}_l^{k(j)} = 0$, $(1 \leq l < \infty)$ if $V(x) = a_0 w(x)$.

This type of theorems has been proved by [11], [7], [8] and others for double well or multiple well potentials. Though their results include one well potential case, we want to treat some more general one well potentials. In the first place we shall prove Theorem 3.1 by a method similar to that used by Simon [11] to prove the tunneling effect. We modify two lemmas used in his proof.

We can take $C^\infty$ functions $j^0(x)$ and $j^1(x)$ such that $0 \leq j^k(x) \leq 1$, $k = 0, 1$, $(j^0(x))^2 + (j^1(x))^2 = 1$ and $j^0(x)$ satisfies

$$j^0(x) = \begin{cases} 
1, & |x| \leq 1, \\
0, & |x| \geq 2. 
\end{cases}$$
Then we put \( J^0(\hbar) = j^0(\hbar^{-\delta}x) \) and \( J^1(\hbar) = j^1(\hbar^{-\delta}x) \) for some constant \( \delta > 0 \). Set
\[
(U(h)f)(x) = h^{d\beta/2}f(h^{\beta}x), \quad f \in L^2(\mathbb{R}^d).
\]

Let \( (\phi_j(x))_{j=1}^{\infty} \) be the orthonormal eigenfunctions of \( H_\kappa \) in (1.8) with eigenvalues \( (\epsilon_j)_{j=1}^{\infty} \) and put \( \psi_j(x) = (J^0(\hbar)U(\hbar)^{-1}\phi_j)(x) \). Then we shall see below that \( (\psi_j(x))_{j=1}^{\infty} \) are asymptotically approximated eigenfunctions for \( H(\hbar) \).

**Lemma 3.1.** Set \( H_\kappa(\hbar) = -\hbar^2\Delta + a_0w(x) \). Then one has
\[
\langle \psi_j, (H(\hbar) - H_\kappa(\hbar))\psi_k \rangle = O(\hbar^{\beta(\kappa + m + 1)}).
\]

**Proof.** Simple calculation leads us to the identity
\[
\langle \psi_j, (H(\hbar) - H_\kappa(\hbar))\psi_k \rangle
\]
\[
= \int_{\mathbb{R}^d} (V(x) - a_0w(x))\psi_j(x)\overline{\psi_k(x)} \, dx
\]
\[
= \int_{\mathbb{R}^d} (V(x) - a_0w(x))J^0(\hbar)U(\hbar)^{-1}\phi_j(x)J^0(\hbar)U(\hbar)^{-1}\phi_k(x) \, dx.
\]

Here \( \text{supp} \, J^0(\hbar) \) is a neighborhood of the origin in \( \mathbb{R}^d \) and \( V_0 \) satisfies the condition (2) in (1.7), so we have
\[
\int_{|x| < 2\hbar^\theta} (V_0 - a_0w(x))U(\hbar)^{-1}\phi_j(x)U(\hbar)^{-1}\phi_k(x) \, dx
\]
\[
= \int_{|x| < 2\hbar^\theta} w(x)|x|O(1)U(\hbar)^{-1}\phi_j(x)U(\hbar)^{-1}\phi_k(x) \, dx
\]
\[
= \int_{|y| < 2\hbar^{\beta\theta}} w(\hbar^{\beta\theta}y) |y|O(1)\phi_j(y)\overline{\phi_k(y)} \, dy
\]
\[
= \hbar^{\beta(\kappa + m + 1)} \int_{|y| < 2\hbar^{\beta\theta}} w(y)|y|O(1)\phi_j(y)\overline{\phi_k(y)} \, dy.
\]

Since by the exponential decay property of \( (\phi_j(y))_{j=1}^{\infty} \), we have
\[
\left| \int_{|y| < 2\hbar^{\beta\theta}} w(y)|y|O(1)\phi_j(y)\overline{\phi_k(y)} \, dy \right| \leq \|w\| \|y\| \|\phi_j\| \|\phi_k\| < \infty,
\]
we obtain
\[
\langle \psi_j, (H(\hbar) - H_\kappa(\hbar))\psi_k \rangle = O(\hbar^{\beta(\kappa + m + 1)}).
\]
LEMMA 3.2. We have asymptotic orthogonality of the asymptotically approximated eigenfunctions \((\psi_j(x))_{j=1}^\infty\)
\[
\langle \psi_j, \psi_k \rangle = \delta_{jk} + O(\exp(-ch^{\delta-\beta}))
\]
for an arbitrary constant \(\delta\) with \(0 < \delta < \beta\), where \(c\) is a positive constant and \(\delta_{jk}\) is Kronecker's delta.

PROOF. One can verify this lemma by a similar method used to prove Lemma 3.1 and the exponential decay property of \((\phi_j)_{j=1}^\infty\). \(\square\)

PROOF OF THEOREM 3.1. To prove Theorem 3.1 we shall show that we can get the value \(\bar{e}_j\) as both the upper bound and the lower bound.

(1) \(\lim \sup_{h \to 0} E_{k(j)}(h)/h^2 \leq \bar{e}_j\).

First of all, we shall estimate \(\langle \psi_j, H(h)\psi_k \rangle\), using the same notations as in Section 1. To this end we estimate \(\langle \psi_j, H_k(h)\psi_k \rangle\).

Recall the fact that \((\phi_j)_{j=1}^\infty\) are the eigenfunctions of \(H_k\) with eigenvalues \((e_j)_{j=1}^\infty\). Then we have
\[
\langle \psi_j, H_k(h)\psi_k \rangle = \langle J^0(h)U^{-1}(h)\phi_j, J^0(h)H_k(h)U^{-1}(h)\phi_k \rangle
\]
\[
= \frac{1}{2} \langle J^0(h)U^{-1}(h)\phi_j, J^0(h)H_k(h)U^{-1}(h)\phi_k \rangle
\]
\[
+ \frac{1}{2} \langle J^0(h)H_k(h)U^{-1}(h)\phi_j, J^0(h)U^{-1}(h)\phi_k \rangle + \langle \psi_j, h^2(\nabla J^0(h))^2\psi_k \rangle
\]
\[
= \frac{1}{2} \langle \psi_j, h^2 e_k \psi_k \rangle + \frac{1}{2} \langle h^2 e_j \psi_j, \psi_k \rangle + \langle \psi_j, h^2(\nabla J^0(h))^2\psi_k \rangle.
\]
Since we have \((\nabla J^0(h))^2 = O(h^{-2\delta})\) by the definition of \(J^0(h)\), we get, for any constant \(\delta < (2 - \alpha)/2 = \beta\), the semiclassical estimate
\[
\langle \psi_j, H_k(h)\psi_k \rangle = \langle \psi_j, h^2 e_k \psi_k \rangle \delta_{jk} + O(h^{2-2\delta}).
\]
Thus we have by Lemmas 3.1 and 3.2,
\[
(3.1) \quad \langle \psi_j, H(h)\psi_k \rangle = h^2 e_k \delta_{jk} + O(h^{(2-2\delta)\wedge \beta(k+m+1)}).
\]
From Lemma 3.2 we conclude that \((\psi_k)_{k=1}^\infty\) span an \(r\)-dimensional subspace for small \(h\). Then we can find, for arbitrary \((\xi_j)_{j=1}^r \subseteq L^2(\mathbb{R}^d)\) and for sufficiently small \(h\), a linear combination \(\psi\) of \((\psi_1, \psi_2, \ldots, \psi_r)\) such that \(\psi \in [\xi_1, \xi_2, \ldots, \xi_r]^\perp\). Note \(H(h)\) has only pure discrete spectrum, then the semiclassical estimate (3.1) enables us to use the min-max principle to estimate the upper bound for \(E_{k(j)}(h)\).
(2) \( \liminf_{\hbar \to 0} E_{k(j)}(\hbar) / \hbar^\alpha \geq \tilde{e}_j \). We use the following localization formula with the semiclassical parameter to obtain the lower bound.

**Lemma 3.3.** One has the formula

\[
H(\hbar) = J^1(\hbar)H(\hbar)J^1(\hbar) + J^0(\hbar)H(\hbar)J^0(\hbar) - \sum_{a=0}^{1} \hbar^2 (\nabla \psi_a(\hbar))^2
\]

in the form sense.

**Proof.** It is easy to see for an arbitrary \( C^\infty \) function \( f \)

\[
[f, [f, H(\hbar)]] = -2\hbar^2 (\nabla f)^2.
\]

Then taking \( J^1(\hbar) \) and \( J^0(\hbar) \) as \( f \) and summing them up, we obtain the formula. \( \square \)

From the condition for \( V_0(x) \), we have the following asymptotic evaluation

\[
\| J^0(\hbar)(H(\hbar) - H_{\kappa}(\hbar))J^0(\hbar) \| = O(\hbar^{\delta(\kappa+m+1)}).
\]

Then we have

\[
J^0(\hbar)H(\hbar)J^0(\hbar) \geq J^0(\hbar)R(\hbar)J^0(\hbar) + \hbar^\alpha e(J^0(\hbar))^2 + O(\hbar^{\delta(\kappa+m+1)}),
\]

where \( R(\hbar) \) is the restriction of \( H_{\kappa}(\hbar) \) to the span of all eigenfunctions of the \( H_{\kappa}(\hbar) \) with eigenvalues lying below \( \hbar^\alpha e \) for \( e \in (\tilde{e}_{j-1}, \tilde{e}_j) \) and the rank of \( R(\hbar) \) is at most \( 1 + \sum_{j=1}^{J-1} m_j \). Moreover, since \( |x| \geq c_{\hbar} \) on \( \text{supp } J^1(\hbar) \), we see for any \( \delta \) satisfying \( \delta(\kappa + m) < \alpha \)

\[
J^1(\hbar)H(\hbar)J^1(\hbar) \geq c \chi(x)|x|^{k+m}(J^1(\hbar))^2 + c(1 - \chi(x))
\]

\[
\geq \hbar^{\delta(\kappa+m)} c(J^1(\hbar))^2 \geq \hbar^\alpha e(J^1(\hbar))^2,
\]

with sufficiently small \( \hbar \) and every \( e \in (\tilde{e}_{j-1}, \tilde{e}_j) \), where \( \chi(x) \) is a \( C^\infty \) cut-off function with \( 0 \leq \chi(x) \leq 1 \) in \( \mathbb{R}^d \) and \( \text{supp } \chi(x) \subseteq \{ x \in \mathbb{R}^d : |x| \leq 1 \} \).

From Lemma 3.3, summing up and using \( (\nabla \psi_a(\hbar))^2 = O(\hbar^{-2\beta}) \), \( \alpha = 0, 1 \), we obtain for \( \alpha/(\kappa + m + 1) < \delta < \beta \),

\[
H(\hbar) \geq \hbar^\alpha e1 + J^0(\hbar)R(\hbar)J^0(\hbar) + O(\hbar^{2-2\beta})^{\delta(\kappa+m+1)},
\]

where \( 1 \) is the identity operator. This inequality shows the lower bound.
From (1) and (2) we have proved Theorem 3.1 by taking the constant $\delta$ so as to satisfy $\beta(\kappa + m)/(\kappa + m + 1) < \delta < \beta$, noting $\beta(\kappa + m)/(\kappa + m + 1) = \alpha/(\kappa + m + 1)$.

Next we proceed to obtain the asymptotic expansion of the eigenvalue of the Schrödinger operator. We shall recall some notations used in the proof of Theorem 3.1. We put

$$ P_j(h) = \frac{i}{2\pi} \oint_{(\kappa \varepsilon_j, z) = h^\varepsilon} (H(h) - z)^{-1} dz, $$

where $\varepsilon > 0$ is so small that there are no other eigenvalues in the disc $\{ z \in \mathbb{C} \mid z - h^\varepsilon \leq h^\varepsilon \}$. For higher order perturbation the next lemma is crucial.

**Lemma 3.4.** $\|(1 - P_j(h))\psi_k\| \to 0$ as $h \to 0$ for every positive integer $j$, where $k \in (k_1(j), k_1(j), \ldots, k_m(j)) = (k_1(j), k_1(j) + 1, \ldots, k_1(j) + m - 1)$.

**Proof.** We show the lemma by induction on $j$. Suppose the lemma has been proved for all $i < j$. Then for every $i$ with $i < j$, $P_i(h)\psi_s - \psi_s \to 0$ as $h \to 0$ for $s \in (s_1(i), s_2(i), \ldots, s_m(i))$. From Lemma 3.2, we see that $(\psi_k^s)_{k=1}^{m_i}$ is linearly independent and hence $(P_i(h)\psi_k^s)_{i=1}^{m_i}$ span an $m_i$-dimensional subspace $\text{Ran} P_i(h)$. Take an orthonormal basis $(u_l)_{l=1}^{m_i}$ of $\text{Ran} P_i(h)$. Then we can write

$$ u_l = \sum_{p=1}^{m_i} a_l^p P_i(h)\psi_{s_p}. $$

Then for $k \in (k_1(j), k_2(j), \ldots, k_m(j))$ we have

$$ P_i(h)\psi_k = \sum_{l=1}^{m_i} \langle P_i(h)\psi_k, u_l \rangle u_l $$

$$ = \sum_{l=1}^{m_i} \langle P_i(h)\psi_k, \sum_{p=1}^{m_i} a_l^p P_i(h)\psi_{s_p} \rangle \sum_{q=1}^{m_i} a_q^p P_i(h)\psi_{s_q} $$

$$ = \sum_{l=1}^{m_i} \sum_{p=1}^{m_i} \sum_{q=1}^{m_i} a_l^p a_q^q \langle \psi_k, P_l(h)\psi_{s_p} \rangle P_q(h)\psi_{s_q}. $$

On the other hand, since $\|u_l\| = 1$, we have from Lemma 3.2 $|a_l^p| \leq C$, where $C$ is independent of small $h$. Then it follows from the assumption of the induction and Lemma 3.2 that

$$ \langle \psi_k, P_l(h)\psi_{s_p} \rangle = \langle \psi_k, (P_l(h) - 1)\psi_{s_p} \rangle + \langle \psi_k, \psi_{s_p} \rangle \to 0, $$

as $h \to 0$. Therefore we have that $P_l(h)\psi_k \to 0$ as $h \to 0$ from every $i$ with $i < j$ and for $k \in (k_1(j), k_2(j), \ldots, k_m(j))$. That is, $P(-\infty, \varepsilon_j - \varepsilon)\psi_k \to 0$ as $h \to 0$ for
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every positive \( \varepsilon \), where \( P(\lambda) \) is the spectral measure of \( \hbar^{-2}H(h) \). If we preserve the consistency with the fact that \( \langle \psi_k, \hbar^{-2}H(h) \psi_k \rangle \to \tilde{e}_j \), we conclude that \( \| P(\tilde{e}_j - \varepsilon, \tilde{e}_j + \varepsilon) \psi_k \| \) converges to 1 for \( k \in (k_1(j), k_2(j), \ldots, k_m(j)) \), which implies the lemma for \( j \).

We are going to prove Theorem 3.2, first in the case \( \tilde{e}_j \) is simple and then in the case \( \tilde{e}_j \) is degenerate.

(1) The case \( \tilde{e}_j \) is simple.

In this case we have \( m_j = 1 \). Let \( k = k_1(j) = k_m(j) \). Put

\[
\tilde{H}(h) = \hbar^{-2}U(h)H(h)U(h)^{-1},
\]

\[
\tilde{P}_j(h) = \frac{i}{2\pi} \int_{|\tilde{e}_j - z| = \varepsilon} (\tilde{H}(h) - z)^{-1} \, dz.
\]

If \( \phi_k \) is the \( k \)-th eigenfunction of \( H_k \) in (1.8) with the eigenvalue \( e_k = \tilde{e}_j \), then by Lemma 3.4 we have \( \tilde{P}_j(h)\phi_k \to \phi_k \) as \( h \to 0 \). Thus \( \langle \phi_k, \tilde{P}_j(h)\phi_k \rangle \) is convergent to 1 and so it is non-vanishing. Note the trivial relation

\[
\hbar^{-2}E_{k(j)}(h) = \frac{\langle \tilde{H}(h)\phi_k, \tilde{P}_j(h)\phi_k \rangle}{\langle \phi_k, \tilde{P}_j(h)\phi_k \rangle}.
\]

Then for the proof of Theorem 3.2 we need further to obtain the \( L^2 \)-asymptotic expansion of \( \tilde{P}_j(h)\phi_k \).

**Lemma 3.5.** For each fixed positive integer \( l \), \( \langle x \rangle^l (H_k - z)^{-1} \langle x \rangle^{-l} \) is a bounded operator.

**Proof.** The case \( l = 0 \) is trivial. Let \( l = 1 \). Then we can show the lemma noting that

\[
[\langle x \rangle, (H_k - z)^{-1}] = (H_k - z)^{-1} [H_k, \langle x \rangle] (H_k - z)^{-1}
\]

and \( \partial_j \) is \( H_k \) bounded. Assume the case \( l = k \) is valid. Then we can show the case \( l = k + 1 \) in the same way as the case \( l = 1 \).

**Proof of Theorem 3.2** (The simple case). Note \( \hbar^{-2}U(h)H_k(h)U(h)^{-1} = H_k \).

If \( V(x) = a_0 w(x) \) then from (3.2) we have \( \hbar^{-2}E_{k(j)}(h) = e_k = \tilde{e}_j \). Therefore \( c_l^{(k)} = 0 \), \( (1 \leq l < \infty) \) in the case \( V(x) = a_0 w(x) \). If \( V(x) \neq a_0 w(x) \) we expand the resolvent of \( \tilde{H}(h) \) as a geometric series

\[
(H_k - z)^{-1} \phi_k = \sum_{n=0}^{l-1} t_n(h) + r_l(h),
\]
where
\[ t_n(h) = (-1)^n(H_K - z)^{-1} \{ \tilde{V}(H_K - z)^{-1} \}^n \phi_k, \]
\[ r_l(h) = (-1)^l(\tilde{H}(h) - z)^{-1} [ \tilde{V}(H_K - z)^{-1} ]^l \phi_k, \]
\[ \tilde{V} = h^{-\alpha}(V(h^\beta x) - a_0 w(h^\beta x)). \]

Therefore we need to estimate \( \| t_n(h) \| \) and \( \| r_l(h) \| \).

Recall \( V_0(x) \) has an asymptotic expansion in (1.7) in a neighborhood of the origin. Let \( \chi(x) \) be an \( C^\infty \) function such that
\[ \chi(x) = \begin{cases} 1, & |x| \leq 1/2, \\ 0, & |x| \geq 1, \end{cases} \]
and put \( \chi_h = \chi(h^\beta x) \). Then we have
\[ \chi_h \tilde{V} \sim h^{-\alpha} w(h^\beta x) \sum_{|\gamma|=1}^\infty a_j h^{j|\gamma|} x^\gamma \]
as \( h \to 0 \), that is, near \( x = 0 \). This implies that \( \chi_h \tilde{V} \) takes for \( l > 0 \) the form
\[ \chi_h \tilde{V} = \chi_h Q_l(h; x) + R_l(h; x), \]
where
\[ Q_l(h; x) = h^{-\alpha} w(h^\beta x) \sum_{|\gamma|=1}^{l-1} a_j h^{j|\gamma|} x^\gamma. \]

Then we have on \( \text{supp} \chi(h^\beta x) \)
\[ |R_l(h; x)| \leq C_R h^{l|\beta|} x^{(\kappa+m+l)}, \]
where \( C_R \) is some positive constant. Put
\[ \tilde{t}_n(h) = (-1)^n(H_K - z)^{-1} \{ \chi_h \tilde{V}(H_K - z)^{-1} \}^n \phi_k, \]
\[ \tilde{r}_l(h) = (-1)^l(\tilde{H}(h) - z)^{-1} [ \chi_h \tilde{V}(H_K - z)^{-1} ]^l \phi_k. \]

We obtain by Lemma 3.5 and exponential decay property of \( \phi_k \),
\[ \| \tilde{r}_l(h) \| = \| (-1)^l(\tilde{H}(h) - z)^{-1} \{ \chi_h \tilde{V}(H_K - z)^{-1} \}^l \phi_k \|
= O(h^{l|\beta|}). \]
On the other hand, we have

\[(3.5)\]
\[r_I(h) - \tilde{r}_I(h) = (-1)^l (\tilde{H}(h) - z)^{-1} (1 - \chi_h) \tilde{V}(H_k - z)^{-1} \cdots \tilde{V}(H_k - z)^{-1} \phi_k \]
\[+ (-1)^l (\tilde{H}(h) - z)^{-1} \chi_h \tilde{V}(H_k - z)^{-1} (1 - \chi_h) \tilde{V}(H_k - z)^{-1} \cdots \tilde{V}(H_k - z)^{-1} \phi_k \]
\[+ \cdots + (-1)^l (\tilde{H}(h) - z)^{-1} \chi_h \tilde{V}(H_k - z)^{-1} \chi_h \tilde{V} \cdots (1 - \chi_h) \tilde{V}(H_k - z)^{-1} \phi_k.\]

Noting \(|\tilde{V}| \leq C h^{-a} |x|^{(\kappa + m + 1) \vee \rho} \), the exponential decay property of \(\phi_k\),

\[\|(1 - \chi_h) |x|^{-N} \|_\infty = O(h^{N\rho}) \] for all \(N > 0\) and Lemma 3.5 implies

\[\|r_I(h) - \tilde{r}_I(h)\| = \|(-1)^l (\tilde{H}(h) - z)^{-1} ((1 - \chi_h) |x|^{-N}) (|x|^{-N} \tilde{V}) \]
\[\times \langle x \rangle^{2N} (H_k - z)^{-1} \langle x \rangle^{-2N} \langle |x|^{-N} \tilde{V} \rangle \langle x \rangle^{3N} (H_k - z)^{-1} \]
\[\cdots \tilde{V} \langle x \rangle^{(l+1)N} (H_k - z)^{-1} \langle x \rangle^{-l+1} \langle |x|^{-N} \tilde{V} \rangle \langle x \rangle^{l+1} \phi_k \|
\[+ \cdots + \|(-1)^l (H_k(h) - z)^{-1} (|x|^{-N} \chi_h \tilde{V}) \langle x \rangle^N (H_k - z)^{-1} \langle x \rangle^{-N} \]
\[\times \langle x \rangle^{-2N} \chi_h \tilde{V} \times \cdots (1 - \chi_h) |x|^{-N} \langle |x|^{-N} \tilde{V} \rangle \langle x \rangle^{-l+1} \langle |x|^{l+1} \rangle \phi_k \|
\[= O(h^{-(l+1)\rho}) ,\]

for all \(N \geq [(\kappa + m + 1) \vee \rho] + 1\).

Hence we conclude that

\[\|r_I(h) - \tilde{r}_I(h)\| = O(h^\infty)\]

so that \(\|r_I(h)\| = O(h^{\rho})\) from (3.4).

Similarly we have \(\|t_n(h) - \tilde{t}_n(h)\| = O(h^\infty)\).

Moreover we put

\[\tilde{t}_n(h) = (-1)^n (H_k - z)^{-1} \{Q(h; x) (H_k - z)^{-1}\}^n \phi_k.\]

Then it is seen from (3.3) that

\[\|\tilde{t}_n(h) - \tilde{t}_n(h)\| = O(h^{\rho})\]

holds for all \(1 \leq n \leq l - 1\). Since \(\tilde{t}_n(h)\) is a polynomial in \(h^\rho\), this yields the asymptotic expansion of \(E_{k(j)}\).
(2) The case \( \tilde{e}_j \) is degenerate.
We prove Theorem 3.2 in the degenerate case.

**Lemma 3.6.** Let \( C(h) \) be an \( r \times r \) Hermitian matrix whose elements have asymptotic expansion in \( h^\beta \) for \( \beta > 0 \). Then the eigenvalues of \( C(h) \) have asymptotic expansion in \( h^\beta \).

**Proof.** See [11, Lemma 5.2].

**Proof of Theorem 3.2 (The degenerate case).** Since the multiplicity of \( \tilde{e}_j \) is \( m_j \), we can take \( m_j \) eigenfunctions of \( H_x \), \( (\phi_{pq}^{m_j})_{p=1}^{m_j} \). We construct \( m_j \) eigenfunctions of \( H_x(h) \), \( \phi_{pq}^{m_j}(h) = U(h)^{-1}\phi_{pq}^{m_j} \) for \( p \in (1, 2, \ldots, m_j) \) such that \( \langle \phi_{pq}^{m_j}(h), P_j(h)\phi_{pq}^{m_j}(h) \rangle \rightarrow \delta_{pq} \) for \( p, q \in (1, 2, \ldots, m_j) \) as \( h \to 0 \). As in the proof of Theorem 3.2 we can show that the matrices

\[
\Delta(h) = \langle \phi_{pq}^{m_j}(h), P_j(h)\phi_{pq}^{m_j}(h) \rangle, \quad M(h) = \langle \phi_{pq}^{m_j}(h), H(h)P_j(h)\phi_{pq}^{m_j}(h) \rangle
\]

have the asymptotic expansion in \( h^\beta \) for \( p, q \in (1, 2, \ldots, m_j) \), noting \( \Delta(h) = (\delta_{pq}) + o(h^\beta) \).

Therefore \( \Delta(h)^{-1/2}M(h)\Delta(h)^{-1/2} \) has asymptotic expansion in \( h^\beta \). By Lemma 3.6 we conclude the eigenvalues \( (\lambda_{pq}^{m_j}(h))_{p=1}^{m_j} \) have asymptotic expansion in \( h^\beta \). Moreover if \( V(x) = a_0w(x) \) then \( M(h) = \tilde{\phi}_{pq}, \Delta(h) = \delta_{pq} \), that is, \( h^{-a}E_{k(j)}(h) = \tilde{\phi}_j, \ k_1(j) \leq k(j) \leq k_1(j) + m_j - 1 \). Hence \( c_l^{k(j)} = 0, \ (1 \leq l < \infty) \) in the case \( V(x) = a_0w(x) \).

4. **Proof of Theorem 1.1 and Example**

In this section we prove Theorem 1.1. This can be done by using Theorem 2.1 and Theorem 3.2.

**Proof of Theorem 1.1.** Recall \( E_1(h) \) and \( E_2(h) \) are the two smallest eigenvalues of \( H(h) \). Applying Theorem 2.1 and min-max principle, we have

\[
\exp(-E_j(h)) - \mu_j(h) = O(h^{(x+m)^2}), \quad h \to 0, \quad j = 1, 2.
\]

Hence

\[
\mu_2(h)/\mu_1(h) = \exp(-(E_2(h) - E_1(h))) + O(h^{(x+m)^2})
\]

\[
= 1 - (E_2(h) - E_1(h)) + O(h^{(x+m)^2}), \quad h \to 0.
\]

This is a generalization of the estimate (1.4).
Applying Theorem 3.2, we have the asymptotic expansion of $E_j(h)$ and $E_2(h)$ such that

$$E_j(h) \sim h^2 \left( e_j + \sum_{k=1}^{\infty} c_k^j h^k \right), \quad j = 1, 2,$$

where $c_k^j = 0$, $(1 \leq k < \infty, j = 1, 2)$ if $V(x) = a_0 w(x)$. Since the ground state of the Schrödinger operator $H(h)$ is simple, it follows that

$$(4.2) \quad E_1(h) - E_2(h) \sim (e_1 - e_2) h^2 + (c_1^1 - c_1^2) h^{1+\beta} + (c_2^1 - c_2^2) h^{1+2\beta} + O(h^{2+3\beta}),$$

where $c_1^1 - c_1^2 = 0$ if $V(x) = a_0 w(x)$.

If $k + m = a + \beta$, where $\alpha$ and $\beta$ are the same notations as used in Theorem 3.1, then $k + m < \sqrt{2}$ (resp. $k + m \geq \sqrt{2}$) if and only if $\kappa + m < \sqrt{2}$ (resp. $\kappa + m \geq \sqrt{2}$). Then from (4.1) and (4.2) we obtain for the semiclassical eigenvalue splitting of $K(h)$ the expressions in (1.9) and $\Xi = c_1^2 - c_1^1 = 0$ if $V(x) = a_0 w(x)$.

**Example.** Consider the Kac operator $K(h)$ with potential $V(x) = |x|^\sigma \sqrt{1 + |x|^2}$, $0 < \sigma < \infty$. Using a cut-off function $\chi(x)$ with $0 \leq \chi(x) \leq 1$ which is supported in $\{x \in \mathbb{R}^d : |x| \leq 1\}$, we put $V_0(x) = \chi(x) V(x)$ and $V_1(x) = (1 - \chi(x)) V(x)$. Then $V(x)$ satisfies the assumptions (1.6) and (1.7) with $m = [\sigma] - 1$, $\kappa = \sigma - m$ and $\rho = \sigma + 1$. So we can apply Theorem 2.1. We have from Theorem 1.1 with Theorem 3.2

$$\frac{\mu_2(h)}{\mu_1(h)} = \begin{cases} 1 - (e_2 - e_1) h^2 + O(h^\rho), & \sigma < \sqrt{2}, \\ 1 - (e_2 - e_1) h^2 - \Xi h^{1+\beta} + O(h^{\sigma+2}), & \sigma \geq \sqrt{2}, \end{cases}$$

as $h \to 0$, where $e_1$ and $e_2$ are the first two eigenvalues of the Schrödinger operator $-\Delta + |x|^\sigma$ and $\alpha = 2\sigma/(\sigma + 2)$, $\beta = 2/(\sigma + 2)$.

Acknowledgment

I am heartily grateful to Professor Takashi Ichinose and Professor Hideo Tamura for helpful discussions and constant encouragement. I also thank the referee for his useful comment concerning the estimate for (3.5).

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