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Quantitative estimates for Schrödinger and Dirichlet semigroups

by

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Abstract:

The objectives of this article are:

- An explanation of a link between semiclassical limits and the spending time of the Brownian motion in a cone.
- A quantitative comparison for resolvents of Schrödinger and Dirichlet operators in the large coupling limit.

1. Assumptions and introduction

Let H_0 be the selfadjoint realization of $-\frac{1}{2}\Delta$ in $L^2(\mathbf{R}^d)$. Let $V = V_+ - V_-$ be a Kato-class potential. The positive part of the potential is splitted into two parts. For this splitting we introduce a region $\Gamma \subset \mathbf{R}^d$, Γ is a closed subset of $\mathbf{R}^d$ with a positive Lebesgue measure and a piecewise C^1 -boundary. Then we define

$$\begin{aligned} V_\Gamma &:= V_+ 1_\Gamma & \text{with} & & V_\Gamma(x) &\geq V_0 > 0 & \text{for all } x \in \Gamma, \text{ and} \\ V_\Sigma &:= V_+ 1_\Sigma \end{aligned}$$

where $\Sigma = \mathbf{R}^d \setminus \Gamma$ is the complement of Γ . $1_\Gamma, 1_\Sigma$ are the corresponding indicator functions of Γ and Σ , respectively.

It is known that there exists a strong resolvent limit of the operators $H_0 - V_- + V_\Sigma + V_\Gamma$ as V_0 tends to infinity (see e.g. [Bau, Dem]). This limit is the Friedrichs extension of

$$H_0 + V \upharpoonright L^2(\Sigma) \cap \text{dom}(H_0 + V) .$$

We denote this Friedrichs extension by $(H_0 - V_- + V_\Sigma)_\Sigma$. If $V_- \equiv 0$ and $V_\Sigma \equiv 0$ this is the Dirichlet Laplacian $(H_0)_\Sigma$. These operators are defined in $L^2(\Sigma)$. In order to compare them with the Schrödinger operator $H_0 + V$ we have to introduce an embedding operator $Jf := f \upharpoonright \Sigma$, $f \in L^2(\mathbf{R}^d)$.

We are interested in a quantitative estimate of

$$J(\hbar^2 H_0 + V + a)^{-1} - ((\hbar^2 H_0 - V_- + V_\Sigma)_\Sigma + a)^{-1} J \quad (1)$$

for small $\hbar$ and for unbounded Γ such that for instance N -body situations are included.

Instead of considering the difference in (1) we study here the corresponding large coupling problem. Up to an factor $\hbar^{-2}$ the norm of the resolvent difference in (1) is given by

$$\|J \left(H_0 - \frac{1}{\hbar^2} V_- + \frac{1}{\hbar^2} V_\Sigma + \frac{1}{\hbar^2} V_\Gamma + \frac{a}{\hbar^2} \right)^{-1} - \left((H_0 - \frac{1}{\hbar^2} V_- + \frac{1}{\hbar^2} V_\Sigma)_\Sigma + \frac{a}{\hbar^2} \right)^{-1} J\| . \quad (2)$$

The final aim of the present article is to give an explicit bound for the norm in (2) for small $\hbar$.

2. Link to the spending time of the Brownian motion in a cone

Using the Laplace transform and the Feynman-Kac representation the operator norm in (2) is smaller than

$$\begin{aligned}
& \int_0^\infty d\lambda e^{-\frac{\alpha\lambda}{\hbar^2}} \| J e^{-\lambda(H_0 - \frac{1}{\hbar^2}V_- + \frac{1}{\hbar^2}V_\Sigma + \frac{1}{\hbar^2}V_\Gamma)} - e^{-\lambda(H_0 - \frac{1}{\hbar^2}V_- + \frac{1}{\hbar^2}V_\Sigma)} J \| \\
& \leq \int_0^\infty d\lambda e^{-\frac{\alpha\lambda}{\hbar^2}} \sup_{x \in \Sigma} E_x \left\{ e^{-\frac{1}{\hbar^2} \int_0^\lambda V_\Sigma(\omega(s)) ds} \right. \\
& \quad \left. e^{\frac{1}{\hbar^2} \int_0^\lambda V_-(\omega(s)) ds} e^{-\frac{1}{\hbar^2} \int_0^\lambda V_\Gamma(\omega(s)) ds} \chi\{\omega : T_{\lambda, \Gamma}(\omega) > 0\} \right\} ,
\end{aligned} \tag{3}$$

where $T_{\lambda, \Gamma}(\omega) := \text{meas}\{s, s \leq \lambda, \omega(s) \in \Gamma\}$ is the spending time of the Brownian trajectory $\omega(\cdot)$ in the singularity region Γ . $E_x\{\cdot\}$ is the expectation with respect to the Wiener measure.

Because V_- is assumed to be in Kato's class we have

$$\sup_{x \in \Sigma} E_x \left\{ e^{\frac{1}{\hbar^2} \int_0^\lambda V_-(\omega(s)) ds} \right\} \leq B e^{\lambda A / \hbar^2}$$

with positive constants B, A . Moreover $V_\Sigma \geq 0$ and $V_\Gamma \geq V_0 1_\Gamma$. Take $\beta := \frac{V_0}{\hbar^2}$ and $\hbar < 1$. Then the integral in (3) can be estimated by

$$\begin{aligned}
& \int_0^\infty d\lambda e^{-(\alpha-A)\lambda} \\
& \left[\sup_{x \in \Sigma} E_x \left\{ e^{-\int_0^\lambda 1_\Gamma(\omega(s)) ds} \chi\{\omega : T_{\lambda, \Gamma}(\omega) > 0\} \right\} \right]^\alpha
\end{aligned} \tag{4}$$

with some positive α , $\alpha < 1$.

The main task is to estimate

$$\sup_{x \in \Sigma} E_x \left\{ e^{-\beta \int_0^\lambda 1_\Gamma(\omega(s)) ds} \chi\{\omega : T_{\lambda, \Gamma} > 0\} \right\} . \tag{5}$$

Let $A_\Gamma(\omega)$ be the first hitting time of the Brownian motion in Γ , i.e.

$$A_\Gamma(\omega) := \inf\{s, \omega(s) \in \Gamma\} .$$

If A_Γ is near to λ one has to take into account that $\int_{A_\Gamma}^\lambda 1_\Gamma(\omega(s)) ds$ becomes small. Therefore we split the integration in (5), i.e. the supremum in (5) is estimated by

$$\sup_{x \in \Sigma} E_x \{ \chi\{\omega : \lambda - \varepsilon \leq A_\Gamma(\omega) \leq \lambda\} \} \tag{6}$$

$$+ \sup_{x \in \Sigma} E_x \left\{ e^{-\beta \int_{A_\Gamma}^\lambda 1_\Gamma(\omega(s)) ds} \chi\{\omega : A_\Gamma(\omega) \leq \lambda - \varepsilon\} \right\} . \tag{7}$$

For uniform Lipschitz continuous $\delta\Gamma$ the term in (6) is smaller than

$$c \left(1 + \frac{1}{\sqrt{\lambda}}\right) \sqrt{\varepsilon} . \tag{8}$$

The proof is given in [Dem, Jes, Kir]. It will not be repeated here. The conditions are somewhat technical. But they allow the nice class of R -smooth boundaries introduced

by van den Berg [vdB]. These are boundaries where one can find for any $x_0 \in \delta\Gamma$ balls of radius R such that one ball is in Γ the other is in Σ and the intersection is exactly $\{x_0\}$.

Therefore it remains to consider the summand in (7). Because the trajectories are in Σ until the time $A_\Gamma(\omega)$ it follows from the strong Markov property

$$\begin{aligned} & \sup_{x \in \Sigma} E_x \left\{ e^{-\beta \int_{A_\Gamma}^\lambda 1_\Gamma(\omega(s)) ds} \chi\{\omega : A_\Gamma \leq \lambda - \varepsilon\} \right\} \\ & \leq \sup_{x \in \Sigma} E_x \left\{ E_{\omega(A_\Gamma)} \left\{ e^{-\beta \int_0^{\lambda - A_\Gamma} 1_\Gamma(\tilde{\omega}(s)) ds} \chi\{\tilde{\omega} : A_\Gamma \leq \lambda - \varepsilon\} \right\} \right\} \\ & \leq \sup_{y \in \delta\Gamma} E_y \left\{ e^{-\beta \int_0^\varepsilon 1_\Gamma(\omega(s)) ds} \right\}. \end{aligned} \quad (9)$$

Now we choose the singularity region Γ in such a way that it contains always a certain cone K of finite height with the vertex on $\delta\Gamma$, i.e. we assume that Γ satisfies the cone condition. Using the fact that the Brownian motion is invariant with respect to rotations and translations, the supremum in (9) is equal to

$$E_{y_0} \left\{ e^{-\beta \int_0^\varepsilon 1_K(\omega(s)) ds} \right\}, \quad (10)$$

where y_0 is any point on $\delta\Gamma$. In the following we choose $y_0 = 0$.

Consequently we have explained the possible link between the semiclassical problem in (2) and the Laplace transform of the spending time of the Brownian motion in a cone (10).

3. Quantitative estimates

The final aim is to give a quantitative estimate for the rate of convergence of the resolvent difference in (2) in terms of small $\hbar$. Because of (8) and (10) it is clear that this difference tends to zero if $\hbar \rightarrow 0$ or $\beta \rightarrow \infty$. In (8) we have already a quantitative rate for small ε , $0 < \varepsilon < \lambda$.

It remains to find a rate for

$$E_0 \left\{ e^{-\beta T_{\varepsilon, K}} \right\} \quad (11)$$

(see (10)) for large β and small ε , where the choice of an appropriate ε is free. In (11) K is a cone of a finite height, say of height l . Let C be the cone extending K to infinity, then the difference

$$E_0 \left\{ e^{-\beta T_{\varepsilon, K}} \right\} - E_0 \left\{ e^{-\beta T_{\varepsilon, C}} \right\} \leq c e^{-l^2/4\varepsilon}. \quad (12)$$

Therefore it suffices to consider the spending time in the whole cone C , i.e.

$$E_0 \left\{ e^{-\beta T_{\varepsilon, C}} \right\}. \quad (13)$$

For estimating the Laplace transform in (13) we used intensively the article by Meyre [Mey]. The details are given in [Dem, Jes, Kir]. One crucial step is to estimate the distribution of

$$T_{\varepsilon, C}(\omega) < g(\varepsilon)$$

for some real-valued function g , ε small. It turns out that there are positive constants α , η , c such that

$$P_0 \{T_{\varepsilon, c} < \eta \varepsilon^{1+\alpha}\} \leq \frac{c}{|\log \varepsilon|^{1-\alpha}}. \quad (14)$$

Then the final consequence is

$$E_0 \{e^{-\beta T_{\varepsilon, c}}\} \leq \frac{c}{(\log(\beta \varepsilon^{\frac{3}{2}-\gamma}))^\gamma} \quad (15)$$

with $0 < \gamma < \frac{1}{2}$, $0 < \varepsilon < \varepsilon_0$, and $\beta \varepsilon^{\frac{3}{2}-\gamma} > K_0 > 0$.

From the inequality in (15) an appropriate choice of ε is obvious. According to (8), (12), and (15) one can choose $\varepsilon = \beta^\delta$ with any small $\delta > 0$. Hence (7) can be estimated by

$$\sup_x E_x \left\{ e^{-\beta \int_{A_\Gamma}^\lambda 1_{\Gamma(\omega(s))} ds} \chi\{\omega : A_\Gamma \leq \lambda - \varepsilon\} \right\} \leq c \cdot (\log \beta)^{-\gamma} \quad (16)$$

with $0 < \gamma < 1/2$.

4. Results

Hence we are able to give a quantitative estimate for (2), i.e. for

$$\begin{aligned} \Delta(\hbar, \Gamma) := & \|J(H_0 - \frac{1}{\hbar^2} V_- + \frac{1}{\hbar^2} V_\Sigma + \frac{1}{\hbar^2} V_\Gamma + \frac{a}{\hbar^2})^{-1} \\ & - ((H_0 - \frac{1}{\hbar^2} V_- + \frac{1}{\hbar^2} V_\Sigma)_\Sigma + \frac{a}{\hbar^2})^{-1} J\|. \end{aligned}$$

Let Γ be a singularity region with a uniform Lipschitz continuous boundary $\delta\Gamma$, satisfying the cone condition. For $\hbar < 1$ it follows

$$\Delta(\hbar, \Gamma) \leq c \cdot (-\log \hbar)^{-\gamma}, \quad (17)$$

$0 < \gamma < \frac{1}{2}$. This characterization of Γ includes for instance N -body singularity regions, where Γ is a union of sets $B \times \mathbf{R}^{3N-3}$, with certain compact $B \subset \mathbf{R}^3$.

On the other hand, for more regular Γ the rate of convergence in (17) can be improved. For instance, if Γ is the half-space $\mathbf{R}_+ \times \mathbf{R}^{n-1}$, one has

$$\Delta(\hbar, \mathbf{R}_+ \times \mathbf{R}^{n-1}) \leq c \cdot \hbar^{2/3}. \quad (18)$$

This estimate is a consequence of

$$E_0 \left\{ e^{-\frac{1}{\hbar^2} T_{\varepsilon, \mathbf{R}_+ \times \mathbf{R}^{n-1}}} \right\} \leq c \frac{\hbar}{\sqrt{\varepsilon}}. \quad (19)$$

Moreover, if $\Sigma = \mathbf{R}^n \setminus \Gamma$ is a concave set one can choose the half space for the cone C considered above. In that case we obtain.

$$\Delta(\hbar, \Gamma) \leq c \cdot \hbar^{1/2}. \quad (20)$$

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