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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

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

where $\Sigma = \mathbf{R}^d \setminus \Gamma$ is the complement of Γ. 1_Γ, 1_Σ 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

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

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

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

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

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

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

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

where $T_{\lambda,\Gamma}(\omega) := \text{meas}\{s, s \leq \lambda, \omega(s) \in \Gamma\}$ is the spending time of the Brownian trajectory $\omega(.)$ in the singularity region Γ. $E_x\{.\}$ is the exspectation 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

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

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

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

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

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

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

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

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 $\hbar \to 0$ or $\beta \to \infty$. In (8) we have already a quantitative rate for small ε, $0 < \varepsilon < \lambda$.

It remains to find a rate for

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

(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

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

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

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

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

$$P_0\left\{T_{\varepsilon,C} < \eta\ \varepsilon^{1+\alpha}\right\} \leq \frac{c}{|\log\varepsilon|^{1-\alpha}} \ . \tag{14}$$

Then the final consequence is

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

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

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

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

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

$0 < \gamma < \frac{1}{2}$. 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

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

This estimate is a consequence of

$$E_0\left\{e^{-\frac{1}{\hbar^2}\mathrm{T}_{\varepsilon,\mathbf{R}_+\times\mathbf{R}^{n-1}}}\right\} \leq c\frac{\hbar}{\sqrt{\varepsilon}} \ . \tag{19}$$

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.

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

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References

[Bau, Dem] H. Baumgärtel, M. Demuth: Decoupling by a projection, Rep. Math. Phys. **15** (1979), 173–186.

[Dem, Jes, Kir] M. Demuth, F. Jeske, W. Kirsch: On the rate of convergence for large coupling limits in quantum mechanics, Preprint, Max–Planck–Institut, Bonn, MPI **92–29** (1992).

[Mey] T. Meyre: Étude asymptotique du temps passé par le mouvement brownien dans un cône, Ann. Inst. Henri Poincaré **27** (1991), 107–124

[vdB] M. van den Berg: On the asymptotics of the heat equation and bounds on traces associated with the Dirichlet Laplacian, J. Funct. Anal. **71** (1987), 279–293.