MICHAEL DEMUTH
FRANK JESKE
WERNER KIRSCH

Quantitative estimates for Schrödinger and Dirichlet semigroups

Journées Équations aux dérivées partielles (1992), p. 1-6
<http://www.numdam.org/item?id=JEDP_1992____A17_0>

Quantitative estimates for Schrödinger and Dirichlet semigroups

by

M. Demuth*, F. Jeske**, W. Kirsch**

* Max–Planck–Arbeitsgruppe, Fachbereich Mathematik,
Universität Potsdam, Am Neuen Palais 10,
D–1571 Potsdam (Germany)

** Fakultät für Mathematik, Ruhr–Universität,
D–4630 Bochum 1 (Germany)

Supported by Deutsche Forschungsgemeinschaft

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

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

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

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

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

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

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

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

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

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

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

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

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.

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

Acknowlegdement: One of the authors (M.D.) wants to thank the professors D. Robert and P. Bolley for the kind invitation and for the stimulating and pleasant atmosphere during the conference on "Parial Differential Equations" in St.–Jean-de-Monts, 1992.

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.