A diamagnetic inequality for semigroup differences

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Barry Simon and 100DM

The integrated density of states (IDS)

Schrödinger operator:

$$H := H(V) := -\frac{1}{2}\Delta + V_\omega =: H(0, V),$$

or, with a magnetic vector potential A,

$$H := H(A, V) := \frac{1}{2}(-i\nabla - A)^2 + V_\omega$$

on $L^2(\mathbb{R}^d)$.

- To model disordered systems, the potential V is often taken to be a random potential, e.g.,

$$V(x) = V_\omega(x) = \sum_{n\in\mathbb{N}} f(x - x_n(\omega))$$

where x_n are randomly distributed points in $\mathbb{R}^d$, or

$$V(x) = V_\omega(x) = \sum_{n\in\mathbb{Z}^d} \lambda_n(\omega) f(x - x_n)$$

where the (λ_n) are i.i.d. random variables. We will assume that $V \in L^1_{\text{loc}}(\mathbb{R}^d)$ and $v \geq 0$, for simplicity.

- The magnetic vector potential A gives rise to a magnetic field $B := dA$. Again, B can be thought of as given by a random process or is fixed.

Let $\Lambda \subset \mathbb{R}^d$ be an open set. $H_\Lambda^{\#}(A, V_\omega)$ is the restriction of $H(A, V_\omega)$ to Λ with Dirichlet ($\# = D$), respectively Neumann ($\# = N$), boundary conditions.

Definition (IDS) *The finite volume integrated density of states for Dirichlet, respectively Neumann, boundary conditions is given by*

$$\rho_{\Lambda,\omega}^{\#}(s) := \frac{1}{|\Lambda|} \#\{\text{eigenvalues } \lambda_j(H_\Lambda^{\#}(A, V_\omega)) \leq s\}$$

$$\rho_\omega^{\#} := \lim_{\Lambda \to \mathbb{R}^d} \rho_{\Lambda,\omega}^{\#}$$

Natural questions

Question 1: Do the limits $\rho_\omega^{\#}$ exist?

Question 2: If so, how are they related? In particular, are they the same (= independence of the boundary conditions)?

Fact:

- $\Lambda \to |\Lambda|\rho_{\Lambda,\omega}^D$ (resp. $|\Lambda|\rho_{\Lambda,\omega}^N$) is a sub (resp. super) additive ergodic process.

This implies that the macroscopic limits

$$\rho_\omega^{\#} = \lim_{\Lambda \to \mathbb{R}^d} \rho_{\Lambda,\omega}^{\#}$$

exist almost surely and are *non-random*, i.e.,

$$\rho_\omega^{\#} = \mathbb{E}[\rho_\omega^{\#}] \text{ almost all } \omega$$

(= self-averaging property of the IDS).

Independence of the Boundary conditions

We will fix some potential V and magnetic vector potential A and have the the finite volume IDS $\rho_\Lambda^\#$ for these fixed potentials.
It will turn out that the independence of the boundary conditions of the macroscopic limits of $\rho_\Lambda^\#$ is independent of their existence!

Let $f : \mathbb{R} \to \mathbb{R}$ be a nice function, then

$$\int f(E)\, d\rho_\Lambda^\#(E) = \frac{1}{|\Lambda|} \mathrm{tr}_{L^2(\Lambda)}[f(H_\Lambda^\#(A,V))].$$

for $\# =$N (Neumann), resp. $=$D (Dirichlet) boundary conditions.

- We will often write $\mathrm{tr}[f(H_\Lambda^\#(A,V))]$ instead of $\mathrm{tr}_{L^2(\Lambda)}[f(H_\Lambda^\#(A,V))]$ as long as there can be no confusion.

- Choosing $f(E) = \mathrm{e}^{-tE}$ we get the Laplace transforms of the measures $d\rho_\Lambda^\#$, i.e., the Laplace transform is the trace of the corresponding semigroup.

Theorem 1 (S. Nakamura, S.-i. Doi et al). *Take* $\Lambda = [-L, L]^d$, V, $B = dA$ *uniformly bounded, and* $f \in \mathcal{C}_0^1(\mathbb{R})$. *Then*

$$|\mathrm{tr}\,[f(H_\Lambda^N(A,V)) - f(H_\Lambda^D(A,V))]| \le C\frac{|\partial\Lambda|}{|\Lambda|} = \frac{C}{L}.$$

Sketch (of Nakamura's proof):

Recall the Krein spectral shift:

$$\mathrm{tr}[f(A_1) - f(A_2)] = \int f'(E)\,\xi_{A_1,A_2}(E)\,dE$$

with

$$\left\|\xi_{A_1,A_2}\right\|_{L^1} \le \|A_1 - A_2\|_1 .$$

Take $A_1 := (H_\Lambda^N + M)^{-p}$, $A_2 := (H_\Lambda^D + M)^{-p}$, then

$$f(H_\Lambda^N) = g(A_1) \text{ with } f(E) = g((E+m)^{-p}).$$

So using Krein, it is enough to show that

$$\left\|(H_\Lambda^N + M)^{-p} - (H_\Lambda^D + M)^{-p}\right\|_1 \le C|\partial\Lambda|.$$

However, this is rather tricky and requires a good knowledge of the domains of the restricted operators, which is complicated. ∎

A completely different approach:

Theorem 2 (Barry Simon, 100DM). *Let* $\Lambda \subset \mathbb{R}^d$ *be any open set,* $A \in L^2_{\text{loc}}$, $V \geq 0$, $V \in L^1_{\text{loc}}$. *Then*

a) $|(\mathrm{e}^{-tH_\Lambda^N(A,V)} f)(x)| \leq (\mathrm{e}^{-tH_\Lambda^N(0,V)}|f|)(x)$ *for* $x \in \Lambda$

b)
$$\begin{aligned} &\Big|\Big((\mathrm{e}^{-tH_\Lambda^N(A,V)} - \mathrm{e}^{-tH_\Lambda^D(A,V)})f\Big)(x)\Big| \\ &\qquad \leq \Big((\mathrm{e}^{-tH_\Lambda^N(0,V)} - \mathrm{e}^{-tH_\Lambda^D(0,V)})|f|\Big)(x) \\ &\qquad\qquad \underset{V\geq 0}{\leq} \Big((\mathrm{e}^{-tH_\Lambda^N(0,0)} - \mathrm{e}^{-tH_\Lambda^D(0,0)})|f|\Big)(x). \end{aligned}$$

In particular,

$$\begin{aligned} &\mathrm{tr}\Big(\mathrm{e}^{-tH_\Lambda^N(A,V)} - \mathrm{e}^{-tH_\Lambda^D(A,V)}\Big) \\ &\qquad \leq \mathrm{tr}\Big(\mathrm{e}^{-tH_\Lambda^N(0,0)} - \mathrm{e}^{-tH_\Lambda^D(0,0)}\Big) = O(|\partial\Lambda|). \end{aligned}$$

(Weyl asymptotic for the free case!)

Motivation: The Feynman-Kac-Itô formula

$$(e^{-tH_\Lambda^D(A,V)}f)(x) = \mathbb{E}^x[\mathrm{e}^{-iS^t(A)(b)-\int_0^t V(b_s)ds}\chi_{\Lambda_t}(b)f(b_t)],$$

where $t \to b_t$ is a Brownian motion process,

$$S^t(A) := \int_0^t A(b_s)\,db_s + \frac{1}{2}\int_0^t \mathrm{div}A(b_s)\,ds$$

is the “line integral” of A along a Brownian path, and we integrate only over the region

$$\Lambda_t := \{b|\, b_s \in \Lambda \text{ for all } 0 \le s \le t\}.$$

With Neumann boundary conditions:

$$(\mathrm{e}^{-tH_\Lambda^N(A,V)}f)(x) = \widetilde{\mathbb{E}}^x\Big[\mathrm{e}^{-iS^t(A)(\tilde{b})-\int_0^t V(\tilde{b}_s)ds}f(\tilde{b}_t)\Big]$$

where $t \to \tilde{b}_t$ is the so-called reflected Brownian motion (in Λ).

Note that, at least morally, $\tilde{b} = b$ for paths $b \in \Lambda_t$ (if Brownian motion did not hit the boundary up to time t it could not have been reflected, yet.)

Assuming this, we immediately get

$$
\begin{aligned}
&|(\mathrm{e}^{-tH_\Lambda^N(A,V)} - \mathrm{e}^{-tH_\Lambda^D(A,V)})f| = \\
&\quad = \Big|\widetilde{\mathbb{E}}^x\Big[\mathrm{e}^{-iS^t(A)(\tilde{b})-\int_0^t V(\tilde{b}_s)ds}\underbrace{(1-\chi_{\Lambda_t}(\tilde{b}))}_{\geq 0} f(\tilde{b}_t)\Big]\Big| \\
&\quad \leq \widetilde{\mathbb{E}}^x\Big[\mathrm{e}^{-\int_0^t V(\tilde{b}_s)ds}(1-\chi_{\Lambda_t}(\tilde{b}))|f(\tilde{b}_t)|\Big] \\
&\quad = (\mathrm{e}^{-tH_\Lambda^N(0,V)} - \mathrm{e}^{-tH_\Lambda^D(0,V)})|f| \\
&\quad = \widetilde{\mathbb{E}}^x\Big[\underbrace{\mathrm{e}^{-\int_0^t V(\tilde{b}_s)ds}}_{\leq 1}(1-\chi_{\Lambda_t}(\tilde{b}))|f(\tilde{b}_t)|\Big] \\
&\quad \leq \widetilde{\mathbb{E}}^x\Big[(1-\chi_{\Lambda_t}(\tilde{b}))|f(\tilde{b}_t)|\Big] \\
&\quad = (\mathrm{e}^{-tH_\Lambda^N(0,0)} - \mathrm{e}^{-tH_\Lambda^D(0,0)})|f|
\end{aligned}
$$

$\blacksquare$

Sketch of the proof of Theorem 2:

a) $\Rightarrow$ b): Take a potential $W \geq 0$. We have duHamel's formula, for $A, A+B \geq 0$

$$\mathrm{e}^{-tA} - \mathrm{e}^{-t(A+B)} =$$

$$= \int_0^t \underbrace{\frac{d}{ds}\Big(\mathrm{e}^{-sA}\mathrm{e}^{-(t-s)(A+B)}\Big)}_{=\mathrm{e}^{-sA}(-A+A+B)\mathrm{e}^{-(t-s)(A+B)}} \, ds$$

$$= \int_0^t \mathrm{e}^{-sA} B \mathrm{e}^{-(t-s)(A+B)} \, ds.$$

Choose $A = H_\Lambda^N(A,0)$, $B = W$, i.e., $A + B = H_\Lambda^N(A,W)$. Then

$$\Big|(\mathrm{e}^{-tH_\Lambda^N(A,0)} - \mathrm{e}^{-tH_\Lambda^N(A,W)})f\Big|$$

$$\leq \int_0^t \underbrace{\Big|\mathrm{e}^{-sH_\Lambda^N(A,0)} W \mathrm{e}^{-(t-s)(H_\Lambda^N(A,W))} f\Big|}_{\leq \mathrm{e}^{-sH_\Lambda^N(0,0)}|W|\mathrm{e}^{-(t-s)(H_\Lambda^N(0,W))}|f|} \, ds$$

$$\underset{W\geq 0}{=} (\mathrm{e}^{-tH_\Lambda^N(0,0)} - \mathrm{e}^{-tH_\Lambda^N(0,W)})|f|$$

Now reconstruct Dirichlet b.c.: Set $W(x) := W_n(x) := n 1_{\Lambda^c}(x)$ and note that (morally)

$$\mathrm{s-}\lim_{n\to\infty} \mathrm{e}^{-tH_\Lambda^N(A,W_n)} = \mathrm{e}^{-tH_\Lambda^D(A,0)}$$

Proof of a): Let $D = \nabla - iA$, $u_\varepsilon := \sqrt{|u|^2 + \varepsilon^2}$, and $s_\varepsilon := \frac{u}{u_\varepsilon}$. Then the quadratic form domain of the operator with magnetic field and Neumann b. c. is the domain of D.

Lemma 3 (Quadratic form version of Kato's inequality). $u \in \mathcal{D}(D) \Rightarrow |u| \in \mathcal{D}(\nabla)$ *and for* $\varphi \geq 0$, $\varphi \in \mathcal{D}(\nabla)$, $u \in \mathcal{D}(D)$ *we have*

$$\begin{aligned} \mathrm{Re}(\overline{D(s_\varepsilon \varphi)} \cdot Du) &\geq \nabla\varphi \nabla u_\varepsilon \\ &= |s_\varepsilon| \nabla\varphi \nabla |u| \end{aligned}$$

Remark: $\nabla u_\varepsilon = \frac{1}{u_\varepsilon} u_\varepsilon \nabla u_\varepsilon = \frac{1}{u_\varepsilon} \nabla u_\varepsilon^2 = \frac{1}{u_\varepsilon} \nabla |u|^2 = \frac{|u|}{u_\varepsilon} \nabla u_\varepsilon = |s_\varepsilon| \nabla |u|$.

How to use this Lemma:
Note that $\overline{s_\varepsilon} u = |s_\varepsilon||u|$, hence we have

$$\langle s_\varepsilon \varphi, u \rangle = \int |s_\varepsilon| \varphi |u| \, dx \geq 0,$$

and, using the above bound, we see

$$\begin{aligned} &\int |s_\varepsilon| \Big(\nabla\varphi \nabla |u| + \lambda \varphi |u| \Big) \, dx \\ &\leq \mathrm{Re}\Big(\langle D(s_\varepsilon \varphi), Du \rangle + \lambda \langle s_\varepsilon \varphi, u \rangle \Big) \\ &= \mathrm{Re} \langle s_\varepsilon \varphi, v \rangle \leq \langle |s_\varepsilon| \varphi, |v| \rangle \leq \langle \varphi, |v| \rangle \end{aligned}$$

for all $\lambda > 0$ and $u = (H_\Lambda^N(A, 0) + \lambda)^{-1} v$.

Taking $\varepsilon \to 0$, we get

$$\begin{aligned}
&\langle (H_\Lambda^N(0,0) + \lambda)\varphi, |u|\rangle \\
&\quad = \langle \nabla\varphi, \nabla|u|\rangle + \lambda\langle \varphi, |u|\rangle \\
&\quad \le \langle \varphi, |v|\rangle.
\end{aligned}$$

Now choose $\varphi = (H_\Lambda^N(0,0) + \lambda)^{-1}\psi$, $\psi \ge 0$. Then

$$\begin{aligned}
&\langle \psi, |(H_\Lambda^N(A,0) + \lambda)^{-1}v|\rangle \\
&\quad \le \langle (H_\Lambda^N(0,0) + \lambda)^{-1}\psi, |v|\rangle \\
&\quad = \langle \psi, (H_\Lambda^N(0,0) + \lambda)^{-1}|v|\rangle
\end{aligned}$$

for all $\psi \ge 0$ and $v \in L^2(\Lambda)$. I.e.,

$$|(H_\Lambda^N(A,0) + \lambda)^{-1}v| \le H_\Lambda^N(0,0) + \lambda)^{-1}|v|$$

and

$|(H_\Lambda^N(A,0)+\lambda)^{-n}v| \le H_\Lambda^N(0,0)+\lambda)^{-n}|v|$ for all $n \in \mathbb{N}$.

The result for the Neumann semigroup follows, since

$$\mathrm{e}^{-tH_\Lambda^N} = \operatorname*{s-lim}_{n\to\infty} \left(\frac{n}{t}\right)^n \left(H^N + \frac{n}{t}\right)^{-n}.$$

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