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 \( (\lambda_n) \) 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 $\Lambda$ 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 ($\equiv$ independence of the boundary conditions)?

Fact:

- $\Lambda \rightarrow |\Lambda|\rho^D_{\Lambda,\omega}$ (resp. $|\Lambda|\rho^N_{\Lambda,\omega}$) is a sub (resp. super) additive ergodic process.

This implies that the macroscopic limits

$$\rho^\#_\omega = \lim_{\Lambda \rightarrow \mathbb{R}^d} \rho^\#_{\Lambda,\omega}$$

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

$$\rho^\#_\omega = \mathbb{E}[\rho^\#_\omega]$$

almost all $\omega$ ($\equiv$ 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 \( f : \mathbb{R} \rightarrow \mathbb{R} \) be a nice function, then

\[
\int f(E) \, d\rho^\#_\Lambda(E) = \frac{1}{|\Lambda|} \text{tr}_{L^2(\Lambda)}[f(H^\#_\Lambda(A, V))].
\]

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

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

- Choosing \( f(E) = e^{-tE} \) 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 \( f \in C^1_0(\mathbb{R}) \). Then 

\[
|\text{tr} [f(H_N^\Lambda(A, V)) - f(H_D^\Lambda(A, V))]| \leq C \frac{\partial |\Lambda|}{|\Lambda|} = \frac{C}{L}.
\]

Sketch (of Nakamura’s proof):
Recall the Krein spectral shift:

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

with 

\[
\|\xi_{A_1, A_2}\|_{L^1} \leq \|A_1 - A_2\|_1.
\]

Take \( A_1 := (H_N^\Lambda + M)^{-p}, A_2 := (H_D^\Lambda + M)^{-p} \), then 

\[
f(H_N^\Lambda) = g(A_1) \text{ with } f(E) = g((E + m)^{-p}).
\]

So using Krein, it is enough to show that 

\[
\|(H_N^\Lambda + M)^{-p} - (H_D^\Lambda + M)^{-p}\|_1 \leq C |\partial \Lambda|.
\]

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) $|(e^{-tH^N_\Lambda(A,V)} f)(x)| \leq (e^{-tH^N_\Lambda(0,V)} |f|)(x)$ for $x \in \Lambda$

b) $|((e^{-tH^N_\Lambda(A,V)} - e^{-tH^D_\Lambda(A,V)}) f)(x)|$

\[
\leq \left( (e^{-tH^N_\Lambda(0,V)} - e^{-tH^D_\Lambda(0,V)}) |f| \right)(x)
\]

\[
\leq V \geq 0 \left( (e^{-tH^N_\Lambda(0,0)} - e^{-tH^D_\Lambda(0,0)}) |f| \right)(x).
\]

In particular,

\[
\text{tr}(e^{-tH^N_\Lambda(A,V)} - e^{-tH^D_\Lambda(A,V)})
\]

\[
\leq \text{tr}(e^{-tH^N_\Lambda(0,0)} - e^{-tH^D_\Lambda(0,0)}) = O(|\partial \Lambda|).
\]

(Weyl asymptotic for the free case!)
Motivation: The Feynman-Kac-Itô formula

\[(e^{-tH^D_\Lambda(A,V)} f)(x) = \mathbb{E}^x \left[ e^{-iS_t(A)(b) - \int_0^t V(b_s)ds} \chi_{\Lambda_t}(b) f(b_t) \right],\]

where \( t \to b_t \) is a Brownian motion process,

\[S_t(A) := \int_0^t A(b_s) \, db_s + \frac{1}{2} \int_0^t \text{div} A(b_s) \, ds\]

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

\[\Lambda_t := \{ b | b_s \in \Lambda \text{ for all } 0 \leq s \leq t \} .\]

With Neumann boundary conditions:

\[(e^{-tH^N_\Lambda(A,V)} f)(x) = \tilde{\mathbb{E}}^x \left[ e^{-iS_t(A)(\tilde{b}) - \int_0^t V(\tilde{b}_s)ds} f(\tilde{b}_t) \right],\]

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

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

\[ |(e^{-tH^N(A,V)} - e^{-tH^D(A,V)})f| = \]

\[ = \left| \mathbb{E}^x \left[ e^{-iS^t(A)(\tilde{b})} - \int_0^t V(\tilde{b}_s)ds \underline{(1 - \chi \Lambda_t(\tilde{b}))} f(\tilde{b}_t) \right] \right| \]

\[ \leq \mathbb{E}^x \left[ e^{-\int_0^t V(\tilde{b}_s)ds} (1 - \chi \Lambda_t(\tilde{b}))|f(\tilde{b}_t)| \right] \]

\[ = (e^{-tH^N(0,V)} - e^{-tH^D(0,V)})|f| \]

\[ = \mathbb{E}^x \left[ e^{-\int_0^t V(\tilde{b}_s)ds} (1 - \chi \Lambda_t(\tilde{b}))|f(\tilde{b}_t)| \right] \]

\[ \leq \mathbb{E}^x \left[ (1 - \chi \Lambda_t(\tilde{b}))|f(\tilde{b}_t)| \right] \]

\[ = (e^{-tH^N(0,0)} - e^{-tH^D(0,0)})|f| \]
Sketch of the proof of Theorem 2:

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

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

$$= \int_0^t \frac{d}{ds} \left( e^{-sA} e^{-(t-s)(A+B)} \right) ds$$

$$= e^{-sA}(-A+A+B)e^{-(t-s)(A+B)}$$

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

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

$$\left| (e^{-tH_N^\Lambda(A,0)} - e^{-tH_N^\Lambda(A,W)})f \right|$$

$$\leq \int_0^t \left| e^{-sH_N^\Lambda(A,0)} W e^{-(t-s)(H_N^\Lambda(A,W))}f \right| ds$$

$$\leq e^{-sH_N^\Lambda(0,0)}|W|e^{-(t-s)(H_N^\Lambda(0,W))}|f|$$

$$= (e^{-tH_N^\Lambda(0,0)} - e^{-tH_N^\Lambda(0,W)})|f|$$

$W \geq 0$

Now reconstruct Dirichlet b.c.: Set $W(x) := W_n(x) := n1_\Lambda^c(x)$ and note that (morally)

$$s - \lim_{n \to \infty} e^{-tH_N^\Lambda(A,W_n)} = e^{-tH_D^\Lambda(A,0)}$$
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

$$\Re(D(s_\varepsilon \varphi) \cdot Du) \geq \nabla \varphi \nabla u_\varepsilon = |s_\varepsilon| \nabla |u|$$

**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

$$\int |s_\varepsilon| \left( \nabla \varphi \nabla |u| + \lambda \varphi |u| \right) \, dx$$

$$\leq \Re \left( \langle D(s_\varepsilon \varphi), Du \rangle + \lambda \langle s_\varepsilon \varphi, u \rangle \right)$$

$$= \Re \langle s_\varepsilon \varphi, v \rangle \leq \langle |s_\varepsilon| \varphi, |v| \rangle \leq \langle \varphi, |v| \rangle$$

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

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Taking \( \varepsilon \to 0 \), we get
\[
\langle (H^N_{\Lambda}(0,0) + \lambda)\varphi, |u| \rangle
= \langle \nabla \varphi, \nabla |u| \rangle + \lambda \langle \varphi, |u| \rangle
\leq \langle \varphi, |v| \rangle.
\]

Now choose \( \varphi = (H^N_{\Lambda}(0,0) + \lambda)^{-1}\psi, \psi \geq 0 \). Then
\[
\langle \psi, |(H^N_{\Lambda}(A,0) + \lambda)^{-1}v| \rangle
\leq \langle ((H^N_{\Lambda}(0,0) + \lambda)^{-1}\varphi, |v| \rangle
= \langle \psi, (H^N_{\Lambda}(0,0) + \lambda)^{-1}|v| \rangle
\]
for all \( \psi \geq 0 \) and \( v \in L^2(\Lambda) \). I.e.,
\[
|(H^N_{\Lambda}(A,0) + \lambda)^{-1}v| \leq H^N_{\Lambda}(0,0) + \lambda)^{-1}|v|
\]
and
\[
|(H^N_{\Lambda}(A,0) + \lambda)^{-n}v| \leq H^N_{\Lambda}(0,0) + \lambda)^{-n}|v| \text{ for all } n \in \mathbb{N}.
\]

The result for the Neumann semigroup follows, since
\[
e^{-tH^N_{\Lambda}} = s - \lim_{n \to \infty} \left( \frac{n}{t} \right)^n (H^N_{\Lambda} + \frac{n}{t})^{-n}.
\]