

A diamagnetic inequality for semigroup differences

(Birmingham, March 26-30, 2002)

Barry Simon and 100DM

Abstract: We give a simple proof of the fact that the integrated density of states is independent of the boundary conditions used in its construction.

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*

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

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

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:

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

This implies that the macroscopic limits

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

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 $V \geq 0$ and magnetic vector potential $A \in L^2_{\text{loc}}(\mathbb{R}^d)$ and have 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 and $B = dA$ continuous and uniformly bounded, and $f \in \mathcal{C}_0^1(\mathbb{R})$. Then

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

Remark:

- Nakamura needs continuity and uniform boundedness in his proof.
- This was relaxed to $0 \leq V \in L_{\mathrm{loc}}^1(\mathbb{R}^d)$ and $A \in L_{\mathrm{loc}}^2(\mathbb{R}^d)$ by Doi et al.
- Hupfer et al extend it to certain unbounded potentials.

Sketch (of Nakamura's proof):

Recall that with the help of the Krein spectral shift function one can write

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

where

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

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

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

and hence, using Krein,

$$\text{tr}[f(H_\Lambda^N) - f(H_\Lambda^D)] = \int g'(E) \xi_{A_1, A_2}(E) dE$$

So using the L^1 bound on ξ , it is enough to show that

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

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

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

$$b) \left| \left((e^{-tH_\Lambda^N(A,V)} - e^{-tH_\Lambda^D(A,V)}) f \right)(x) \right| \\ \leq \left((e^{-tH_\Lambda^N(0,V)} - e^{-tH_\Lambda^D(0,V)}) |f| \right)(x) \\ \stackrel{V \geq 0}{\leq} \left((e^{-tH_\Lambda^N(0,0)} - e^{-tH_\Lambda^D(0,0)}) |f| \right)(x).$$

In particular,

$$0 \leq \text{tr} \left(e^{-tH_\Lambda^N(A,V)} - e^{-tH_\Lambda^D(A,V)} \right) \\ \leq \text{tr} \left(e^{-tH_\Lambda^N(0,0)} - e^{-tH_\Lambda^D(0,0)} \right) = O(|\partial\Lambda|).$$

(Weyl asymptotic for the free case!)

Remark: So the difference of the Laplace transforms of ρ_Λ^N and ρ_Λ^D is $O\left(\frac{|\partial\Lambda|}{|\Lambda|}\right)$.

Thus we have independence of the boundary conditions in the macroscopic limit $\Lambda \rightarrow \mathbb{R}^d$.

Motivation: The Feynman-Kac-Itô formula

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

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

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

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

$$\Lambda_t := \{b \mid b_s \in \Lambda \text{ for all } 0 \leq s \leq t\}.$$

With Neumann boundary conditions:

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

where $t \rightarrow \tilde{b}_t$ 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

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

■

Sketch of the proof of Theorem 2:

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

$$\begin{aligned}
 e^{-tA} - e^{-t(A+B)} &= \\
 &= \int_0^t \underbrace{\frac{d}{ds} \left(e^{-sA} e^{-(t-s)(A+B)} \right)}_{= e^{-sA}(-A+A+B)e^{-(t-s)(A+B)}} ds \\
 &= \int_0^t e^{-sA} B e^{-(t-s)(A+B)} ds.
 \end{aligned}$$

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

$$\begin{aligned}
 & \left| (e^{-tH_\Lambda^N(A, 0)} - e^{-tH_\Lambda^N(A, W)}) f \right| \\
 & \leq \int_0^t \underbrace{\left| e^{-sH_\Lambda^N(A, 0)} W e^{-(t-s)(H_\Lambda^N(A, W))} f \right|}_{\leq e^{-sH_\Lambda^N(0, 0)} |W| e^{-(t-s)(H_\Lambda^N(0, W))} |f|} ds \\
 & \stackrel{W \geq 0}{=} (e^{-tH_\Lambda^N(0, 0)} - e^{-tH_\Lambda^N(0, W)}) |f|
 \end{aligned}$$

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

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

Proof of a): Let $D = \nabla - iA$. Then the quadratic form domain of $H_{\Lambda}^N(A, 0)$ is the domain of D .

Lemma 3 (Kato's inequality (bilinear version)).

Let $u_{\varepsilon} := \sqrt{|u|^2 + \varepsilon^2}$, and $s_{\varepsilon} := \frac{u}{u_{\varepsilon}}$. Then $u \in \mathcal{D}(D) \Rightarrow |u_{\varepsilon}|, |u| \in \mathcal{D}(\nabla)$. Moreover, for $\varphi \geq 0$, $\varphi \in \mathcal{D}(\nabla)$, $u \in \mathcal{D}(D)$ with $\varphi \lesssim 1 + |u|$ we have $s_{\varepsilon}\varphi \in \mathcal{D}(D)$ and

$$\begin{aligned} \operatorname{Re}(\overline{D(s_{\varepsilon}\varphi)} \cdot Du) &= \varphi \frac{|Du|^2 - |\nabla u_{\varepsilon}|^2}{u_{\varepsilon}} + |s_{\varepsilon}| \nabla \varphi \nabla |u| \\ &\geq |s_{\varepsilon}| \nabla \varphi \nabla |u| \end{aligned}$$

Remark:

- All proofs of Kato's inequality start by proving $|Du| \geq |\nabla u_{\varepsilon}|$.
-

$$\nabla s_{\varepsilon} = \nabla \frac{u}{u_{\varepsilon}} = \frac{\nabla u - s_{\varepsilon} \nabla u_{\varepsilon}}{u_{\varepsilon}},$$

hence

$$\begin{aligned} D(s_{\varepsilon}\varphi) &= \varphi(\nabla s_{\varepsilon} - iAs_{\varepsilon}) + s_{\varepsilon}\nabla\varphi \\ &= \varphi \frac{Du - s_{\varepsilon}\nabla u_{\varepsilon}}{u_{\varepsilon}} + s_{\varepsilon}\nabla\varphi \in L^2 \end{aligned}$$

as long as $\varphi/u_{\varepsilon} \in L^{\infty}$.

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

$$\begin{aligned} & \int |s_\varepsilon|(\nabla\varphi\nabla|u| + E\varphi|u|) dx \\ & \leq \operatorname{Re}(\langle D(s_\varepsilon\varphi), Du \rangle + E\langle s_\varepsilon\varphi, u \rangle) \\ & = \operatorname{Re}\langle s_\varepsilon\varphi, (H_\Lambda^N(A, 0) + E)u \rangle \\ & \leq \langle |s_\varepsilon|\varphi, |(H_\Lambda^N(A, 0) + E)u| \rangle \\ & = \langle |s_\varepsilon|\varphi, |v| \rangle \leq \langle \varphi, |v| \rangle \end{aligned}$$

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

Taking $\varepsilon \rightarrow 0$, we get

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

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

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

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

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

and by induction

$$|(H_\Lambda^N(A, 0) + E)^{-n}v| \leq (H_\Lambda^N(0, 0) + E)^{-n}|v| \text{ for all } n \in \mathbb{N}$$

The diamagnetic inequality for the Neumann semi-group follows, since

$$e^{-tH_\Lambda^N} = \text{s-}\lim_{n \rightarrow \infty} \left(\frac{n}{t}\right)^n \left(H_\Lambda^N + \frac{n}{t}\right)^{-n}.$$

■