A diamagnetic inequality for semigroup differences

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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*

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

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

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:

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

This implies that the macroscopic limits

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

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

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

Remark:

- Nakamura needs continuity and uniform boundedness in his proof.
- This was relaxed to $0 \le V \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ and $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d)$ 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

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

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

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

and hence, using Krein,

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

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.

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A completely different approach:

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

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

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

In particular,

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

(Weyl asymptotic for the free case!)

Remark: So the difference of the Laplace transforms of ρ^N_Λ and ρ^D_Λ is $O(\frac{|\partial\Lambda|}{|\Lambda|})$.
Thus we have independence of the boundary conditions in the macroscopic limit $\Lambda \to \mathbb{R}^d$.

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

$$|(\mathrm{e}^{-tH_\Lambda^N(A,V)} - \mathrm{e}^{-tH_\Lambda^D(A,V)})f| =$$

$$= \left|\widetilde{\mathbb{E}}^x\Big[\mathrm{e}^{-iS^t(A)(\tilde{b})-\int_0^t V(\tilde{b}_s)ds}\underbrace{(1-\chi_{\Lambda_t}(\tilde{b}))}_{\geq 0}f(\tilde{b}_t)\Big]\right|$$

$$\leq \widetilde{\mathbb{E}}^x\Big[\mathrm{e}^{-\int_0^t V(\tilde{b}_s)ds}(1-\chi_{\Lambda_t}(\tilde{b}))|f(\tilde{b}_t)|\Big]$$

$$= (\mathrm{e}^{-tH_\Lambda^N(0,V)} - \mathrm{e}^{-tH_\Lambda^D(0,V)})|f|$$

$$= \widetilde{\mathbb{E}}^x\Big[\underbrace{\mathrm{e}^{-\int_0^t V(\tilde{b}_s)ds}}_{\leq 1 \text{ if } V\geq 0}(1-\chi_{\Lambda_t}(\tilde{b}))|f(\tilde{b}_t)|\Big]$$

$$\leq \widetilde{\mathbb{E}}^x\Big[(1-\chi_{\Lambda_t}(\tilde{b}))|f(\tilde{b}_t)|\Big]$$

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

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Sketch of the proof of Theorem 2:

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

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

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

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

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

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

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

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

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

$$\operatorname*{s-lim}_{n\to\infty} e^{-tH_\Lambda^N(A,W_n)} = e^{-tH_\Lambda^D(A,0)}$$

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*

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

Remark:

- All proofs of Kato's inequality start by proving $|Du| \geq |\nabla u_\varepsilon|$.
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$$\nabla s_\varepsilon = \nabla \frac{u}{u_\varepsilon} = \frac{\nabla u - s_\varepsilon \nabla u_\varepsilon}{u_\varepsilon},$$
  hence
$$D(s_\varepsilon\varphi) = \varphi(\nabla s_\varepsilon - iAs_\varepsilon) + s_\varepsilon \nabla\varphi$$
$$= \varphi \frac{Du - s_\varepsilon \nabla u_\varepsilon}{u_\varepsilon} + s_\varepsilon \nabla\varphi \in L^2$$
  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

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

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

Taking $\varepsilon \to 0$, we get

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

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

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

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 semigroup follows, since

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

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