Equality of bulk and edge Hall conductance revisited

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Abstract

The integral quantum Hall effect can be explained either as resulting from bulk or edge currents (or, as it occurs in real samples, as a combination of both). This leads to different definitions of Hall conductance, which agree under appropriate hypotheses, as shown by Schulz-Baldes et al. by means of K-theory. We propose an alternative proof based on a generalization of the index of a pair of projections to more general operators. The equality of conductances is an expression of the stability of that index as a flux tube is moved from within the bulk across the boundary of a sample.

The model and the result

The simultaneous quantization of bulk and edge conductance is essential to the QHE in finite samples, as explained in [8, 13]. In these two references that property is established in the context of an effective field theory description, resp. of a microscopic treatment suitable to the integral QHE. The present paper is placed in the latter setting as well.

In our model H is a discrete Schrödinger operator on the single-particle Hilbert space $\ell^2(\mathbb{Z}\times\mathbb{N})$ over the upper half-plane. It is obtained from the restriction (with e.g. Dirichlet boundary conditions) of a 'bulk' Hamiltonian H_B acting on $\ell^2(\mathbb{Z}\times\mathbb{Z})$. These assumptions are spelled out in detail at the end of this section. The spectrum of H_B (but not that of H, as a rule) has an open gap Δ containing the Fermi energy:

$$\Delta \cap \sigma(H_B) = \varnothing \ . \tag{1}$$

Let P_B be the Fermi projection: $P_B = E_{(-\infty,\mu]}(H_B)$ for any $\mu \in \Delta$.

A real-valued function $g \in C^\infty(\mathbb{R})$ with $g(\lambda) = 1$ (resp. 0) for λ large and negative (resp. positive) will be called a *switch function*. We remark that $P_B = g(H_B)$ if the switch function has supp $g' \subset \Delta$.

Theorem 1 *Assume the hypotheses as described and, in particular, (1). Let*

$$\sigma_B = \frac{1}{2\pi}\ \mathrm{Ind}(UP_BU^*, P_B)\ , \tag{2}$$

where $U = U(\vec{r}) = \mathrm{e}^{\mathrm{i}\arg\vec{r}}$ *be the* **bulk Hall conductance***; and let*

$$\sigma_E = -\,\mathrm{tr}\,(g'(H)\mathrm{i}[H, \chi(x)])\ , \tag{3}$$

where g *and* χ *are switch functions with* $\operatorname{supp} g' \subset \Delta$*, be the* **edge Hall conductance***. Then*

$$\sigma_B = \sigma_E\ . \tag{4}$$

In particular, σ_E *is independent of* g *and* χ *as stated.*

Remarks. 1) $\mathrm{Ind}(P, Q)$ is the index of a pair of projections, see [2], from where also the definition of σ_B is taken, except for a change of sign. In other words, their definition of σ_B agrees with the Kubo formula (6.18) for σ_{12}, whereas ours with σ_{21}. Or equivalently: their definition is such that for a Landau Hamiltonian with magnetic field $B > 0$ and electron charge $e = +1$ one has $\sigma_B > 0$, see Remark 6.7c. Ours is opposite.

2) $U(\vec{r})$ can be replaced, without affecting σ_B, by

$$U(\vec{r}) = \mathrm{e}^{\mathrm{i}\varphi(\arg\vec{r})}\ , \tag{5}$$

where $\varphi : S^1 \to S^1$ is a continuous function with winding number 1. This follows by continuity from the additivity [2] and stability of the index:

$$\|Q - P\| < 1\ \Rightarrow\ \mathrm{Ind}(Q, P) = 0\ .$$

3) The rationale for the definition (3) is that $-\mathrm{i}[H, \chi(x)]$ is the current operator in x-direction (for $\chi(x) = \theta(-x)$, it is the current across $x = 0$). For $-g'(H) = E_{[\mu_1,\mu_2]}(H)/(\mu_2 - \mu_1)$ (3) is (up to the sign) the expected current in 1-particle density matrix $E_{[\mu_1,\mu_2]}(H)$, corrisponding to filled edge levels $[\mu_1, \mu_2] \subset \Delta$, divided by the potential difference. For the above Landau Hamiltonian the current is positive, since the electrons run in the positive x-direction near the boundary. Thus σ_E is, like σ_B, negative.

The result (4) was proven in [13] and, more extensively, in [11] using non-commutative geometry and K-theory. (However, the quantization of σ_E was shown there without making use of these tecniques). The present proof makes use of basic functional analysis. While their result is established using and extending tools developed in [4], ours bears a similar relation to [2].

We conclude this section by specifying the Schrödinger Hamiltonians H used here. Lattice points are denoted as $\vec{r} = (x, y)$, corresponding Kronecker states as $\delta_{\vec{r}} \in \ell^2(\mathbb{Z}\times\mathbb{N})$ and matrix elements as $H(\vec{r}_1, \vec{r}_2) = (\delta_{\vec{r}_1}, H\delta_{\vec{r}_2})$. We assume H to be a self-adjoint operator with short-range off-diagonal hopping terms:

$$\sup_{\vec{r}_1}\sum_{\vec{r}_2} |H(\vec{r}_1, \vec{r}_2)|(\mathrm{e}^{\mu_0|\vec{r}_1-\vec{r}_2|} - 1) < \infty \tag{6}$$

for some $\mu_0 > 0$. The bulk Hamiltonian H_B is of the same form, except that the lattice is $\mathbb{Z} \times \mathbb{Z} = \mathbb{Z}^2$. It should restrict to H on the upper half-plane under some largely arbitrary boundary condition. More precisely, let $J : \ell^2(\mathbb{Z} \times \mathbb{N}) \to \ell^2(\mathbb{Z}^2)$ denote the extension by 0. We assume that the 'edge term'

$$E = JH - H_B J : \; \ell^2(\mathbb{Z} \times \mathbb{N}) \to \ell^2(\mathbb{Z}^2)$$

satisfies

$$\sum_{\vec{r}\,' \in \mathbb{Z} \times \mathbb{N}} |E(\vec{r}, \vec{r}\,')| \le C \mathrm{e}^{-\mu_0 |y|} \tag{7}$$

for all $\vec{r} = (x, y) \in \mathbb{Z}^2$. For instance, for Dirichlet boundary conditions,

$$E(\vec{r}, \vec{r}\,') = \begin{cases} -H_B(\vec{r}, \vec{r}\,') \, , & (y < 0) \, , \\ 0 \, , & (y \ge 0) \, , \end{cases}$$

whence (7) follows from (6) for H_B at the expense of making μ_0 smaller.

The trace ideals of operators on the Hilbert space $\ell^2(\mathbb{Z} \times \mathbb{N})$ or $\ell^2(\mathbb{Z}^2)$, depending on the context, are denoted as $\mathcal{J}_p$, $(1 \le p < \infty)$, with norm $\| \cdot \|_p$. Universal constants are denoted by C.

Idea and outline of the proof

We consider the gauge transformation (5) with φ having supp $\varphi' \subset [\pi/4, 3\pi/4]$, so that $U(\vec{r}) - 1$ is supported in a wedge pointing upwards. We shall compare two modifications thereof. The first one, $\breve{U}_a$, is obtained from (5) by changing $U(\vec{r})$ to 1 for $y < a$.

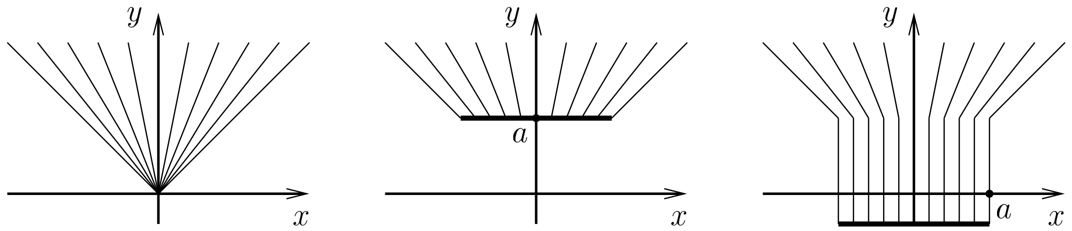

Figure 1: Isolines of U, $\breve{U}_a$, $\widehat{U}_a$

The second one, $\widehat{U}_a$, is obtained from $\breve{U}_a$ by pulling the line of fluxes at $y = a$ across the boundary, as in the figure.

Morally, the Hall conductance σ_B is given as

$$\frac{1}{2\pi} \operatorname{tr} (\widetilde{U}_a g(H) \widetilde{U}_a^* - g(H)) \tag{8}$$

with either $\widetilde{} = \breve{}, \widehat{}$. Indeed, in both cases the heuristic argument, explained in more detail in [2], Sect. 5, is that the trace in (8) counts the number of electrons which are pulled to infinity as the gauge field is switched on adiabatically starting from zero to a flux quantum, see Fig. 1. That number may also by computed by integrating the current

$$\vec{\jmath} = \sigma_B \varepsilon \vec{E} \tag{9}$$

(with ε denoting a rotation by $\pi/2$) over time and across a large circle $\mathcal{C}$ enclosing the flux. Here $\vec{E} = \mathrm{i}\partial_t \nabla(\log \widetilde{U}_a)$ is the electric field accompanying the change of magnetic field, and is the same on $\mathcal{C}$ in the two cases. Since the phenomenological equation (9) is valid only well inside the sample, it is crucial that the isolines of the gauge transformation run to infinity through the upper half-plane, so that $\vec{E}$ vanishes where $\mathcal{C}$ crosses the boundary of the sample.

It appears reasonable, even without recourse to (9), that for $\widetilde{\ } = \breve{\ }$ and $a \to \infty$ (8) tends to σ_B as defined in (2). As for $\widehat{U}_a$ note that

$$\widehat{U}_a(\vec{r}) = \mathrm{e}^{2\pi \mathrm{i} \chi_a(\vec{r})},$$

where $\chi_a(\vec{r})$ is a single-valued function over the sample and, for $\vec{r}$ close to the boundary,

$$\chi_a(\vec{r}) = \chi_a(x) = \chi(x/a)$$

is a switch function. This suggests that

$$\begin{aligned} \frac{1}{2\pi} \operatorname{tr}\left(\widehat{U}_a g(H) \widehat{U}_a^* - g(H)\right) &= \frac{1}{2\pi} \int_0^{2\pi} d\varphi \frac{d}{d\varphi} \operatorname{tr}\left[\mathrm{e}^{\mathrm{i}\varphi\chi_a} g(H) \mathrm{e}^{-\mathrm{i}\varphi\chi_a} - g(H)\right] \\ &= -\operatorname{tr}\left(\mathrm{i}[g(H), \chi_a]\right) = -\operatorname{tr}\left(g'(H)\mathrm{i}[H, \chi_a]\right) = \sigma_E \ , \end{aligned}$$

where the last two traces are formally equal since the operators inside differ by a commutator.

The trouble with this explanation for $\sigma_B = \sigma_E$ is that none of the traces starting with (8), except for the last one, is well-defined. In fact, one has the weaker property $\widetilde{U}_a g(H) \widetilde{U}_a^* - g(H) \in \mathcal{J}_3$ for g a switch function (but notice that as a rule even this fails if g is taken as a step function, a fact related to Theorem 3.11 in [2]).

Put differently: the formal eigenvalue sum represented by (8) is not absolutely convergent, but exhibits strong cancellations between small eigenvalues of opposite sign (which are exact except for $\lambda = \pm 1$ in a bulk situation, where $g(H_B) = P_B$ is a projection [3]). Let therefore $f_t(\lambda)$ be an odd function with $f_t(1) = 1$ interpolating between λ^3 (as $t = 0$) and λ (as $t = \infty$). For definiteness we take

$$f_t(\lambda) = \frac{(1+t)\lambda^3}{1 + t\lambda^2} \ . \tag{10}$$

We regard $\lim_{t\to\infty} \operatorname{tr} f_t(A)$ as a replacement for $\operatorname{tr} A$, when the latter is not defined. But first we pass to a more general setting.

We consider a fixed bounded operator P (typically not a projection!) on a Hilbert space $\mathcal{H}$ equipped with a fixed orthonormal basis $\mathcal{B}$. Our standing assumptions are: let

$$Q = UPU^* \ , \tag{11}$$

where U is a unitary operator satisfying

$$\mathcal{B} \text{ is an eigenbasis for } U \,, \tag{12}$$
$$Q - P \in \mathcal{J}_3 \,, \tag{13}$$
$$(Q-P)(P-P^2) \,,\; (P-P^2)(Q-P) \in \mathcal{J}_1 \,, \tag{14}$$
$$p(Q) - p(P) \in \mathcal{J}_1 \,, \tag{15}$$

for any polynomial $p(\lambda)$ with $p(0) = p(1) = 0$ and $\deg p \le 3$. This implies

$$\mathrm{tr}\,\big(p(Q) - p(P)\big) = 0 \,, \tag{16}$$

as it is seen be evaluating the trace in an eigenbasis of U. Specifically, (16) will be used for the polynomials $p(\lambda) = \lambda - \lambda^2$ and $p(\lambda) = (1-2\lambda)(\lambda - \lambda^2) = \lambda - 3\lambda^2 + 2\lambda^3$, which span the above space of polynomials.

As an abstract replacement for (8) we have

Lemma 2 *Assume (11–15) and $P = P^*$. Then*

$$\lim_{t\to\infty} \mathrm{tr}\; f_t(Q-P) = \mathrm{tr}\,\Big(\frac{3}{2}\{Q-P, (Q-Q^2) + (P-P^2)\} + (Q-P)^3\Big) \equiv K(U) \,. \tag{17}$$

The proof of Theorem 1 will not depend on Lemma 2, except for the fact that $K(U)$ is well-defined. The limit (17) will thus be proved only towards the end of the paper.

The heuristic discussion following (8) is now substantiated in terms of $K(U)$.

Lemma 3 *Let $Q_i = U_i P U_i^*$, $(i = 1,2)$ satisfy (12–15) and assume*

$$U_2 - U_1 \in \mathcal{J}_1 \,. \tag{18}$$

Then $K(U_1) = K(U_2)$.

We now turn to the application to the quantum Hall effect.

Lemma 4 *i) The assumptions (12–15) hold true for $\mathcal{H} = \ell^2(\mathbb{Z}\times\mathbb{N}), B = \{\delta_{\vec r}\}_{\vec r\in\mathbb{Z}\times\mathbb{N}}$,*

$$P = g(H) \,, \qquad U = \widetilde{U}_a \,, \qquad Q_a = \widetilde{U}_a g(H) \widetilde{U}_a^* \tag{19}$$

with $\widetilde{\ } = \breve{\ }, \widehat{\ }$ and g as in Theorem 1.

ii) Assumption (18) applies to $U_i = \widetilde{U}_a$, with separate choices of a and $\widetilde{\ } = \breve{\ }, \widehat{\ }$ for $i = 1,2$.

Therefore, $K(\widetilde{U}_a)$ is independent of a and $\widetilde{\ }$.

Lemma 5 *Let (19) with $\widetilde{\ } = \breve{\ }$. Then*

$$\lim_{a\to\infty} \mathrm{tr}\,(Q_a - P)^3 = 2\pi\sigma_B \,, \tag{20}$$
$$\lim_{a\to\infty} \frac{3}{2}\,\mathrm{tr}\,\{Q_a - P, (P-P^2) + (Q_a - Q_a^2)\} = 0 \,. \tag{21}$$

Lemma 6 *Let (19) with $\widetilde{\ } = \widehat{\ }$. Then*

$$\lim_{a\to\infty} \mathrm{tr}\,(Q_a - P)^3 = 0 \,, \tag{22}$$
$$\lim_{a\to\infty} \frac{3}{2}\,\mathrm{tr}\,\{Q_a - P, (P-P^2) + (Q_a - Q_a^2)\} = 2\pi\sigma_E \,. \tag{23}$$

Proof of Theorem 1. Is immediate from Lemmas 3–6. □

The details

The starting point to the proofs of Lemma 2 and 3 are two identities from [2] valid for projections $P = P^2$ and $Q = Q^2$. They are

$$(Q - P) - (Q - P)^3 = [QP, PQ] = [QP, [P, Q - P]] \,, \tag{24}$$

$$[P, (Q - P)^2] = [Q, (Q - P)^2] = 0 \,. \tag{25}$$

The first was used there for it yields the case $n = 0$ of

$$\mathrm{tr}\,(Q - P)^{2n+3} = \mathrm{tr}\,(Q - P)^{2n+1}$$

for $Q - P \in \mathcal{J}_{2n+1}$. The second yields the extension to $n \in \mathbb{N}$. For later purpose we remark that they similarly yield

$$\mathrm{tr}\ f_t(Q - P) = \mathrm{tr}\,(Q - P)^3 \tag{26}$$

for $0 \leq t < \infty$ if $P - Q \in \mathcal{J}_3$. Indeed: since

$$f_t(\lambda) - \lambda^3 = \frac{t\lambda^2}{1 + t\lambda^2}(\lambda - \lambda^3) \tag{27}$$

we have

$$f_t(Q - P) - (Q - P)^3 = t\big[QP, [P, \frac{(Q - P)^3}{1 + t(Q - P)^2}]\big]$$

with the inner commutator being trace class, whence (26).

Our primary concern here is however a generalization of (24, 25) to arbitrary bounded operators P, Q. More precisely, we take the half-difference between (24) and its "particle-hole" reversed variant ($P \to 1 - P$, $Q \to 1 - Q$), and correct the result by the appropriate terms involving $P - P^2$ and $Q - Q^2$:

$$\begin{aligned}(Q - P) - (Q - P)^3 \;=\;& \frac{1}{2}[QP, PQ] - \frac{1}{2}\big[(1 - Q)(1 - P), (1 - P)(1 - Q)\big] \\ &+ (1 - 2Q)(Q - Q^2) - (1 - 2P)(P - P^2) \\ &+ \frac{3}{2}\{Q - P, Q - Q^2 + P - P^2\} \,.\end{aligned} \tag{28}$$

In the new setting (25) is replaced with

$$\big[P, (Q - P)^2\big] = \big[Q, (Q - P)^2\big] = \big[Q - P, (Q - Q^2) - (P - P^2)\big] \,. \tag{29}$$

These relations are conveniently stated in terms of the operators

$$A = Q - P \,, \qquad B = 1 - P - Q \tag{30}$$

introduced in [10, 3], for which

$$\{A, B\} = 2\big[(Q - Q^2) - (P - P^2)\big] \,, \tag{31}$$

$$1 - A^2 - B^2 = 2\big[(Q - Q^2) + (P - P^2)\big] \,. \tag{32}$$

Then (28) reads (with equality line by line)

$$\begin{aligned} A - A^3 &= \frac{1}{4}[B,[B,A]] \\ &\quad + \frac{1}{4}\{B,\{A,B\}\} - \frac{1}{4}\{A, 1 - A^2 - B^2\} \\ &\quad + \frac{3}{4}\{A, 1 - A^2 - B^2\} \end{aligned} \tag{33}$$

and (29) (after multiplication by 2)

$$[A^2, B] = [A, \{A, B\}] \ . \tag{34}$$

Proof of Lemma 3. We remark that

$$\big\{Q - P, (Q - Q^2) + (P - P^2)\big\} = 2\big\{Q - P, P - P^2\big\} + \{Q - P, p(Q) - p(P)\}$$

with $p(\lambda) = \lambda - \lambda^2$, is trace class by our assumptions (14, 15). Thus $K(U)$ in (17) is well-defined. Let $A_i = Q_i - P$, $(i = 1, 2)$, and similarly for B_i. We take the difference between (33) (or (28)) in the two cases. In a mixed notation we have

$$\begin{aligned} A_i \big|_1^2 - A_i^3 \big|_1^2 &= \frac{1}{4}\big[B_i, [B_i, A_i]\big] \big|_1^2 \\ &\quad + \big[p(Q_i) - p(P)\big] \big|_1^2 \\ &\quad + \frac{3}{2}\big\{Q_i - P, (Q_i - Q_i^2) + (P - P^2)\big\} \big|_1^2 \end{aligned} \tag{35}$$

with $p(\lambda) = (1 - 2\lambda)(\lambda - \lambda^2)$. We note that $A_2 - A_1 = -(B_2 - B_1) = Q_2 - Q_1 \in \mathcal{J}_1$ with $\mathrm{tr}\,(Q_2 - Q_1) = 0$. Indeed, by (18),

$$Q_2 - Q_1 = U_2 P U_2^* - U_1 P U_1^* = (U_2 - U_1) P U_2^* + U_1 P (U_2 - U_1)^* \tag{36}$$

is trace class, and the trace is seen to vanish using the basis $\mathcal{B}$. Writing

$$\big[B_i, [B_i, A_i]\big] \big|_1^2 = \big[B_2, [B_2, A_2 - A_1]\big] + \big[B_2, [B_2 - B_1, A_1]\big] + \big[B_2 - B_1, [B_1, A_1]\big]$$

we see that the first term on the r.h.s. of (35) is trace class with vanishing trace. So is the next one due to (16). □

Proof of Lemma 4. Eq. (12) is evident, since the $\widetilde{U}_a$ are multiplication operators. Let $U(\vec{r})$ be given by (5) as in Figure 1. Since $U - \widetilde{U}_a$ has compact support as a function, it is trace class as an operator. Thus (ii) holds true and it suffices to prove (13–15) for U instead of $\widetilde{U}_a$, cf. (36). The $(\vec{r}_1, \vec{r}_2)$-matrix element of $(Q - P)U = Ug(H) - g(H)U$ is

$$g(H)(\vec{r}_1, \vec{r}_2)\big(U(\vec{r}_1) - U(\vec{r}_2)\big) \ ,$$

so (13) follows from (A.5),

$$\big|U(\vec{r}_1) - U(\vec{r}_2)\big| \le C \frac{|\vec{r}_1 - \vec{r}_2|}{1 + |\vec{r}_1|}$$

and (A.4) with $p = 3$. To prove (15), we note that $G = p \circ g$ has supp $G \subset \Delta$. Hence (A.7) applies. Writing the matrix element of $(p(Q) - p(P))U = UG(H) - G(H)U$ as before, the claim follows. As mentioned, the verification of (14) could equally be done on the basis of U instead of $\widetilde{U}_a$. However we prefer to do this for $\widetilde{\ } = \check{\ }, \widehat{\ }$ explicitly, since this will provide estimates, stated in the lemma below, which will be useful in the proofs of Lemma 5, 6. Technically, the first part of (14) is just the case $b = 0$ in (37) below. The second part follows by taking the adjoint. □

The rough reason for

$$(Q_a - P)(P - P^2) = \big(\widetilde{U}_a g(H) \widetilde{U}_a^* - g(H)\big)\big(g(H) - g(H)^2\big)$$

to be trace class is that supp $(\widetilde{U}_a - 1)$ has compact intersection (possibly empty) with the boundary.

Lemma 7 *Let $F_b = F_b(y)$ be the characteristic function of the neighborhood $\{\vec{r} | y < b\}$ of the boundary. Then, in the notation (19),*

$$\|(Q_a - P)(1 - F_b)(P - P^2)\|_1 \le C(1 + a)\mathrm{e}^{-\kappa b} , \tag{37}$$

$$\|(Q_a - P)(1 - F_b)(Q_a - Q_a^2)\|_1 \le C(1 + a)\mathrm{e}^{-\kappa b} \tag{38}$$

for both $\widetilde{\ } = \check{\ }, \widehat{\ }$ and some $\kappa > 0$. For $b \le a/2$ we furthermore have

$$\|(Q_a - P)F_b\|_1 \le C_N (1 + a)^{-N} \tag{39}$$

in case $\widetilde{\ } = \check{\ }$; and

$$\|(Q_a - P)F_b\|_1 \le C \cdot b , \tag{40}$$

$$\|(Q_a - P)F_b\|_2 \le C(b/a)^{1/2} \tag{41}$$

in case $\widetilde{\ } = \widehat{\ }$.

Proof. We set $G(H) = P - P^2 = g(H) - g(H)^2$ and estimate (37) as

$$\begin{aligned} \|(Q_a - P)(1 - F_b)G(H)\|_1 &= \|(Q_a - P)(1 - F_b)\mathrm{e}^{-\kappa y}\mathrm{e}^{\kappa y} G(H)\|_1 \\ &\le \mathrm{e}^{-\frac{\kappa}{2} b} \|(Q_a - P)\mathrm{e}^{-\frac{\kappa}{2} y}\|_1 \|\mathrm{e}^{\kappa y} G(H)\| , \end{aligned}$$

where the last norm is finite due to (A.7). The operator $T = (Q_a - P)\mathrm{e}^{-\frac{\kappa}{2} y}\widetilde{U}_a$ has kernel

$$T(\vec{r}_1, \vec{r}_2) = g(H)(\vec{r}_1, \vec{r}_2)\big(\widetilde{U}_a(\vec{r}_1) - \widetilde{U}_a(\vec{r}_2)\big)\mathrm{e}^{-\frac{\kappa}{2} y_2}$$

with

$$|\widetilde{U}_a(\vec{r}_1) - \widetilde{U}_a(\vec{r}_2)| \le C_k \big(1 + (|x_2| - a - y_2)_+\big)^{-k} \big(1 + |\vec{r}_1 - \vec{r}_2|\big)^k . \tag{42}$$

In fact if $|x_2| < a + y_2$, the first factor on the r.h.s. is bounded below by 1, while the l.h.s. is bounded above by 2. In the opposite case $|x_2| \ge a + y_2$, we distinguish between $|x_1| \ge a + y_1$, whence the l.h.s. vanishes (see Fig. 1), and $|x_1| < a + y_1$, where

$\sqrt{2}|\vec{r}_1 - \vec{r}_2| \geq |x_2| - a - y_2$ implies that the r.h.s. is bounded below away from 0. We claim this proves

$$\|T\|_1 = \|(Q_a - P)\mathrm{e}^{-\frac{\kappa}{2}y}\widetilde{U}_a\|_1 \leq C(1+a) \ , \tag{43}$$

and hence (37). To this end we apply (A.4) with $p = 1$: using (A.5) with $N + k$ instead of N we have

$$\begin{aligned}\sum_{\vec{r}\in\mathbb{Z}\times\mathbb{N}} |T(\vec{r}+\vec{s},\vec{r})| &\leq C(1+|\vec{s}|)^{-N}\sum_{\vec{r}}\big(1+(|x|-a-y)_+\big)^{-k}\cdot \mathrm{e}^{-\frac{\kappa}{2}y} \\ &\leq C(1+|\vec{s}|)^{-N}\sum_{y=0}^{\infty}(1+a+y)\mathrm{e}^{-\frac{\kappa}{2}y} \leq C(1+|\vec{s}|)^{-N}\cdot(1+a) \ ,\end{aligned}$$

for $k \geq 2$. This is summable w.r.t. $\vec{s} \in \mathbb{Z}^2$ for $N \geq 3$. Taking (37) with $\widetilde{U}_a^*$ instead of $\widetilde{U}_a$ yields (38).

Let now $b \leq a/2$ for the rest of the proof. The proof of (39) is just like that of (43), which we supplement with $\breve{U}_a(\vec{r}_1) - \breve{U}_a(\vec{r}_2) = 0$ if $y_2 < a/2$ and $|\vec{r}_1 - \vec{r}_2| \leq a/2$. This yields for $T = (Q_a - P)F_b\breve{U}_a$

$$\begin{aligned}\sum_{\vec{r}} |T(\vec{r}+\vec{s},\vec{r})| &\leq C(1+|\vec{s}|)^{-N}\sum_{y=0}^{\infty}(1+a+y)F_b(y) \\ &\leq C(1+|\vec{s}|)^{-N}(1+a)^2 \ ,\end{aligned}$$

and $= 0$ if $|\vec{s}| < a/2$. Thus

$$\|T\|_1 \leq C(1+a)^2 \sum_{\vec{s}:|\vec{s}|\geq a/2}(1+|\vec{s}|)^{-N} \leq C(1+a)^2(1+a)^{-(N-2)}.$$

Let finally $\widetilde{\ } = \widehat{\ }$, where

$$\big|\widehat{U}_a(\vec{r}_1) - \widehat{U}_a(\vec{r}_2)\big| \leq C\frac{|\vec{r}_1 - \vec{r}_2|}{a + |\vec{r}_2|} \ . \tag{44}$$

This holds true for $a = 1$ and $\vec{r}_1, \vec{r}_2 \in \mathbb{R}^2$, and follows by scaling, $\widehat{U}_a(\vec{r}) = \widehat{U}_1(\vec{r}/a)$, for $a > 0$. To estimate $T = (Q_a - P)F_b\widehat{U}_a$ we use (44) for $|x_2| < 3a$ and (42) for $|x_2| \geq 3a$ (with $N + 1$, resp. $N + k$ in (A.5)). Thus

$$\begin{aligned}\sum_{\vec{r}\in\mathbb{Z}\times\mathbb{N}} |T(\vec{r}+\vec{s},\vec{r})| &\leq C(1+|\vec{s}|)^{-N}\sum_{y=0}^{b-1}\Big(\sum_{|x|<3a}\frac{1}{a} + \sum_{|x|\geq 3a}\big(1+(|x|-a-y)_+\big)^{-k}\Big) \\ &\leq C(1+|\vec{s}|)^{-N}b\Big(6 + 2\sum_{m=a}^{\infty}(1+m)^{-k}\Big) \ ,\end{aligned}$$

where we used $|x| - a - y \geq 3a - 2a = a$. Similarly,

$$\begin{aligned}\sum_{r\in\mathbb{Z}\times\mathbb{N}} |T(\vec{r}+\vec{s},\vec{r})|^2 &\leq C(1+|\vec{s}|)^{-2N}b\Big(\frac{1}{a} + \sum_{m=a}^{\infty}(1+m)^{-2k}\Big) \\ &\leq C(1+|\vec{s}|)^{-2N}\cdot b/a \ .\end{aligned}$$

□

Proof of Lemma 5. Let $A = Q_a - P = \breve{U}_a g(H)\breve{U}_a^* - g(H)$, $A_B = \breve{U}_a g(H_B)\breve{U}_a^* - g(H_B) = \breve{U}_a P_B \breve{U}_a^* - P_B$ and $D = (A - A_B)\breve{U}_a$, where $g(H) \equiv Jg(H)J^*$ is now meant as an operator on $\ell^2(\mathbb{Z}\times\mathbb{Z})$, simply extended by zero. The kernel of D,

$$D(\vec{r}_1,\vec{r}_2) = \big(Jg(H)J^* - g(H_B)\big)(\vec{r}_1,\vec{r}_2)\big(\breve{U}_a(\vec{r}_1) - \breve{U}_a(\vec{r}_2)\big) ,$$

satisfies (up to a factor 2) the bound (A.6), and vanishes if both $\vec{r}_1,\vec{r}_2$ are outside of the wedge. Thus (A.4) with $p = 1$ shows

$$\|D\|_1 \le C\mathrm{e}^{-\kappa a} .$$

Writing $A^3 - A_B^3 = A^2(A - A_B) + A(A - A_B)A_B + (A - A_B)A_B^2$, this proves

$$\lim_{a\to\infty}(\mathrm{tr}\ A^3 - \mathrm{tr}\ A_B^3) = 0 .$$

But, see [2],

$$\mathrm{tr}\ A_B^3 = \mathrm{Ind}\big(\breve{U}_a P_B \breve{U}_a^*, P_B\big) \tag{45}$$

is independent of a due to the stability of the index ([10], Theorem 5.26) under compact perturbations (or use Lemma 3 above instead). In particular (45) equals $2\pi\sigma_B$ as defined. This proves (20). To prove (21), we let $b \le a/2$ and note that by (37, 38, 39)

$$\begin{aligned}
&\|(Q_a - P)(P - P^2 + Q_a - Q_a^2)\|_1 \\
&\qquad \le \|(Q_a - P)(1 - F_b)(P - P^2 + Q_a - Q_a^2)\|_1 + 2\|(Q_a - P)F_b\|_1 \\
&\qquad \le C(1 + a)\mathrm{e}^{-\kappa b} + C_N(1 + a)^{-N} .
\end{aligned}$$

Upon choosing e.g. $b = a^{1/2}$, this tends to 0 as $a \to \infty$. □

As a preparation to the proof of Lemma 6 we have:

Lemma 8 *Eq. (3) is well-defined and independent of χ and g as stated in Theorem 1. In particular,*

$$\sigma_E = -\lim_{a\to\infty} \mathrm{tr}\,(g'(H)\mathrm{i}[H, \chi_a(x)]) , \tag{46}$$

where $\chi_a(x) = \chi(x/a)$.

Proof. Eq. (3) is well-defined by (A.8). By taking differences of switch functions, independence amounts to

$$\text{(i)}\quad \mathrm{tr}\,\big(g'(H)\mathrm{i}[H, X(x)]\big) = 0 , \qquad \text{(ii)}\quad \mathrm{tr}\,\big(G'(H)\mathrm{i}[H, \chi(x)]\big) = 0 ,$$

where $X, G \in C_0^\infty(\mathbb{R})$ with supp $G \subset \Delta$. These statements are verified as follows:

i) Since $g'(H)X(x) \in \mathcal{J}_1$ by (A.7, A.4) we have $\mathrm{tr}\,\big(g'(H)[H, X]\big) = \mathrm{tr}\,\big(g'(H)HX\big) - \mathrm{tr}\,\big(g'(H)XH\big) = 0$ by cyclicity. This already proves (46).

ii) $\big([G(H),\chi]\big)(\vec r_1,\vec r_2)=G(H)(\vec r_1,\vec r_2)\big(\chi(\vec r_2)-\chi(\vec r_1)\big)$. By (A.7, A.4), $[G(H),\chi]\in\mathcal{J}_1$ and hence

$$\operatorname{tr}[G(H),\chi(x)]=0\ . \tag{47}$$

We then pick $\widetilde G\in C_0^\infty$ with supp $\widetilde G\subset\Delta$ and $\widetilde G G=G$. Then (47) may also be written, using cyclicity and (A.9) as

$$\operatorname{tr}[\widetilde G G,\chi]=\operatorname{tr}\big([G,\chi]\widetilde G\big)+\operatorname{tr}\big([\widetilde G,\chi]G\big)=\operatorname{tr}\big([H,\chi](G'\widetilde G+\widetilde G'G)\big)=\operatorname{tr}\big([H,\chi]G'\big)\ .$$

□

Proof of Lemma 6. Let $A=Q_a-P$. Then, by (A.5) and (44),

$$|A(\vec r_1,\vec r_2)|=\big|g(H)(\vec r_1,\vec r_2)\big(\widehat U_a(\vec r_1)-\widehat U_a(\vec r_2)\big)\big|\le C_N\big(1+|\vec r_1-\vec r_2|\big)^{-N}\ \frac{|\vec r_1-\vec r_2|}{a+|\vec r_1|}\ ,$$

so that by (A.4) $\|A^3\|_1=\|A\|_3^3\le Ca^{-1}$. This proves (22).

For $b\le a/2$ we have

$$F_b(y)\widehat U_a(\vec r)=F_b(y)\mathrm{e}^{2\pi\mathrm{i}\chi_a(x)}\ ,$$

where $\chi_a(x)=\chi(x/a)$ is a switch function. We then have, using (37, 38),

$$\begin{aligned}&\frac{3}{2}\operatorname{tr}\{Q_a-P,P-P^2+Q_a-Q_a^2\} &&(48)\\ &\quad=3\operatorname{tr}\,F_b(Q_a-P)F_b(P-P^2+Q_a-Q_a^2)+O((1+a)\mathrm{e}^{-\kappa b})\\ &\quad=3\operatorname{tr}\,F_b\big(P(2\pi)-P(0)\big)F_b\big(P(0)-P(0)^2+P(2\pi)-P(2\pi)^2\big)+O((1+a)\mathrm{e}^{-\kappa b})\ ,\end{aligned}$$

where $P(\varphi)=\mathrm{e}^{\mathrm{i}\varphi\chi_a(x)}g(H)\mathrm{e}^{-\mathrm{i}\varphi\chi_a(x)}$. We now apply the fundamental theorem of calculus to

$$P(2\pi)-P(0)=\int_0^{2\pi}d\varphi\,\frac{d}{d\varphi}P(\varphi)=-\int_0^{2\pi}d\varphi\,\mathrm{e}^{\mathrm{i}\varphi\chi_a}\mathrm{i}[g(H),\chi_a]\mathrm{e}^{-\mathrm{i}\varphi\chi_a}\ . \tag{49}$$

We remark that in (37, 38, 40, 41) one can, by the same proof, replace Q_a-P by $\mathrm{i}[g(H),\chi_a]$:

$$\|\mathrm{i}[g(H),\chi_a]F_b\|_2\le C(b/a)^{1/2}\ , \tag{50}$$
$$\|\mathrm{i}[g(H),\chi_a](1-F_b)(g(H)-g(H)^2)\|_1\le C(1+a)\mathrm{e}^{-\kappa b}\ . \tag{51}$$

Thus

$$\sup_{0\le\varphi,\varphi'\le 2\pi}\|\big(P(\varphi')-P(\varphi)\big)F_b\|_2\le C(b/a)^{1/2}\ ,$$

so that by writing

$$\begin{aligned}&\big(P(\varphi')-P(\varphi')^2\big)-\big(P(\varphi)-P(\varphi)^2\big)=\\ &\qquad\qquad\big(P(\varphi')-P(\varphi)\big)\big(1-P(\varphi')\big)-P(\varphi)\big(P(\varphi')-P(\varphi)\big)\end{aligned}$$

we infer

$$\sup_{0\le\varphi,\varphi'\le 2\pi}\|F_b\big[\big(P(\varphi')-P(\varphi')^2\big)-\big(P(\varphi)-P(\varphi)^2\big)\big]F_b\|_2\le C(b/a)^{1/2}\ .$$

Using this with $\varphi'=0,2\pi$, (49, 50) and the Cauchy-Schwarz inequality we find that (48) equals, up to errors $O(b/a)+O((1+a)\mathrm{e}^{-\kappa b})$,

$$\begin{aligned}
-6\int_0^{2\pi} & d\varphi\ \mathrm{tr}\ \big(F_b\mathrm{i}[g(H),\chi_a]F_b\big(g(H)-g(H)^2\big)\big)\\
&=-6\cdot 2\pi\ \mathrm{tr}\ \big(\mathrm{i}[g(H),\chi_a]\big(g(H)-g(H)^2\big)\big)\\
&=-2\pi\cdot 6\ \mathrm{tr}\ \big(\mathrm{i}[H,\chi_a]g'(H)\big(g(H)-g(H)^2\big)\big)=-2\pi\ \mathrm{tr}\ \big(\mathrm{i}[H,\chi_a]\widetilde{g}'(H)\big)\ ,
\end{aligned}$$

where F_b has been dropped using (51) and (A.9) been used. We remark that $\widetilde{g}=3g^2-2g^3$ is also a switch function. We finally pick e.g. $b=a^{1/2}$ so that the error mentioned above vanishes as $a\to\infty$. Thus (23) follows from Lemma 8. □

Proof of Lemma. 2. This is a variant of the argument leading to (26) in the case of projections. Let, in the general case, A,B be as in (30, 19). Then, by (27),

$$\begin{aligned}
f_t(A)-A^3 &= (1-R_t)(\text{r.h.s. of }(33))\\
&= \frac{1}{4}\big((1-R_t)[B,[B,A]]-R_t\{B,\{A,B\}\}\big)\\
&\quad -\frac{1}{2}R_t\{A,1-A^2-B^2\}\\
&\quad +\frac{1}{4}\{B,\{A,B\}\}-\frac{1}{4}\{A,1-A^2-B^2\}\\
&\quad +\frac{3}{4}\{A,1-A^2-B^2\}\\
&\equiv L_1+L_2+L_3+L_4 \qquad \text{(linewise)},
\end{aligned}$$

where

$$1-R_t=tA^2(1+tA^2)^{-1}\ , \tag{52}$$

resp. $R_t=(1+tA^2)^{-1}$. Note that since $A=A^*$

$$\mathrm{s}-\lim_{t\to\infty}t^{1/2}AR_t=0\ , \tag{53}$$

$$\mathrm{s}-\lim_{t\to\infty}R_t=\Pi\ , \tag{54}$$

where Π is the projection onto the null space of A.

1) We claim $\lim_{t\to\infty}\mathrm{tr}\ L_1=0$. To this end we consider the first term in the corresponding bracket first:

$$(1-R_t)[B,[B,A]]=[B,(1-R_t)[B,A]]+[B,R_t][B,A]\ . \tag{55}$$

Since $A\in\mathcal{J}_3$ and $1-R_t\in\mathcal{J}_{3/2}$ we have $(1-R_t)[B,A]\in\mathcal{J}_1$ by the Hölder inequality. Thus $\mathrm{tr}\,[B,(1-R_t)[B,A]]=0$. The last term in (55) is by (34)

$$\begin{aligned}
[B,R_t][B,A] &= tR_t[A^2,B]R_t\cdot[B,A]\\
&= tR_t[A,\{A,B\}]R_t[B,A]\\
&= tR_tA\{A,B\}R_t(-2AB+\{A,B\})-tR_t\{A,B\}AR_t(2BA-\{A,B\})\\
&= -2tR_tA\{A,B\}R_tAB-2tR_t\{A,B\}AR_tBA\\
&\quad +tR_t\{A,\{A,B\}\}R_t\{A,B\}\ .
\end{aligned}$$

All terms are trace class since $\{A, B\}$ is by (31, 15) with $p(\lambda) = 2(\lambda - \lambda^2)$. We recall that

$$\begin{aligned} X_n \xrightarrow{s} 0,\ Y \in \mathcal{J}_1 \ &\Rightarrow\ \|X_n Y\|_1 \to 0 , \\ X_n^* \xrightarrow{s} 0,\ Y \in \mathcal{J}_1 \ &\Rightarrow\ \|Y X_n\|_1 \to 0 . \end{aligned} \tag{56}$$

Thus the first two terms on the r.h.s. do not contribute to the trace as $t \to \infty$ by (53) (use cyclicity for the second). Similarly, in the last term

$$tR_t(A^2B + 2ABA + BA^2)R_t\{A, B\} ,$$

the middle term thereof does not. Using cyclicity of the trace on the remaining ones, as well as (52), we find for $t \to \infty$

$$\begin{aligned} \mathrm{tr}\,(1 - R_t)[B, [B, A]] &= \mathrm{tr}\ BR_t\{A, B\}(1 - R_t) + \mathrm{tr}\ B(1 - R_t)\{A, B\}R_t + o(1) \\ &= \mathrm{tr}\ BR_t\{A, B\} + \mathrm{tr}\ B\{A, B\}R_t + o(1) \\ &= \mathrm{tr}\ R_t\{B, \{A, B\}\} + o(1) , \end{aligned}$$

where we used $R_t\{A, B\}R_t \underset{t\to\infty}{\longrightarrow} \Pi\{A, B\}\Pi = 0$ in trace norm, a consequence of (54, 56). The traces of the two terms in L_1 thus compensate one another in the limit $t \to \infty$.

2) We note that $\{A, 1 - A^2 - B^2\} \in \mathcal{J}_1$ by (30, 32, 14). Again by (54) we have

$$-2 \lim_{t\to\infty} \mathrm{tr}\ L_2 = \mathrm{tr}\ \Pi\{A, 1 - A^2 - B^2\} = \mathrm{tr}\ \Pi\{A, 1 - A^2 - B^2\}\Pi = 0$$

since $\Pi = \Pi^2$.

3) L_3 equals the second line of the r.h.s. of (28), as seen from (33). Hence $\mathrm{tr}\ L_3 = 0$ follows from (16) for $p(\lambda) = (1 - 2\lambda)(\lambda - \lambda^2)$.

We can now summarize:

$$\lim_{t\to\infty} \mathrm{tr}\ f_t(A) = \mathrm{tr}\ A^3 + \frac{3}{4}\,\mathrm{tr}\,\{A, 1 - A^2 - B^2\} ,$$

which is (17). □

As a final remark, we note that $\lim_{t\to\infty} \mathrm{tr}\ f_t(UPU^* - P)$, if existent, is invariant under trace class perturbations of U. This follows from (A.3). Similarly, as a possible replacement for Lemma 5, one has, without making recourse to Lemma 2,

$$\lim_{a\to\infty} \mathrm{tr}\ f_t\big(\breve{U}_a g(H)\breve{U}_a^* - g(H)\big) = 2\pi\sigma_B$$

uniformly in $t \geq 1$. This follows from the proof of Lemma 5 together with (26) and (A.2).

A Appendix

Lemma A.1 *Let $X = X^*, Y = Y^*$ and $t \geq 0$. For $X \in \mathcal{J}_3$,*

$$\|f_t(X)\|_1 \leq (1 + t)\|X\|_3^3 . \tag{A.1}$$

If $X - Y \in \mathcal{J}_1$, then

$$\|f_t(X) - f_t(Y)\|_1 \leq 3(1 + t^{-1})\|X - Y\|_1 \tag{A.2}$$

and

$$\lim_{t\to\infty} \mathrm{tr}\,\big(f_t(X) - f_t(Y)\big) = \mathrm{tr}\,(X - Y) . \tag{A.3}$$

Proof. Eq. (A.1) is evident from (10). From

$$f_t(\lambda) = (1+t^{-1})\big[\lambda - \frac{\lambda}{1+t\lambda^2}\big]$$

and from

$$X(1+tY^2) - (1+tX^2)Y = X - Y - tX(X-Y)Y$$

we find

$$f_t(X) - f_t(Y) = (1+t^{-1})\big[X - Y - (1+tX^2)^{-1}(X-Y-tX(X-Y)Y)(1+tY^2)^{-1}\big] .$$

Using $\|(1+tX^2)^{-1}\| \le 1$, $\|t^{1/2}X(1+tX^2)^{-1}\| \le 1$ we obtain (A.2). Using furthermore

$$\begin{aligned} \mathrm{s-}\lim_{t\to\infty} t^{1/2}X(1+tX^2)^{-1} &= 0 , \\ \mathrm{s-}\lim_{t\to\infty} (1+tX^2)^{-1} &= \Pi_X , \end{aligned}$$

where Π_X is the projection onto the null space of X, together with (56), we obtain

$$f_t(X) - f_t(Y) \underset{t\to\infty}{\longrightarrow} X - Y - \Pi_X(X-Y)\Pi_Y = X - Y$$

in trace norm. □

Lemma A.2 *For $1 \le p < \infty$,*

$$\|T\|_p \le \sum_{\vec{s}} \Big(\sum_{\vec{r}\in\mathbb{Z}\times\mathbb{N}} |T(\vec{r}+\vec{s},\vec{r})|^p \Big)^{1/p} . \tag{A.4}$$

Proof. The case $p = 3$ is Eq. (4.11) in [1], and the proof given there applies to $1 \le p < \infty$. □

Lemma A.3 *i) Let $g \in C^\infty(\mathbb{R})$ with* supp g' *compact. Then, for any N,*

$$|g(H)(\vec{r}_1,\vec{r}_2)| \le C_N(1+|\vec{r}_1-\vec{r}_2|)^{-N} . \tag{A.5}$$

ii) If furthermore supp $g' \subset \Delta$*, then, for some $\kappa > 0$,*

$$\big|\big(Jg(H)J^* - g(H_B)\big)(\vec{r}_1,\vec{r}_2)\big| \le C_N(1+|\vec{r}_1-\vec{r}_2|)^{-N}\mathrm{e}^{-\kappa\min(|y_1|,|y_2|)} , \tag{A.6}$$

unless both $y_1, y_2 < 0$.
iii) If $G \in C_0^\infty(\mathbb{R})$ with supp $G \subset \Delta$*, then*

$$\big|G(H)(\vec{r}_1,\vec{r}_2)\big| \le C_N(1+|\vec{r}_1-\vec{r}_2|)^{-N}\mathrm{e}^{-\kappa(y_1+y_2)}. \tag{A.7}$$

In particular, $\mathrm{e}^{\kappa y}G(H)$ is a bounded operator.

Lemma A.4 *Let $\chi', g', G \in C_0^\infty$ with* supp $G \subset \Delta$*. Then*

$$[H,\chi(x)]G(H) , \quad [g(H),\chi(x)]G(H) \in \mathcal{J}_1 \tag{A.8}$$

and

$$\mathrm{tr}\,([g(H),\chi(x)]G(H)) = \mathrm{tr}\,([H,\chi(x)]g'(H)G(H)) . \tag{A.9}$$

In [6], Chapter 2, or [12], Lemma B.1 the Helffer-Sjöstrand formula

$$g(H) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \partial_{\bar{z}} \tilde{g}(z)(H - z)^{-1} dx dy , \qquad (z = x + \mathrm{i}y) , \tag{A.10}$$

is proven in the sense of a norm convergent integral for H a self-adjoint operator on a Hilbert space $\mathcal{H}$ and, say, $g \in C_0^\infty$, where $\partial_{\bar{z}} = \partial_x + \mathrm{i}\partial_y$ and $\tilde{g}$ is a quasi-analytic extension of g. For definiteness, let

$$\tilde{g}(z) = \sum_{k=0}^{N} g^{(k)}(x) \frac{(\mathrm{i}y)^k}{k!} \chi(y) ,$$

with $N \geq 1$, and hence

$$\partial_{\bar{z}} \tilde{g}(z) = g^{(N+1)}(x)(\mathrm{i}y)^N \chi(y) + \mathrm{i} \sum_{k=0}^{N} g^{(k)}(x) \frac{(\mathrm{i}y)^k}{k!} \chi'(y) , \tag{A.11}$$

where $\chi \in C_0^\infty$ is even and equals 1 in a neighborhood $(-\delta, \delta)$ of $y = 0$. In Lemma A.3 one is mainly interested in functions with supp g', but not supp g, compact. The difference is of little importance, since, if H were bounded above or below, one could trade the one for the other by adding a constant to g and changing it outside of the spectrum. As we however do not want to resort to this assumption, we maintain that (A.10) still holds in the strong sense.

Proof of Lemma A.3. We claim that

$$g(H)\psi = \frac{1}{2\pi} \int dx \Big(\int dy \partial_{\bar{z}} \tilde{g}(z)(H - z)^{-1} \psi \Big) \tag{A.12}$$

for all $\psi \in \mathcal{H}$ and $g' \in C_0^\infty$. By the functional calculus it suffices to show that, if ψ is dropped and H replaced by $a \in \mathbb{R}$, the r.h.s. is (a) well-defined as an improper Riemann integral, and (b) agrees with $g(a)$. Indeed, all of $\partial_{\bar{z}} \tilde{g}$, except for the $k = 0$ term in (A.11), has compact support $K \subset \mathbb{R}^2$, and

$$|\partial_{\bar{z}} \tilde{g}(z) - \mathrm{i}g(x)\chi'(y)| \leq C|y|^N , \tag{A.13}$$

so that the analysis of [6, 12] still applies, except for the contribution from $\mathrm{i}g(x)\chi'(y)$. The latter equals, using that χ' is odd,

$$\begin{aligned}
&\frac{\mathrm{i}}{2\pi} \int dx g(x) \Big(\int_0^\infty dy \chi'(y)[(a - x - \mathrm{i}y)^{-1} - (a - x + \mathrm{i}y)^{-1}] \Big) \\
&\qquad = -\frac{1}{\pi} \int dx g(x) \Big(\int_0^\infty dy\, y \chi'(y)[(a - x)^2 + y^2]^{-1} \Big) ,
\end{aligned}$$

which is absolutely convergent. This proves (a); part (b) follows as, e.g., in [6, 12].

Let $R(\vec{r}_1, \vec{r}_2; z) = (H - z)^{-1}(\vec{r}_1, \vec{r}_2)$ be the Green function. We shall use the Combes-Thomas [5] estimates

$$|R(\vec{r}_1, \vec{r}_2; x + \mathrm{i}y)| \leq \frac{2}{|y|} \mathrm{e}^{-\mu|\vec{r}_1 - \vec{r}_2|} , \tag{A.14}$$

$$\int |R(\vec{r}_1, \vec{r}_2; x + \mathrm{i}y) - R(\vec{r}_1, \vec{r}_2; x - \mathrm{i}y)| dx \leq 12\sqrt{2}\pi \mathrm{e}^{-\mu|\vec{r}_1 - \vec{r}_2|} , \tag{A.15}$$

which hold true provided

$$\sup_{\vec{r}_0\in\mathbb{Z}\times\mathbb{N}}\sum_{\vec{r}}|H(\vec{r}_0,\vec{r}_0+\vec{r})|(\mathrm{e}^{\mu|\vec{r}|}-1)\le|y|/2\ . \tag{A.16}$$

They have been proven in this form in [1], Appendix D, Eqs. (D.3, D.4, D.11). Since $(\mathrm{e}^{\mu|\vec{r}|}-1)\le(\mu/\mu_0)(\mathrm{e}^{\mu_0|\vec{r}|}-1)$ for $0\le\mu\le\mu_0$ we may take, by (6), $\mu=c|y|$ for $y\in\operatorname{supp}\chi$, where $c>0$ is some small constant.

i) The contribution to (A.5) from the $k=0$ term in (A.11) is, through (A.12),

$$\frac{\mathrm{i}}{2\pi}\int dxg(x)\Bigl(\int_0^\infty dy\chi'(y)\bigl(R(\vec{r}_1,\vec{r}_2;x+\mathrm{i}y)-R(\vec{r}_1,\vec{r}_2;x-\mathrm{i}y)\bigr)\Bigr)\ ,$$

and is bounded in modulus by

$$6\sqrt{2}\|g\|_\infty\int_0^\infty dy|\chi'(y)|\mathrm{e}^{-c|y||\vec{r}_1-\vec{r}_2|}\le C\mathrm{e}^{-c\delta|\vec{r}_1-\vec{r}_2|}\ ,$$

by using (A.15). The remaining contribution is bounded using (A.14, A.13) as

$$C\int_K dxdy|\chi'(y)||y|^N\frac{2}{|y|}\mathrm{e}^{-c|y||\vec{r}_1-\vec{r}_2|}\le C_N(1+c|\vec{r}_1-\vec{r}_2|)^{-N}\ ,$$

since K is compact.

ii) It suffices to establish a bound of the form $C\mathrm{e}^{-2\kappa|y_1|}$ if $y_2\ge0$ for the l.h.s. of (A.6). In fact by applying that estimate to $\bar{g}$ we can interchange y_1 and y_2 in the bound, and hence replace it by $C\mathrm{e}^{-2\kappa\min(|y_1|,|y_2|)}$ for y_1, y_2 as specified in the lemma. Moreover, we can also bound (A.6) by a constant times $(1+|\vec{r}_1-\vec{r}_2|)^{-2N}$ in virtue of (A.5), which applies to H_B as well. Then (A.6) follows since $\min(a,b)\le(ab)^{1/2}$ for $a,b>0$.

For $y_2\ge0$ the matrix element (A.6) is $(Jg(H)-g(H_B)J)(\vec{r}_1,\vec{r}_2)$. We use the resolvent identity $J(H-z)^{-1}-(H_B-z)^{-1}J=-(H_B-z)^{-1}E(H-z)^{-1}$ in (A.12) and distinguish as before between the contribution, I, to (A.6) from $\mathrm{i}g(x)\chi'(y)$, and the rest, II. Using again that χ' is odd and

$$\begin{aligned}&(H_B-z)^{-1}E(H-z)^{-1}-(H_B-\bar{z})^{-1}E(H-\bar{z})^{-1}=\\&\qquad[(H_B-z)^{-1}-(H_B-\bar{z})^{-1}]E(H-z)^{-1}+(H_B-\bar{z})^{-1}E[(H-z)^{-1}-(H-\bar{z})^{-1}]\end{aligned}$$

we have

$$\begin{aligned}I=-\frac{\mathrm{i}}{2\pi}\int dxg(x)\Bigl(\int_0^\infty dy\chi'(y)\sum_{\substack{\vec{r}\in\mathbb{Z}^2\\ \vec{r}\,'\in\mathbb{Z}\times\mathbb{N}}}&\Delta R_B(\vec{r}_1,\vec{r};x+\mathrm{i}y)E(\vec{r},\vec{r}\,')R(\vec{r}\,',\vec{r}_2;x+\mathrm{i}y)\\&+R_B(\vec{r}_1,\vec{r};x-\mathrm{i}y)E(\vec{r},\vec{r}\,')\Delta R(\vec{r}\,',\vec{r}_2;x+\mathrm{i}y)\Bigr)\ ,\end{aligned}$$

where $\Delta R(\vec{r}_1,\vec{r}_2;z)=R(\vec{r}_1,\vec{r}_2;z)-R(\vec{r}_1,\vec{r}_2;\bar{z})$. We use (A.14) for R, R_B and (A.15) for ΔR, ΔR_B, and bound $\mathrm{e}^{-c\delta|\vec{r}\,'-\vec{r}_2|}$ by 1. The result is

$$\begin{aligned}|I|&\le\sum_{\substack{\vec{r}\in\mathbb{Z}^2\\ \vec{r}\,'\in\mathbb{Z}\times\mathbb{N}}}|E(\vec{r},\vec{r}\,')||F_I(\vec{r}_1,\vec{r},\vec{r}\,',\vec{r}_2)|\ ,\\|F_I|&\le\frac{\|g\|_\infty}{2\pi}\Bigl(\int_0^\infty dy|\chi'(y)|\Bigr)12\sqrt{2}\pi\cdot\frac{2}{\delta}\mathrm{e}^{-c\delta|\vec{r}_1-\vec{r}|}\cdot2\ ,\end{aligned}$$

so that by (7) $|I| \le C \sum_{\vec r\in\mathbb{Z}^2} \mathrm{e}^{-\mu_0|y|}\mathrm{e}^{-c\delta|\vec r_1-\vec r|}$. We may at this point assume $\mu_0 < c\delta$ and use $|y| \ge |y_1| - |\vec r_1 - \vec r|$, so that

$$|I| \le C\mathrm{e}^{-\mu_0|y_1|} \sum_{\vec r\in\mathbb{Z}^2} \mathrm{e}^{-(c\delta-\mu_0)|\vec r_1-\vec r|} \le C\mathrm{e}^{-\mu_0|y_1|} \,. \tag{A.17}$$

Before turning to II we note that $|y|$ in (A.14, A.16) can be replaced with $\mathrm{dist}\,(x+\mathrm{i}y, \sigma(H))$. This follows by inspection of the proof, Eqs. (D.8-D.10) in [1]. By the spectral condition (1) and the assumption of (ii) we have $\mathrm{dist}\,(z, \sigma(H_B)) \ge d$ for some $d > 0$ and all $z \in \mathrm{supp}\ \partial_{\bar z}\tilde g$. Therefore,

$$II = -\frac{1}{2\pi}\int_K dxdy(\partial_{\bar z}\tilde g(z) - \mathrm{i}g(x)\chi'(y)) \sum_{\substack{\vec r\in\mathbb{Z}^2\\ \vec r\,'\in\mathbb{Z}\times\mathbb{N}}} R_B(\vec r_1, \vec r; x+\mathrm{i}y)E(\vec r, \vec r\,')R(\vec r\,', \vec r_2; x+\mathrm{i}y)$$

can be estimated as

$$\begin{aligned} |II| &\le \sum_{\substack{\vec r\in\mathbb{Z}^2\\ \vec r\,'\in\mathbb{Z}\times\mathbb{N}}} |E(\vec r, \vec r\,')||F_{II}(\vec r_1, \vec r, \vec r\,', \vec r_2)| \,,\\ |F_{II}| &\le C\int_K dxdy|y|^N \frac{2}{d}\mathrm{e}^{-cd|\vec r_1-\vec r|}\cdot\frac{2}{|y|} \le C\mathrm{e}^{-cd|\vec r_1-\vec r|} \,. \end{aligned}$$

We conclude as in (A.17).

iii) In this case $G(H_B) = 0$, and (A.7) follows from (A.6). The final remark follows e.g. from Holmgren's bound [7]: $\|A\| \le \max(\sup_{\vec r_1}\sum_{\vec r_2}|A(\vec r_1, \vec r_2)|, \sup_{\vec r_2}\sum_{\vec r_1}|A(\vec r_1, \vec r_2)|)$.□

Proof of Lemma A.4. By $\|[H,\chi]G(H)\|_1 \le \|[H,\chi]\mathrm{e}^{-\kappa y}\|_1\|\mathrm{e}^{\kappa y}G(H)\|$ and (A.7) we are left to show that $T = [H,\chi]\mathrm{e}^{-\kappa y}$ is trace class. Its kernel is

$$T(\vec r_1, \vec r_2) = H(\vec r_1, \vec r_2)(\chi(x_2) - \chi(x_1))\mathrm{e}^{-\kappa y_2} \,.$$

Since

$$|\chi(x_2) - \chi(x_1)| \le C\frac{|x_2 - x_1|(1 + |x_2 - x_1|)}{1 + x_2^2} \le C\frac{\mathrm{e}^{\mu_0|x_2-x_1|} - 1}{1 + x_2^2}$$

we have by (6)

$$\sum_{\vec s} |T(\vec r + \vec s, \vec r)| \le C\frac{\mathrm{e}^{-\kappa y}}{1 + x^2} \,,$$

which is summable w.r.t. $\vec r = (x, y) \in \mathbb{Z}\times\mathbb{N}$. The first part of (A.8) thus follows by (A.4) with $p = 1$. The same proof with H replaced by $g(H)$, except that (A.5) is used instead of (6), implies the second part of (A.8).

Eq. (A.12) implies, see [12], Eqs. (B.10, B. 14),

$$[g(H), \chi] = -\frac{1}{2\pi}\int dx\Big(\int dy\partial_{\bar z}\tilde g(z)(H - z)^{-1}[H, \chi](H - z)^{-1}\Big) \,, \tag{A.18}$$

$$g'(H) = -\frac{1}{2\pi}\int dx\Big(\int dy\partial_{\bar z}\tilde g(z)(H - z)^{-2}\Big) \,, \tag{A.19}$$

where the integrals are again meant in the strong sense. For the two sides of (A.9) we may write

$$\begin{aligned}\operatorname{tr}([g(H),\chi(x)]G(H)) &= \operatorname{tr}(E_\Delta(H)[g(H),\chi(x)]G(H)E_\Delta(H))\ ,\\ \operatorname{tr}([H,\chi(x)]g'(H)G(H)) &= \operatorname{tr}(E_\Delta(H)[H,\chi(x)]g'(H)G(H)E_\Delta(H))\ .\end{aligned}$$

We now multiply (A.19) from the left by $[H,\chi]$, and both (A.18, A.19) by $E_\Delta(H)$ from the left and by $G(H)E_\Delta(H)$ from the right. The integrals then become absolutely convergent in trace class norm. This follows from (A.13) and from

$$\begin{aligned}\|E_\Delta(H-z)^{-1}[H,\chi](H-z)^{-1}GE_\Delta\|_1 &\le \|[H,\chi]G\|_1\|(H-z)^{-1}E_\Delta\|^2\ ,\\ \|E_\Delta[H,\chi](H-z)^{-2}GE_\Delta\|_1 &\le \|[H,\chi]G\|_1\|(H-z)^{-2}E_\Delta\|\ ,\end{aligned}$$

since $\|(H-x-\mathrm{i}y)^{-p}E_\Delta\|\le C|x|^{-p}$ for large x. The traces can thus be carried inside the integral representations, where they are seen to be equal by cyclicity. □

After completion of this work we learned from A. Klein that Lemma A.3(i) appeared in [9].

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