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A Jensen inequality for partial traces and applications to partially semiclassical limits

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Abstract

We prove a matrix inequality for convex functions of a Hermitian matrix on a bipartite space. As an application, we reprove and extend some theorems about eigenvalue asymptotics of Schrödinger operators with homogeneous potentials. The case of main interest is where the Weyl expression is infinite and a partially semiclassical limit occurs.

Keyword Jensen's inequality · Partial traces · Semiclassical limits

Mathematics Subject Classification 47A63 · 15A45 · 35P20

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1 Introduction and main results

1.1 A Jensen inequality for partial traces

A simple, yet very useful inequality says that if H is a Hermitian matrix in a finite-dimensional Hilbert space $\mathcal{H}$ and f is a convex function defined on the convex hull of the spectrum of H, then for any normalized $\psi \in \mathcal{H}$

$$f\left(\langle\psi|H|\psi\rangle\right) \leq \langle\psi|f(H)|\psi\rangle\,. \tag{1}$$

This well-known result easily follows from Jensen's inequality, applied to the spectral measure of H, see, e.g., [5, Proof of Theorem 2.9] or [6, Lemma 3.2].

Our goal in this paper is to extend this inequality to the bipartite setting where $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ is the tensor product of two spaces. As usual, we denote by Tr_j, $j = 1, 2$, the partial traces. For background on these matters, we refer to [5, Section 5] and [6, Chapter 2]. The extension is motivated by a specific application that we also discuss here.

The inequality that we will prove says that for any normalized $\varphi \in \mathcal{H}_1$, and self-adjoint H on $\mathcal{H}_1 \otimes \mathcal{H}_2$

$$\mathrm{Tr}_2\, f(\langle\varphi|H|\varphi\rangle) \leq \langle\varphi|\mathrm{Tr}_2\, f(H)|\varphi\rangle\,, \tag{2}$$

where $\langle\varphi|H|\varphi\rangle$ on the left side denotes the operator $\mathrm{Tr}_1[(|\varphi\rangle\langle\varphi| \otimes \mathbb{1}_{\mathcal{H}_2})H]$ on $\mathcal{H}_2$. Clearly, when the space $\mathcal{H}_2$ is trivial, inequality (2) reduces to (1).

In fact, we will prove the following extension of (2), where $|\varphi\rangle\langle\varphi|$ is replaced by a density matrix (that is, a nonnegative operator of unit trace).

Theorem 1 *Let $\mathcal{H}_1$, $\mathcal{H}_2$ be finite-dimensional Hilbert spaces, let H be a Hermitian matrix in $\mathcal{H}_1 \otimes \mathcal{H}_2$ and let f be a convex function on the convex hull of the spectrum of H. Then for any density matrix ρ on $\mathcal{H}_1$*

$$\mathrm{Tr}_2\, f(\mathrm{Tr}_1(\rho\otimes\mathbb{1})^{\frac{1}{2}} H (\rho\otimes\mathbb{1})^{\frac{1}{2}}) \leq \mathrm{Tr}_1\, \rho^{\frac{1}{2}}\, (\mathrm{Tr}_2\, f(H))\, \rho^{\frac{1}{2}}\,.$$

Since the partial trace Tr_1 is cyclic with respect to operators that act trivially on $\mathcal{H}_2$, we can write the inequality in the theorem equivalently as

$$\mathrm{Tr}_2\, f(\mathrm{Tr}_1(\rho\otimes\mathbb{1})H) \leq \mathrm{Tr}_1\, \rho\, \mathrm{Tr}_2\, f(H)\,.$$

We will prove this theorem in Sect. 2.

1.2 Partially semiclassical limits

Our interest in inequality (2) comes from what we call a *partially semiclassical limit* and from three recent papers, discussed below, where this limit appears naturally in applications. We are concerned with the asymptotic behavior of eigenvalues of differential operators. The leading term in these asymptotics is often given by Weyl's law, but in our applications this expression for the leading term given by Weyl's law is infinite. In some situations where this happens, an asymptotic separation of variables occurs. For one group of variables, Weyl's law is applicable and these variables become 'semiclassical', while the complementary set of variables remains 'quantum', that is, there appear differential operators that act with respect to the 'quantum variables' and depend parametrically on the 'semiclassical variables'. We call this phenomenon a 'partially semiclassical limit' and give more references where this is studied later on in this introduction.

The description may seem vague at this point, but we hope it becomes clearer after stating Theorems 2 and 3. We emphasize that these theorems are known, at least under certain additional regularity assumptions, and that our goal is to provide simple proofs for them, in the spirit of works of Berezin [2] and Lieb [13], based on inequalities (1) and (2).

Both theorems concern Schrödinger operators

$$H = -\Delta + V \qquad \text{in } L^2(\mathbb{R}^d)$$

with potentials $V \geq 0$ that are homogeneous of positive degree. More specifically, we are interested in the asymptotic growth as $\lambda \to \infty$ of the number $N(\lambda, H)$ of eigenvalues $< \lambda$, counting multiplicities. The following constant appears in the limits,

$$C_{\gamma,d} := (4\pi)^{-\frac{d}{2}}\, \gamma^{-1} \frac{\Gamma(\frac{\mathrm{d}}{\gamma})}{\Gamma(\frac{\mathrm{d}}{\gamma} + \frac{d}{2} + 1)} .$$

The first theorem, which we state as a warmup, involves a standard semiclassical limit.

Theorem 2 *Let $d \in \mathbb{N}$ and $\gamma > 0$. Let $0 \leq V \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ be homogeneous of degree γ. Then,*

$$\lim_{\lambda\to\infty} \lambda^{-\frac{d(\gamma+2)}{2\gamma}} N(\lambda, H) = C_{\gamma,d} \int_{\mathbb{S}^{d-1}} V(\omega)^{-\frac{\mathrm{d}}{\gamma}}\, \mathrm{d}\omega .$$

We emphasize that this theorem is valid whether or not the integral on the right side is finite. In the next theorem, we consider a situation where it is infinite (see Remark 7), which gives rise to a partially semiclassical limit. We write $d = m + n$, $\gamma = \alpha + \beta$ and denote coordinates in $\mathbb{R}^{m+n}$ by $(x, y) \in \mathbb{R}^m \times \mathbb{R}^n$.

Theorem 3 *Let $n, m \in \mathbb{N}$ and $\alpha, \beta > 0$ with $m\alpha^{-1} > n\beta^{-1}$. Let $0 \leq V \in L^1_{\mathrm{loc}}(\mathbb{R}^{n+m})$ be separately homogeneous of degrees α and β with respect to x and y, respectively. Then,*

$$\lim_{\lambda\to\infty} \lambda^{-\frac{m(\alpha+\beta+2)}{2\alpha}} N(\lambda, H) = C_{\frac{2\alpha}{\beta+2},m} \int_{\mathbb{S}^{m-1}} \mathrm{Tr}\Big((-\Delta_{y'} + V(\omega, y'))^{-\frac{m(\beta+2)}{2\alpha}}\Big)\, \mathrm{d}\omega .$$

As before, the theorem is valid whether or not the integral on the right side is finite. Also, a similar theorem holds when $m\alpha^{-1} < n\beta^{-1}$ by switching the roles of x and y.

One can also compute the asymptotics when $m\alpha^{-1} = n\beta^{-1}$, but they do not involve a partially semiclassical limit; see the references given below.

Theorem 2 describes a semiclassical limit, since the leading term

$$C_{\gamma,d}\, \lambda^{\frac{d(\gamma+2)}{2\gamma}} \int_{\mathbb{S}^{d-1}} V(\omega)^{-\frac{d}{\gamma}}\, \mathrm{d}\omega = \iint_{\mathbb{R}^d\times\mathbb{R}^d} \mathbb{1}(|\xi|^2 + V(x) < \lambda)\, \frac{\mathrm{d}x\, \mathrm{d}\xi}{(2\pi)^d} \tag{3}$$

is given by an integral over semiclassical phase space. In contrast, Theorem 3 describes a partially semiclassical limit, since the leading term

$$\begin{aligned} &C_{\frac{2\alpha}{\beta+2},m}\lambda^{\frac{m(\alpha+\beta+2)}{2\alpha}} \int_{\mathbb{S}^{m-1}} \mathrm{Tr}\Big((-\Delta_{y'} + V(\omega, y'))^{-\frac{m(\beta+2)}{2\alpha}}\Big)\, \mathrm{d}\omega \\ &\quad = \iint_{\mathbb{R}^m\times\mathbb{R}^m} N(\lambda, |\xi|^2 - \Delta_y + V(x, y))\, \frac{\mathrm{d}x\, \mathrm{d}\xi}{(2\pi)^m} \end{aligned} \tag{4}$$

is given by an integral over part of the semiclassical phase space, namely $\mathbb{R}^m \times \mathbb{R}^m$. Associated to each given $(x, \xi) \in \mathbb{R}^m \times \mathbb{R}^m$ is an effective Schrödinger operator $|\xi|^2 - \Delta_y + V(x, y)$ in $L^2(\mathbb{R}^n)$, and the limit depends on the spectrum of these operators.

The proof of identities (3) and (4) follows by straightforward computations with beta functions, using also the explicit expression for the volume of the unit ball. Similar computations appear in the proofs of Theorems 4 and 5, and here we omit the details.

The partially semiclassical limit phenomenon has been studied since the early 1960s, and we refer to [3, Chapter 5, Section: Commentary and references to the literature] for many references. Those include, in particular, results by Solomyak and Vulis concerning a power-like degeneration of the coefficients of an operator close to the boundary of a domain; see [3, Theorem 5.19]. See also [22]. The same phenomenon in the setting of Schrödinger operators was studied by Robert [17] and by Simon [20]. The latter studied the operators $-\Delta + |x|^\alpha |y|^\beta$ in $L^2(\mathbb{R}^2)$ with $\alpha, \beta > 0$, which is a special case of Theorem 3 with $m = n = 1$. In Solomyak's paper [21], Theorems 2 and 3 appear under certain additional technical assumptions (continuity of V in both cases; $d \geq 3$ and finiteness of the integral in Theorem 3; nonvanishing of V outside the set $(\mathbb{R}^m \times \{0\}) \cup (\{0\} \times \mathbb{R}^n)$). Simon [20] and Solomyak [21] also study the case $m\alpha^{-1} = n\beta^{-1}$.

The three recent papers that motivated us are [7, 11, 16]. In [16], the author computes the asymptotic number of low-lying states in a two-dimensional confined Stark effect and finds an asymptotic separation of variables. In [7], the authors compute the asymptotic growth of eigenvalues for manifolds whose metric degenerates near the boundary. In passing, we also mention the related paper [8] where techniques from [16] and [7] are combined. In [11], two of us computed the asymptotic number of eigenvalues of Laplace operators less than λ_j on a sequence of convex bounded open sets Ω_j satisfying $\lambda_j^{\frac{d}{2}} |\Omega_j| \gg 1 \sim \lambda_j^{\frac{1}{2}} r_{\mathrm{in}}(\Omega_j)$. (Here $r_{\mathrm{in}}(\Omega_j)$ is the inradius of Ω_j.) The results obtained in the present paper allow us to reprove the asymptotics in [11] in the case of Dirichlet boundary conditions, but do not appear to yield the results obtained in [11] for Neumann boundary conditions; the approach in [11], based on Dirichlet–Neumann bracketing, gives a unified proof.

We emphasize again that in the present paper, while we remove some unnecessary assumptions from [21], we do not strive at obtaining the most general results. Rather, we aim to present an approach to partially semiclassical limits that maintains as close as possible a parallel with methods that yield semiclassical limits, and would like to present our method in the simplest possible setting. For this reason, we first present the method in the setting of Theorem 2, which only uses arguments that are already present in the semiclassical limit literature. Then, we show how a natural extension of these arguments leads, through Theorem 1, to Theorem 3.

Our proof is based on heat kernel asymptotics and coherent states. The idea of deducing asymptotics for $N(\lambda, H)$ as $\lambda \to \infty$ from asymptotics for $\operatorname{Tr} e^{-tH}$ as $t \to 0$ goes back to Carleman [4] and is based on a Tauberian theorem. (More precisely, Carleman used the closely related resolvent trace asymptotics instead of heat trace asymptotics.) We recall the Hardy–Littlewood–Karamata Tauberian theorem (see, e.g., [18, Theorem 10.3]), which says that if μ is a nonnegative measure on $[0, \infty)$ whose Laplace transform is finite on $(0, \infty)$ and if $p, C \geq 0$, then

$$\lim_{\lambda\to\infty} \lambda^{-p}\mu([0,\lambda)) = C \qquad \text{if and only if} \qquad \lim_{t\to 0} t^p \int_{[0,\infty)} e^{-t\lambda}\mathrm{d}\mu(\lambda) = \Gamma(p+1)\, C\,.$$

Denoting

$$C'_{\gamma,d} := \Gamma\left(\tfrac{\mathrm{d}}{\gamma} + \tfrac{d}{2} + 1\right) C_{\gamma,d} = (4\pi)^{-\frac{d}{2}}\, \gamma^{-1}\Gamma\left(\tfrac{\mathrm{d}}{\gamma}\right),$$

we see that Theorems 2 and 3 are equivalent to the following two theorems.

Theorem 4 *Let H be as in Theorem 2. Then,*

$$\lim_{t\to 0} t^{\frac{d(\gamma+2)}{2\gamma}} \operatorname{Tr} e^{-tH} = C'_{\gamma,d} \int_{\mathbb{S}^{d-1}} V(\omega)^{-\frac{\mathrm{d}}{\gamma}}\, \mathrm{d}\omega\,.$$

Theorem 5 *Let H be as in Theorem 3. Then,*

$$\lim_{t\to 0} t^{\frac{m(\alpha+\beta+2)}{2\alpha}} \operatorname{Tr} e^{-tH} = C'_{\frac{2\alpha}{\beta+2},m} \int_{\mathbb{S}^{m-1}} \operatorname{Tr}\Big((-\Delta_{y'} + V(\omega,y'))^{-\frac{m(\beta+2)}{2\alpha}}\Big)\, \mathrm{d}\omega\,.$$

To emphasize the (partially) semiclassical character of these asymptotics, we note that we can write

$$C'_{\gamma,d}\, t^{-\frac{d(\gamma+2)}{2\gamma}} \int_{\mathbb{S}^{d-1}} V(\omega)^{\frac{\mathrm{d}}{\gamma}}\, \mathrm{d}\omega = \iint_{\mathbb{R}^d\times\mathbb{R}^d} e^{-t(|\xi|^2+V(x))}\, \frac{\mathrm{d}x\,\mathrm{d}\xi}{(2\pi)^d}$$

and

$$\begin{aligned} &C'_{\frac{2\alpha}{\beta+2},m}\, t^{-\frac{m(\alpha+\beta+2)}{2\alpha}} \int_{\mathbb{S}^{m-1}} \operatorname{Tr}\Big((-\Delta_{y'} + V(\omega,y'))^{-\frac{m(\beta+2)}{2\alpha}}\Big)\, \mathrm{d}\omega \\ &\quad = \iint_{\mathbb{R}^m\times\mathbb{R}^m} \operatorname{Tr}_{L^2(\mathbb{R}^n)}\Big(e^{-t(|\xi|^2-\Delta_y+V(x,y))}\Big)\, \frac{\mathrm{d}x\,\mathrm{d}\xi}{(2\pi)^m}\,. \end{aligned}$$

These identities will be derived in the course of the proof of Theorems 4 and 5.

From now on, we will focus on the proofs of the latter two theorems. The advantage of working with heat traces is that the ‘difficult’ upper bound comes for free by means of the Golden–Thompson inequality. In the setting of Theorem 2, this is the standard Golden–Thompson inequality, while in that of Theorem 5 it is a partial variant of it, noted by Simon in [20].

As an aside, we mention that we could also consider the asymptotics of $\mathrm{Tr}(H-\lambda)_-^\gamma$ for some $\gamma \geq \frac{3}{2}$. On the one hand, by a Tauberian-type argument this would give the asymptotics of $N(H,\lambda)$. On the other hand, we could use the sharp Lieb–Thirring inequality (for operator-valued potentials [12] in the setting of Theorem 3) to obtain the ‘difficult’ upper bound by the limiting expression. For a recent implementation of this idea in a special case, see [1].

Thus, the only thing that needs to be proved is the lower bound in Theorems 4 and 5. As we will show, this can be accomplished rather easily using coherent states. It is for this purpose that we need (1) in the proof of Theorem 4. Our new inequality (2) plays the analogous role in the proof of Theorem 5.

This proof of the lower bound in Theorem 5 using coherent states differs from that of Simon who uses the Feynman–Kac formula. We hope that our proof retains some of the elegance of Simon’s proof of the upper bound. The use of coherent states in the context of eigenvalue asymptotics goes back at least to the celebrated papers by Berezin [2] and Lieb [13]. The usefulness of this method is further explained in [14, 19]; see also [9] for a recent application to Weyl laws for Schrödinger operators on domains under minimal assumptions on the potential.

2 Proof of Theorem 1

We work under the assumptions of Theorem 1, that is, let $\mathcal{H}_1, \mathcal{H}_2$ be finite-dimensional Hilbert spaces, let H be a Hermitian matrix in $\mathcal{H}_1 \otimes \mathcal{H}_2$ and let ρ be a density matrix on $\mathcal{H}_1$. We set

$$K := \mathrm{Tr}_1 (\rho \otimes \mathbb{1})^{\frac{1}{2}} H (\rho \otimes \mathbb{1})^{\frac{1}{2}}$$

and chose an orthonormal basis $(v_1, \ldots, v_N)$ of $\mathcal{H}_2$ consisting of eigenvectors of K. Then, for any convex function f on the convex hull of the spectrum of H,

$$\mathrm{Tr}_2\, f(K) = \sum_{n=1}^{N} \langle v_n | f(K) | v_n \rangle = \sum_{n=1}^{N} f(\langle v_n | K | v_n \rangle)\,. \tag{5}$$

Now we write

$$\rho = \sum_{m=1}^{M} \lambda_m |u_m\rangle\langle u_m|$$

with an orthonormal basis $(u_1, \ldots, u_M)$ of $\mathcal{H}_1$. Then, for any $v \in \mathcal{H}_2$, we have

$$\begin{aligned}\langle v|K|v\rangle &= \sum_{m=1}^{M} \big\langle u_m \otimes v \big| (\rho \otimes \mathbb{1})^{\frac{1}{2}} H (\rho \otimes \mathbb{1})^{\frac{1}{2}} \big| u_m \otimes v \big\rangle \\ &= \sum_{m=1}^{M} \lambda_m \, \langle u_m \otimes v \, | H | \, u_m \otimes v \rangle \, .\end{aligned}$$

We fix $n \in \{1, \ldots, N\}$ and apply this identity with $v = v_n$. Using Jensen's inequality twice, we find

$$\begin{aligned}f(\langle v_n|K|v_n\rangle) &= f\left(\sum_{m=1}^{M} \lambda_m \, \langle u_m \otimes v_n \, | H | \, u_m \otimes v_n \rangle\right) \\ &\le \sum_{m=1}^{M} \lambda_m \, f\left(\langle u_m \otimes v_n \, | H | \, u_m \otimes v_n \rangle\right) \\ &\le \sum_{m=1}^{M} \lambda_m \, \langle u_m \otimes v_n \, | f(H) | \, u_m \otimes v_n \rangle \, .\end{aligned}$$

Here, the first application of Jensen's inequality uses $\lambda_m \ge 0$ and $\sum_{m=1}^{M} \lambda_m = \operatorname{Tr}_1 \rho = 1$, while the second application is inequality (1). Summing this inequality with respect to n, interchanging the two sums and recalling (5), we obtain

$$\begin{aligned}\operatorname{Tr}_2 f(K) &\le \sum_{m=1}^{M} \lambda_m \sum_{n=1}^{N} \langle u_m \otimes v_n \, | f(H) | \, u_m \otimes v_n \rangle \\ &= \sum_{m=1}^{M} \lambda_m \langle u_m | \operatorname{Tr}_2 f(H) | u_m \rangle \\ &= \operatorname{Tr}_1 \rho^{\frac{1}{2}} \left(\operatorname{Tr}_2 f(H)\right) \rho^{\frac{1}{2}} \, .\end{aligned}$$

This completes the proof of the claimed inequality.

Remark 6 We will need an extension of Theorem 1 to the infinite-dimensional setting. We assume that the operator H and the function f are nonnegative and that the operator $\operatorname{Tr}_1 (\rho \otimes \mathbb{1})^{\frac{1}{2}} H (\rho \otimes \mathbb{1})^{\frac{1}{2}}$ has discrete spectrum. Then, the above proof goes through unchanged, except that now N and/or M are possibly infinite. Since all quantities are nonnegative under our assumptions, all manipulations are allowed even if some of the sums are infinite. There are more subtle extensions to the infinite-dimensional context, but this one is good enough for our purposes.

3 Semiclassical limit: proof of Theorem 4

In this section, we prove Theorem 4 and thereby also Theorem 2. It serves as a warmup for the next section and is included mostly for pedagogical purposes. In particular, we want to highlight the role of inequality (1) in this proof, which in the next section will be replaced by the new inequality (2).

We proceed by proving an upper and a lower bound on $\operatorname{Tr} e^{-tH}$. To do so, we argue similarly as in [19], but a different choice of coherent states will allow us to relax the assumptions on V imposed there.

The *upper bound* follows immediately from the Golden–Thompson inequality; see, e.g., [6, Theorem 4.49]. Specifically,

$$\operatorname{Tr} e^{-tH} \leq \operatorname{Tr} e^{t\Delta/2} e^{-tV} e^{t\Delta/2} = (4\pi t)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{-tV(x)}\, \mathrm{d}x\,.$$

Introducing spherical coordinates $x = r\omega$ with $r > 0$, $\omega \in \mathbb{S}^{d-1}$ and then changing variables by letting $s = tr^\gamma$, we obtain

$$\begin{aligned}\int_{\mathbb{R}^d} e^{-tV(x)}\, \mathrm{d}x &= \int_{\mathbb{S}^{d-1}} \int_0^\infty e^{-tr^\gamma V(\omega)} r^{d-1}\, \mathrm{d}r\, \mathrm{d}\omega \\ &= \gamma^{-1} t^{-\frac{d}{\gamma}} \int_{\mathbb{S}^{d-1}} \int_0^\infty e^{-sV(\omega)} s^{\frac{d}{\gamma}-1}\, \mathrm{d}s\, \mathrm{d}\omega \\ &= \gamma^{-1} t^{-\frac{d}{\gamma}}\, \Gamma\left(\frac{d}{\gamma}\right) \int_{\mathbb{S}^{d-1}} V(\omega)^{-\frac{d}{\gamma}}\, \mathrm{d}\omega\,.\end{aligned}$$

This proves the upper bound. To express it as semiclassical bound and connect it with the lower bound that follows, we note that

$$(4\pi t)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{-tV(x)}\, \mathrm{d}x = \iint_{\mathbb{R}^d\times\mathbb{R}^d} e^{-t(|\xi|^2+V(x))}\, \frac{\mathrm{d}x\, \mathrm{d}\xi}{(2\pi)^d}\,.$$

For the *lower bound*, we fix a symmetric decreasing function $g \in H^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ with $\|g\|_{L^2(\mathbb{R}^d)} = 1$ and compact support, and we set, for $(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d$,

$$\psi_{\xi,x}(x') := e^{i\xi\cdot x}\, g(x'-x)\,.$$

Then, by a well-known consequence of Plancherel's theorem,

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} |\psi_{\xi,x}\rangle\langle\psi_{\xi,x}|\, \frac{\mathrm{d}x\, \mathrm{d}\xi}{(2\pi)^d} = \mathbb{1}_{L^2(\mathbb{R}^d)}\,. \tag{6}$$

Thus,

$$\operatorname{Tr} e^{-tH} = \iint_{\mathbb{R}^d\times\mathbb{R}^d} \operatorname{Tr}\left(|\psi_{\xi,x}\rangle\langle\psi_{\xi,x}| e^{-tH}\right) \frac{\mathrm{d}x\, \mathrm{d}\xi}{(2\pi)^d}$$

and, by Jensen's inequality (1) (generalized to the infinite-dimensional setting),

$$\operatorname{Tr}\big(|\psi_{\xi,x}\rangle\langle\psi_{\xi,x}|e^{-tH}\big) \geq e^{-t\langle\psi_{\xi,x}|H|\psi_{\xi,x}\rangle}\,.$$

Standard computations with coherent states (see, e.g, [15, Chapter 12] or [9, 19]) imply that

$$\langle\psi_{\xi,x}|H|\psi_{\xi,x}\rangle = |\xi|^2 + \|\nabla g\|^2_{L^2(\mathbb{R}^d)} + g^2 * V(x)\,.$$

Thus, we have shown that

$$\begin{aligned}\operatorname{Tr} e^{-tH} &\geq e^{-t\|\nabla g\|^2_{L^2(\mathbb{R}^d)}} \iint_{\mathbb{R}^d\times\mathbb{R}^d} e^{-t(|\xi|^2+g^2*V(x))}\,\frac{\mathrm{d}x\,\mathrm{d}\xi}{(2\pi)^d}\\ &= (4\pi t)^{-\frac{d}{2}} e^{-t\|\nabla g\|^2_{L^2(\mathbb{R}^d)}} \int_{\mathbb{R}^d} e^{-t(g^2*V)(x)}\,\mathrm{d}x\,.\end{aligned}$$

Similarly as in the proof of the upper bound, we introduce spherical coordinates $x = r\omega$ and change variables $s = tr^\gamma$ to obtain

$$\begin{aligned}\int_{\mathbb{R}^d} e^{-t(g^2*V)(x)}\,\mathrm{d}x &= \int_{\mathbb{S}^{d-1}}\int_0^\infty e^{-t(g^2*V)(r\omega)} r^{d-1}\,\mathrm{d}r\,\mathrm{d}\omega\\ &= \gamma^{-1} t^{-\frac{\mathrm{d}}{\gamma}} \int_{\mathbb{S}^{d-1}}\int_0^\infty e^{-t(g^2*V)((s/t)^{\frac{1}{\gamma}}\omega)} s^{\frac{\mathrm{d}}{\gamma}-1}\,\mathrm{d}s\,\mathrm{d}\omega\,.\end{aligned}$$

It follows from Fatou's lemma that

$$\liminf_{t\to 0} t^{\frac{d}{2}+\frac{\mathrm{d}}{\gamma}} \operatorname{Tr} e^{-tH} \geq (4\pi)^{-\frac{d}{2}}\gamma^{-1} \int_{\mathbb{S}^{d-1}}\int_0^\infty \liminf_{t\to 0} e^{-t(g^2*V)((s/t)^{\frac{1}{\gamma}}\omega)} s^{\frac{\mathrm{d}}{\gamma}-1}\,\mathrm{d}s\,\mathrm{d}\omega\,. \tag{7}$$

It follows by Lebesgue's differentiation theorem that, for a.e. $\omega \in \mathbb{S}^{d-1}$,

$$\begin{aligned}\lim_{\varepsilon\to 0} \varepsilon^\gamma (g^2 * V)(\varepsilon^{-1}\omega) &= \lim_{\varepsilon\to 0}\int_{\mathbb{R}^d} \varepsilon^{-d} g^2((\omega - x')/\varepsilon)\ \varepsilon^\gamma V(x'/\varepsilon)\,\mathrm{d}x'\\ &= \lim_{\varepsilon\to 0}\int_{\mathbb{R}^d} \varepsilon^{-d} g^2((\omega - x')/\varepsilon)\ V(x')\,\mathrm{d}x'\\ &= V(\omega)\,.\end{aligned}$$

(Note that due to the fact that g is symmetric decreasing, by the layer cake formula [15] the convolution with g^2 can be written as a superposition of convolutions with characteristic functions of balls, and therefore, Lebesgue's differentiation theorem is applicable. Initially, this theorem gives convergence for a.e. $x \in \mathbb{R}^d$, but since V is homogeneous this implies convergence for a.e. ω with respect to surface measure on $\mathbb{S}^{d-1}$.) Setting $\varepsilon = (t/s)^{\frac{1}{\gamma}}$, we deduce that

$$\int_0^\infty \liminf_{t\to 0} e^{-t(g^2*V)((s/t)^{\frac{1}{\gamma}}\omega)} s^{\frac{\mathrm{d}}{\gamma}-1}\,\mathrm{d}s = \int_0^\infty e^{-sV(\omega)} s^{\frac{\mathrm{d}}{\gamma}-1}\,\mathrm{d}s = \Gamma(\tfrac{\mathrm{d}}{\gamma})\, V(\omega)^{-\frac{\mathrm{d}}{\gamma}}\,.$$

When inserted in (7), this completes the proof of the claimed lower bound.

Remark 7 We claimed that for potentials of the form considered in Theorem 3 the integral in Theorem 2 is infinite. Let us justify this. Consider $F \in L^1(\mathbb{S}^{m-1} \times \mathbb{S}^{n-1})$ such that $V(x, y) = |x|^\alpha |y|^\beta F(x/|x|, y/|y|)$. We parametrize $\omega \in \mathbb{S}^{m+n-1} \subset \mathbb{R}^m \times \mathbb{R}^n$ as $(\Omega \sin\varphi, \Theta \cos\varphi)$ with $\Omega \in \mathbb{S}^{m-1}$, $\Theta \in \mathbb{S}^{n-1}$ and $\varphi \in [0, \frac{\pi}{2}]$. For the corresponding surface measure, we have $\mathrm{d}\omega = (\sin\varphi)^{m-1}(\cos\varphi)^{n-1}\,\mathrm{d}\Omega\,\mathrm{d}\Theta\,\mathrm{d}\varphi$ and consequently

$$\int_{\mathbb{S}^{m+n-1}} V(\omega)^{-\frac{m+n}{\alpha+\beta}}\,\mathrm{d}\omega = c \iint_{\mathbb{S}^{m-1}\times\mathbb{S}^{n-1}} F(\Omega, \Theta)^{-\frac{m+n}{\alpha+\beta}}\,\mathrm{d}\Omega\,\mathrm{d}\Theta$$

with

$$c = \int_0^{\frac{\pi}{2}} (\sin\varphi)^{m-1-\frac{(m+n)\alpha}{\alpha+\beta}} (\cos\varphi)^{n-1-\frac{(m+n)\beta}{\alpha+\beta}}\,\mathrm{d}\varphi\,.$$

The claim now follows from the fact that $c = \infty$ for the range of parameters in Theorem 3. Indeed, if $\frac{m}{\alpha} \geq \frac{n}{\beta}$ (resp. $\frac{m}{\alpha} \leq \frac{n}{\beta}$), then the integral diverges at $\varphi = \frac{\pi}{2}$ (resp. $\varphi = 0$).

4 Partially semiclassical limit: proof of Theorem 5

We now turn to the main application of our new inequality (2), namely the proof of Theorem 5 (and thereby also that of Theorem 3).

As in the previous section, we proceed by proving an upper and a lower bound on $\operatorname{Tr} e^{-tH}$. The upper bound is already contained in Simon's paper [20], but we repeat the short argument to emphasize the similarity of the upper and lower bounds.

For the *upper bound*, we apply the Golden–Thompson inequality, separating $-\Delta_x$ from the rest of the operator H. This is what Simon calls the 'sliced Golden–Thompson inequality'. We obtain

$$\begin{aligned}\operatorname{Tr} e^{-tH} &\leq \iint_{\mathbb{R}^m\times\mathbb{R}^m} \operatorname{Tr}_{L^2(\mathbb{R}^n)}\big(e^{-t(|\xi|^2-\Delta_y+V(x,y))}\big)\,\frac{\mathrm{d}x\,\mathrm{d}\xi}{(2\pi)^m} \\ &= (4\pi t)^{-\frac{m}{2}} \int_{\mathbb{R}^m} \operatorname{Tr}_{L^2(\mathbb{R}^n)}\big(e^{-t(-\Delta_y+V(x,y))}\big)\,\mathrm{d}x\,.\end{aligned}$$

Introducing spherical coordinates $x = r\omega$ with $r > 0$, $\omega \in \mathbb{S}^{m-1}$, we obtain

$$\int_{\mathbb{R}^m} \operatorname{Tr}_{L^2(\mathbb{R}^n)}\big(e^{-t(-\Delta_y+V(x,y))}\big)\,\mathrm{d}x = \int_{\mathbb{S}^{m-1}}\int_0^\infty \operatorname{Tr}_{L^2(\mathbb{R}^n)}\big(e^{-t(-\Delta_y+r^\alpha V(\omega,y))}\big) r^{m-1}\,\mathrm{d}r\,\mathrm{d}\omega\,.$$

Changing variables $y = g^{-\frac{1}{\beta+2}}y'$, we see that $-\Delta_y + r^\alpha V(\omega, y)$ is unitarily equivalent to $g^{\frac{2}{\beta+2}}(-\Delta_{y'} + r^\alpha g^{-1} V(\omega, y'))$ in $L^2(\mathbb{R}^n)$. We apply this observation with $g = r^\alpha$ and find

$$\operatorname{Tr}_{L^2(\mathbb{R}^n)}\big(e^{-t(-\Delta_y+r^\alpha V(\omega,y))}\big) = \operatorname{Tr}_{L^2(\mathbb{R}^n)}\Big(e^{-tr^{\frac{2\alpha}{\beta+2}}K_\omega}\Big)$$

with the operator $K_\omega := -\Delta_{y'} + V(\omega, y')$ in $L^2(\mathbb{R}^n)$. Changing variables $s = tr^{\frac{2\alpha}{\beta+2}}$, we obtain

$$\begin{aligned}
\int_0^\infty \operatorname{Tr}_{L^2(\mathbb{R}^n)}\big(e^{-t(-\Delta_y + r^\alpha V(\omega,y))}\big) r^{m-1}\,\mathrm{d}r &= \int_0^\infty \operatorname{Tr}_{L^2(\mathbb{R}^n)}\Big(e^{-tr^{\frac{2\alpha}{\beta+2}} K_\omega}\Big) r^{m-1}\,\mathrm{d}r \\
&= \frac{\beta+2}{2\alpha} t^{-\frac{m(\beta+2)}{2\alpha}} \int_0^\infty \operatorname{Tr}_{L^2(\mathbb{R}^n)}\big(e^{-sK_\omega}\big) s^{\frac{m(\beta+2)}{2\alpha}-1}\,\mathrm{d}s \\
&= \frac{\beta+2}{2\alpha} t^{-\frac{m(\beta+2)}{2\alpha}} \Gamma\big(\tfrac{m(\beta+2)}{2\alpha}\big) \operatorname{Tr}_{L^2(\mathbb{R}^n)}\Big(K_\omega^{-\frac{m(\beta+2)}{2\alpha}}\Big).
\end{aligned}$$

To summarize, we have shown that

$$\operatorname{Tr} e^{-tH} \leq C'_{\frac{2\alpha}{\beta+2},m}\, t^{-\frac{m(\alpha+\beta+2)}{2\alpha}} \int_{\mathbb{S}^{m-1}} \operatorname{Tr}_{L^2(\mathbb{R}^n)}\Big(K_\omega^{-\frac{m(\beta+2)}{2\alpha}}\Big)\,\mathrm{d}\omega\,,$$

which is the claimed upper bound.

We now turn to the proof of the *lower bound*. We fix a symmetric decreasing function $g \in H^1(\mathbb{R}^m)$ with $\|g\|_{L^2(\mathbb{R}^m)} = 1$ and set, for $(x, \xi) \in \mathbb{R}^m \times \mathbb{R}^m$,

$$\psi_{\xi,x}(x') = e^{i\xi\cdot x}\, g(x'-x)\,.$$

Then, by (6) with d replaced by m, we find

$$\operatorname{Tr} e^{-tH} = \iint_{\mathbb{R}^m\times\mathbb{R}^m} \operatorname{Tr}_{L^2(\mathbb{R}^m)}\Big(|\psi_{\xi,x}\rangle\langle\psi_{\xi,x}|\operatorname{Tr}_{L^2(\mathbb{R}^n)} e^{-tH}\Big)\frac{\mathrm{d}x\,\mathrm{d}\xi}{(2\pi)^m}\,.$$

We now apply Theorem 1 with $\varphi(E) = e^{-tE}$ and $\rho = |\psi_{\xi,x}\rangle\langle\psi_{\xi,x}|$ (see also Remark 6) and obtain

$$\operatorname{Tr}_{L^2(\mathbb{R}^m)}\big(|\psi_{\xi,x}\rangle\langle\psi_{\xi,x}|\operatorname{Tr}_{L^2(\mathbb{R}^n)} e^{-tH}\big) \geq \operatorname{Tr}_{L^2(\mathbb{R}^n)} e^{-t\langle\psi_{\xi,x}|H|\psi_{\xi,x}\rangle}\,.$$

Note that $\langle\psi_{\xi,x}|H|\psi_{\xi,x}\rangle$ is an operator in $L^2(\mathbb{R}^n)$. Using standard computations with coherent states, we find

$$\langle\psi_{\xi,x}|H|\psi_{\xi,x}\rangle = -\Delta_y + |\xi|^2 + \|\nabla g\|^2_{L^2(\mathbb{R}^m)} + \widetilde{V}(x,y)\,,$$

where

$$\widetilde{V}(x,y) := \int_{\mathbb{R}^m} g(x-x')^2 V(x',y)\,\mathrm{d}x'\,.$$

Thus, we have shown that

$$\begin{aligned}
\operatorname{Tr} e^{-tH} &\geq \iint_{\mathbb{R}^m\times\mathbb{R}^m} \operatorname{Tr}_{L^2(\mathbb{R}^n)}\big(e^{-t(-\Delta_y+|\xi|^2+\|\nabla g\|^2_{L^2(\mathbb{R}^m)}+\widetilde{V}(x,y))}\big)\frac{\mathrm{d}x\,\mathrm{d}\xi}{(2\pi)^m} \\
&= (4\pi t)^{-\frac{m}{2}} e^{-t\|\nabla g\|^2_{L^2(\mathbb{R}^m)}} \int_{\mathbb{R}^m} \operatorname{Tr}_{L^2(\mathbb{R}^n)}\big(e^{-t(-\Delta_y+\widetilde{V}(x,y))}\big)\,\mathrm{d}x\,.
\end{aligned}$$

We now proceed similarly as in the upper bound. We introduce spherical coordinates $x = r\omega$, change variables by letting $y = r^{-\frac{\alpha}{\beta+2}} y'$ and $s = tr^{\frac{2\alpha}{\beta+2}}$. This gives

$$\begin{aligned}
&\int_{\mathbb{R}^m} \mathrm{Tr}_{L^2(\mathbb{R}^n)}\, e^{-t(-\Delta_y+\widetilde{V}(x,y))}\,\mathrm{d}x \\
&\quad = \int_{\mathbb{S}^{m-1}} \int_0^\infty \mathrm{Tr}_{L^2(\mathbb{R}^n)} \Big(e^{-t(-\Delta_y+\widetilde{V}(r\omega,y))}\Big) r^{m-1}\,\mathrm{d}r\,\mathrm{d}\omega \\
&\quad = \int_{\mathbb{S}^{m-1}} \int_0^\infty \mathrm{Tr}_{L^2(\mathbb{R}^n)} \Big(e^{-tr^{\frac{2\alpha}{\beta+2}}(-\Delta_{y'}+r^{-\alpha}\widetilde{V}(r\omega,y'))}\Big) r^{m-1}\,\mathrm{d}r\,\mathrm{d}\omega \\
&\quad = \frac{\beta+2}{2\alpha}\, t^{-\frac{m(\beta+2)}{2\alpha}} \int_{\mathbb{S}^{m-1}} \int_0^\infty \mathrm{Tr}_{L^2(\mathbb{R}^n)} \Big(e^{-sK_\omega^{(\varepsilon_{s,t})}}\Big) s^{\frac{m(\beta+2)}{2\alpha}-1}\,\mathrm{d}s\,\mathrm{d}\omega\,,
\end{aligned}$$

where $\varepsilon_{s,t} := (t/s)^{\frac{\beta+2}{2\alpha}}$ and

$$K_\omega^{(\varepsilon)} := -\Delta_{y'} + \varepsilon^\alpha\, \widetilde{V}(\varepsilon^{-1}\omega, y') \qquad \text{in } L^2(\mathbb{R}^n)\,.$$

We shall show below that for a.e. $\omega \in \mathbb{S}^{m-1}$ and every $s > 0$

$$\liminf_{\varepsilon\to 0} \mathrm{Tr}_{L^2(\mathbb{R}^n)}\, e^{-sK_\omega^{(\varepsilon)}} \geq \mathrm{Tr}\, e^{-sK_\omega} \tag{8}$$

with the same operator K_ω as in the upper bound. Therefore, by Fatou's lemma,

$$\begin{aligned}
\liminf_{t\to 0} t^{\frac{m(\alpha+\beta+2)}{2\alpha}}\, \mathrm{Tr}\, e^{-tH} &\geq \frac{\beta+2}{2\alpha(4\pi)^{\frac{m}{2}}} \int_{\mathbb{S}^{m-1}} \int_0^\infty \liminf_{t\to 0} \mathrm{Tr}_{L^2(\mathbb{R}^n)} \Big(e^{-sK_\omega^{(\varepsilon_{s,t})}}\Big) s^{\frac{m(\beta+2)}{2\alpha}-1}\, ds\,\mathrm{d}\omega \\
&\geq \frac{\beta+2}{2\alpha(4\pi)^{\frac{m}{2}}} \int_{\mathbb{S}^{m-1}} \int_0^\infty \mathrm{Tr}_{L^2(\mathbb{R}^n)} (e^{-sK_\omega}) s^{\frac{m(\beta+2)}{2\alpha}-1}\,\mathrm{d}s\,\mathrm{d}\omega \\
&= C'_{\frac{2\alpha}{\beta+2},m} \int_{\mathbb{S}^{m-1}} \mathrm{Tr}_{L^2(\mathbb{R}^n)} \Big(K_\omega^{-\frac{m(\beta+2)}{2\alpha}}\Big)\,\mathrm{d}\omega\,.
\end{aligned}$$

This is the claimed lower bound.

It remains to prove (8). To this end, we use the following lemma.

Lemma 8 *Let A_j, $j \in \mathbb{N}$, and A be self-adjoint, lower-bounded operators in a Hilbert space with a common form core $\mathcal{Q}$ and assume that for all $\psi \in \mathcal{Q}$ we have $\limsup_{j\to\infty} \langle\psi|A_j|\psi\rangle \leq \langle\psi|A|\psi\rangle$. Then,*

$$\liminf_{j\to\infty} \mathrm{Tr}\, e^{-A_j} \geq \mathrm{Tr}\, e^{-A}\,.$$

The following proof of the lemma relies on the Gibbs variational principle (see, e.g., [5, Theorem 2.13] or [6, Theorem 7.45]), which says that for any self-adjoint, lower semibounded operator H

$$\inf_{\rho \text{ density matrix}} \Big(\mathrm{Tr}\, \rho^{\frac{1}{2}} H \rho^{\frac{1}{2}} + \mathrm{Tr}\, \rho \ln \rho\Big) = -\ln \mathrm{Tr}\, e^{-H}\,,$$

where the infimum is taken over all density matrices with $\operatorname{Tr}\rho\ln\rho > -\infty$. Note that $\operatorname{Tr}\rho^{\frac{1}{2}}H\rho^{\frac{1}{2}}$ is well defined, but possibly $+\infty$.

Proof Let ρ be a finite rank density matrix with range in $\mathcal{Q}$. Then, by assumption,

$$\operatorname{Tr}\rho^{\frac{1}{2}}A\rho^{\frac{1}{2}} + \operatorname{Tr}\rho\ln\rho \geq \limsup_{j\to\infty}\left(\operatorname{Tr}\rho^{\frac{1}{2}}A_j\rho^{\frac{1}{2}} + \operatorname{Tr}\rho\ln\rho\right).$$

Bounding the right side from below by the Gibbs variational principle, we find

$$\operatorname{Tr}\rho^{\frac{1}{2}}A\rho^{\frac{1}{2}} + \operatorname{Tr}\rho\ln\rho \geq -\liminf_{j\to\infty}\ln\operatorname{Tr}e^{-A_j}.$$

By density this lower bound extends to any density matrix ρ with $\operatorname{Tr}\rho\ln\rho > -\infty$. Taking the infimum over all such ρ and employing again the Gibbs variational principle, we arrive at

$$-\ln\operatorname{Tr}e^{-A} \geq -\liminf_{j\to\infty}\ln\operatorname{Tr}e^{-A_j},$$

which is the claimed inequality. □

Let us provide an alternative proof of Lemma 8, which was suggested to us by the referee. It relies on the fact that

$$\operatorname{Tr}e^{-H} = \sup\left\{\sum_n e^{-\langle\psi_n|H|\psi_n\rangle} : (\psi_n) \text{ finite orthonormal system}\right\}. \tag{9}$$

Indeed, $\leq$ is clear by taking (ψ_n) consisting of eigenfunctions of H and $\geq$ follows by applying (1) with $f(E) = e^{-E}$ to $\psi = \psi_n$ and summing over n.

With (9) at hand, we notice that for all finite orthonormal systems (ψ_n), we have

$$\liminf_{j\to\infty}\operatorname{Tr}e^{-A_j} \geq \liminf_{j\to\infty}\sum_n e^{-\langle\psi_n|A_j|\psi_n\rangle} \geq \sum_n e^{-\langle\psi_n|A|\psi_n\rangle}.$$

Taking the supremum over (ψ_n) on the right side and using (9), we arrive again at the conclusion of Lemma 8.

We return to the proof of (8). By Fubini's theorem and homogeneity of V, there is a full measure subset of $\mathbb{S}^{m-1}$ such that for any ω from this set and any $\varepsilon > 0$ the function $y' \mapsto \varepsilon^\alpha\widetilde{V}(\varepsilon^{-1}\omega, y')$ is locally integrable on $\mathbb{R}^n$. Since it is also nonnegative, it follows that $C_c^\infty(\mathbb{R}^n)$ is a form core for $K_\omega^{(\varepsilon)}$; see, e.g., [10, Proposition 4.1]. We claim that for $\psi \in C_c^\infty(\mathbb{R}^n)$ we have

$$\lim_{\varepsilon\to 0}\langle\psi|\varepsilon^\alpha\widetilde{V}(\varepsilon^{-1}\omega,\cdot)|\psi\rangle = \langle\psi|V(\omega,\cdot)|\psi\rangle. \tag{10}$$

Once we have shown (10), we can apply Lemma 8 with $A_j = sK_\omega^{(\varepsilon_j)}$ and obtain (8).

To prove (10), we set $W(x) := \int_{\mathbb{R}^n} V(x, y)|\psi(y)|^2\, dy$ and note that (10) is equivalent to

$$\lim_{\varepsilon\to 0} \varepsilon^{\alpha}(g^2 * W)(\varepsilon^{-1}\omega) = W(\omega)\,.$$

This holds for a.e. $\omega \in \mathbb{S}^{m-1}$ as shown in the proof of the lower bound in Theorem 4. This concludes the proof.

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