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Unity-resolving states and generalised Golden–Thompson bounds on partition functions

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Abstract. It is shown that certain sets of normalised unity-resolving (e.g. coherent) states in Hilbert space serve to generate upper bounds on the partition function of a given Hamiltonian in that space. These bounds may be viewed as generalisations of bounds derived previously by Golden, Thompson, Hepp and Lieb. The new bounds are compared to the original Golden–Thompson bound by proving several theorems and by computing explicit examples.

1. Introduction

Due to the complexity of quantum statistical problems one is in most cases forced to find some approximations to the relevant physical quantities. A standard non-perturbative tool of increasing popularity is the use of rigorous bounds or estimates for these quantities. The value of such bounds is at least two-fold. On the one hand, they often allow one to prove general (convexity) properties of thermodynamic potentials and rigorous (non-)existence theorems (cf for example Griffiths 1972), and on the other hand, they often provide calculable variational-type approximations, reflecting the main physical properties of the model under consideration. Perhaps the most prominent example of this kind is given by the mean field approximation which is based on the Rayleigh–Ritz–Peierls–Bogolyubov upper bound for the free energy (cf for example Huber 1969, 1970).

While it is true that upper bounds for the free energy are frequently encountered, the situation is different for lower bounds. Among the few examples for lower bounds we refer to the inequality

$$\operatorname{Tr} \mathrm{e}^{-\beta(A+B)} \leqslant \operatorname{Tr}(\mathrm{e}^{-\beta A}\, \mathrm{e}^{-\beta B}) \tag{1.1}$$

for the partition function $\operatorname{Tr} \mathrm{e}^{-\beta H}$ of a Hamiltonian of the form $H = A + B$. This inequality has been first derived by Golden (1965) and Thompson (1965) (cf also Breitenecker and Grümm 1972, Ruskai 1972, Lieb 1973a, Reed and Simon 1978).

The aim of the present paper is to present a generalisation of the right-hand side of (1.1) which is based on a 'pseudo-diagonal representation' of the operator B with respect to a general set of normalised 'unity-resolving' states in Hilbert space. If these states are chosen to be the eigenstates of B, the pseudo-diagonal representation of B coincides with its spectral resolution and the bound given in (1.1) is recovered. If in the

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case of the Hilbert space $L^2(\mathbb{R})$ boson coherent states are chosen, the corresponding pseudo-diagonal representation of B is analogous to the P representation (Cahill and Glauber 1969) of statistical operators often used in quantum optics. The corresponding upper bound on the partition function generalises a bound derived by Lieb (1973b) and Hepp and Lieb (1973) and used by them to discuss the classical limit of quantum spin systems and the equilibrium statistical mechanics of matter interacting with radiation, with particular emphasis on the Dicke maser.

Other problems where similar (upper and/or lower) bounds have been recently applied include the Peierls transition in (quasi-)one-dimensional electron–phonon systems (Brandt and Leschke 1974, Siegl 1979) and the density of states in disordered electronic systems (Luttinger 1976, Gross 1977).

The main advantages of the present generalised Golden–Thompson bound with respect to the original Golden–Thompson bound are:

(i) its flexibility due to the possibility of choosing different sets of unity-resolving states,

(ii) the fact that it is often easier to compute,

(iii) the fact that it is in some cases closer to the exact partition function.

The plan of this paper is as follows. In § 2 the notions of a set of unity-resolving states and of the corresponding pseudo-diagonal representation of a given operator are introduced and illustrated by way of examples. Section 3 is devoted to the proof of the generalised Golden–Thompson inequality which is our main result. Special cases of this inequality are discussed in § 4. In § 5 the generalised and the original Golden–Thompson bounds are systematically compared to each other. We show that the Golden–Thompson bound is better than the generalised Golden–Thompson bound in several limiting cases. That the converse relation may also hold is demonstrated by deriving a special criterion and by computing explicit examples.

2. Unity-resolving states and pseudo-diagonal representations of operators

The starting point of our considerations is a set $\{|i\rangle\}$ of normalised but not necessarily orthogonal states $|i\rangle$ in a separable Hilbert space $\mathscr{H}$ of finite or infinite dimension. We assume that these states provide a resolution of unity in the sense that

$$\sum_i w_i|i\rangle\langle i| = 1 \tag{2.1}$$

with certain non-negative weights w_i. If i represents a continuous label, the sum is to be understood as an appropriate integral (Klauder 1963). If the cardinal number of the set of non-vanishing weights w_i in (2.1) exceeds the dimension of $\mathscr{H}$ $(=\Sigma_i w_i)$, the set $\{|i\rangle\}$ is overcomplete.

We are interested in cases where a linear (self-adjoint) operator B acting in $\mathscr{H}$ is represented as

$$B = \sum_i w_i b_i|i\rangle\langle i| \tag{2.2}$$

with some (real) c-numbers b_i. We shall refer to this representation as the pseudo-diagonal representation of B with respect to the set $\{|i\rangle\}$. For given $\{|i\rangle\}$ and $\{w_i\}$ fulfilling (2.1) this representation may not exist even for 'simple' operators; if it exists, it need not be unique and there seems to be no general procedure to obtain a set $\{b_i\}$.

For illustrative purposes and for later use we offer the following examples.

(i) *Complete orthonormal sets.* Any complete orthonormal set $\{|i\rangle\}$ in $\mathscr{H}$ fulfils (2.1) with $w_i = 1$ for all i. The representation (2.2) exists if and only if B commutes with all projections $|i\rangle\langle i|$. Clearly, in that case (2.2) coincides with the spectral or diagonal resolution of B, the b_i being the uniquely determined (though often not known) eigenvalues.

Other sets, for which the b_i may be explicitly calculated for many operators, are given by non-orthogonal and overcomplete states, the most prominent being the

(ii) *Sets of coherent states.* According to Klauder (1963) and Perelomov (1977), with any Lie group of unitary transformations and any fixed normalised reference state in Hilbert space there is associated a set of continuously labelled states which are nowadays usually called coherent. We briefly describe two examples, namely the boson coherent states and the spin coherent states associated with the translation group and the rotation group, respectively, where we restrict ourselves to a single degree of freedom for the sake of notational transparency†.

As to the boson coherent states, the underlying Lie algebra may be characterised by the unit operator 1, an annihilation operator a and its adjoint creation operator a^+ acting in the Hilbert space $\mathscr{H} = L^2(\mathbb{R})$ of square integrable complex-valued functions of a real variable and fulfilling the canonical commutation relation:

$$aa^+ - a^+a = 1. \tag{2.3}$$

With any c-number α there is associated a boson coherent state

$$|\alpha\rangle := \exp(\alpha a^+ - \alpha^* a)|0\rangle \tag{2.4}$$

generated from the normalised ground state $|0\rangle$ of a^+a. These states enjoy the properties

$$\langle\alpha|\alpha'\rangle = \exp\left(\alpha^*\alpha' - \frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2}\right) \tag{2.5}$$

$$\int \frac{\mathrm{d}^2\alpha}{\pi} |\alpha\rangle\langle\alpha| = 1 \tag{2.6}$$

$$a|\alpha\rangle = \alpha|\alpha\rangle \tag{2.7}$$

where $\int \mathrm{d}^2\alpha$ means $\int_{-\infty}^{\infty} \mathrm{d}\,\mathrm{Re}\,\alpha \int_{-\infty}^{\infty} \mathrm{d}\,\mathrm{Im}\,\alpha$.

If one substitutes for $|0\rangle$ in (2.4) an arbitrary normalised state $|\psi\rangle$, the normalisation $\langle\alpha|\alpha\rangle = 1$ and the resolution of unity (2.6) remain valid (Klauder 1963).

The pseudo-diagonal coherent state representation of a given operator $B = B(a, a^+)$ is

$$B = \int \frac{\mathrm{d}^2\alpha}{\pi} b(\alpha)|\alpha\rangle\langle\alpha|. \tag{2.8}$$

The (generalised) function $b(\alpha)$ may be obtained by substituting α for a and α^* for a^+ in the antinormal-ordered form of B, the latter resulting (if it exists as a convergent operator power series) by bringing with the help of (2.3) all a to the left of all a^+. For further details, especially for questions of convergence, see Cahill and Glauber (1969).

† For more general coherent states, their properties, some of their applications, and relevant earlier references the reader is again referred to Perelomov (1977).

Important operators B for which $b(\alpha)$ is explicitly known include all polynomials and the exponential of a general quadratic form in a and a^+ (Wilcox 1967, Mehta 1977).

The underlying Lie algebra for the spin coherent states consists of the unit operator and the three components S_x, S_y, S_z of a spin operator $\boldsymbol{S}$ ($\boldsymbol{S}^2 = J(J+1)$, J fixed) acting in the $(2J+1)$-dimensional Hilbert space $\mathscr{H} = \mathbb{C}^{2J+1}$ and obeying angular momentum commutation relations ($\hbar = 1$)

$$S_xS_y - S_yS_x = \mathrm{i}S_z \qquad \text{and cyclically.} \tag{2.9}$$

With any pair $\Omega := (\theta, \phi)$ of real numbers θ and ϕ $(0 \leq \theta \leq \pi, 0 \leq \phi < 2\pi)$ there is associated a spin coherent state:

$$|\Omega\rangle := \exp\left(\frac{\theta}{2}(\mathrm{e}^{\mathrm{i}\phi}S_- - \mathrm{e}^{-\mathrm{i}\phi}S_+)\right)|J\rangle \tag{2.10}$$

generated from the normalised ground state $|J\rangle$ of $-S_z$, where as usual

$$S_\pm := S_x \pm \mathrm{i}S_y. \tag{2.11}$$

The properties analogous to (2.5) and (2.6) are

$$\langle\Omega|\Omega'\rangle = \left(\cos\frac{\theta}{2}\cos\frac{\theta'}{2} + \mathrm{e}^{\mathrm{i}(\phi'-\phi)}\sin\frac{\theta}{2}\sin\frac{\theta'}{2}\right)^{2J} \tag{2.12}$$

$$\frac{2J+1}{4\pi}\int \mathrm{d}\Omega\, |\Omega\rangle\langle\Omega| = 1 \tag{2.13}$$

where $\int \mathrm{d}\Omega$ means $\int_0^\pi \mathrm{d}\theta \sin\theta \int_0^{2\pi} \mathrm{d}\phi$.

Every operator $B = B(\boldsymbol{S})$ has a pseudo-diagonal coherent state representation:

$$B = \frac{2J+1}{4\pi}\int \mathrm{d}\Omega\, b(\Omega)|\Omega\rangle\langle\Omega| \tag{2.14}$$

where the function $b(\Omega)$ may always be chosen to be infinitely differentiable (Lieb 1973b). This choice, however, does not ensure uniqueness as the following example for $J = \frac{1}{2}$ demonstrates:

$$S_\pm = \int \frac{\mathrm{d}\Omega}{2\pi}\frac{3}{2}\sin\theta\, \mathrm{e}^{\pm\mathrm{i}\phi}|\Omega\rangle\langle\Omega| = \int \frac{\mathrm{d}\Omega}{2\pi}\frac{4}{\pi}\mathrm{e}^{\pm\mathrm{i}\phi}|\Omega\rangle\langle\Omega|. \tag{2.15}$$

Since there is no property analogous to (2.7) there is no construction recipe for $b(\Omega)$ based on (re)ordering; useful formulae are, however, given by Lieb (1973b).

3. Generalised Golden–Thompson bound

In this section we are going to derive for self-adjoint operators A and B bounded from below the following generalisation of the Golden–Thompson inequality (1.1):

$$\mathrm{Tr}\,\mathrm{e}^{-\beta(A+B)} \leq \mathrm{Tr}(\mathrm{e}^{-\beta A}P_B) =: Z_{\mathrm{GGT}} \tag{3.1}$$

where the operator P_B is defined by

$$P_B := \sum_i w_i\, \mathrm{e}^{-\beta b_i}|i\rangle\langle i|. \tag{3.2}$$

The sets $\{|i\rangle\}$, $\{w_i\}$, $\{b_i\}$ are assumed to fulfil (2.1) and (2.2), and $\beta > 0$ has the physical meaning of an inverse temperature.

To prove (3.1) we start from the Lie–Trotter-type formula

$$e^{-\beta(A+B)} = \lim_{n\to\infty} \left(e^{-(\beta/n)A} \sum_i w_i\, e^{-(\beta/n)b_i} |i\rangle\langle i|\right)^n \tag{3.3}$$

being valid because $\Sigma_i w_i\, e^{-(\beta/n)b_i}|i\rangle\langle i|$ equals $e^{-(\beta/n)B}$ up to first order in $1/n$. The trace of (3.3) yields (with $i_0 := i_n$)

$$\mathrm{Tr}\, e^{-\beta(A+B)} = \lim_{n\to\infty} \sum_{i_1} \ldots \sum_{i_n} \prod_{j=1}^{n} K_{\beta/n}(i_j, i_{j-1}). \tag{3.4}$$

Interpreting the 'transfer matrix'

$$K_\tau(i, i') := \langle i|e^{-\tau A}|i'\rangle (w_i w_{i'})^{1/2}\, e^{-\tau b_{i'}} \tag{3.5}$$

as the matrix representation of an operator K_τ in the Hilbert space† $\mathscr{L}$ of square summable c-number sequences $\{z_i\}_{i=1}^{\infty}$ we can rewrite (3.4):

$$\mathrm{Tr}\, e^{-\beta(A+B)} = \lim_{n\to\infty} \mathrm{Tr}_{\mathscr{L}} K^n_{\beta/n} \tag{3.6}$$

where $\mathrm{Tr}_{\mathscr{L}}$ means the trace in $\mathscr{L}$, in contrast to $\mathrm{Tr} \equiv \mathrm{Tr}_{\mathscr{H}}$. The inequality (3.1) is thus equivalent to the inequality

$$\lim_{n\to\infty} \mathrm{Tr}_{\mathscr{L}} K^n_{\beta/n} \leqslant \mathrm{Tr}_{\mathscr{L}} K_\beta. \tag{3.7}$$

In order to prove (3.7) we start from the factorisation

$$K_\tau = L_\tau M_\tau \tag{3.8}$$

where the self-adjoint operators L_τ and M_τ are defined by the matrices

$$\begin{aligned} L_\tau(i, i') &:= \langle i|\, e^{-\tau A}|i'\rangle (w_i w_{i'})^{1/2} \\ M_\tau(i, i') &:= \delta_{ii'}\, e^{-\tau b_i} \end{aligned} \tag{3.9}$$

and enjoy the (semi-)group properties

$$L_\tau L_{\tau'} = L_{\tau+\tau'} \qquad M_\tau M_{\tau'} = M_{\tau+\tau'}. \tag{3.10}$$

We note that it is sufficient to prove (3.7) for the subsequence $n = 2^m$ ($m \in \mathbb{N}$) and recall the following 'iterated Schwarz-type inequality' also due to Golden (1965) and Thompson (1965):

$$|\mathrm{Tr}_{\mathscr{L}}(PQ)^n| \leqslant \mathrm{Tr}_{\mathscr{L}} P^n Q^n \qquad \text{for } n = 2^m (m \in \mathbb{N}) \tag{3.11}$$

valid for any two self-adjoint operators P and Q acting in $\mathscr{L}$. Putting together (3.8), (3.10) and (3.11) we obtain for $n = 2^m$:

$$|\mathrm{Tr}_{\mathscr{L}} K^n_{\beta/n}| \leqslant \mathrm{Tr}_{\mathscr{L}}(L^n_{\beta/n} M^n_{\beta/n}) = \mathrm{Tr}_{\mathscr{L}}(L_\beta M_\beta) = \mathrm{Tr}_{\mathscr{L}} K_\beta \tag{3.12}$$

which completes the proof of (3.7) and hence of (3.1).

† If i is a continuous label, $K_\tau(i, i')$ is actually a transfer kernel and the summations are integrations. In that case the space $\mathscr{L}$ in which K_τ acts is the space $L^2(\{i\})$ of square integrable functions defined on the label set $\{i\}$, e.g. the two-dimensional real plane for boson coherent states or the surface of the three-dimensional unit sphere for spin coherent states.

4. Special cases

Choosing appropriate unity-resolving states and/or operators we may obtain from (3.1) several more or less well-known inequalities, some of which we are going to list in the following.

(i) If the states $|i\rangle$ in (3.1) are assumed to be orthogonal (which implies that they are eigenstates of B) the original Golden–Thompson inequality is reproduced.

(ii) If the states $|i\rangle$ are chosen to be the boson coherent states (2.4), the inequality (3.1) reads

$$\operatorname{Tr} e^{-\beta(A+B)} \leqslant \int \frac{d^2\alpha}{\pi} \langle\alpha| e^{-\beta A} |\alpha\rangle e^{-\beta b(\alpha)} \tag{4.1}$$

with the 'antinormal symbol' $b(\alpha)$ of B defined by (2.8). This inequality has been reported earlier by one of us (Leschke 1979).

(iii) For $A = 0$ the inequality (3.1) reduces to

$$\operatorname{Tr} e^{-\beta B} \leqslant \sum_i w_i e^{-\beta b_i} \tag{4.2}$$

which for $i = \Omega$ and $i = \alpha$ was derived by Lieb (1973b) and Hepp and Lieb (1973), respectively. In fact, their method of proof provided the basis of our proof of the generalised Golden–Thompson inequality. It is, however, interesting to note that (4.2) may be proved more simply as we now proceed to demonstrate.

Denoting by $\{|n\rangle\}$ a complete set of orthonormal eigenstates of B and using (2.2) we have

$$\operatorname{Tr} e^{-\beta B} = \sum_n \exp(-\beta\langle n|B|n\rangle) = \sum_n \exp\Big(-\beta \sum_i b_i w_i |\langle n|i\rangle|^2\Big). \tag{4.3}$$

Since $w_i|\langle n|i\rangle|^2$ defines for fixed n a probability measure μ on the label set $\{i\}$, we can employ Jensen's inequality (Hardy *et al* 1967)

$$e^{\langle\zeta\rangle} \leqslant \langle e^{\zeta}\rangle \tag{4.4}$$

where $\langle\ \rangle$ denotes the mean value with respect to μ and ζ is any real random variable on $\{i\}$. The result is

$$\operatorname{Tr} e^{-\beta B} \leqslant \sum_i w_i e^{-\beta b_i} \sum_n |\langle n|i\rangle|^2 \tag{4.5}$$

which is (4.2) in view of

$$\sum_n |\langle n|i\rangle|^2 = \langle i|i\rangle = 1. \tag{4.6}$$

5. Comparison

The purpose of this section is to compare the generalised Golden–Thompson bound Z_{GGT} given in (3.1) to the original Golden–Thompson bound Z_{GT} given in (1.1) in order to see which one is closer to the true partition function Z of the 'total Hamiltonian' $A+B$.

We list the following statements. The GT bound is better than or equivalent to the GGT bound (i.e. $Z_{GT} \leq Z_{GGT}$):

(i) if A and B commute,

(ii) if P_B and B commute (being true, e.g. in the case of boson coherent states, if B is a function only of $a + a^+$ or $a - a^+$ or $(a^+ - \delta^*)(a - \delta)$ for any c-number δ),

(iii) if the temperature $1/\beta$ is sufficiently high and the b_i are bounded (implying that B is bounded)†,

(iv) if in the case of boson coherent states B is a polynomial of a and a^+, $\mathrm{Tr}\, \mathrm{e}^{-\beta_c A}$ exists for some $\beta_c > 0$, and the temperature is sufficiently low.

Although in these cases the GT bound is better than the GGT bound we want to stress that the GGT bound is often easier to compute. In other cases the GGT bound may also be better than the GT bound, which we will illustrate below by a criterion for the discrete label case and by two examples. We first comment on the proofs of statements (i)–(iv).

(i) In this case one simply observes $Z_{GT} = Z$.

(ii) In this case P_B is diagonal with respect to a complete set $\{|n\rangle\}$ of orthogonal eigenstates $|n\rangle$ of B. Hence

$$\begin{aligned} P_B &= \sum_n |n\rangle\langle n|P_B|n\rangle\langle n| \\ &= \sum_n |n\rangle\langle n| \sum_i w_i\, \mathrm{e}^{-\beta b_i}|\langle n|i\rangle|^2. \end{aligned} \tag{5.1}$$

Using (4.4) we get

$$\begin{aligned} P_B &\geq \sum_n |n\rangle\langle n| \exp\Big(-\beta \sum_i w_i b_i |\langle n|i\rangle|^2\Big) \\ &= \sum_n |n\rangle\langle n| \exp(-\beta\langle n|B|n\rangle) = \mathrm{e}^{-\beta B}. \end{aligned} \tag{5.2}$$

Averaging this operator inequality with the 'density matrix' $\mathrm{e}^{-\beta A}$ yields the desired result.

(iii) We show that up to order β^2 the operator $P_B - \mathrm{e}^{-\beta B}$ is non-negative:

$$\begin{aligned} \lim_{\beta\to 0} \frac{2}{\beta^2}(P_B - \mathrm{e}^{-\beta B}) & \\ &= \sum_i w_i b_i^2 |i\rangle\langle i| - B^2 \\ &= \sum_i w_i[(B - b_i)|i\rangle\langle i|][(B - b_i)|i\rangle\langle i|]^+ \geq 0. \end{aligned} \tag{5.3}$$

(iv) If B is a c-number multiple of unity the statement is obvious due to (i). We therefore can exclude this case. Since B is a polynomial and bounded from below, $b(\alpha)$ is a polynomial and has a minimum:

$$b_0 := \min_\alpha b(\alpha). \tag{5.4}$$

† We believe that statement (iii) holds true also for some (A-dependent) class of unbounded operators B which we are unfortunately not able to characterise in a simple non-technical way.

Otherwise one would have a contradiction to Ritz's principle valid for any normalised $|\psi\rangle$:

$$\epsilon_B \leqslant \langle\psi|B|\psi\rangle = \int \frac{d^2\alpha}{\pi} b(\alpha)|\langle\alpha|\psi\rangle|^2 \tag{5.5}$$

with ϵ_B being the ground-state energy of B.

Now we observe that

$$B = \int \frac{d^2\alpha}{\pi} b(\alpha)|\alpha\rangle\langle\alpha| > b_0 \int \frac{d^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = b_0 1 \tag{5.6}$$

where equality is excluded because $b(\alpha)$ is non-constant. Taking the ground-state expectation value we obtain

$$\epsilon_B > b_0. \tag{5.7}$$

Furthermore, it follows from Ritz's principle that

$$e^{-\beta B} \leqslant e^{-\beta\epsilon_B} 1. \tag{5.8}$$

As a consequence, we have for $\beta \geqslant \beta_c$:

$$\mathrm{Tr}(e^{-\beta A}\, e^{-\beta B}) \leqslant e^{-\beta\epsilon_B}\, \mathrm{Tr}\, e^{-\beta A}. \tag{5.9}$$

On the other hand, we have from the spectral resolution of A

$$e^{-\beta A} \geqslant e^{-\beta\lambda} E_\lambda \tag{5.10}$$

for any real λ, where E_λ is the spectral projection† of A corresponding to the interval $(-\infty, \lambda)$. Combining (5.9) and (5.10) we get

$$\Delta Z := Z_{\mathrm{GGT}} - Z_{\mathrm{GT}} \geqslant e^{-\beta\lambda}\, \mathrm{Tr}(E_\lambda P_B) - e^{-\beta\epsilon_B}\, \mathrm{Tr}\, e^{-\beta A}. \tag{5.11}$$

Without loss of generality we can assume

$$b_0 = 0 \qquad \epsilon_A = 0 \tag{5.12}$$

where ϵ_A is the ground-state energy of A. For the special choice $\lambda = \epsilon_B/2$, (5.11) leads to

$$\begin{aligned}\Delta Z &\geqslant e^{-\beta\epsilon_B/2}[\mathrm{Tr}(E_{\epsilon_B/2}P_B) - e^{-\beta\epsilon_B/2}\, \mathrm{Tr}\, e^{-\beta A}] \\ &\geqslant e^{-\beta\epsilon_B/2}[\langle\psi|P_B|\psi\rangle - e^{-\beta\epsilon_B/2}\, \mathrm{Tr}\, e^{-\beta A}]\end{aligned} \tag{5.13}$$

where $|\psi\rangle$ is a normalised state in the subspace onto which $E_{\epsilon_B/2}$ projects. Since $\mathrm{Tr}\, e^{-\beta A}$ and $\langle\psi|P_B|\psi\rangle$ are monotonically decreasing functions of β (for $\beta \geqslant \beta_c$) the RHS of (5.13) becomes positive for sufficiently large β if $\langle\psi|P_B|\psi\rangle$ decreases slower than exponentially, i.e. if

$$\lim_{\beta\to\infty} e^{\beta\delta}\langle\psi|P_B|\psi\rangle = \infty \qquad \text{for all } \delta > 0. \tag{5.14}$$

For given δ there exists, due to the continuity of $b(\alpha)$, a region R_δ of the α plane such

† Formally $E_\lambda = \theta(\lambda - A)$, where θ is the Heaviside step function.

that $b(\alpha)<\delta/2$ for all $\alpha\in R_\delta$. Hence:

$$\begin{aligned}e^{\beta\delta}\langle\psi|P_B|\psi\rangle &= \int \frac{d^2\alpha}{\pi}\, e^{\beta(\delta-b(\alpha))}|\langle\psi|\alpha\rangle|^2\\ &\geq \int_{R_\delta} \frac{d^2\alpha}{\pi}\, e^{\beta(\delta-b(\alpha))}|\langle\psi|\alpha\rangle|^2\\ &\geq \mu_\delta\, e^{\beta\delta_b}\end{aligned}\tag{5.15}$$

where

$$\delta_b := \inf_{\alpha\in R_\delta}(\delta-b(\alpha))\geq\delta/2\tag{5.16}$$

and the integral

$$\mu_\delta := \int_{R_\delta}\frac{d^2\alpha}{\pi}|\langle\psi|\alpha\rangle|^2>0$$

does not vanish since $\langle\psi|\alpha\rangle\, e^{|\alpha|^2/2}$ is a non-constant analytic function of α (Klauder 1963) and thus has at most isolated zeros. This completes the proof of (5.14) and thus of statement (iv).

We are now going to show that in the case of a discrete label set $\{i\}$ either of the two bounds may be the better one for low temperatures. To this end we first estimate the A-expectation value:

$$\langle\,.\,\rangle_A := \operatorname{Tr} e^{-\beta A}(\,.\,)/\operatorname{Tr} e^{-\beta A}\tag{5.17}$$

of $P_B - e^{-\beta B}$. Using (5.8) and

$$P_B \geq w_i\, e^{-\beta b_i}|i\rangle\langle i| \qquad \text{for any } i\tag{5.18}$$

we obtain:

$$\langle P_B - e^{-\beta B}\rangle_A \geq w_i\, e^{-\beta b_i}\langle |i\rangle\langle i|\rangle_A - e^{-\beta\epsilon_B}.\tag{5.19}$$

Let us now look for an index i such that the RHS of (5.19) can become positive in the limit $\beta\to\infty$. For this purpose we note that for any normalised $|\psi\rangle$

$$\langle\psi|B|\psi\rangle \geq b_{i_\psi}\tag{5.20}$$

where i_ψ is an index such that

$$b_{i_\psi} = \min_i\{b_i | w_i\langle i|\psi\rangle\neq 0\}.\tag{5.21}$$

The proof of (5.20) is as follows:

$$\begin{aligned}\langle\psi|B|\psi\rangle &= \sum_i w_i b_i|\langle i|\psi\rangle|^2\\ &= \sum_i{}' w_i b_i|\langle i|\psi\rangle|^2\\ &\geq b_{i_\psi}\sum_i{}' w_i|\langle i|\psi\rangle|^2\\ &= b_{i_\psi}\sum_i w_i|\langle i|\psi\rangle|^2 = b_{i_\psi}\end{aligned}$$

where the prime denotes summation over all indices i such that $b_i\geq b_{i_\psi}$.

Choosing the normalised ground state $|\psi_0\rangle$ of B for $|\psi\rangle$ in (5.20) we obtain

$$\epsilon_B \geqslant b_{i_0} \qquad \text{with } i_0 := i_{\psi_0}. \tag{5.22}$$

We now recall that

$$\langle |i\rangle\langle i|\rangle_A \overset{\beta\to\infty}{\to} |\langle\varphi_0|i\rangle|^2 \tag{5.23}$$

where $|\varphi_0\rangle$ is a normalised ground state of A. Choosing $i = i_0$ in (5.19) we see that the RHS of (5.19) becomes positive for $\beta \to \infty$ if the following two conditions hold:

$$\epsilon_B \neq b_{i_0} \tag{5.24}$$

and

$$\langle\varphi_0|i_0\rangle \neq 0. \tag{5.25}$$

In this case the GT bound is better than the GGT bound for sufficiently low temperatures.

We now demonstrate, by way of an example, that the converse relation between the two bounds may hold if one of the above conditions is violated. We consider a two-dimensional (spin-$\frac{1}{2}$) Hilbert space spanned by two orthonormal states $|1\rangle$ and $|2\rangle$. These states, supplemented by the two states

$$\begin{aligned} |3\rangle &:= \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \\ |4\rangle &:= \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle) \end{aligned} \tag{5.26}$$

form an overcomplete set with

$$\tfrac{1}{2}\sum_{i=1}^{4} |i\rangle\langle i| = 1. \tag{5.27}$$

We define two operators A and B by

$$\begin{aligned} A &:= \mu_1|1\rangle\langle 1| + \mu_2|2\rangle\langle 2| \\ B &:= \frac{b}{4}(-|1\rangle\langle 1| + |2\rangle\langle 2| - |1\rangle\langle 2| - |2\rangle\langle 1|) \end{aligned} \tag{5.28}$$

where the real numbers μ_1, μ_2 and b are assumed to fulfil

$$\mu_1 > \mu_2 \qquad b > 0. \tag{5.29}$$

The pseudo-diagonal representation of B reads

$$B = \tfrac{1}{2}\sum_{i=1}^{4} b_i|i\rangle\langle i| \tag{5.30}$$

where

$$b_4 := -b_1 := b \qquad b_2 := b_3 := 0. \tag{5.31}$$

The eigenvalues $\lambda_\pm$ and corresponding normalised eigenstates $|\pm\rangle$ of B are given by

$$
\begin{aligned}
&\lambda_\pm = \pm\frac{b}{2\sqrt{2}}\\
&|+\rangle = \sin\frac{\pi}{8}|1\rangle - \cos\frac{\pi}{8}|2\rangle\\
&|-\rangle = \cos\frac{\pi}{8}|1\rangle + \sin\frac{\pi}{8}|2\rangle.
\end{aligned}
\tag{5.32}
$$

The index i_0 defined in (5.21) and (5.22) therefore equals 1 and the condition (5.25) is violated. The GT and GGT bounds corresponding to A and B are easily calculated to be

$$
\begin{aligned}
Z_{\mathrm{GT}} = {}& \exp[-\beta(\mu_1+\lambda_+)]\sin^2\frac{\pi}{8} + \exp[-\beta(\mu_1+\lambda_-)]\cos^2\frac{\pi}{8}\\
&+\exp[-\beta(\mu_2+\lambda_+)]\cos^2\frac{\pi}{8} + \exp[-\beta(\mu_2+\lambda_-)]\sin^2\frac{\pi}{8}
\end{aligned}
\tag{5.33}
$$

and

$$Z_{\mathrm{GGT}} = \tfrac{1}{2}\,\mathrm{e}^{-\beta\mu_1}(\mathrm{e}^{\beta b} + \tfrac{1}{2}\,\mathrm{e}^{-\beta b} + \tfrac{1}{2}) + \tfrac{1}{2}\,\mathrm{e}^{-\beta\mu_2}(\tfrac{3}{2} + \tfrac{1}{2}\,\mathrm{e}^{-\beta b}). \tag{5.34}$$

Comparing the leading exponentials of the two bounds for $\beta \to \infty$ one finds in that limit

$$Z_{\mathrm{GGT}} \lesseqgtr Z_{\mathrm{GT}} \Leftrightarrow \mu_1 - \mu_2 \gtreqless \left(1 - \frac{1}{2\sqrt{2}}\right) b. \tag{5.35}$$

The crucial feature of the above example (and similar ones) lies in the fact that all states $|i\rangle$ corresponding to b_i below the ground-state energy of B (in the above example, only the state $|1\rangle$) are orthogonal to the ground state of A.

In order to demonstrate that in the case of boson coherent states the GGT bound may be better than the GT bound for intermediate temperatures we offer the following example. We define in the (Fock-)Hilbert space of a single boson mode two operators of the harmonic oscillator type:

$$
\begin{aligned}
A &:= \epsilon(a^+ + \mathrm{i}\delta)(a - \mathrm{i}\delta)\\
B &:= \omega a^+ a + \frac{\eta}{2}(a^2 + (a^+)^2)
\end{aligned}
\tag{5.36}
$$

in terms of the annihilation operator a and the creation operator a^+. The real numbers ϵ, δ, ω and η are assumed to fulfil

$$\epsilon > 0 \qquad \omega > \eta \geqslant 0. \tag{5.37}$$

Under these conditions both operators are bounded from below and have finite partition functions.

The operator P_B associated via (3.2) with B and the boson coherent states (2.4) reads

$$P_B = \int \frac{\mathrm{d}^2\alpha}{\pi}\,\mathrm{e}^{-\beta b(\alpha)}|\alpha\rangle\langle\alpha| \tag{5.38}$$

with

$$b(\alpha) = \omega(|\alpha|^2 - 1) + \frac{\eta}{2}(\alpha^2 + \alpha^{*2}) \tag{5.39}$$

being the 'antinormal symbol' of B. We have calculated the GT bound on $\mathrm{Tr}\, e^{-\beta(A+B)}$ with the help of the normal-ordered form of $e^{-\beta B}$ and the antinormal-ordered form of $e^{-\beta A}$ given, for example, in Wilcox (1967) and Mehta (1977). The result is

$$\begin{aligned} Z_{\mathrm{GT}} &= \mathrm{Tr}(e^{-\beta A}\, e^{-\beta B}) \\ &= \frac{c\, e^{-u\delta^2}}{[(uv - v - u)^2 - (s - su)^2]^{1/2}} \exp\left(\frac{(v - s - 1)(u\delta)^2}{uv - us - u - v + s}\right) \end{aligned} \tag{5.40}$$

where we have used the abbreviations:

$$\begin{aligned} u &:= 1 - e^{-\beta\epsilon} \qquad \Omega := (\omega^2 - \eta^2)^{1/2} \\ c &:= e^{\beta\omega/2}\left(\cosh \beta\Omega + \frac{\omega}{\Omega}\sinh \beta\Omega\right)^{-1/2} \\ v &:= \left(\omega + \Omega \tanh \frac{\beta\Omega}{2}\right)(\omega + \Omega \coth \beta\Omega)^{-1} \\ s &:= \eta(\omega + \Omega \coth \beta\Omega)^{-1}. \end{aligned} \tag{5.41}$$

The GGT bound may be found from (5.38), (5.39) and the normal-ordered form of $e^{-\beta A}$:

$$\begin{aligned} Z_{\mathrm{GGT}} &= \mathrm{Tr}(e^{-\beta A} P_B) \\ &= \frac{e^{\beta\omega - u\delta^2}}{[(u + \beta\omega)^2 - (\beta\eta)^2]^{1/2}} \exp\left(\frac{(u\delta)^2}{u + \beta(\omega - \eta)}\right). \end{aligned} \tag{5.42}$$

In order to simplify things let us ask how Z_{GT} and Z_{GGT} look for

$$\beta\omega \gg 1 \qquad \eta/\omega \ll 1. \tag{5.43}$$

Neglecting terms of order $(\eta/\omega)^2$ we have in that limit

$$v \approx 1 \qquad c \approx 1 \qquad s \approx \eta/2\omega \tag{5.44}$$

and hence from (5.40) and (5.42):

$$\begin{aligned} Z_{\mathrm{GT}} &\approx e^{-u\delta^2} \exp[(u\delta)^2 \eta/2\omega] \\ Z_{\mathrm{GGT}} &\approx \frac{e^{\beta\omega - u\delta^2}}{\beta\omega} \exp\left[\frac{(u\delta)^2}{\beta\omega}\left(1 + \frac{\eta}{\omega}\right)\right]. \end{aligned} \tag{5.45}$$

Assuming

$$\beta\eta > 2 \tag{5.46}$$

we see from these expressions that Z_{GGT} is better than Z_{GT} (i.e. $Z_{\mathrm{GGT}} < Z_{\mathrm{GT}}$) if

$$u|\delta| \gtrsim \beta\omega\left(\frac{\beta\eta}{2} - 1\right)^{-1/2}. \tag{5.47}$$

The important feature of the above example lies in the fact that B and P_B do not commute. This allows us to find a region R of the α plane such that for intermediate β

$$\langle\alpha|P_B|\alpha\rangle < \langle\alpha|e^{-\beta B}|\alpha\rangle \qquad \text{for } \alpha\in R. \tag{5.48}$$

In fact, the operator B as given in (5.36) is the simplest polynomial with this property. If the operator A is now such that the function $f_A(\alpha)$ in the representation

$$e^{-\beta A} = \int \frac{d^2\alpha}{\pi} f_A(\alpha)|\alpha\rangle\langle\alpha| \tag{5.49}$$

is concentrated in R, it follows from (5.48) that Z_{GGT} is better than Z_{GT}. In particular, for the operator A in (5.36) $f_A(\alpha)$ is a Gaussian centred around $i\delta$.

6. Concluding remarks

We have shown that certain sets of normalised unity-resolving states in Hilbert space serve to generate upper bounds (3.1) on the partition function $\operatorname{Tr} e^{-\beta H}$ of a Hamiltonian of the form $H = A + B$. We have called each of these bounds a generalised Golden–Thompson bound (GGT bound) because it reduces to the Golden–Thompson bound $\operatorname{Tr}(e^{-\beta A}\, e^{-\beta B})$ if the unity-resolving states are chosen to be the eigenstates of B. Other important choices for the unity-resolving states are all kinds of coherent states. In particular, in the case of boson or spin coherent states our bound generalises results of Lieb (1973b) and Hepp and Lieb (1973). We want to stress that the GGT bound has built into it a considerable amount of flexibility which can be used to optimise it. One degree of flexibility is present already in the original Golden–Thompson bound, namely the possibility to subdivide a given H into A and B in different ways. An additional degree of flexibility stems from the fact that one is free to choose different sets of unity-resolving states. As an example for a systematic variation of these sets we mention the possibility of varying a set of coherent states by varying its underlying reference state. Thereby one gets a variational principle for the free energy from below in contrast to the more common Rayleigh–Ritz–Peierls–Bogolyubov principles, giving upper bounds on the free energy. We finally remark that many of our results have an obvious generalisation to the case where additional degrees of freedom are coupled to the ones considered by us.

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Note added in proof. After completion of this work we became aware of Berezin's inequalities (Berezin F A 1972 *Math. USSR Sbornik* **17** 269–77, Berezin F A 1972 *Math. USSR Izvestija* **6** 1117–51) which generalise the Hepp–Lieb inequalities to arbitrary sets of unity-resolving states (cf equation (4.2) of this work) and to arbitrary convex operator functions. Furthermore, we want to draw the reader's attention to the interesting Princeton preprint 'The Classical Limit of Quantum Partition Functions' by B Simon (to be published in *Commun. Math. Phys.*) which contains related material and in particular extends the work of Lieb (1973b) on the classical limit of quantum SO(3) spin systems to general compact Lie groups.

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