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Boundary Conditions for Quantum Lattice Systems

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Abstract For classical lattice systems, the Dobrushin-Lanford-Ruelle theory of boundary conditions states that the restriction of a global equilibrium state to a subsystem can be obtained as an integral over equilibrium states of the subsystem alone. The Hamiltonians for the subsystem are obtained by fixing a configuration for the variables in the complement of the subsystem, or more generally, by evaluating the full interaction Hamiltonian with respect to a state for the complement. We provide examples showing that the quantum mechanical version of this statement is false. It fails even if the subsystem is classical, but embedded into a quantum environment. We suggest an alternative characterization of the local restrictions of global equilibrium states by inequalities involving only local data.

I. Introduction

It is well-known that basic phenomena in statistical physics such as phase transitions, critical behaviour, and symmetry breaking cannot be modelled by finite systems as studied in classical or quantum mechanics. On the other hand, infinite systems can rarely be handled directly by finite computations. Therefore it is a fundamental task of statistical mechanics to develop techniques by which properties of infinite systems can be inferred from a study of finite subsystems. For the equilibrium statistical mechanics of classical systems on a lattice there is a standard tool for performing precisely such a step, namely the

Dobrushin-Lanford-Ruelle (DLR) theory of boundary conditions [**1**]. It says that the effect of the ambient infinite system on a finite subsystem can be parametrized adequately by a choice of "boundary conditions" for the finite subsystem. Here, boundary conditions are identified with configurations of the particles outside the finite subsystem in consideration. They can then be used to classify the pure phases, or to select a particular pure phase in the event of a broken symmetry. In specific models such as, e.g., the two-dimensional Ising model, a small selection of boundary conditions suffices to obtain all phases.

The notion of boundary condition as a configuration in the boundary region of a finite subsystem is the starting point both for proofs of existence of a phase transition and proofs of its opposite, the uniqueness of the equilibrium state. An example of the first is the Peierls argument [**2**] where one shows that the configuration of a small subsystem (a single spin), strongly depends on the configurations of the boundary region. An example of the other usage is the Dobrushin-Shlosman unicity argument [**3**]. In this case, the influence of variations in boundary conditions is proven to become negligible when one surrounds a small system by larger and larger intermediate regions.

It is one aim of the present paper to show, by way of explicit examples, that, while the basic statement of the DLR-theory has a straightforward generalization to the case of quantum lattice systems, this generalization, along with some of its natural modifications, turns out to be false. But our intention is not merely to disprove a single statement. Rather, we believe that a careful study of examples may be helpful for the development of the much needed tools of quantum statistical mechanics which would be capable to serve some of the functions of the classical DLR-theory. The energy-entropy inequalities [**4,5**] described in Sec. IV are a promising step in this direction: they form a set of strictly local constraints on the restrictions of possible equilibrium states, which approaches an exact characterization of equilibrium states as the local region under consideration becomes larger and larger. For the restrictions to classical subsystems, an efficient evaluation of these conditions is possible (see Sec. V), but, for the case of general quantum systems, better techniques of extracting information from these inequalities are still to be developed.

The term boundary condition, especially as used in the context of quantum statistical mechanics, carries several meanings, often not too clearly defined. "Free boundary conditions" refer to a special way of constructing finite volume Hamiltonians from an interaction potential, namely as the sum over all potential terms localized in the given region. There are always many different interaction potentials representing the same infinite volume Hamiltonian ("equivalent potentials" [**1**]), which in this language lead to different "free boundary conditions" for the same Hamiltonian. Some properties, like the presence or absence of frustration [**6,7**], or the invariance of local Hamiltonians under the action of a symmetry group or quantum group [**8**], depend very sensitively to this choice. "Periodic boundary conditions" arise when a lattice is shaped into a torus. The translation symmetry of the infinite lattice is then approximated by cyclic shifts. Another type of "boundary condition" is obtained by adding an overall small external field, which is removed afterwards [**9**]. Such fields are usually introduced for driving the system in a pure phase of broken symmetry. Typically, all these additional terms to the Hamiltonian leave the thermodynamic quantities unchanged. In the description of continuous systems "boundary conditions" are used to specify the Hamiltonian as a self-adjoint operator [**10**]. This can

be used to confine the system to a particular region, or to introduce hard-core repulsion. In principle, this is equivalent to adding strongly repulsive potentials to the Hamiltonian. Finally, conditions that select particular ground states in situations with degeneracy are also called boundary conditions. An example of such usage occurs in valence-bond-solid models [**11**].

For simplicity, we will only consider finite systems in this paper. The difficulties that we demonstrate for describing the local restrictions of equilibrium states will certainly not be lifted by considering infinite systems. (This could only happen if more structure, like translation invariance, is incorporated into the scheme). However, the notions that we introduce for finite systems can be generalized in a straightforward manner to the infinite systems obtained in the thermodynamical limit. The adequate tools for doing so are the DLR-equations for classical lattice systems, the KMS-condition [**10**] for quantum spin systems, and the energy-entropy inequalities for both. The basic input, namely the interaction between the lattice spins, now translates into a relative Hamiltonian for the classical systems, and a derivation that generates the dynamics for quantum spin systems. There is an, apparently local, description of equilibrium states for quantum spin systems known as the Gibbs condition [**12**] (see also Sect. 6.2 of [**10**]). Unfortunately, it involves a variation over all global extensions of the local state, and is therefore of little practical help.

The paper is organized as follows: in Sec. II we briefly review the local "DLR-characterization" of equilibrium states of classical systems in terms of boundary conditions. Sec. III introduces the corresponding notions for quantum spin systems. In Sec. IV we recall the characterization of equilibrium states in terms of energy-entropy inequalities, while Sec. V examines the consequences of these inequalities for the restrictions of global equilibrium states to a classical subsystem. Sec. VI contains the major part of our results, a succession of examples showing the failure of the direct quantum analogue of the DLR-theory. Where feasible we also discuss the consequences of the energy-entropy inequalities.

II. Boundary conditions for classical equilibrium states

In this section we will only consider finite, discrete classical systems, described by finite configuration spaces. We will concentrate on a distinguished subsystem, called the inner system, with configuration space X. The configuration space of the global system is $X \times Y$, where Y is the configuration space of the outer system. We assume that we have a complete knowledge of the contribution of the particles in the inner system to the total energy H_{tot}, meaning that we write

$$H_{\text{tot}} = H + V \quad , \quad \begin{array}{l} H \text{ fixed function on } X \times Y \text{ and} \\ V \text{ only depending on } Y \quad . \end{array} \tag{1}$$

The function $(x,y) \in X \times Y \mapsto H(x,y)$ is the basic information that is at our disposal, whereas the size of the outer system and the interaction V is supposed to be less well-known. The minimal choice of outer system is fixed by requiring that H actually depends on the configurations in this minimal exterior region. More precisely we say that y and y' in Y are equivalent iff for all $x \in X$, $H(x,y) = H(x,y')$. The quotient of Y by this equivalence relation is called the set of the boundary configurations Y_{bd} and it is the minimal exterior configuration space that has to be considered. We will sometimes refer to it as the boundary system.

The equilibrium state of the global system at inverse temperature $\beta = 1/kT$ is given by the canonical Gibbs distribution, which assigns the probability

$$\mu(x,y) = e^{-\beta H_{\mathrm{tot}}(x,y)}/\mathcal{Z} \tag{2}$$

to the configuration (x,y). The normalization factor is the canonical partition function $\mathcal{Z} = \sum_{x,y} e^{-\beta H_{\mathrm{tot}}(x,y)}$. Unless we explicitly discuss temperature behaviour, we assume that β is included in the Hamiltonian, and therefore put $\beta = 1$.

The restriction μ_{int} of μ to X is easily computed. It assigns to $x \in X$ the probability of $\{(x,y) | \, y \in Y\}$:

$$\begin{aligned} \mu_{\mathrm{int}}(x) &= \sum_{y \in Y} \mu(x,y) = \sum_{y \in Y} \frac{e^{-H_{\mathrm{tot}}(x,y)}}{\mathcal{Z}} \\ &= \sum_{y \in Y} \frac{\mathcal{Z}^y \, e^{-V(y)}}{\mathcal{Z}} \, \frac{e^{-H^y(x)}}{\mathcal{Z}^y} = \sum_{y \in Y} \lambda(y) \, \mu^y(x) \quad , \end{aligned} \tag{3}$$

where

$$\mu^y(x) = e^{-H^y(x)}/\mathcal{Z}^y \tag{4}$$

is the Gibbs distribution on X defined by the averaged Hamiltonian

$$H^y(x) = H(x,y) \quad , \tag{5}$$

and where the $\lambda(y)$ are positive numbers adding up to 1. Thus formula (3) says that the global equilibrium state, reduced to the inner system X, is a convex combination of equilibrium states μ^y of the inner subsystem for averaged Hamiltonians H^y. The configurations $y \in Y_{\mathrm{bd}}$ can be viewed as boundary conditions, defining the averaged Hamiltonians H^y. Formula (3) solves the problem of giving a simple characterization of the equilibrium distributions, reduced to the inner system, in terms of the basic interaction H. It is a basic tool in proving both absence and occurrence of phase transitions.

It is easily seen that all the Gibbs distributions μ^y are themselves limits of restrictions of equilibrium distributions of the global system to X. Indeed, it suffices to consider the minimal system $X \times Y_{\mathrm{bd}}$ and to take $V = \lambda \, e_y$ (where the function e_y takes the value 1 on y and zero elsewhere), and consider the limit $\lambda \to -\infty$. This makes the configuration $y \in Y_{\mathrm{bd}}$ infinitely attractive to the outer system, and yields a sequence of equilibrium

states, whose restrictions converge to μ^y. This procedure is reminiscent of the way one finds the Dirichlet boundary conditions for the Schrödinger equation in a finite region, by introducing larger and larger confining potentials.

The set of restrictions of global equilibrium states μ, determined by Hamiltonians H_{tot} satisfying (1), is convex. This is easily seen as follows: if Y and Y' are two outer configuration spaces for the subsystem, consider then $Y'' = Y \cup Y'$ and the total Hamiltonian $H''_{\text{tot}} = H + V''$, where $V''(y) = V(y)$ if y belongs to Y and $V''(y) = V'(y) + C$ else. By varying the constant $C \in \mathbb{R}$, we can produce any convex combination of the restrictions of the equilibrium distributions corresponding to H_{tot} and H'_{tot}. Taking the conclusions of the last three paragraphs together, we arrive at the following statement, whose quantum versions form the subject of this paper:

for a measure μ on X the following two statements are equivalent:
(1) μ can be approximated by the restriction of Gibbs distributions for Hamiltonians in the class (1).
(2) μ is a convex combination of the Gibbs distributions μ^y, formed with Hamiltonians H^y (5)*, averaged with one outside configuration $y \in Y_{\text{bd}}$.*

Especially suggestive in this equivalence is the identification of the "extreme" elements μ^y of the set so described: in terms of the reduced equilibrium distributions (1), these are obtained by making the outside potential V very large, whereas in (2) the same elements play the role of the extreme boundary in the sense of convex sets.

This suggestive picture loses a bit of its appeal when we consider more general, less "extreme" averages of the Hamiltonian H: rather than evaluating H on a single external configuration $y \in H$, we can also consider

$$H^\rho(x) = \sum_{y \in Y_{\text{bd}}} \rho(y)\, H(x,y) \quad , \tag{6}$$

where ρ is a probability distribution on Y_{bd}. Such boundary conditions arise naturally when considering random systems. They will also appear when we couple classical systems to quantum outer systems. One can easily find examples in which the equilibrium states of such averaged Hamiltonians H^ρ are *not* contained in the convex set described above (see Example 1 for an illustration).

Besides equilibrium distributions, *ground states* can be considered as well. A distribution μ is a global ground state if it minimizes the energy functional $\mu \mapsto \mu(H_{\text{tot}})$. As this functional is obviously affine, the ground states form a face of the simplex of probability measures on $X \times Y$, and the same is of course true for their restriction to the inner system X. By an argument quite similar to that for equilibrium states, one verifies that the set of reduced ground states, when Y and V vary as in (1), is still a face of the probability measures on X. A configuration $x_0 \in X$ is an extreme reduced ground state iff there is a $y_0 \in Y_{\text{bd}}$ such that

$$H(x, y_0) \geq H(x_0, y_0) \quad \text{for all } x \in X \quad .$$

The situation is quite analogous to that for equilibrium states: in order to characterize reduced ground states, it suffices to minimize the energy of the averaged Hamiltonians H^y (5) where y runs over the configurations of the boundary region Y_{bd}.

III. Extension to quantum systems

There are two essential properties of classical systems that underlie the description of equilibrium states of global systems in terms of local Gibbs distributions. Firstly, all probability distributions on a composite system are convex combinations of product measures, namely the point measures described by pairs of configurations. This allows conditioning as in equation (3). Secondly, for functions f and g, $\exp(f+g) = \exp f \exp g$. Both properties totally fail when we pass to quantum systems.

Quantum systems are described in terms of algebras of observables rather than configurations. The observables of a discrete, fully quantum mechanical system form a matrix algebra, say, the algebra $\mathcal{M}_d$ of complex $d \times d$-matrices. On the other hand, the observables of a discrete classical system with finite configuration space X are the complex-valued functions $\mathcal{C}(X)$ on X. This is an Abelian algebra, which can be identified with the diagonal $d \times d$ matrices, d being the number of points in X. In this paper, we only consider finite-dimensional algebras of observables. All such algebras decompose into sums of matrix algebras and may also describe quantum-classical hybrid systems. Probability distributions are expressed in algebraic language as linear functionals, called *states*, which assign to each observable its expectation value. On a finite-dimensional algebra $\mathcal{A}$ all such functionals are of the form

$$\omega(A) = \mathrm{Tr}(D_\omega A) \quad ,$$

where the density matrix D_ω is positive, and $\mathrm{Tr}\, D_\omega = 1$.

We consider systems split into an "inner" and an "outer" subsystem. On the level of the algebras, this translates into a tensor product structure of the global algebra of observables $\mathcal{A} = \mathcal{A}_{\mathrm{int}} \otimes \mathcal{A}_{\mathrm{ext}}$: the elements of $\mathcal{A}$ can be written as finite linear combinations of elementary tensors $A \otimes B$, $A \in \mathcal{A}$, $B \in \mathcal{B}$. $A \mapsto A \otimes B$ and $B \mapsto A \otimes B$ are linear and the multiplication in $\mathcal{A}$ is given by

$$(A_1 \otimes B_1)(A_2 \otimes B_2) = A_1 A_2 \otimes B_1 B_2 \quad .$$

As in the classical case, we will assume that we have a complete knowledge of the interaction of the particles in the inner system with the exterior. More precisely

$$\begin{aligned} &H \in \mathcal{A}_{\mathrm{int}} \otimes \mathcal{A}_{\mathrm{bd}} \quad \text{is a fixed Hermitian operator and} \\ &H_{\mathrm{tot}} = H + \mathbb{1} \otimes V, \quad V = V^* \in \mathcal{A}_{\mathrm{ext}} \supset \mathcal{A}_{\mathrm{bd}} \quad . \end{aligned} \tag{7}$$

Here, $\mathcal{A}_{\mathrm{bd}}$ denotes the smallest $*$-subalgebra of $\mathcal{A}_{\mathrm{ext}}$ such that $H \in \mathcal{A}_{\mathrm{int}} \otimes \mathcal{A}_{\mathrm{bd}}$. For classical systems $\mathcal{A}_{\mathrm{bd}}$ is precisely $\mathcal{C}(Y_{\mathrm{bd}})$. The equilibrium state ω of the global system is given by the Gibbs density matrix

$$D_\omega = e^{-H_{\mathrm{tot}}}/\mathcal{Z} \quad . \tag{8}$$

The normalization factor $\mathcal{Z}$ is the canonical partition function. We can restrict the state ω to the inner system to obtain the state ω_{int} on $\mathcal{A}_{\mathrm{int}}$:

$$\omega_{\mathrm{int}}(A) = \omega(A \otimes \mathbb{1}), \quad A \in \mathcal{A}_{\mathrm{int}} \quad . \tag{9}$$

The density matrix of $\omega_{\rm int}$ is the partial trace of the one for ω with respect to $\mathcal{A}_{\rm ext}$. We now define the set $\mathcal{E}_{\rm R}$ of reduced equilibrium states

$$\mathcal{E}_{\rm R} = \overline{\left\{\omega_{\rm int} \,\middle|\, \omega \text{ equilibrium state for } H_{\rm tot} \text{ as in (7)}\right\}} \quad , \tag{10}$$

where the bar denotes the closure. The set $\mathcal{E}_{\rm R}$ is completely determined by H and we will sometimes explicitly refer to that dependence by writing $\mathcal{E}_{\rm R} = \mathcal{E}_{\rm R}(H)$. By the same argument as in Sec. II, $\mathcal{E}_{\rm R}$ is a convex set and we are interested in the following question: can one give a simple description of $\mathcal{E}_{\rm R}$ in terms of H?

There are two natural ways of averaging the Hamiltonian H: either against pure or against arbitrary states ρ on $\mathcal{A}_{\rm bd}$ (compare with (5) and (6)). In either case, the averaged Hamiltonian is obtained as

$$\mathbb{E}^{\rho}(H) = \sum_i \rho(B_i)\, A_i \quad ,$$

where $H = \sum_i A_i \otimes B_i$ with $A_i \in \mathcal{A}_{\rm int}$ and $B_i \in \mathcal{A}_{\rm bd} \subset \mathcal{A}_{\rm ext}$. The sets of Gibbs states on $\mathcal{A}_{\rm int}$ corresponding to these averaged Hamiltonians will be denoted by

$$\mathcal{E}_{\rm AH}^{\rm pure} = \left\{\omega \,\middle|\, \text{equilibrium state for } \mathbb{E}^{\rho}(H) \quad , \ \rho \text{ pure} \quad \right\} \tag{11}$$

and

$$\mathcal{E}_{\rm AH} = \left\{\omega \,\middle|\, \text{equilibrium state for } \mathbb{E}^{\rho}(H) \quad , \ \rho \text{ arbitrary}\right\} \quad . \tag{12}$$

In [1], the set of pure states on $\mathcal{A}_{\rm bd}$ is considered as a candidate for quantum boundary conditions. As in the classical case, this choice can be made plausible by considering perturbations of the Hamiltonian by large potentials: let P be a minimal projection in $\mathcal{A}_{\rm ext}$ and consider the Hamiltonians $H_{\rm tot}(\lambda) = H + \lambda \mathbb{1} \otimes P$. Note that P, taken as a density matrix, also determines a pure state ρ on $\mathcal{A}_{\rm ext}$. We claim that, as $\lambda \to -\infty$, the restrictions of the equilibrium states for $H_{\rm tot}(\lambda)$ to $\mathcal{A}_{\rm int}$ converge to the equilibrium state for $\mathbb{E}^{\rho}(H)$. In order to verify this, we consider $\lambda^{-1}H$ as a small perturbation of $-\mathbb{1} \otimes P$, obtaining eigenvectors $\psi_\alpha(\lambda)$, and eigenvalues $\eta_\alpha(\lambda)$, which depend analytically on λ^{-1}. Note that the eigenspaces of $\mathbb{1} \otimes P$ are highly degenerate, and we must chose the basis in $0^{\rm th}$ order such that $\psi_\alpha(\infty)$, $\alpha = 1, \ldots, d$ is the eigenbasis of the operator $(\mathbb{1} \otimes P)H(\mathbb{1} \otimes P)$ and the remaining $\psi_\alpha(\infty)$ are an eigenbasis of $(\mathbb{1} \otimes (\mathbb{1} - P))H(\mathbb{1} \otimes (\mathbb{1} - P))$. Let η'_α denote the eigenvalues of these operators. Then the equilibrium state ω^λ is given by

$$\omega^\lambda(A) = \frac{1}{\mathcal{Z}(\lambda)} \sum_\alpha e^{-\lambda \eta_\alpha(\lambda)} \frac{\langle \psi_\alpha(\lambda),\, A\psi_\alpha(\lambda)\rangle}{\|\psi_\alpha(\lambda)\|^2} \quad .$$

The exponent is

$$\lambda\eta_\alpha(\lambda) = \begin{cases} -\lambda + \eta'_\alpha + \mathbf{O}(\lambda^{-1}) & \text{for } \alpha = 1, \ldots, d \\ \eta'_\alpha + \mathbf{O}(\lambda^{-1}) & \text{for } \alpha > d \end{cases} \quad .$$

Hence the terms with $\alpha > d$ are negligible in the sum and, after cancelling the factor e^{λ} between the sum and $\mathcal{Z}(\lambda)$, we can take the limit $\lambda \to -\infty$, obtaining

$$\omega^{\infty}(A) = \frac{1}{\mathcal{Z}(\infty)} \sum_{\alpha=1}^{d} e^{-\eta'_\alpha} \langle \psi_\alpha(\infty),\, A\psi_\alpha(\infty) \rangle$$
$$= (1/\mathcal{Z})\, \mathrm{Tr}\, e^{-(\mathbb{1}\otimes P)H(\mathbb{1}\otimes P)} A \quad .$$

An infinite system generalization of this result can be found in [**13**]. Now, if P is the one-dimensional projection onto the vector φ, the 1-eigenspace of $(\mathbb{1} \otimes P)$ consists precisely of the vectors $\psi \otimes \varphi$ where ψ is in the Hilbert space of the inner system. By identifying $\psi \otimes \varphi$ with ψ, the operator $(\mathbb{1} \otimes P)H(\mathbb{1} \otimes P)$ becomes $\mathbb{E}^{\rho}(H)$, hence ω^{∞} is the Gibbs state with this Hamiltonian, as claimed.

As any state on $\mathcal{A}_{\mathrm{bd}}$ can be extended to a pure state on $\mathcal{A}_{\mathrm{ext}}$ for some suitable embedding of $\mathcal{A}_{\mathrm{bd}}$ into a $\mathcal{A}_{\mathrm{ext}}$, it follows that

$$\mathrm{conv}\, \mathcal{E}_{\mathrm{AH}} \subset \mathcal{E}_{\mathrm{R}} \quad . \tag{13}$$

Obviously, $\mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}} \subset \mathcal{E}_{\mathrm{AH}}$ and the states in $\mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}}$ can be obtained by restricting in the construction of above to the case $\mathcal{A}_{\mathrm{ext}} = \mathcal{A}_{\mathrm{bd}}$.

In the classical case we found that $\mathcal{E}_{\mathrm{R}} = \mathrm{conv}\, \mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}}$. In Sec. VI we will examine whether the converse inclusion of (13) holds, i.e., whether we have

$$\mathcal{E}_{\mathrm{R}} \subset \mathrm{conv}\, \mathcal{E}_{\mathrm{AH}} \quad . \tag{14}$$

We will refer to this as the *DLR-inclusion.* By (13) it is in fact equivalent to the equality $\mathcal{E}_{\mathrm{R}} = \mathrm{conv}\, \mathcal{E}_{\mathrm{AH}}$.

A state ω of the global system is a *ground state* of H_{tot} if it minimizes the energy $\omega(H_{\mathrm{tot}})$. For a fixed H_{tot}, the ground states form a closed convex set, which is even a face of the state space. Restricting a pure state of the global system $\mathcal{A}_{\mathrm{int}} \otimes \mathcal{A}_{\mathrm{ext}}$ to the inner system will in general destroy its purity. The set $\mathcal{G}_{\mathrm{R}}$ of reduced ground states is similar to $\mathcal{E}_{\mathrm{R}}$

$$\mathcal{G}_{\mathrm{R}} = \overline{\left\{ \omega_{\mathrm{int}} \,\middle|\, \omega \text{ ground state for } H_{\mathrm{tot}} \text{ as in (7)} \right\}} \quad . \tag{15}$$

It is a closed convex set that contains the convex hulls of the sets $\mathcal{G}_{\mathrm{AH}}^{\mathrm{pure}}$ and $\mathcal{G}_{\mathrm{AH}}$ which are defined as the sets of ground states on $\mathcal{A}_{\mathrm{int}}$ with respect to the averaged Hamiltonians $\mathbb{E}^{\rho}(H)$, where ρ varies either over the pure or over the general states on $\mathcal{A}_{\mathrm{bd}}$.

IV. Energy-entropy inequalities

An equilibrium state can be characterized as a solution of the variational principle of thermodynamics:

$$\omega \mapsto F(\omega) = U(\omega) - S(\omega)$$

attains its minimum at the Gibbs state. F is the free energy, it is the difference between the internal energy $U(\omega)$ and the entropy $S(\omega) = -\operatorname{Tr} D_\omega \ln D_\omega$. It is possible to characterize equilibrium states by a set of inequalities that express in a differential form that the Gibbs state minimizes the mean free energy [**14**]. Consider a quantum system described by the $d \times d$ matrices $\mathcal{M}_d$ and let H be the Hamiltonian of the system. For any observable $A \in \mathcal{M}_d$, the Gibbs state ω satisfies the "energy-entropy inequalities"

$$\omega(A^*[H,A]) \geq \omega(A^*A) \ln \frac{\omega(A^*A)}{\omega(A\,A^*)} \quad . \tag{16}$$

Conversely, if (16) holds for any choice of $A \in \mathcal{M}_d$, then ω is the Gibbs state defined by H. The main advantage of these inequalities, which express the energy-entropy balance in equilibrium, is that they involve the Hamiltonian in a linear way.

Consider now again the situation of Sec. III. Any equilibrium state ω of the global system will satisfy the energy-entropy inequalities (16). In particular, the inequalities must hold for $A \in \mathcal{A}_{\text{int}}$ and therefore:

$$\omega(A^*[H_{\text{tot}},A]) = \omega(A^*[H,A]) \geq \omega(A^*A) \ln \frac{\omega(A^*A)}{\omega(A\,A^*)}, \quad A \in \mathcal{A}_{\text{int}} \quad . \tag{17}$$

Note that the left hand side involves only the restriction of ω to $\mathcal{A}_{\text{int}} \otimes \mathcal{A}_{\text{bd}}$, whereas the right hand side involves only the restriction to $\mathcal{A}_{\text{int}}$. In either case, this condition is "local" in the sense that it does not require knowledge of the global state on $\mathcal{A}_{\text{ext}}$. Moreover, if this condition is satisfied for $\mathcal{A}_{\text{int}}$ varying over the observable algebras of *arbitrary* bounded regions, the inequalities (16) hold on the whole algebra, and hence ω must be an equilibrium state. Thus at least some of the key requirements for a useful replacement of the DLR-equations in the quantum case are satisfied by the partial energy-entropy inequalities (17).

We denote by $\mathcal{E}_{\text{EE}}$ the set of states on $\mathcal{A}_{\text{int}}$ defined by

$$\mathcal{E}_{\text{EE}} = \left\{ \omega \,\middle|\, \exists\, \omega\tilde{}\ \text{extending}\ \omega\ \text{and satisfying (17)} \right\} \quad .$$

The set $\mathcal{E}_{\text{EE}}$ is a closed convex set and it contains $\mathcal{E}_{\text{R}}$. Indeed, in order to show convexity, let ω and ω' be states in $\mathcal{E}_{\text{EE}}$. We can then find extensions $\omega\tilde{}$ and $\omega'\tilde{}$ on $\mathcal{A}_{\text{int}} \otimes \mathcal{A}_{\text{bd}}$ that satisfy

$$\omega^{(\prime)}\tilde{}(A^*[H,A]) \geq \omega^{(\prime)}(A^*A) \ln \frac{\omega^{(\prime)}(A^*A)}{\omega^{(\prime)}(A\,A^*)}, \quad A \in \mathcal{A}_{\text{int}} \quad .$$

For $\lambda \in [0,1]$, $\lambda\omega\tilde{} + (1-\lambda)\omega'\tilde{}$ extends $\lambda\omega + (1-\lambda)\omega'$ and for $A \in \mathcal{A}_{\text{int}}$:

$$\begin{aligned}
&\left(\lambda\omega\tilde{} + (1-\lambda)\omega'\tilde{}\right)\left(A^*[H,A]\right) \\
&\quad = \lambda\omega\tilde{}(A^*[H,A]) + (1-\lambda)\omega'\tilde{}(A^*[H,A]) \\
&\quad \geq \lambda\omega(A^*A) \ln \frac{\omega(A^*A)}{\omega(A\,A^*)} + (1-\lambda)\omega'(A^*A) \ln \frac{\omega'(A^*A)}{\omega'(A\,A^*)} \\
&\quad = -\left(\lambda\omega(A^*A) \ln \frac{\omega(A\,A^*)}{\omega(A^*A)} + (1-\lambda)\omega'(A^*A) \ln \frac{\omega'(A\,A^*)}{\omega'(A^*A)}\right) \\
&\quad \geq -\left(\lambda\omega(A^*A) + (1-\lambda)\omega'(A^*A)\right) \ln \frac{\lambda\omega(A\,A^*) + (1-\lambda)\omega'(A\,A^*)}{\lambda\omega(A^*A) + (1-\lambda)\omega'(A^*A)} \\
&\quad = \left(\lambda\omega(A^*A) + (1-\lambda)\omega'(A^*A)\right) \ln \frac{\lambda\omega(A^*A) + (1-\lambda)\omega'(A^*A)}{\lambda\omega(A\,A^*) + (1-\lambda)\omega'(A\,A^*)} \quad .
\end{aligned}$$

There are versions of the energy-entropy inequalities for classical and hybrid systems too. The inequalities (16) are of no use in this case because in a classical system all commutators vanish and $A^*A = AA^*$. Hence (16) is trivially satisfied as $0 \geq 0$. We therefore consider in the next section a more general type of inequality that also covers hybrid systems.

V. Systems with a classical interior algebra

With the exception of Example 3, all examples in Sec. VI will be "hybrid systems" with a classical inside system with n = finitely many configurations, i.e., we have $\mathcal{A}_{\text{int}} = \mathcal{C}(\{1,\ldots,n\})$. The interaction is given by a Hermitian element $H \in \mathcal{A}_{\text{int}} \otimes \mathcal{A}_{\text{ext}}$, i.e., by a Hermitian-valued function $x \mapsto H(x) \in \mathcal{A}_{\text{ext}}$. The subalgebra $\mathcal{A}_{\text{bd}} \subset \mathcal{A}_{\text{ext}}$ is the algebra generated by $\mathbb{1}$, and all $H(x)$. The perturbation $\mathbb{1} \otimes V$ by a potential $V = V^* \in \mathcal{A}_{\text{ext}}$ is represented by the corresponding x-independent function. The reduced equilibrium states of the total Hamiltonian $H_{\text{tot}} = H + \mathbb{1} \otimes V$ are then the probability distributions

$$\mu^V_{\text{RE}}(x) = \frac{1}{\mathcal{Z}} \operatorname{Tr}\Big(e^{-(H(x)+V)}\Big) \quad , \quad x = 1,\ldots,n \quad , \tag{18}$$

where $\mathcal{Z}$ is the normalization factor making this a probability distribution. If ρ is a state on $\mathcal{A}_{\text{ext}}$, the averaged Hamiltonian $\mathbb{E}^\rho(H)$ is the function $h = \mathbb{E}^\rho(H) \in \mathcal{C}(\{1,\ldots,n\})$ taking the value $h(x) = \rho(H(x))$ at x. (Note that only the restriction $\rho\restriction\mathcal{A}_{\text{bd}}$ enters this expression). This leads to a probability distribution of the form

$$\mu^\rho_{\text{AH}}(x) = \frac{1}{\mathcal{Z}}\, e^{-\rho(H(x))} \quad , \quad x = 1,\ldots,n \quad . \tag{19}$$

General states ω on $\mathcal{A}_{\text{int}} \otimes \mathcal{A}_{\text{ext}}$ are given by (not normalized) positive functionals ω^x on $\mathcal{A}_{\text{ext}}$:

$$\omega = \sum_x \delta_x \otimes \omega^x \quad , \tag{20}$$

where δ_x is the evaluation at x. If $e_x \in X$ denotes the function which is 1 at x and 0 otherwise, we can expand the observables A of this system as

$$A = \sum_x e_x \otimes A(x) \quad , \tag{21}$$

where the $A(x)$ are elements of $\mathcal{A}_{\text{ext}}$. Thus observables are identified with $\mathcal{A}_{\text{ext}}$-valued functions on X, and the algebraic operations are defined pointwise in x. In particular, A is Hermitian iff $A(x)^* = A(x)$ for all x, and the identity element is the function which is equal to $\mathbb{1} \in \mathcal{A}$ for all x. The expectation of an observable (21) in the state (20) is computed as

$$\omega(A) = \sum_{x \in X} \omega^x(A(x)) \quad .$$

With the identity element for A, we find the normalization condition

$$\sum_{x\in X} \omega^x(\mathbb{1}) = 1 \quad .$$

The useful energy-entropy inequalities in this situation are

$$\omega^x\Big(A^*\big(H(y)\,A - A\,H(x)\big)\Big) \geq \omega^x(A^*A)\,\ln\frac{\omega^x(A^*A)}{\omega^y(A\,A^*)} \quad , \tag{22}$$

$x, y = 1, \ldots, n$ and $A \in \mathcal{A}_{\text{ext}}$. From this, we find restricted energy-entropy inequalities analogous to (17). We have to evaluate (22) for $A = \alpha\mathbb{1}$. Thus $A\,A^* = A^*A$, and a factor α^2 can be cancelled from (22). Hence, for a classical inner system, the suitable definition for $\mathcal{E}_{\text{EE}}$ is the set of all probability measures μ_{EE} on $\{1, \ldots, n\}$ for which there exist non-negative functionals ω^x on $\mathcal{A}_{\text{ext}}$ with $\mu_{\text{EE}}(x) = \omega^x(\mathbb{1})$ and such that

$$\omega^x\big(H(y) - H(x)\big) \geq \mu_{\text{EE}}(x)\,\ln\frac{\mu_{\text{EE}}(x)}{\mu_{\text{EE}}(y)}, \quad x,\ y = 1, \ldots, n \quad . \tag{23}$$

It is sometimes convenient to work with the logarithms of probabilities, i.e., to describe a state μ on $\mathcal{A}_{\text{int}}$ by the $n-1$ numbers

$$(\widetilde{\ln}\,\mu)(x) = \ln\big(\mu(x)\big) - \ln\big(\mu(1)\big) \quad , \quad \text{for} \quad x = 2, \ldots, n \quad . \tag{24}$$

The image of the various sets $\mathcal{E}_{\text{XX}} \subset \mathbb{R}^{n-1}$ under this map will be denoted by $\widetilde{\ln}\,\mathcal{E}_{\text{XX}}$. In this logarithmic scale $\mathcal{E}_{\text{AH}}$ becomes

$$\widetilde{\ln}\,\mathcal{E}_{\text{AH}} = \Big\{\xi \in \mathbb{R}^{n-1}\Big|\ \xi_x = \rho\big(H(1) - H(x)\big)\Big\} \quad , \tag{25}$$

where ρ runs over all states of $\mathcal{A}_{\text{bd}}$. This is an affine image of the state space of $\mathcal{A}_{\text{bd}}$. Note that this set is always convex but, due to the non-linearity of exp, $\mathcal{E}_{\text{AH}}$ itself is not (compare Figure 1).

When $\mathcal{A}_{\text{int}}$ is classical, we can also give a fairly explicit description of $\mathcal{E}_{\text{EE}}$. Since we want to interpret (23) as a condition for the probability distribution $\mu_{\text{EE}}(x) = \omega^x(\mathbb{1})$, it is convenient to write the positive linear functionals ω^x determining ω as $\omega^x = \mu_{\text{EE}}(x) \cdot \rho^x$, where the ρ^x are now states on $\mathcal{A}_{\text{ext}}$. Note that no $\mu_{\text{EE}}(y)$ can vanish: since $\omega \neq 0$, some $\mu_{\text{EE}}(x)$ must be non-zero, and by (23) $\ln(\mu_{\text{EE}}(x)/\mu_{\text{EE}}(y))$ is not infinite. Hence we may divide (23) by $\mu_{\text{EE}}(x)$ and we find

$$\ln\mu_{\text{EE}}(y) + \rho^x(H(y)) \geq \ln\mu_{\text{EE}}(x) + \rho^x(H(x)) \quad . \tag{26}$$

In these terms, the energy-entropy condition on μ_{EE} is that, for every x, there is a state ρ^x on $\mathcal{A}_{\text{ext}}$ such that (26) holds for all y. We consider first the case $x = 1$. Then, using the equations (24) and (25), we conclude that there is a vector $\xi \in \widetilde{\ln}\,\mathcal{E}_{\text{AH}}$, namely $\xi_y = \rho^x(H(1) - H(y))$, such that $\widetilde{\ln}\,\mu_{\text{EE}} - \xi$ lies in the cone C_1 of coordinatewise positive

vectors in $\mathbb{R}^{n-1}$. In shorthand notation, this is written as $\widetilde{\ln}\,\mu_{\rm EE} \in \widetilde{\ln}\,\mathcal{E}_{\rm AH} + C_1$, where, as usual, the sum on the right is to be interpreted as $\left\{\xi+\eta \,\middle|\, \xi \in \widetilde{\ln}\,\mathcal{E}_{\rm AH},\ \eta \in C_1\right\}$. The conditions for $x > 1$ can be written in a similar form after subtracting $\ln \mu_{\rm EE}(1) + \rho^x(H(1))$ from both sides of the inequality when $x \neq y$. Thus, with the cones

$$C_x = \begin{cases} \{\xi \in \mathbb{R}^{n-1} \,|\, \forall y\ \xi_y \geq 0\} & x = 1 \\ \{\xi \in \mathbb{R}^{n-1} \,|\, \forall y\ \xi_y \geq \xi_x \text{ and } \xi_x \leq 0\} & x > 1 \end{cases}, \tag{27}$$

we get the formula

$$\widetilde{\ln}\,\mathcal{E}_{\rm EE} = \bigcap_{x=1}^{n} (\widetilde{\ln}\,\mathcal{E}_{\rm AH} + C_x) \quad . \tag{28}$$

This construction is illustrated below in Example 5 (see Figure 4). An amazing feature of this set is that both $\widetilde{\ln}\,\mathcal{E}_{\rm EE}$ and its exponentiated version $\mathcal{E}_{\rm EE}$ are convex (see Sec. IV for the second statement). This seems to be in conflict with the non-linearity of the map $\widetilde{\ln}$. However, this conflict is resolved by considering the special form of the cones (27): the cone C_x corresponds to that subset of the state space in which $\ln \mu(x) \leq \ln \mu(y)$ for all y. Such inequalities survive exponentiation, i.e., the cone $C_x + \widetilde{\ln}\,\mu$ at μ corresponds in the state space to the set of probability distributions μ' such that $\mu'(x)/\mu(x) \leq \mu'(y)/\mu(y)$ for all y, which is a convex set.

VI. Examples

Since our main aim is to demonstrate the failure of the DLR-inclusion in the quantum case, our main results are in the form of examples demonstrating the success or failure of these ideas in various situations. We have chosen a succession of examples to illustrate various degrees of failure of the DLR-inclusion $\mathcal{E}_{\rm R} \subset \operatorname{conv} \mathcal{E}_{\rm AH}$. Mathematically, the strongest result is the last example, in which both the inside system $\mathcal{A}_{\rm int}$, and the boundary algebra $\mathcal{A}_{\rm bd}$ are classical, and $\mathcal{A}_{\rm ext}$ is the algebra of 3×3-matrices. However, this example is rather indirect, so we will give simpler, direct examples as well, hoping to help the reader to develop an intuition of what exactly goes wrong. We emphasize that, while we treat only finite systems, our results are equally valid for infinite outside systems. In fact, every example that we give can easily be enlarged to an example with infinite outside. In the same spirit we are looking mostly for examples with classical $\mathcal{A}_{\rm int}$: usually these can be expanded easily to examples with non-commutative $\mathcal{A}_{\rm int}$. Moreover, they are simpler to treat and, being closer to the classical DLR-situation, they bring the failure of the quantum generalization into sharper focus. In producing the examples we found the help of a computer algebra program [**15**] a very valuable tool.

The symbols in the heading of each example are a shorthand for the type of algebras used. Thus "Q5C3" is an example with a quantum inside with $\mathcal{A}_{\rm int} = \mathcal{M}_5$, and an interaction H contained in a subalgebra of $\mathcal{A}_{\rm int} \otimes \mathcal{A}_{\rm bd}$, which is isomorphic to $\mathcal{A}_{\rm int} \otimes \mathcal{C}(\{1,2,3\})$, i.e., the inside system interacts with 3 classical configurations. Of course, we will mostly assume that the whole algebra $\mathcal{A}_{\rm ext}$ is not commutative, since otherwise

the DLR-theory would simply be valid. If the number of configurations or Hilbert space dimensions is irrelevant, we just write "n". Each example begins with a short description of the model and of the claims about various inclusions to be seen in this example (set in *italics*), followed by the verification of these claims and some additional remarks.

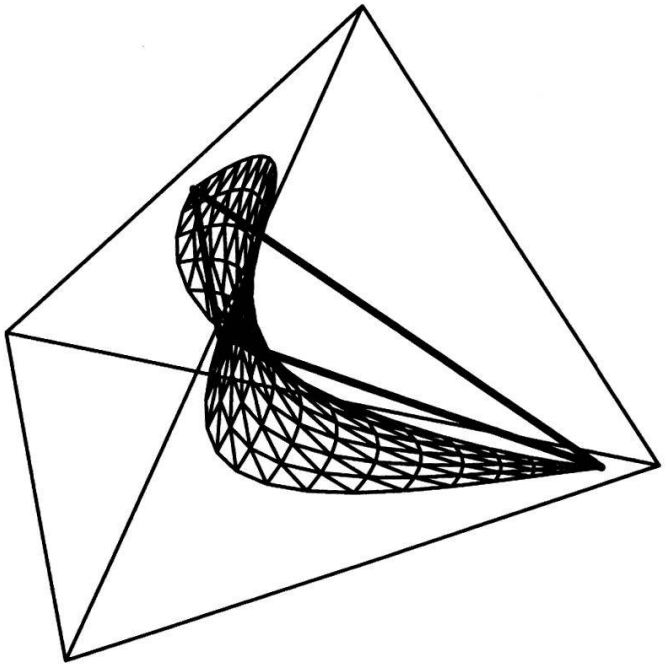

Figure 1 (for Example 1): state space of $C(\{1,2,3,4\})$ with $\mathcal{E}_{\mathrm{AH}}$ embedded. The triangle is $\mathrm{conv}\,\mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}} = \mathcal{E}_{\mathrm{R}}$.

Example 1: C4C3; $\mathcal{A}_{\mathrm{ext}}$ classical

With this example, where $\mathcal{A}_{\mathrm{ext}}$ is Abelian, we demonstrate that $\mathrm{conv}\,\mathcal{E}_{\mathrm{AH}} \not\subset \mathrm{conv}\,\mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}}$. *It also serves to illustrate the lack of any definite convexity properties of the map which takes Hamiltonians to Gibbs distributions (see Figure 1). Explicitly, the interaction is given by the matrix $H(x,y)$, $x = 1,2,3,4$, $y = 1,2,3$, as*

$$H = \begin{pmatrix} 0 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \\ 1 & 0 & -1 \end{pmatrix} .$$

The numerical evaluation in this example is straightforward, and the result is shown in Figure 1. We include this example mainly to illustrate a remark made in Sec. II, namely that, due to the non-linearity of the exponentiation map, general averaged Hamiltonians (6) do not give equilibrium states inside the DLR-triangle $\mathcal{E}_{\mathrm{R}}$, which is also marked in the figure.

Example 2: C2Qn

When the inside system is a single Ising spin and the outside is arbitrary, the DLR-inclusion holds, namely

$$\mathcal{E}_{\mathrm{R}} = \mathcal{E}_{\mathrm{AH}} = \mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}} \quad .$$

The Hamiltonian is specified by two Hermitian $H(1), H(2) \in \mathcal{M}_n$. Then, by (25), $\widetilde{\ln}\,\mathcal{E}_{\mathrm{AH}}$ is just the set of numbers $\rho(H(1) - H(2))$, where ρ ranges over all states of $\mathcal{A}_{\mathrm{ext}}$. Thus $\widetilde{\ln}\,\mathcal{E}_{\mathrm{AH}}$ is the interval $[\eta_-, \eta_+]$, with endpoints given by the largest and smallest eigenvalues of $H(1) - H(2)$, i.e., the smallest η_+ and the largest η_- such that $\eta_- \mathbb{1} \leq H(1) - H(2) \leq \eta_+ \mathbb{1}$. Moreover, the same interval is obtained if we restrict the states ρ to be pure, i.e., $\mathcal{E}_{\mathrm{AH}} = \mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}} = [\eta_-, \eta_+]$.

On the logarithmic scale, $\mu_{\mathrm{RE}}^V \in \mathcal{E}_{\mathrm{R}}$ from (10), is given by the single number

$$\eta(V) = \ln \mathrm{Tr} \exp -(H(2) + V) - \ln \mathrm{Tr} \exp -(H(1) + V) \quad .$$

Now the function $A \mapsto \ln \mathrm{Tr} \exp(-A)$ is monotonely decreasing with respect to the operator ordering for A. Moreover, $\ln \mathrm{Tr} \exp(-A - \eta \mathbb{1}) = \ln \mathrm{Tr} \exp(-A) - \eta$. Since $H(2) \leq H(1) - \eta_- \mathbb{1}$, we get $\eta(V) \geq \eta_-$. Similarly, we get the upper bound $\eta(V) \leq \eta_+$. Hence $\mathcal{E}_{\mathrm{R}} \subset [\eta_-, \eta_+] = \mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}}$, and, from the general arguments in Sec. III concerning large potentials, we get the inclusion $\mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}} \subset \mathcal{E}_{\mathrm{R}}$, and hence equality.

Example 3: Q2Q2

We now replace the Ising spin of the inside system by a quantum mechanical spin-$\frac{1}{2}$, i.e., we take $\mathcal{A}_{\mathrm{int}} = \mathcal{M}_2$. For the outside, we will also have $\mathcal{A}_{\mathrm{ext}} = \mathcal{M}_2$, and define the Hamiltonian by

$$H(\alpha, \gamma) = \sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2 + \gamma\, \sigma_3 \otimes \sigma_3 - \alpha\, \sigma_3 \otimes \mathbb{1} \quad , \tag{29}$$

where $\alpha > 0$ and $\gamma \geq 0$ are parameters, and σ_i, $i = 1, 2, 3$ are the usual Pauli matrices. We claim that, in this model, the reduced equilibrium state $\omega_{\mathrm{int}}^0 \in \mathcal{E}_{\mathrm{R}}\big(\beta H(\alpha, \gamma)\big)$, where the superscript 0 denotes that the potential V is vanishing, is not contained in $\mathrm{conv}\, \mathcal{E}_{\mathrm{AH}}\big(\beta H(\alpha, \gamma)\big)$. *Hence the DLR-inclusion fails in the following cases:*

(1) $\beta = 3$, $\alpha = .3$, $\gamma = .05$ (see Figure 2)
(2) $\gamma = 0$, and all $\beta > 0$,
(3) for $0 \leq \gamma \leq .8$, and $\beta = \infty$, i.e., for ground states.

What makes this operator tractable is that it commutes with SU(2)-rotations around the 3-axis. In the joint eigenbasis of $\sigma_3 \otimes \mathbb{1}$ and $\mathbb{1} \otimes \sigma_3$ it corresponds to the matrix

$$H(\alpha, \gamma) = \begin{pmatrix} -\alpha + \gamma & 0 & 0 & 0 \\ 0 & -\alpha - \gamma & 2 & 0 \\ 0 & 2 & \alpha - \gamma & 0 \\ 0 & 0 & 0 & \alpha + \gamma \end{pmatrix} \quad .$$

The partition function for $H(\alpha,\gamma)$ and the expectation of $\sigma_3 \otimes \mathbb{I}$ are readily computed:

$$\begin{aligned} \mathcal{Z}(\beta,\alpha,\gamma) &= \operatorname{Tr} e^{-\beta H(\alpha,\gamma)} = 2e^{-\beta\gamma}\ \cosh(\beta\alpha) + 2e^{\beta\gamma}\ \cosh(\beta R_1) \\ \omega^0_{\mathrm{int}}(\sigma_3) &= \frac{1}{\beta}\frac{\partial}{\partial\alpha}\ln \mathcal{Z}(\beta,\alpha,\gamma) \\ &= \frac{\alpha e^{\beta(\alpha+2\gamma)}\left(e^{2\beta R_1}-1\right) + R_1 e^{\beta R_1}\left(e^{2\alpha\beta}-1\right)}{R_1\left(e^{\beta(\alpha+2\gamma)} + e^{\beta R_1} + e^{\beta(2\alpha+R_1)} + e^{\beta(\alpha+2\gamma+2R_1)}\right)} \quad , \end{aligned} \tag{30}$$

where $R_1 = \sqrt{4+\alpha^2}$. Since $H(\alpha,\gamma)$ commutes with rotations around the 3-axis, so does ω^0_{int}, and hence it is completely determined by the expectation of σ_3.

If $\rho = \frac{1}{2}\begin{pmatrix} 1+x_3 & x_1-ix_2 \\ x_1+ix_2 & 1-x_3 \end{pmatrix}$, with $x_i \in \mathbb{R}$ and $\sum_i x_i^2 \leq 1$, is a 2×2-density matrix, we find

$$\mathbb{E}^\rho(H(\alpha,\gamma)) = \begin{pmatrix} -\alpha+\gamma x_3 & x_1-ix_2 \\ x_1+ix_2 & \alpha-\gamma x_3 \end{pmatrix} \quad .$$

The equilibrium state $\omega^\rho_{\mathrm{AH}}$ of $\mathbb{E}^\rho(H(\alpha,\gamma))$ can be evaluated with the formula

$$\frac{e^{-\beta H}}{\operatorname{Tr} e^{-\beta H}} = \frac{1}{2}\mathbb{I} - \frac{\tanh\beta\sqrt{\det H}}{2\sqrt{\det H}}\ H \tag{31}$$

for H a traceless 2×2-matrix. $\mathcal{E}_{\mathrm{AH}}$ is now a body in the state space of $\mathcal{M}_2$, parametrized by the triple (x_1,x_2,x_3) determining ρ. It is the image of an ellipsoid in the space of 2×2 Hamiltonians under the non-linear map (31). This map preserves the symmetry under rotations around the 3-axis, hence $\mathcal{E}_{\mathrm{AH}}$ will also have this symmetry. Figure 2 shows a section of $\mathcal{E}_{\mathrm{AH}}$ in the $(1,3)$-plane of the state space. It has to be completed by rotating it around the vertical axis, thus making $\mathcal{E}_{\mathrm{AH}}$ the shape of a mushroom. The point marked on the axis is ω^0_{int}. It is clearly not contained in the convex hull of $\mathcal{E}_{\mathrm{R}}$.

At high temperature (small β) one can expand all exponentials, and one finds that, in first order in β and as long as $\gamma \neq 0$, the convex hull of $\mathcal{E}_{\mathrm{AH}}$ does contain ω^0_{int}. However, if $\gamma = 0$, the first orders coincide, and we get

$$\omega^\rho_{\mathrm{AH}}(\sigma_3) - \omega^0_{\mathrm{int}}(\sigma_3) \geq \frac{\alpha}{3}(2-x_1^2-x_2^2)\ \beta^3 + \mathbf{O}(\beta^5) > 0 \quad .$$

Hence the DLR-inclusion fails even for small β, and it can be seen numerically that, with $\gamma = 0$, it fails for all $\beta \geq 0$.

In the opposite direction, as β grows, the points in $\mathcal{E}_{\mathrm{AH}}$ move radially out to the extreme boundary of the state space and, in the limit, we obtain the pure ground states of the Hamiltonians $\mathbb{E}^\rho(H(\alpha,\gamma))$. Hence, for $\beta = \infty$

$$\omega^\rho_{\mathrm{AH}}(\sigma_3) = \frac{\alpha-\gamma x_3}{\sqrt{x_1^2+x_2^2+(\alpha-\gamma x_3)^2}} \geq \frac{\sqrt{\alpha^2-\gamma^2}}{\sqrt{1+\alpha^2-\gamma^2}} \quad ,$$

where the second expression is the minimum of the first with respect to variation of the x_i, attained for $x_1^2+x_2^2 = 1-x_3^2$ and $x_3 = \gamma/\alpha$. The limit $\beta\to\infty$ of ω^0_{int} can be obtained

directly from (30): of all the exponents appearing in this equation, $\beta(\alpha + 2\gamma + 2R_1)$ is clearly the largest, so the limit is α/R_1, or

$$\omega^0_{\rm int}(\sigma_3) = \frac{\alpha}{\sqrt{4+\alpha^2}} \quad .$$

Hence, for all ρ, we have

$$\omega^\rho_{\rm AH}(\sigma_3) > \omega^0_{\rm int}(\sigma_3) \quad \text{for } \beta = \infty \text{ and } 0 \le \gamma < \tfrac{\sqrt{3}}{2}\alpha \quad .$$

Thus the DLR-inclusion fails in general for quantum ground states. For this conclusion it is crucial that both systems are non-classical. In our further examples we will always take $\mathcal{A}_{\rm int}$ Abelian. The pure states of the tensor product $\mathcal{A}_{\rm int} \otimes \mathcal{A}_{\rm ext}$, such as the extremal ground states of H, are then product states and can be found by minimizing $\mathbb{E}^\rho(H)$ for each ρ. Thus, for classical $\mathcal{A}_{\rm int}$, the ground state DLR-inclusion holds.

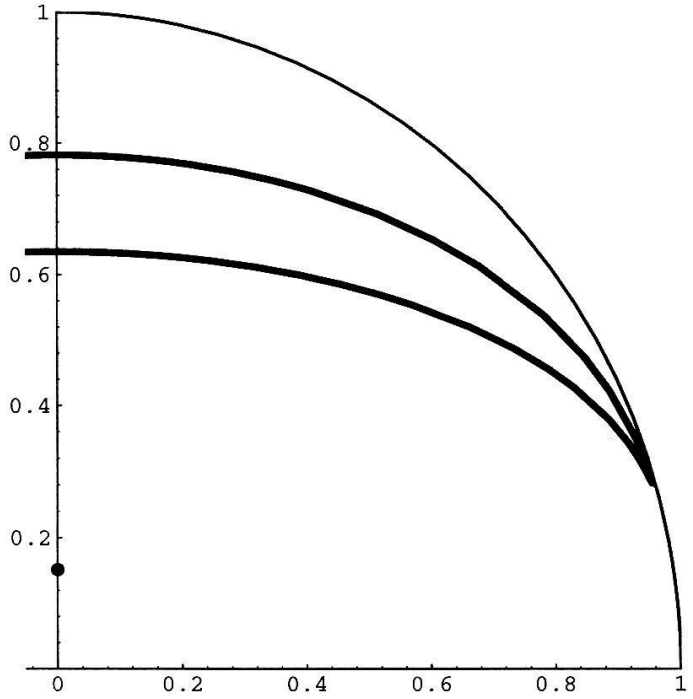

Figure 2 (for Example 3): section of state space, with $\mathcal{E}_{\rm AH}$ marked ($\beta = 3$, $\alpha = 0.3$, $\gamma = 0.05$). The point on the vertical axis is $\omega^0_{\rm int}$. It is not contained in the convex hull of $\mathcal{E}_{\rm AH}$.

Example 4: QnCm; $\mathcal{A}_{\rm ext} = \mathcal{A}_{\rm bd} \otimes \mathcal{B}$

The DLR-inclusion $\mathcal{E}_{\rm R} = \operatorname{conv} \mathcal{E}^{\rm pure}_{\rm AH}$ holds when the boundary algebra is purely classical and when the exterior algebra $\mathcal{A}_{\rm ext}$ factorizes into a tensor product $C(Y_{\rm bd}) \otimes \mathcal{B}$, $\mathcal{B}$ arbitrary.

From the general argument of Sec. II we always have $\operatorname{conv} \mathcal{E}^{\rm pure}_{\rm AH} \subset \mathcal{E}_{\rm R}$. Conversely, with $H_{\rm tot} = H + \mathbb{1} \otimes V$, H and V functions from $Y_{\rm bd}$ to $\mathcal{A}_{\rm int}$ and $\mathcal{B}$, we have for any $A \in \mathcal{A}_{\rm int}$

$$\sum_{y \in Y_{\rm bd}} \operatorname{Tr}_{\mathcal{A}_{\rm int} \otimes \mathcal{B}} \left(e^{-(H+V)} A \right) = \sum_{y \in Y_{\rm bd}} \operatorname{Tr}_{\mathcal{B}} \left(e^{-V(y)} \right) \operatorname{Tr}_{\mathcal{A}_{\rm int}} \left(e^{-H(y)} A \right) \quad .$$

But this precisely means that $\mathcal{E}_{\mathrm{R}} \subset \operatorname{conv} \mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}}$. From Example 1 it becomes clear that generally $\operatorname{conv} \mathcal{E}_{\mathrm{AH}}^{\mathrm{pure}}$ is strictly contained in $\operatorname{conv} \mathcal{E}_{\mathrm{AH}}$. Therefore the inclusion $\operatorname{conv} \mathcal{E}_{\mathrm{AH}} \subset \mathcal{E}_{\mathrm{R}}$, that holds if we allow for general embeddings of $\mathcal{C}(Y_{\mathrm{bd}})$ in an exterior algebra $\mathcal{A}_{\mathrm{ext}}$, is reversed if we restrict ourselves to product systems $\mathcal{A}_{\mathrm{int}} \otimes \mathcal{C}(Y_{\mathrm{bd}}) \otimes \mathcal{B}$.

A special case of this example is the case where all of $\mathcal{A}_{\mathrm{ext}}$ is classical. The representation of equilibrium states by conditioning with respect to a classical outside is reminiscent of the work [**16**]. In that project one also considers quantum systems split into inner and outer region. The aim is then to represent general quantum states as integrals of states conditioned with respect to a classical subalgebra in the outside region. In the present, finite-dimensional setting, this is a trivial operation.

Example 5: C3Q2; $\mathcal{A}_{\mathrm{ext}} = \mathcal{M}_2$

By Example 2, the smallest non-trivial case of a classical inside algebra is $\mathcal{A}_{\mathrm{int}} = \mathcal{C}(\{1,2,3\})$ *and we stay with* $\mathcal{A}_{\mathrm{ext}} = \mathcal{M}_2$ *i.e., we consider only the subset* $\mathcal{E}_{\mathrm{R}}(\mathcal{M}_2) \subset \mathcal{E}_{\mathrm{R}}$ *of reduced equilibrium states coming from potentials* $V \in \mathcal{M}_2$. *Thus* H *is given by three* 2×2*-matrices, which we choose as*

$$H(1) = 0 \quad , \quad H(2) = \frac{3}{2}\sigma_3 \quad , \quad \textit{and} \quad H(3) = \frac{3}{2}\sigma_1 \quad .$$

In this example, we will determine the three sets $\mathcal{E}_{\mathrm{AH}} \subset \mathcal{E}_{\mathrm{R}}(\mathcal{M}_2) \subset \mathcal{E}_{\mathrm{EE}}$ *explicitly and show that both inclusions are strict (see Figure 3).*

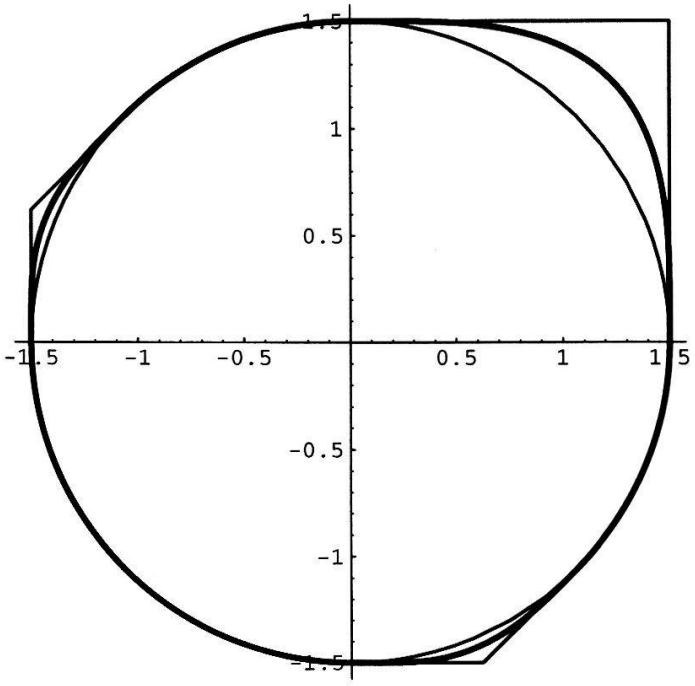

Figure 3 (for Example 5): state space of $\mathcal{M}_2$ in logarithmic scale; inner circle is $\widetilde{\ln}\, \mathcal{E}_{\mathrm{AH}}$, extension by curves is $\widetilde{\ln}\, \mathcal{E}_{\mathrm{R}}(\mathcal{M}_2)$, angles determine $\widetilde{\ln}\, \mathcal{E}_{\mathrm{EE}}$.

The averaged Hamiltonians $\mathbb{E}^{\rho}(H)$ depend only on the two expectations $\rho(\sigma_3)$ and $\rho(\sigma_1)$, and therefore form a two-dimensional disc in the space of Hamiltonians. Note that,

because $\rho(\sigma_2)$ does not enter, we get the same disc when Hamiltonians are averaged only by pure states ρ. The disc of Hamiltonians is (up to a factor) identical with $\widetilde{\ln}\,\mathcal{E}_{\mathrm{AH}}$ (see the circle in Figure 3).

In the logarithmic scale μ^V_{RE} is given by a point in the plane with coordinates

$$\eta(V) = \widetilde{\ln}\,\mu^V_{\mathrm{RE}} = \begin{pmatrix} \ln \mathrm{Tr}\, \exp(-H(2) - V) - \ln \mathrm{Tr}\, \exp(-V) \\ \ln \mathrm{Tr}\, \exp(-H(3) - V) - \ln \mathrm{Tr}\, \exp(-V) \end{pmatrix} .$$

By choosing some random V, it is easy to convince oneself that in this example $\mathcal{E}_{\mathrm{R}}(\mathcal{M}_2) \not\subset \mathcal{E}_{\mathrm{AH}}$, i.e., we get points outside the circle in Figure 3. The precise determination of $\mathcal{E}_{\mathrm{R}}(\mathcal{M}_2)$ is more difficult. Consider the map $V \mapsto \eta(V)$. We know that, as $\lambda \to \infty$, $\eta(\lambda V)$ approaches a point in $\mathcal{E}_{\mathrm{AH}}$. Therefore the boundary points of $\mathcal{E}_{\mathrm{R}}(\mathcal{M}_2)$ must be of the form $\eta(V)$ with finite V, and at such points the map η must be singular, more precisely, the rank of the Jacobian must be one. It turns out that this can happen only in the plane $V = x\sigma_1 + z\sigma_3$, along three disjoint arcs. Each of these arcs extends to infinity, and describes a piece of the boundary of $\mathcal{E}_{\mathrm{R}}(\mathcal{M}_2)$ connecting with the boundary of $\mathcal{E}_{\mathrm{AH}}$. Solving for the critical points in the (x, z)-plane can only be done numerically and the result is shown in Figure 3.

In this example we can also evaluate the energy-entropy inequalities (23). Using the general method outlined in Sec. V, we obtain $\widetilde{\ln}\,\mathcal{E}_{\mathrm{EE}}$ as the intersection of the three convex sets shown in Figure 4. The result is also included in Figure 3 for easier comparison.

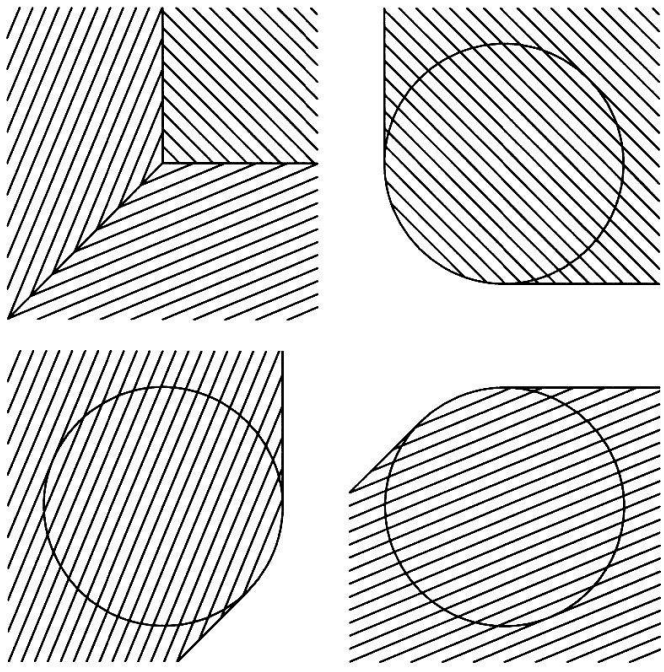

Figure 4 (for Example 5): upper left: the cones C_1, C_2, C_3 from (27). Remaining panels: $\widetilde{\ln}\,\mathcal{E}_{\mathrm{AH}} + C_i$, $i = 1, 2, 3$. The intersection of these sets is shown in Figure 3.

Example 6: C3C2

In the previous example the algebra $\mathcal{A}_{\rm bd}$ was non-Abelian. We now move still closer to the classical DLR-situation by requiring this algebra to be Abelian too. We will retain the choice $\mathcal{A}_{\rm int} = C(\{1,2,3\})$ of the previous example, but set $\mathcal{A}_{\rm bd} = C(\{1,2\})$. More generally, the considerations of this example are valid if $\mathcal{A}_{\rm int} = C(\{1,2,3\})$ and if the three operators $H(x) \in \mathcal{A}_{\rm ext}$, determining the interaction, are of the form

$$H(x) = h_0 + a_x h_1 + b_x \mathbb{1} \quad ,$$

for some Hermitian $h_0, h_1 \in \mathcal{A}_{\rm ext}$ and real constants a_x, b_x. We then find that the DLR-inclusion holds, i.e., $\mathcal{E}_{\rm R} = \operatorname{conv} \mathcal{E}_{\rm AH}$. Moreover, the inclusion $\mathcal{E}_{\rm R} \subset \mathcal{E}_{\rm EE}$ is strict (see Figure 5).

Without loss of generality, we can take $a_2 \geq a_1 \geq a_3$. Then we can find a λ, $0 \leq \lambda \leq 1$, such that

$$H(1) = \lambda H(2) + (1-\lambda) H(3) + \tilde{y}\mathbb{1} \quad , \tag{32}$$

where $\tilde{y} = b_1 - \lambda b_2 - (1-\lambda) b_3$. Hence, we have

$$\ln \mu(1) = \lambda \ln \mu(2) + (1-\lambda) \ln \mu(3) - \tilde{y} \quad , \quad \text{for} \quad \mu \in \mathcal{E}_{\rm AH} \quad . \tag{33}$$

Thus $\mathcal{E}_{\rm AH}$ lies on a line in the state space, which appears straight on the logarithmic scale. The set $\mathcal{E}_{\rm AH}$ is parametrized by the expectation $\rho(h_1)$ in arbitrary states ρ of $\mathcal{A}_{\rm ext}$ and the extremal eigenvalues $\eta_\pm$ of h_1 (i.e., the best constants with $\eta_- \mathbb{1} \leq h_1 \leq \eta_+ \mathbb{1}$) determine the $\mathcal{E}_{\rm AH}$ as a segment of that line. An alternative description of the endpoints is by the equation of the line passing through them, or equivalently, by the coefficients c_2, c_3 of the linear inequality

$$\mu(1) \geq c_2 \mu(2) + c_3 \mu(3) \quad , \tag{34}$$

which becomes an equality precisely at these endpoints. Inserting the known endpoints $\mu_\pm$ and solving the linear system, we find

$$c_2 = \frac{e^{\eta_-(a_2-a_1)+\eta_+(a_2-a_1)+(b_2-b_1)} \left(e^{\eta_-(a_3-a_1)} - e^{\eta_+(a_3-a_1)} \right)}{e^{\eta_+(a_2-a_1)+\eta_-(a_3-a_1)} - e^{\eta_-(a_2-a_1)+\eta_+(a_3-a_1)}}$$

$$c_3 = \frac{e^{\eta_-(a_3-a_1)+\eta_+(a_3-a_1)+(b_3-b_1)} \left(e^{\eta_+(a_2-a_1)} - e^{\eta_-(a_2-a_1)} \right)}{e^{\eta_+(a_2-a_1)+\eta_-(a_3-a_1)} - e^{\eta_-(a_2-a_1)+\eta_+(a_3-a_1)}} \quad .$$

The only information we will need from these formulas is that, since $\eta_+ \geq \eta_-$ and $a_2 \geq a_1 \geq a_3$, both constants are positive. This implies that, for all η with $\eta_- \leq \eta \leq \eta_+$,

$$e^{-a_1\eta - b_1} \geq c_2 e^{-a_2\eta - b_2} + c_3 e^{-a_3\eta - b_3} \quad .$$

Indeed, this is an equality for $\eta = \eta_+$ and $\eta = \eta_-$ and follows for the intermediate values by multiplying both sides with $e^{a_1\eta}$ and invoking the convexity of the exponential function. Since $\rho(h_1) \in [\eta_-, \eta_+]$ for all states ρ on $\mathcal{A}_{\rm ext}$, we find that $\mathcal{E}_{\rm AH}$ is the set of probability distributions satisfying equation (33) and inequality (34). (See the thick line in Figure 5).

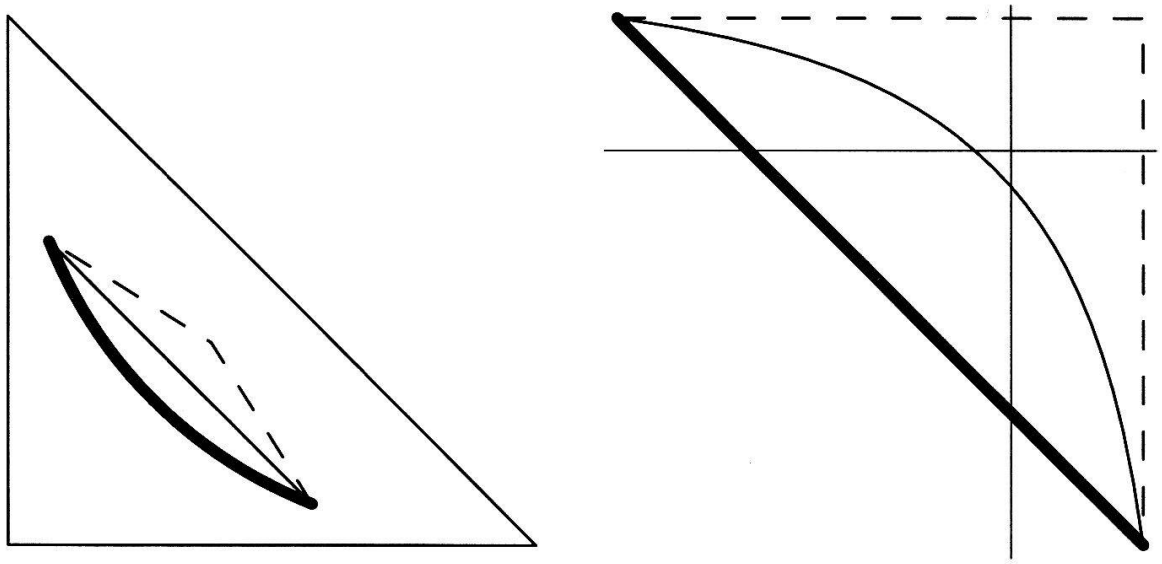

Figure 5 (for Example 6): left panel: state space of $C(\{1,2,3\})$; right panel: same figure in logarithmic coordinates (same orientation). Thick line is $\mathcal{E}_{\mathrm{AH}}$, lens shape is $\mathcal{E}_{\mathrm{R}}$, and dashed corners together with $\mathcal{E}_{\mathrm{AH}}$ are the boundary of $\mathcal{E}_{\mathrm{EE}}$.

On the other hand, since the interval $[\eta_-, \eta_+]$ contains the spectrum of h_1 and both $(H(1) - H(2))$ and $(H(1) - H(3))$ are functions of h_1, we obtain from (32) the operator inequality

$$\mathbb{1} \geq c_2\, e^{H(1)-H(2)} + c_3\, e^{H(1)-H(3)} \quad .$$

Combining this with the Golden-Thompson inequality [**17**], i.e.,

$$\mathrm{Tr} \exp(A + B) \leq \mathrm{Tr}(\exp(A)\, \exp(B)) \quad ,$$

we get

$$\begin{aligned} c_2\, \mathrm{Tr}\, e^{-H(2)-V} &+ c_3\, \mathrm{Tr}\, e^{-H(3)-V} \\ &= c_2\, \mathrm{Tr}\, e^{(H(1)-H(2))-(H(1)+V)} + c_3\, \mathrm{Tr}\, e^{(H(1)-H(3))-(H(1)+V)} \\ &\leq \mathrm{Tr} \left(c_2\, e^{H(1)-H(2)} + c_3\, e^{H(1)-H(3)} \right) e^{-H(1)-V} \\ &\leq \mathrm{Tr}\, e^{-H(1)-V} \quad . \end{aligned}$$

Hence, all probability distributions $\mu \in \mathcal{E}_{\mathrm{R}}$ also satisfy inequality (34). On the other hand, we may use the convexity of the function $A \mapsto \ln \mathrm{Tr} \exp(-A)$, together with (32) to obtain that, for $\mu \in \mathcal{E}_{\mathrm{R}}$,

$$\ln \mu(1) \leq \lambda \ln \mu(2) + (1 - \lambda) \ln \mu(3) - \widetilde{y} \quad .$$

Thus we have shown the DLR-inclusion $\mathcal{E}_{\mathrm{R}} \subset \mathcal{E}_{\mathrm{AH}}$. The determination of $\mathcal{E}_{\mathrm{EE}}$ uses the method described in Sec. V and illustrated in Figure 4.

Example 7: CnC3

The previous example might have nourished the hope that, at least for purely classical interactions ($\mathcal{A}_{\rm bd}$ Abelian), the DLR-inclusion might survive. What we will show now, however, is that $\mathcal{E}_{\rm R} \not\subset \operatorname{conv} \mathcal{E}_{\rm AH}$ in this case. The proof of the following Proposition is based on the failure of a well-known failed conjecture, which was disproved by Gaudin [18].

Proposition. *Let $\mathcal{A}_{\rm ext} = \mathcal{M}_3$, and denote by $\mathcal{D}_3$ the subalgebra of diagonal matrices. There exist an $n \in \mathbb{N}$ and a Hamiltonian $H \in \mathcal{C}(\{1,\ldots,n\}) \otimes \mathcal{D}_3$ such that the DLR-inclusion $\mathcal{E}_{\rm R} \subset \operatorname{conv} \mathcal{E}_{\rm AH}$ does not hold.*

Proof: We will show that the validity of the DLR-inclusion would imply for any Hermitian 3×3-matrix V the existence of a positive measure μ_V on $\mathbb{R}^3$ such that

$$\operatorname{Tr} \exp\left(- \begin{pmatrix} x_1 & 0 & 0 \\ 0 & x_2 & 0 \\ 0 & 0 & x_3 \end{pmatrix} - V \right) = \int \mu_V(d\lambda_1\, d\lambda_2\, d\lambda_3)\; e^{-\sum \lambda_i x_i} \quad . \tag{35}$$

We may paraphrase this by saying that the expression $\operatorname{Tr} \exp A$, considered as a function of the diagonal matrix elements of A, is the Laplace transform of a positive measure. This is precisely the statement investigated by Gaudin [18] and proven to be wrong for suitable V. Hence the DLR-inclusion fails for such V.

It remains to prove (35) assuming the validity of the DLR-inclusion. By $E_i \in \mathcal{D}_3$ we denote the matrix with "1" in the $i^{\rm th}$ place of the diagonal, and all other entries zero. For $x \in \mathbb{R}^3$ we set $H(x) = \sum_{i=1}^3 x_i E_i$. Consider a finite subset $X \subset \mathbb{R}^3$. Then $H(x)$ defines an interaction $H \in \mathcal{C}(X) \otimes \mathcal{D}_3$. The left hand side of equation (35) is $\mu^V_{\rm RE}(x)$, for $x \in X$. On the other hand, the average of H with respect to a state on $\mathcal{M}_3$ (or, equivalently, a state on $\mathcal{D}_3$) is characterized by three numbers $\lambda_i \geq 0$ with $\sum_i \lambda_i = 1$, and $\mathbb{E}^\lambda(H)(x) = \sum_i \lambda_i x_i$. As we assumed the inclusion $\mathcal{E}_{\rm R} \subset \mathcal{E}_{\rm AH}$, we can find a measure μ^X_V with finite support such that equation (35) holds for all $x \in X$ with μ^X_V for μ_V. Now consider the net of finite subsets of $X \subset \mathbb{R}^3$, ordered by inclusion. We may assume that each X contains the origin, so that each one of the associated measures μ^X_V is normalized to the same constant $\operatorname{Tr} \exp(-V)$. Then, by weak*-compactness, we find an accumulation point μ_V of this net of measures and it is clear that equation (35) holds for this measure and all $x \in \mathbb{R}$.

■

Rather than considering the expression $\operatorname{Tr} \exp A$ as a function of its n diagonal elements, one can also study this expression along a single straight line in the space of Hermitian $n \times n$-matrices. The following conjecture about this situation was formulated by Bessis, Moussa, and Villani in 1975 [19]:

Conjecture. *Let A and B be Hermitian $n \times n$-matrices. Then there is a positive measure μ such that*

$$\mathrm{Tr}\, e^{A+tB} = \int \mu(d\beta)\, e^{\beta t} \quad .$$

A, possibly signed, measure μ satisfying this equation always exists and is uniquely determined by A and B. Hence, the issue is only the positivity of this measure. Despite many attempts, this conjecture is still open, even for $n = 3$. It is true for $n = 2$ and whenever A has positive matrix off-diagonal elements in an eigenbasis of B [**19**]. Moreover, it is true for sufficiently small A [**20**]. The measure μ is known to have support in the convex hull of the eigenvalues of B and to have a positive atomic part, supported by the eigenvalues themselves. A review of the existing partial results, together with some new ones, is in preparation [**20**].

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