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# The Gibbs Variational Principle for Inhomogeneous Mean-Field Systems

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*Abstract.* We show the existence of the limiting free-energy density of inhomogeneous (“site- dependent coupling”) mean-field models in the thermodynamic limit, and derive a variational formula for this quantity. The formula requires the minimization of an energy term plus an entropy term as a functional depending on a function with values in the one-particle state space. The minimizing functions describe the pure phases of the system, and all cluster points of the sequence of finite volume equilibrium states have unique integral decomposition into pure phases. Applications are considered; they include the full BCS-model, and random mean-field models.

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## I. Introduction

Since Haag's pioneering paper [18] the BCS model has attracted the attention of many mathematical physicists. Haag and others [26] focussed on the simplifying features of the model in infinite volume, but did not attempt to control the thermodynamic limit. This was done first by Thirring and Wehrl [36] for the strong-coupling limit of the model. The main simplifying feature of this version of the BCS model is that the coupling constants do not depend on momentum, i.e. it is a homogeneous model in the terminology used in this paper, as opposed to the inhomogeneous full BCS model. Progress on the general inhomogeneous case proved to be difficult, and was mostly achieved by N.N.Bogoliubov and his school (see [5] and the references therein). It was only in 1988, in the work of Duffield and Pulé [13], that a rigorous derivation of a variational formula for the free-energy density was given. The Duffield-Pulé method for inhomogeneous mean-field systems, which has also been applied to the Overhauser model [14], the full spin-boson model [30] and some random mean-field models [12], combines Bogoliubov's Approximating Hamiltonian Method [5] with ideas of Cegła, Lewis and Raggio [9]. These authors had shown that a large deviation treatment of the measures arising from the multiplicities of the irreducible representations of  $SU(2)$  in the decomposition of the total spin, combined with the use of the Berezin-Lieb inequalities, streamlines the treatment of the thermodynamics of homogeneous mean-field models such as the strong-coupling BCS model.

Often the term “mean-field” system is used for a sequence of finite systems, indexed by the total particle number  $n$ , such that the interaction is a fixed two-body potential multiplied by  $n^{-1}$ . In the Cegła-Lewis-Raggio approach, and already in [21], the connection between the Hamiltonians for different system size was given instead by expressing the Hamiltonian density for each  $n$  as the same polynomial in the generators of global spin rotations (compare also [6]). This idea can be extended to an arbitrary compact semisimple Lie group, the Large Deviation result necessary for completing the Cegła-Lewis-Raggio method in this general case having been obtained in [10].

An indication that even this generalized notion of mean-field systems misses an essential point came from the work of Petz, Raggio, and Verbeure [29], who managed to treat models in which the Hamiltonian density of the  $n$ -particle system is of the form  $f(X_n)$  with  $X_n = n^{-1}(x \otimes \mathbb{I} \otimes \cdots \otimes \mathbb{I} + \mathbb{I} \otimes x \otimes \mathbb{I} \otimes \cdots \otimes \mathbb{I} + \mathbb{I} \otimes \cdots \otimes \mathbb{I} \otimes x)$  for a fixed one-particle observable  $x$ , and  $f$  a fixed continuous function evaluated on  $X_n$  in the functional calculus (compare also [7]). The function  $f$  did not have to be a polynomial, and  $x$  did not have to be considered as one of the generators of an irreducible representation of a Lie group. In [31] we managed to bring these two sets of examples together into a simple general notion “mean-field” Hamiltonians. We require that the sequence  $H_n$  of Hamiltonian densities be

“approximately symmetric” in the sense that for large  $m$ , and  $n > m$ ,  $H_n$  is approximately obtained by symmetrizing  $H_m$  (considered as an observable of the  $n$ -particle system) with respect to all permutations of the  $n$  sites. This property is obvious for the generators of a product representation, and was shown [31, Appendix] to be preserved under the continuous non-commutative functional calculus.

The Large Deviation methods of [9], with their inherent limitation to models allowing a classical approximation, could be replaced in [31] as in [29] by estimates of quantum relative entropy, as defined by Araki [2,3]. Taking these ingredients together we obtained in [31] a Gibbs Variational Principle characterizing the limiting Gibbs states as states of the infinite volume system. This variational principle can be contracted to a variational principle on the one-particle state space by application of Størmer’s de Finetti-theorem [35].

In the case of inhomogeneous mean-field systems the Hamiltonian of the  $n$ -particle system depends on  $n$  external parameters. This dependence destroys the permutation symmetry, which was the key ingredient of the method developed in [31]. In this paper we show that our method can nevertheless be extended to the inhomogeneous situation. The basic idea for making this extension is the introduction of an auxiliary algebra of functions on the space of external parameters taking values in the one-particle algebra of the system. With respect to this algebra (first used by [4]) permutation symmetry is regained, and the techniques of [31] become applicable.

In order for the limiting free energy and limiting Gibbs states to exist, it is necessary to make an assumption about the asymptotic behaviour of the  $n$  external parameters of the  $n$ -particle system. We show that it suffices to assume that as  $n \rightarrow \infty$  these sets of parameters have a limiting density. This assumption is easily checked in the BCS model, where the external parameters are just the discrete momenta of the finite system belonging to the cutoff region. However, the limiting density assumption is also true with probability one, when the external parameters are random variables distributed according to some ergodic process. Thus our method also covers so-called site-random mean-field models [12]. We would like to stress, however, that we do not make use of probabilistic methods, and indeed our result is stronger than the usual statements of the theory of quenched random systems: we do not only prove convergence of the free energy for almost all samples of a random model, but also describe explicitly a set of measure one, on which convergence holds everywhere. This strengthening of almost everywhere convergence to a pointwise statement is essential for the application to the BCS model, since there the external parameters are explicitly given in terms of the geometry of the finite system.

Under these assumptions we obtain a characterization of the limiting Gibbs states



and a formula for the free energy density in terms of a Gibbs variational principle. As in [31] the variational problem can be contracted to a “one-particle” problem, or more precisely, a variation over functions from the space of external parameters to the state space of the one-particle observable algebra. This result was announced in [32]. A special case of this principle was also obtained by Blobel and Messer [4]. We briefly discuss the relation between their work and ours in section IV.3.

This paper is part of an ongoing project. The class of approximately symmetric sequences as the class of intensive variables appropriate to mean-field systems was also used in [16] to treat the dynamics of homogeneous mean-field systems. An extension to the dynamics of inhomogeneous systems, together with further examples and applications of the present paper, and a detailed discussion of different notions of “mean-field limit” for states can be found in [15]. A survey is to appear in [37].

The paper is organized as follows: the general class of inhomogeneous mean-field models is described in section II, which also contains the main result. The proof is given in section III; it relies on results obtained in [31], but we hope it is reasonably self-contained as to be intelligible. Section IV describes a series of applications.

## II. The models, and the results

To clarify the nature of the models to be considered, we present a specific example. The Hamiltonian of the full BCS-model in its quasi-spin version is given by (compare [13])

$$\mathcal{H}_n^{BCS}(\mathbf{k}_n) = \frac{1}{2} \sum_{i=1}^n \varepsilon(\mathbf{k}_{n,i}) (\mathbb{1} - \sigma_i^z) - \frac{1}{V_n} \sum_{i,j=1}^n \sigma_i^+ U(\mathbf{k}_{n,i}, \mathbf{k}_{n,j}) \sigma_j^- \quad ,$$

where  $\sigma_i^\alpha$  ( $\alpha = \pm, x, y, z$ ) denotes a copy of the Pauli-matrix  $\sigma^\alpha$  acting on the  $i^{\text{th}}$  component of the  $n$ -fold tensor product of the single-particle Hilbert space  $\mathbb{C}^2$ ,  $\mathbf{k}_n$  is a vector with  $n$  components, each taking values in momentum space  $\mathbb{R}^d$ ,  $\varepsilon$  and  $U$  are real-valued functions on  $\mathbb{R}^d$  and  $\mathbb{R}^d \times \mathbb{R}^d$  respectively, and  $V_n$  is the volume available to the  $n$  “spins” (i.e. Cooper pairs). It is assumed that the density  $n/V_n$  converges as  $n \rightarrow \infty$ . In our terminology, this is an inhomogeneous mean-field system. *Inhomogeneous*, because the single-particle energies  $\varepsilon(\mathbf{k}_{n,i})$ , and the inter-particle interactions (i.e. coupling-constants)  $U(\mathbf{k}_{n,i}, \mathbf{k}_{n,j})$  are particle-dependent (here via their momentum); and *mean-field* because of the factor  $1/V_n \propto 1/n$  multiplying the inter-particle interaction. The corresponding *homogeneous* model would be obtained if both  $\varepsilon$  and  $U$  were constant functions.

In order to extract the essential features of the above model, we formulate things in algebraic language. Although this introduces, necessarily, a certain degree of generality which need not be of value in the discussion of every specific physical model, it does help to rid oneself of unnecessary details. Moreover, this language is appropriate to identify and discuss the rôle of permutation symmetry, which, in our opinion, is the key to the mean-field nature of the models.

We introduce basic terminology and notation. We will consider  $C^*$ -algebras  $\mathcal{A}$  with identity  $\mathbb{1}$ , whose state space is denoted by  $K(\mathcal{A})$ . When  $\omega \in \mathcal{A}_+^*$  is a positive linear functional on  $\mathcal{A}$ , we write the state  $\omega(\mathbb{1})^{-1}\omega$  as  $\text{Norm}^{-1}\omega$ . The  $n$ -fold minimal  $C^*$ -tensor product  $\mathcal{A} \otimes \mathcal{A} \otimes \cdots \otimes \mathcal{A}$  of  $\mathcal{A}$  with itself is denoted by  $\mathcal{A}^n$ . The  $C^*$ -inductive limit of these algebras is denoted by  $\mathcal{A}^\infty$ . Whenever convenient,  $\mathcal{A}^n$  will be identified with a subalgebra of  $\mathcal{A}^m$  for  $n \leq m \leq \infty$ . There is a natural action of the permutations of  $\{1, \dots, n\}$  as automorphisms on  $\mathcal{A}^n$ . For  $n < \infty$ ,  $\text{sym}_n : \mathcal{A}^n \rightarrow \mathcal{A}^n$  denotes the corresponding symmetrization projection, i.e. the projection onto the algebra of permutation-invariant elements. The set of symmetric states in  $\mathcal{A}^n$ , i.e. the states  $\varphi \in K(\mathcal{A}^n)$  with  $\varphi \circ \text{sym}_n = \varphi$ , will be denoted by  $K_s(\mathcal{A}^n)$ .  $K_s(\mathcal{A}^\infty)$  is the set of states invariant under all finite permutations of  $\mathbb{N}$ . For any state  $\omega \in K(\mathcal{A})$  and  $n \leq \infty$ , we denote by  $\omega^n = \omega \otimes \omega \otimes \cdots \otimes \omega$  the corresponding symmetric product state on  $\mathcal{A}^n$ .

We take equilibrium states to be defined as KMS states with respect to the one-parameter group  $t \mapsto \alpha_t$  of automorphisms on the observable algebra  $\mathcal{A}$  under consideration. For simplicity of notation we shall always take the inverse temperature  $\beta = 1$ . This is possible since in all thermostatic expressions (i.e. not in the time-evolution) the Hamiltonian appears only in the combination  $\beta H$ . In order to restore physical dimensions in the variational expressions we use later on, it suffices to multiply all entropies by  $T = k\beta^{-1}$ . Since  $\alpha_t$  is not in general of the form  $\alpha_t(A) = \exp(it\mathcal{H})A \exp(-it\mathcal{H})$  with  $\mathcal{H} \in \mathcal{A}$ , we cannot in general make sense of expressions for the Hamiltonian as the one in the beginning of this section. We shall therefore split the generator of the time evolution into a “non-interacting” part generating a one-parameter group  $t \mapsto \alpha_t^0$ , and a perturbation  $h = h^* \in \mathcal{A}$ , which we call the *relative hamiltonian* of the model. If  $\alpha_t^0$  is generated by a Hamiltonian  $\mathcal{H}^0$ , the perturbed time evolution  $\alpha$  is generated by the Hamiltonian  $\mathcal{H} = \mathcal{H}^0 + h$ ; in the general case, we take  $\alpha_t$  to be defined by the integral equation  $\alpha_t(A) = \int_0^t ds \alpha_{t-s}^0(i[h, \alpha_s(A)])$ .

Suppose now that  $\rho$  is a separating state (a state whose GNS vector is separating for the generated von Neumann algebra) of  $\mathcal{A}$ , which is KMS for  $\alpha_t^0$ . Then Araki [1] defines the perturbation of  $\rho$  by the relative Hamiltonian  $h$  as a certain, in general unnormalized linear functional on  $\mathcal{A}$ , which is denoted by  $\rho^h$ . It is then shown [1] that the state

$\text{Norm}^{-1}\rho^h := (\rho^h(\mathbb{I}))^{-1}\rho^h$  is a KMS-state for the perturbed evolution  $\alpha_t$ . The number

$$\mathbb{F}(\rho, h) = -\log \rho^{-h}(\mathbb{I})$$

will be interpreted as the *relative free energy* of the new Gibbs state. A closely related quantity is the *relative entropy*  $\mathbb{S}(\rho, \varphi)$  of a state  $\varphi \in K(\mathcal{A})$  with respect to the separating state  $\rho \in K(\mathcal{A})$ . This was defined by Araki [2,3] for normal states on a von Neumann algebra; the relative entropy for states of  $C^*$ -algebras is obtained by passing to the GNS-representation if the states are quasi-equivalent, and agreeing that it is  $+\infty$  otherwise [3,28]. We have the relation

$$\mathbb{F}(\rho, h) \leq \varphi(h) + \mathbb{S}(\rho, \varphi) \quad ,$$

and the perturbed equilibrium state  $\varphi = \text{Norm}^{-1}\rho^{-h}$  is characterized as the unique state for which equality holds (see Proposition III.1.below). Thus one recovers the usual thermodynamic relation  $F = U - TS$ , where the first term on the right is interpreted as the relative internal energy, and the difference in sign of the entropy results from Araki's sign convention (see below), which makes  $\mathbb{S}(\rho, \varphi)$  positive. We emphasize that the above quantities are “relative” to the choice of a “free” system described by  $\alpha_t^0$  and  $\rho$ . This point of reference can easily be shifted without changing  $\alpha_t$ , and its equilibrium state  $\varphi$ . Explicitly, if we choose instead of  $\rho$  a reference state  $\tilde{\rho} = \text{Norm}^{-1}\rho^k$ , and choose as relative Hamiltonian  $\tilde{h} = h + k$ , then the perturbed dynamics is unchanged, and because of the relation  $(\rho^k)^{-h} = \rho^{k-h}$ , the equilibrium state  $\tilde{\varphi} = \text{Norm}^{-1}\tilde{\rho}^{-\tilde{h}}$  coincides with  $\varphi$ . Moreover,  $\mathbb{F}(\tilde{\rho}, \tilde{h}) = \mathbb{F}(\rho, h) - \mathbb{F}(\rho, -k)$ ,  $\tilde{\varphi}(\tilde{h}) = \varphi(h) + \varphi(k)$ , and  $\mathbb{S}(\tilde{\rho}, \varphi) = \mathbb{S}(\rho, \varphi) - \varphi(k) - \mathbb{F}(\rho, -k)$ . Hence the above equation holds for the new quantities as well, albeit with a different splitting between the contributions of “relative internal energy” and relative entropy.

We illustrate these concepts in the case of a finite dimensional matrix algebra  $\mathcal{M}$ . This will serve as a justification for the terminology, and facilitate the comparison of our sign conventions with those of other authors. A separating state  $\rho \in K(\mathcal{M})$  is given by a density with respect to the trace  $\text{Tr}$  of the form

$$D_\rho = e^k / \text{Tr}(e^k) \quad ,$$

where  $k$  is a self-adjoint element of  $\mathcal{M}$ . The perturbation  $\rho^{-h}$  of this state by the relative Hamiltonian  $h$  then has the density

$$e^{k-h} / \text{Tr}(e^k) \quad ,$$

The relative free energy is just the difference of the “absolute” free energies in the usual sense, taken with  $\beta = 1$ :

$$\mathbb{F}(\rho, h) = -\log(\operatorname{Tr} e^{k-h}) + \log(\operatorname{Tr} e^k) \quad .$$

If  $D_\varphi$  is the density matrix of  $\varphi \in K(\mathcal{A})$ , the relative entropy is

$$\mathbb{S}(\rho, \varphi) = \operatorname{Tr} D_\varphi (\log(D_\varphi) - \log(D_\rho)) \quad .$$

From this it is easy to check the relation between the relative free energy, internal energy, and entropy using  $D_\varphi = \operatorname{Tr} (e^{k-h})^{-1} e^{k-h}$ .

A *homogeneous mean-field* model [31] is now specified by a C\*-algebra  $\mathcal{A}$  and a separating state  $\rho$ . For each  $n$ , the non-interacting system of  $n$  “particles” is specified by the product state  $\rho^n = \rho \otimes \rho \otimes \cdots \otimes \rho$  on  $\mathcal{A}^n$ . That is,  $\rho^n$  is the KMS-state of an “unperturbed” time evolution of the product form  $\alpha_t^{0,n}(A_1 \otimes \cdots \otimes A_n) = (\alpha_t^{0,1} A_1) \otimes \cdots \otimes (\alpha_t^{0,1} A_n)$ . The interaction is introduced by a relative Hamiltonian  $nH_n$  which is a self-adjoint element of  $\mathcal{A}^n$ . The sequence  $H = (H_n)$  of relative Hamiltonian *densities* is assumed to be *approximately symmetric*, that is:

- (i)  $H_n = \operatorname{sym}_n(H_n)$  ;
- (ii) for every  $\varepsilon > 0$ , there exists an  $m \in \mathbb{N}$  such that (MF)  
for every  $n > m$ ,  $\|H_n - \operatorname{sym}_n(H_m \otimes \mathbb{I}_{n-m})\| \leq \varepsilon$  .

Notice that the key requirement is (ii): if (ii) holds true, then we may replace  $H_n$  by  $\operatorname{sym}_n(H_n)$  to satisfy (i) without altering the limiting thermodynamics. Equivalently, an approximately symmetric sequences is characterized by the property [31] that for sufficiently large  $n$ ,  $H_n$  is uniformly approximated by a “strictly symmetric” sequence of the form  $X_n = \operatorname{sym}_n(X_k \otimes \mathbb{I}_{n-k})$  for fixed  $k$ .

We illustrate the definition by the homogeneous version of the BCS-model. Here  $\mathcal{A}$  is the algebra of  $(2 \times 2)$ -matrices with complex entries, and the state  $\rho$  is taken to be the normalized trace. On  $\mathcal{A} \otimes \mathcal{A}$  set

$$H_2 = \frac{\varepsilon}{4} \left( (\mathbb{I} - \sigma^z) \otimes \mathbb{I} + \mathbb{I} \otimes (\mathbb{I} - \sigma^z) \right) + \frac{U}{2\lambda} \left( \sigma^+ \otimes \sigma^- + \sigma^- \otimes \sigma^+ \right) \quad ,$$

where  $\lambda^{-1}$  is the limiting density. Then

$$\|\mathcal{H}_n^{BCS} - n \operatorname{sym}_n(H_2)\| = o(n) \quad ,$$

and this model is indeed a homogeneous mean-field model. Notice that self-interaction terms do not contribute.

For every approximately symmetric sequence  $H = (H_n)$ ,  $H_n \in \mathcal{A}^n$ , and any symmetric state  $\Phi \in K_s(\mathcal{A}^\infty)$  the limiting relative energy density  $\lim_{n \rightarrow \infty} \Phi(H_n)$  exists. In the particular case of a symmetric product state  $\Phi = \varphi^\infty$  with  $\varphi \in K(\mathcal{A})$  we have the limit

$$j(H)(\varphi) = \lim_n \varphi^n(H_n) \quad .$$

Then  $j : H \mapsto j(H)(\cdot) \equiv j(H)$  maps the set of approximately symmetric sequences onto the continuous functions over the state space  $K(\mathcal{A})$  [31].

The ingredients defining an *inhomogeneous mean-field model* are again a  $C^*$ -algebra  $\mathcal{A}$  and a separating state  $\rho$  which specify the non-interacting system. The interaction is introduced by perturbation of  $\rho^n$  with a relative Hamiltonian which is assumed to be of the form  $nH_n(\xi_{n,1}, \dots, \xi_{n,n})$  where the  $n$  parameters  $\xi_{n,1}, \dots, \xi_{n,n}$  take values in a fixed compact space  $X$ , and  $H_n : X^n \rightarrow \mathcal{A}^n$  is a continuous function in the norm topology of  $\mathcal{A}^n$ , i.e. an element of  $\mathcal{C}(X^n, \mathcal{A}^n) \cong \mathcal{C}(X, \mathcal{A})^n$ . The sequence  $(H_n)$  is assumed to be approximately symmetric. The sequence of  $n$ -tuples  $(\xi_{n,1}, \dots, \xi_{n,n}) \equiv \xi_n \in X^n$  is constrained only by the condition, that there exists a *limiting density*  $\mu \in K(\mathcal{C}(X))$ :

$$\frac{1}{n} \sum_{i=1}^n \delta(\xi_{n,i}) \longrightarrow \mu \quad (LD)$$

in the  $w^*$ -topology, where  $\delta(x) \in K(\mathcal{C}(X))$  denotes the evaluation functional at  $x \in X$ . There is a further rather technical assumption on the space  $X$ , which is nevertheless harmless from the point of view of applications. We suppose that  $\mathcal{C}(X)$  admits a *separating state*; equivalently, there exists a finite regular Borel measure on  $X$  whose support is  $X$  itself.

It can be verified that the BCS-model is an inhomogeneous mean-field model, provided the momenta are restricted to take values in some compact subset  $\Omega$ , condition (LD) is satisfied, and, of course, both  $\varepsilon$  and  $U$  are continuous functions. Condition (ii) is met with  $H_2 \in \mathcal{C}(\Omega \times \Omega, \mathcal{A} \otimes \mathcal{A})$  given by

$$\begin{aligned} H_2(\mathbf{k}_1, \mathbf{k}_2) = & \frac{1}{4} \varepsilon(\mathbf{k}_1) (\mathbb{I} - \sigma^z) \otimes \mathbb{I} + \frac{1}{4} \varepsilon(\mathbf{k}_2) \mathbb{I} \otimes (\mathbb{I} - \sigma^z) \\ & + \frac{1}{2\lambda} U(\mathbf{k}_1, \mathbf{k}_2) (\sigma^+ \otimes \sigma^- + \sigma^- \otimes \sigma^+) \quad . \end{aligned} \quad (2.1)$$

Consider an inhomogeneous mean-field model specified by  $(\mathcal{A}, \rho, X, (\xi_n), \mu, (H_n))$ , and set  $\Psi_n := \text{Norm}^{-1}(\rho^n)^{-nH_n(\xi_n)}$  for the Gibbs state of the  $n^{\text{th}}$  system (*we will keep this notation throughout the paper*). Because of the  $\xi_n$ -dependence of  $H_n$ ,  $\Psi_n$  depends on the labelling of the  $n$  points  $\xi_{n,1}, \dots, \xi_{n,n} \in X$ . Therefore, unless we make further assumptions

on the relation between the labellings of successive  $n$ -tuples  $\xi_n$ , we cannot expect these equilibrium states to converge in any sense to a state of  $\mathcal{A}^\infty$ . We shall use the “location in  $X$ -space” itself as a label; this amounts to considering the equilibrium state of the  $n^{\text{th}}$  model not as a state on  $\mathcal{A}^n$ , but as a symmetric state on  $\mathcal{C}(X, \mathcal{A})^n$ . To formalize this idea we introduce the operator  $\Xi_n : \mathcal{C}(X, \mathcal{A})^n \rightarrow \mathcal{A}^n$  of “symmetrized evaluation” at  $\xi_n$ :

$$\Xi_n F := (\text{sym}_n F)(\xi_{n,1}, \dots, \xi_{n,n}) \quad \text{for } F \in \mathcal{C}(X^n, \mathcal{A}^n) \quad .$$

Since  $H_n \in \mathcal{C}(X, \mathcal{A})^n$  is symmetric, the  $n^{\text{th}}$  Hamiltonian density is given by  $H_n(\xi_n) = \Xi_n(H_n)$ . Since  $\Xi_n$  contains a symmetrization its adjoint takes  $K(\mathcal{A}^n)$  into  $K_s(\mathcal{C}(X, \mathcal{A})^n)$ . If the limit of the states  $\Psi_n \circ \Xi_n$  exists (we will state precisely what we mean below), it will be a symmetric state on  $\mathcal{C}(X, \mathcal{A})^\infty$ . Note that the restriction  $(\phi_n \circ \Xi_n)|_{\mathcal{C}(X)^n}$  does not depend on  $\phi_n \in K(\mathcal{A}^n)$ , but only on  $\xi_n$ . Therefore we expect that condition (LD) forces the limit of  $(\Psi_n \circ \Xi_n)$  to lie in the set

$$K_s^\mu := \left\{ \phi \in K_s(\mathcal{C}(X, \mathcal{A})^\infty) \mid \phi|_{\mathcal{C}(X)^\infty} = \mu^\infty \right\} \quad .$$

In the previous paragraph we were speaking loosely of convergence of sequences of states defined on  $\mathcal{A}^n$ . We make this precise as follows. Let  $\nu$  be a subnet of  $\mathbb{N}$ , i.e. a function  $\nu : \mathbf{A} \rightarrow \mathbb{N}$  on a directed set  $(\mathbf{A}, \geq)$  such that for every  $n \in \mathbb{N}$  there exists  $\alpha_0 \in \mathbf{A}$  such that  $\nu(\alpha) \geq n$ , whenever  $\alpha \geq \alpha_0$ . If  $(a_n)_{n \in \mathbb{N}}$  is a sequence in a Hausdorff space, we write  $\lim_{n \rightarrow \nu} a_n$  for  $\lim_{\alpha \in \mathbf{A}} a_{\nu(\alpha)}$  if it exists, and employ a similar notation for superior and inferior limits of sequences of extended-real numbers.

**II.1 Definition.** Let  $(\phi_n)_{n \in \mathbb{N}}$  be a sequence of states  $\phi_n \in K(\mathcal{A}^n)$ . We say that  $(\phi_n)$  is **convergent along a subnet**  $\nu : \mathbf{A} \rightarrow \mathbb{N}$  to a state  $\phi \in K(\mathcal{A}^\infty)$ , if for all  $m \in \mathbb{N}$  and all  $X \in \mathcal{A}^m$ ,  $\phi(X) = \lim_{n \rightarrow \nu} \phi_n(X)$ . Here  $\mathcal{A}^m$  is identified with a subalgebra of  $\mathcal{A}^n$  for all  $m \leq n \leq \infty$ .

Relative entropy, as the difference of two entropies, is an extensive quantity. The interesting quantity in the thermodynamic limit therefore is its density, called the *mean relative entropy*, which is defined for an infinite product state  $\rho^\infty$ , and a symmetric state  $\psi \in K_s(\mathcal{A}^\infty)$  of  $\mathcal{A}^\infty$ , by the limit

$$\mathbb{S}_M(\rho^\infty, \psi) = \lim_{n \rightarrow \infty} n^{-1} \mathbb{S}(\rho^n, \psi|_{\mathcal{A}^n}) \quad ,$$

which is actually a supremum [29,31].



The main result of this paper is the following Gibbs variational principle for inhomogeneous mean-field models.

**II.2 Theorem.** *For any inhomogeneous mean-field model specified by the  $C^*$ -algebra  $\mathcal{A}$ , the separating state  $\rho$ , the compact space  $X$ , the probability measure  $\mu$ , and the sequences  $(\xi_n)$  of parameters, and  $(H_n)$  of relative Hamiltonian densities, satisfying the conditions (MF) and (LD), one has*

$$\lim_{n \rightarrow \infty} n^{-1} \mathbb{F}(\rho^n, nH_n(\xi_n)) = \inf \left\{ \lim_{n \rightarrow \infty} \phi(H_n) + \mathbb{S}_M((\mu \otimes \rho)^\infty, \phi) \mid \phi \in K_s^\mu \right\} \quad (*)$$

$$= \inf \left\{ j(H)(\varphi) + \mathbb{S}(\mu \otimes \rho, \varphi) \mid \varphi \in K(\mathcal{C}(X, \mathcal{A})), \varphi|_{\mathcal{C}(X)} = \mu \right\} \quad (**)$$

Moreover, the first infimum is attained at any  $w^*$ -cluster point of the sequence  $(\Psi_n \circ \Xi_n)$  of symmetric states of  $\mathcal{C}(X, \mathcal{A})^n$ .

The proof of the following result is obtained as in [31].

### II.3 Proposition.

- (1) The subset  $M_* \subset K_s^\mu$  of states maximizing (\*) is convex and compact, and the subset  $M_{**} \subset K(\mathcal{C}(X, \mathcal{A}))$  of states maximizing (\*\*) is non-empty and compact. The extreme points of  $M_*$  are the states  $\varphi^\infty$  with  $\varphi \in M_{**}$ . Every  $\phi \in M_*$  has a unique  $w^*$ -integral decomposition  $\phi = \int \nu(d\varphi) \varphi^\infty$ , where  $\nu$  is a regular Borel probability measure supported by  $M_{**}$ .
- (2) If  $\mathcal{A}$  is separable, and  $X$  is metrizable, then for any extreme point  $\phi$  of  $M_*$  there exists an approximately symmetric sequence  $(\hat{H}_n)$  such that  $\lim_n \|H_n - \hat{H}_n\| = 0$ , and the sequence  $\hat{\Psi}_n \in K_s(\mathcal{C}(X, \mathcal{A})^n)$  defined from  $\hat{H}_n$  is  $w^*$ -convergent to  $\phi$ .
- (3) Suppose that  $\Psi_n$  converges to an extreme point of  $M_*$ , and let  $X_n = X_n^* \in \mathcal{C}(X, \mathcal{A})^n$  be an approximately symmetric sequence. Let  $\mu_n$  denote the probability measure on  $\mathbb{R}$  describing the distribution of the observable  $X_n$  in the state  $\Psi_n$ . Then the sequence  $\mu_n$  is  $w^*$ -convergent to a point measure.

The solution of the variational problem (\*\*) can pose a formidable task. In the rest of this section we shall comment on some simplifications of this problem, which apply in special circumstances. In many applications  $\mathcal{A}$  is separable. In this case every state  $\varphi$  of  $\mathcal{C}(X, \mathcal{A})$  has a unique decomposition of the form

$$\varphi = \int^\oplus \mu_\varphi(dx) \varphi_x \quad ;$$



that is to say, there exists a regular Borel probability measure  $\mu_\varphi$  on  $X$ , and a  $K(\mathcal{A})$ -valued function  $x \mapsto \varphi_x$  such that for every  $F \in \mathcal{C}(X, \mathcal{A})$ ,  $\varphi(F) = \int_X \mu_\varphi(dx) \varphi_x(F(x))$ . The proof is the same as that of Proposition IV.5 in [31]. Then, if  $\mu_\varphi = \mu$ , i.e.,  $\varphi|_{\mathcal{C}(X)} = \mu$ , we have (see III.2.2 below):

$$\mathbb{S}(\mu \otimes \rho, \varphi) = \int_X \mu(dx) \mathbb{S}(\rho, \varphi_x) \quad .$$

Also, the integral decomposition of  $\varphi$  can often be used (see below, and applications in section IV) to express  $j(H)(\varphi)$ .

Suppose, for example, that the Hamiltonian density  $H_n$  can be expressed in terms of finitely many elements  $A_\alpha \in \mathcal{A}$  ( $\alpha = 1, \dots, r$ ). To be specific, consider a *quadratic* model specified by consecutive symmetrization of

$$\begin{aligned} H_2(x_1, x_2) = & \frac{1}{2} \sum_{\alpha=1}^r (\overline{\varepsilon_\alpha(x_1)} A_\alpha \otimes \mathbb{I} + \overline{\varepsilon_\alpha(x_2)} \mathbb{I} \otimes A_\alpha) \\ & + \frac{1}{2} \sum_{\alpha, \beta=1}^r U_{\alpha\beta}(x_1, x_2) A_\alpha^* \otimes A_\beta \quad , \end{aligned} \quad (2.2)$$

where  $\varepsilon_\alpha \in \mathcal{C}(X)$ , and  $U_{\alpha\beta} \in \mathcal{C}(X \times X)$  are such that this expression is hermitian and symmetric. We find

$$\begin{aligned} n \operatorname{sym}_n(H_2 \otimes \mathbb{I}_{n-2})(x_1, x_2, \dots, x_n) = & \sum_{i=1}^n \sum_{\alpha=1}^r \overline{\varepsilon_\alpha(x_i)} (A_\alpha)_i \\ & + \frac{1}{(n-1)} \sum_{i,j=1}^n \sum_{\alpha, \beta=1}^r U_{\alpha\beta}(x_i, x_j) (A_\alpha^*)_i (A_\beta)_j \quad , \end{aligned} \quad (2.3)$$

where  $(A_\alpha)_i$  is a copy of  $A_\alpha$  acting on the  $i^{\text{th}}$  factor of  $\mathcal{A}^n$ . Then for  $\varphi = \int^\oplus \mu(dx) \varphi_x$  we obtain

$$\begin{aligned} j(H)(\varphi) = & \int \mu(dx) \sum_{\alpha=1}^r \overline{\varepsilon_\alpha(x)} \varphi_x(A_\alpha) \\ & + \frac{1}{2} \int \mu(dx) \mu(dy) \sum_{\alpha, \beta=1}^r U_{\alpha\beta}(x, y) \overline{\varphi_x(A_\alpha)} \varphi_y(A_\beta) \quad . \end{aligned} \quad (2.4)$$

Hence the energy term of the variational principle depends only on the function  $x \mapsto \vec{\phi}(x) \in \mathbb{C}^r$ , where  $\vec{\phi}(x) \in \mathbb{C}^r$  denotes the vector with components  $\varphi_x(A_\alpha)$  ( $\alpha = 1, \dots, r$ ). Therefore we need only consider states, which minimize the entropy term among all states with given  $\vec{\phi}(x)$ . For any  $\vec{\phi} \in \mathbb{C}^r$ , let

$$\hat{\mathbb{S}}(\vec{\phi}) = \inf \left\{ \mathbb{S}(\rho, \varphi) \mid \varphi(A_\alpha) = \vec{\phi}_\alpha \quad \text{for } \alpha = 1, \dots, r \right\} \quad ,$$

with the understanding that the infimum over an empty set is  $+\infty$ . Then using the integral decomposition of  $\mathbb{S}(\mu \otimes \rho, \varphi)$ ,  $(**)$  becomes

$$\begin{aligned} \lim_{n \rightarrow \infty} n^{-1} \mathbb{F}(\rho^n, nH_n(\xi_n)) &= \\ &= \inf \left\{ \langle \vec{\varepsilon}, \vec{\phi} \rangle + \langle \vec{\phi}, U\vec{\phi} \rangle + \int \mu(dx) \hat{\mathbb{S}}(\vec{\phi}(x)) \mid \vec{\phi} \in \mathcal{L}^\infty(X, \mu, \mathbb{C}^r) \right\} . \end{aligned}$$

Here  $\mathcal{L}^\infty(X, \mu, \mathbb{C}^r)$  denotes the set of  $\mu$ -essentially bounded  $\mathbb{C}^r$ -valued Borel measurable functions on  $X$ ,  $\langle \cdot, \cdot \rangle$  denotes the inner product  $\langle \vec{\Psi}, \vec{\phi} \rangle = \int \mu(dx) \sum_\alpha \overline{\Psi_\alpha(x)} \phi_\alpha(x)$  on  $\mathcal{L}^2(X, \mu, \mathbb{C}^r)$ , and  $U$  denotes the compact integral operator

$$(U\vec{\phi})_\alpha(x) = \int \mu(dy) \sum_\beta U_{\alpha\beta}(x, y) \vec{\phi}_\beta(y) .$$

This discussion generalizes immediately to more than quadratic models, defined from an  $H_m$  with  $m > 2$ . Note also that for  $r$  large enough any  $H_2 \in \mathcal{C}(X, \mathcal{A})^2$  can be approximated by an expression of the form (2.2), so that there is no essential loss of generality in taking  $r$  finite.

The above discussion shows that the choice of the algebra  $\mathcal{A}$  in a given model is partly a matter of convenience, and one can often replace  $\mathcal{A}$  by a smaller algebra  $\hat{\mathcal{A}}$ . A necessary condition is, of course, that  $H_n \in \hat{\mathcal{A}}^n$  for sufficiently large  $n$ , or  $A_1, \dots, A_r \in \hat{\mathcal{A}}$  in (2.2). In the classical case there is no further requirement, but in the quantum case one has take into account that the entropy inequality  $\mathbb{S}(\rho \mid \hat{\mathcal{A}}, \hat{\varphi}) \leq \inf \left\{ \mathbb{S}(\rho, \varphi) \mid \varphi \mid \hat{\mathcal{A}} = \hat{\varphi} \right\}$  is strict in general, so  $\hat{\mathbb{S}}(\vec{\phi})$  may come out too small when computed relative to a subalgebra  $\hat{\mathcal{A}}$ . A sufficient condition for the reduction from  $\mathcal{A}$  to  $\hat{\mathcal{A}}$  to be valid is the existence of a positive unital projection  $\mathbb{E} : \mathcal{A} \rightarrow \hat{\mathcal{A}}$  with  $\rho \circ \mathbb{E} = \rho$ .

Similar remarks apply to the choice of the compact space  $X$ . As is commonly the case in probability theory, the underlying measure space  $(X, \mu)$  itself is irrelevant, and only the distributions of the random variables  $\varepsilon_\alpha$  and  $U_{\alpha\beta}$  really enter the problem. Suppose that  $H_2$  is given by (2.2) for some bounded, measurable, but not necessarily continuous functions  $\varepsilon_\alpha$  and  $U_{\alpha\beta}$  on some measure space  $(X, \mu)$ . Then the functions  $\varepsilon_\alpha$  and  $U_{\alpha\beta}(x, \cdot)$  generate a  $C^*$ -subalgebra of the algebra of bounded functions on  $X$ , which can be represented as  $\mathcal{C}(\hat{X})$  for some compact set  $\hat{X}$ . The space  $\hat{X}$  arises from  $X$  by identifying all points of  $X$ , which are not distinguished by the functions  $\varepsilon$  and  $U$ . If  $X$  is a compact space and the functions  $\varepsilon$  and  $U$  are continuous to begin with, then the quotient map  $x \mapsto \hat{x}$  is continuous, and the condition (LD) carries over from any sequence  $\xi_n \in X^n$  to its quotients  $\hat{\xi}_n \in \hat{X}^n$ . However, if  $\varepsilon$  or  $U$  is discontinuous, or no topological structure was assumed for  $X$ , (LD) becomes an independent condition for  $\hat{\xi}_n$ . This shows

that the continuity of  $\varepsilon$  and  $U$ , or more generally the continuity  $H_n : X^n \rightarrow \mathcal{A}^n$ , is not in itself vital for our theory, but is needed only to ensure the boundedness of  $H_n$  (together with compactness of  $X$ ) and to formulate an appropriate version of the limiting density assumption.

The choice of the reference state  $\rho$  is also a matter of convenience. In fact, the choices  $\hat{\rho} = \rho^h$  for some  $h = h^* \in \mathcal{A}$ , and  $\hat{H}_n = H_n + \text{sym}_n(h)$  describe exactly the same system as  $\rho$  and  $H_n$ , and as discussed previously, one obtains exactly the same variational principle up to a different splitting of the relative free energy into relative internal energy and relative entropy. If  $\mathcal{A}$  is the algebra of  $(d \times d)$ -matrices, it is convenient to choose the reference state to be the trace  $\tau$  given by:  $\tau(h) = d^{-1} \text{Tr}(h)$ . Then  $\mathbb{S}(\tau, \varphi) = \mathbb{S}(\tau) - \mathbb{S}(\varphi) = \log d - \mathbb{S}(\varphi)$ , where  $\mathbb{S}(\varphi) = -\text{Tr}(D_\varphi \log D_\varphi)$  denotes the “absolute entropy” of the state  $\varphi$  with density matrix  $D_\varphi$ . Then if  $\mathbb{F}(H) = -\log \text{Tr}(\exp(-H)) = \mathbb{F}(\tau, H) - \log d$  denotes the “absolute free energy” of the system with Hamiltonian  $H$ , the variational principle becomes

$$\lim_n \frac{1}{\beta n} \mathbb{F}(\beta n H_n) = \inf_\varphi \left\{ j(H)(\varphi) - \frac{1}{\beta} \int \mu(dx) \mathbb{S}(\varphi_x) \right\}, \quad (2.5)$$

where the infimum is over the states  $\varphi = \int^\oplus \mu(dx) \varphi_x$ .

### III. Proof of the Gibbs Variational Principle

The proof of the variational principle follows the strategy of [29], and [31]; it relies on the relation between free-energy, energy, and entropy known from thermodynamics, and formulated for general states on a  $C^*$ -algebra by Petz [27,28]. The Petz Duality Theorem characterizes the relative free-energy functional  $h \mapsto \log \rho^h(\mathbb{I})$  as the Legendre transform of the relative entropy functional  $\mathbb{S}(\rho, \cdot)$ . Since  $\mathbb{S}(\rho, \psi)$  is also defined for non-normalized positive linear functionals  $\psi \in \mathcal{A}_+^*$ , there is a second version of the Duality Theorem, describing the variation of  $\mathbb{S}(\rho, \psi) - \psi(h)$  over this larger set. We shall need both versions below.

**III.1 Proposition.** *Let  $\mathcal{A}$  be a  $C^*$ -algebra, and  $\rho \in K(\mathcal{A})$  a separating state. Then for  $\varphi \in K(\mathcal{A})$  (resp.  $\psi \in \mathcal{A}_+^*$ ) and  $h = h^* \in \mathcal{A}$ :*

$$\begin{aligned} & \mathbb{S}(\rho, \varphi) + \log \rho^h(\mathbb{I}) - \varphi(h) \geq 0 \\ (\text{resp. } & \mathbb{S}(\rho, \psi) + \rho^h(\mathbb{I}) - \psi(h + \mathbb{I}) \geq 0). \end{aligned}$$

Equality holds if and only if  $\varphi = \rho^h(\mathbb{I})^{-1}\rho^h$  (resp.  $\psi = \rho^h$ ). The following variational formulae hold:

$$\begin{aligned}\mathbb{F}(\rho, h) &= -\log \rho^{-h}(\mathbb{I}) = \inf \{ \varphi(h) + \mathbb{S}(\rho, \varphi) \mid \varphi \in K(\mathcal{A}) \} \quad , \\ \mathbb{S}(\rho, \varphi) &= \sup \{ \varphi(h) - \log \rho^h(\mathbb{I}) \mid h = h^* \in \mathcal{A} \} \quad , \text{ and} \\ \mathbb{S}(\rho, \psi) &= \sup \{ \psi(h + \mathbb{I}) - \rho^h(\mathbb{I}) \mid h = h^* \in \mathcal{A} \} \quad .\end{aligned}$$

**Proof :** The statements about states  $\varphi$  are proven in [27], and we shall reduce the case of unnormalized functionals  $\psi \in \mathcal{A}_+^*$  to these. Any  $\psi \in \mathcal{A}_+^*$  can be written as  $\psi = \lambda\varphi$  with  $\lambda \in \mathbb{R}_+$  and  $\varphi$  a state. Then by the scaling properties of  $\mathbb{S}$  (see [2,3], or the Appendix of [29]) the left hand side of the second inequality can be written as

$$\lambda[\mathbb{S}(\rho, \varphi) + \log \rho^h(\mathbb{I}) - \varphi(h)] + [\lambda \log(\lambda \rho^h(\mathbb{I})^{-1}) - \lambda + \rho^h(\mathbb{I})] \quad .$$

Both brackets are positive, and the second one vanishes only for  $\lambda = \rho^h(\mathbb{I})$ . This proves the inequality and the condition for equality. Proving the variational formula for  $\mathbb{S}(\rho, \psi)$  ( while  $\mathbb{S}(\rho, \psi)$  is finite) is equivalent to showing that the infimum of the above expression with respect to  $h$  vanishes. The substitution  $h \mapsto h + \alpha\mathbb{I}$  does not change the first bracket, and can be used to make the second one vanish. This reduces the statement to the known theorem for states [27]. A similar argument works if  $\mathbb{S}(\rho, \psi) = \infty$ . ■

For arbitrary (not necessarily separating)  $\omega \in \mathcal{A}_+^*$  and  $h = h^* \in \mathcal{A}$ , we define

$$\omega^h(\mathbb{I}) = \sup \{ \psi(h + \mathbb{I}) - \mathbb{S}(\omega, \psi) \mid \psi \in \mathcal{A}_+^* \} \quad ;$$

and remark that the map  $h \mapsto \omega^h(\mathbb{I})$  is continuous in the norm topology of  $\mathcal{A}$ . Moreover, if  $\omega$  is a state,  $\log \omega^h(\mathbb{I}) = \sup \{ \varphi(h) - \mathbb{S}(\omega, \varphi) \mid \varphi \in K(\mathcal{A}) \}$ .

We now describe the main ingredients of the proof of the variational principle. An upper bound on the limit of the relative free-energy density  $n^{-1}\mathbb{F}(\rho^h, nH_n(\xi_n))$  is obtained from III.1 by substituting suitable states  $\chi_n \in K(\mathcal{A}^n)$  for  $\varphi$  in the expression  $\varphi(H_n(\xi_n)) + n^{-1}\mathbb{S}(\rho^n, \varphi)$ ; to establish lower bounds we substitute for  $\varphi$  the equilibrium state  $\Psi_n$  of the  $n^{\text{th}}$  system.

The energy term may be written as  $\varphi(H_n(\xi_n)) = (\varphi \circ \Xi_n)(H_n)$  with  $\varphi \circ \Xi_n \in K_s(\mathcal{C}(X, \mathcal{A})^n)$ . The states  $\chi_n$  used for the upper bound will be constructed so that the sequence  $(\chi_n \circ \Xi_n)$  is  $w^*$ -convergent to a state  $\chi_\infty$  on  $\mathcal{C}(X, \mathcal{A})^\infty$  (III.7.). Then the approximate symmetry of  $H_n$  ensures (Proposition III.3 of [31]) the convergence of the mean energy  $(\chi_n \circ \Xi_n)(H_n)$ . For the lower bound the convergence of  $\Psi_n \circ \Xi_n$  holds along suitable

subnets by  $w^*$ -compactness, and this again ensures the convergence of the mean energy. Turning now to the entropy terms, one expects heuristically that

$$n^{-1} \mathbb{S}(\rho^n, \varphi) \approx n^{-1} \mathbb{S}(\rho^n \circ \Xi_n, \varphi \circ \Xi_n) \quad .$$

Here the inequality " $\geq$ " holds unconditionally, which takes care of the lower bound; for the upper bound equality is achieved by judicious choice of  $\chi_n$  (III.7.). A critical step in the proof is to establish the approximate equality

$$n^{-1} \mathbb{S}(\rho^n \circ \Xi_n, \varphi \circ \Xi_n) \approx n^{-1} \mathbb{S}((\mu \otimes \rho)^n, \varphi \circ \Xi_n) \quad . \quad (\approx)$$

To see the heuristic content of  $(\approx)$  note that, by definition of  $\Xi_n$ , the restriction  $\varphi \circ \Xi_n|_{\mathcal{C}(X)^n} =: \hat{\mu}_n \in K(\mathcal{C}(X^n))$  is independent of  $\varphi \in K(\mathcal{A}^n)$ . In fact,  $\hat{\mu}_n$  is just the symmetrized evaluation at  $\xi_n \in X^n$ , and  $\rho^n \circ \Xi_n = \hat{\mu}_n \otimes \rho^n$ . The difference between the two sides of  $(\approx)$  is the conditional entropy  $n^{-1} \mathbb{S}(\mu^n, \hat{\mu}_n)$  (see III.2.(3) below). By virtue of the limiting density assumption (LD) for the sequence  $\xi_n$  the measures  $\hat{\mu}_n$  and  $\mu_n$  on  $X^n$  are  $w^*$ -close (III.6.). Hence one may expect this conditional entropy to vanish in the limit  $n \rightarrow \infty$ . Unfortunately, however, this expression is typically infinite, because  $\hat{\mu}_n$  is singular with respect to  $\mu^n$ . All states must thus be regularized by a coarse graining operation (III.3.). After coarse graining  $(\approx)$  becomes valid in the limit (III.5.), and the right-hand side converges to the mean relative entropy. The coarse graining is removed at the end of the proof.

We now establish some basic facts about relative entropies in algebras of the form  $\mathcal{C}(X, \mathcal{A})$ . Since this algebra will appear often, we shall from now on use the abbreviation  $\mathcal{B} = \mathcal{C}(X, \mathcal{A})$ . The following Lemma will mostly be applied to  $\mathcal{B}^n = \mathcal{C}(X, \mathcal{A})^n \cong \mathcal{C}(X^n, \mathcal{A}^n)$ .

**III.2 Lemma.** *Let  $\mathcal{A}$  be a  $C^*$ -algebra with unit, and  $\rho \in K(\mathcal{A})$  be separating. Let  $X$  be a compact space and  $\mu \in K(\mathcal{C}(X))$ . Then*

(1) *For  $h \in \mathcal{C}(X, \mathcal{A})$ ,*

$$(\mu \otimes \rho)^h(\mathbb{I}) = \int \mu(dx) \rho^{h(x)}(\mathbb{I}) \quad .$$

(2) *If  $\mathcal{A}$  is separable, and  $\varphi \in K(\mathcal{C}(X, \mathcal{A}))$  is decomposed as  $\varphi = \int^\oplus \mu(dx) \varphi_x$  with  $\varphi_x \in K(\mathcal{A})$ , then  $x \mapsto \mathbb{S}(\rho, \varphi_x)$  is measurable, and*

$$\mathbb{S}(\mu \otimes \rho, \varphi) = \int \mu(dx) \mathbb{S}(\rho, \varphi_x) \quad .$$

(3) *Let  $\varphi \in K(\mathcal{C}(X, \mathcal{A}))$  with  $\varphi|_{\mathcal{C}(X)} = \nu$ . Then,*

$$\mathbb{S}(\mu \otimes \rho, \varphi) = \mathbb{S}(\nu \otimes \rho, \varphi) + \mathbb{S}(\mu, \nu)$$

whenever the left-hand side is finite, and there exists a separating  $\omega \in K(\mathcal{C}(X))$ .

**Proof :** (1) It is a general property of the relative entropy on a C\*-algebra  $\mathcal{D}$  [3,28] that whenever  $\mathbb{S}(\rho, \varphi)$  is finite,  $\varphi$  has a unique extension  $\hat{\varphi}$  to the von Neumann algebra  $\pi_\rho(\mathcal{D})''$  in the GNS representation with respect to  $\rho$ , and  $\mathbb{S}(\hat{\rho}, \hat{\varphi}) = \mathbb{S}(\rho, \varphi)$ . By monotonicity we also have  $\mathbb{S}(\rho, \varphi) = \mathbb{S}(\hat{\rho}|_{\mathcal{M}}, \hat{\varphi}|_{\mathcal{M}})$  for any C\*-algebra  $\mathcal{M}$  with  $\pi_\rho(\mathcal{D}) \subset \mathcal{M} \subset \pi_\rho(\mathcal{D})''$ . Applying these considerations to  $\mathcal{D} = \mathcal{C}(X, \mathcal{A})$  we find that  $\mathbb{S}(\mu \otimes \rho, \varphi)$  may be computed in the C\*-tensor product  $\mathcal{M} := \mathcal{L}^\infty(X, \mu) \otimes \mathcal{A}$ . By definition  $(\mu \otimes \rho)^h(\mathbb{I}) = \sup \{ \psi(h + \mathbb{I}) - \mathbb{S}(\mu \otimes \rho, \psi) \mid \psi \in \mathcal{D}_+^* \}$  for all  $h \in \mathcal{C}(X, \mathcal{A})$ , and this supremum is unchanged if  $\psi$  is allowed to range over  $\mathcal{M}_+^*$ . We may thus prove relation (1) for  $h$  in the algebra  $\mathcal{M}$ , and utilize the fact that every  $h \in \mathcal{M}$  can be approximated uniformly by step functions  $h(x) = \sum_\alpha \chi_\alpha(x) h_\alpha$ , with  $h_\alpha \in \mathcal{A}$ ,  $\chi_\alpha = |\chi_\alpha|^2 \in \mathcal{L}^\infty(X, \mu)$  and  $\sum_\alpha \chi_\alpha = 1$ . The formula is clearly true for constant  $h$ . Since  $\mathcal{M} = \bigoplus_\alpha (\chi_\alpha \otimes \mathbb{I}) \mathcal{M}$ , and a step function is constant on each direct summand in this decomposition, the formula holds for step functions. Finally, the continuity of  $h \mapsto \rho^h(\mathbb{I})$  in the norm topology shows that the formula holds for arbitrary  $h \in \mathcal{M}$ , and hence for  $h \in \mathcal{C}(X, \mathcal{A})$ .

(2) Let  $(A_n)_{n \in \mathbb{N}}$  be a dense sequence in  $\mathcal{A}$ , and define

$$\mathbb{S}_n(\rho, \varphi) = \max_{m \leq n} \{ \varphi(A_m + \mathbb{I}) - \rho^{A_m}(\mathbb{I}) \} \quad .$$

Clearly,  $n \mapsto \mathbb{S}_n(\rho, \varphi)$  is increasing, and  $\mathbb{S}(\rho, \varphi) = \sup_n \mathbb{S}_n(\rho, \varphi)$ . For every  $n$ , the function  $x \mapsto \mathbb{S}_n(\rho, \varphi_x)$  is measurable, hence the pointwise supremum of this sequence of functions is also measurable, and  $\int \mu(dx) \mathbb{S}(\rho, \varphi_x) = \sup_n \int \mu(dx) \mathbb{S}_n(\rho, \varphi_x)$  by monotone convergence. By III.1, and (1),  $\mathbb{S}(\mu \otimes \rho, \varphi) = \sup_h \{ \varphi(h + \mathbb{I}) - (\mu \otimes \rho)^h(\mathbb{I}) \} = \sup_h \left( \int \mu(dx) \{ \varphi_x(h(x) + \mathbb{I}) - \rho^{h(x)}(\mathbb{I}) \} \right) \leq \int \mu(dx) \mathbb{S}(\rho, \varphi_x)$ . To prove the converse inequality, we construct for every  $n$  a measurable step function  $h : X \rightarrow \{A_1, \dots, A_n\}$  such that  $\{ \varphi_x(h(x) + \mathbb{I}) - \rho^{h(x)}(\mathbb{I}) \} = \max_{m \leq n} \{ \varphi_x(A_m + \mathbb{I}) - \rho^{A_m}(\mathbb{I}) \}$  for all  $x \in X$ . Integrating this equation with respect to  $\mu$ , and using part (1), we find  $\mathbb{S}(\mu \otimes \rho, \varphi) \geq \varphi(h + \mathbb{I}) - (\mu \otimes \rho)^h(\mathbb{I}) = \int \mu(dx) \mathbb{S}_n(\rho, \varphi_x)$ . Now the result follows by taking the supremum over  $n$ .

(3) This is the conditional entropy formula of Theorem 2 of [28], applied to the conditional expectation  $\mathbb{E} : \mathcal{C}(X, \mathcal{A}) \rightarrow \mathcal{C}(X) \otimes \mathbb{I}$  given by  $\mathbb{E}(f \otimes A) = \rho(A)f \otimes \mathbb{I}$ . There the claim is proved when  $\mu \otimes \rho$  is separating. Let  $\omega_\varepsilon = (1 - \varepsilon)\mu \otimes \rho + \varepsilon\omega \otimes \rho$ ,  $0 < \varepsilon \leq 1$ , which is separating and preserved by  $\mathbb{E}$ . By monotonicity [3],  $\mathbb{S}(\mu \otimes \rho, \varphi) \geq \mathbb{S}(\varepsilon^{-1}\omega_\varepsilon \otimes \rho, \varphi) = \mathbb{S}(\omega \otimes \rho, \varphi) + \log(\varepsilon)$ , so that  $\mathbb{S}(\omega_\varepsilon \otimes \rho, \varphi)$  is finite. By the theorem mentioned,

$$\mathbb{S}(\omega_\varepsilon \otimes \rho, \varphi) = \mathbb{S}((1 - \varepsilon)\mu + \varepsilon\omega, \nu) + \mathbb{S}(\nu \otimes \rho, \varphi) \quad .$$



Using the lower semicontinuity of  $\mathbb{S}(\cdot, \cdot)$  in the norm topology (Theorem 3.7 (1), of [3]), and the joint convexity (Theorem 3.8 (1), of [3]), we obtain the claim by taking the limit  $\varepsilon \rightarrow 0$ .

■

When  $X$  is a finite set, the conditional entropy  $n^{-1} \mathbb{S}(\mu^n, \hat{\mu}_n)$  cannot diverge, and can be seen to go to zero by a direct application of Stirling's formula. This suggests the use of "coarse-graining", a standard technique for reducing problems on a general probability spaces  $X$  to the finite case. The term "coarse graining" is usually applied to a conditional expectation of  $\mathcal{L}^\infty(X, \mu)$  onto the subalgebra generated by a finite  $\mu$ -measurable partition of  $X$ . However, this kind of discretization does not fit the purpose at hand, because (LD) requires only the  $w^*$ -convergence of certain measures, so that the convergence of expectations of discontinuous (e.g. characteristic) functions cannot be guaranteed. This difficulty is circumvented by using the following class of operators, which is more adapted to the  $C^*$ -algebraic (rather than the  $W^*$ -algebraic) setting.

**III.3 Definition.** Let  $\mu \in K(\mathcal{C}(X))$ . Then a **continuous coarse-graining** of  $X$  with respect to  $\mu$  is a map  $\gamma : \mathcal{C}(X) \rightarrow \mathcal{C}(X)$  of the form

$$(\gamma f)(x) = \sum_{i \in I} g_i(x) \nu_i(f) \quad ,$$

where  $I$  is a finite set,  $g_i \in \mathcal{C}(X)$  is positive with  $\sum_i g_i = 1$ ,  $\nu_i \in K(\mathcal{C}(X))$  with  $\sum_i \mu(g_i) \nu_i = \mu$ , and if  $\mu(g_i) \neq 0$ , then  $\nu_i(\cdot) = \mu(h_i \cdot)$ , with  $h_i \in \mathcal{C}(X)$ . The set of such operators will be denoted by  $\Gamma_\mu$ .

For many purposes coarse graining operators with  $\nu_i(f) = \mu(g_i)^{-1} \mu(g_i f)$  are sufficient. These correspond to hermitian operators in  $\mathcal{L}^2(X, \mu)$ , but we shall not have any use for this property. When  $\gamma \in \Gamma_\mu$ , the symbol  $\gamma$  will also stand for the operator  $\gamma \otimes \text{id}_A : \mathcal{B} \rightarrow \mathcal{B}$  (recall that  $\mathcal{B} = \mathcal{C}(X, \mathcal{A}) \cong \mathcal{C}(X) \otimes \mathcal{A}$ ). For  $n \leq \infty$ ,  $\gamma^n$  will denote the  $n^{\text{th}}$  tensor power of  $\gamma$ , considered either as an operator on  $\mathcal{C}(X)^n$  or on  $\mathcal{B}^n$ .

**III.4 Lemma.**

(1) Let  $n \leq \infty$ ,  $\varepsilon > 0$ ,  $r \in \mathbb{N}$ ,  $B_1, \dots, B_r \in \mathcal{B}^n$ . Then there is  $\gamma \in \Gamma_\mu$  such that

$$\|\gamma^n(B_i) - B_i\| \leq \varepsilon \quad \text{for } i = 1, \dots, r \quad .$$

(2) Let  $H = (H_n)_{n \in \mathbb{N}}$  with  $H_n \in \mathcal{B}^n$  be an approximately symmetric sequence. Then there is  $\gamma \in \Gamma_\mu$  such that  $\|\gamma^n(H_n) - H_n\| \leq \varepsilon$  uniformly for sufficiently large  $n$ . Hence for all  $\varphi \in K(\mathcal{B})$ :

$$|(jH)(\varphi \circ \gamma) - (jH)(\varphi)| \leq \varepsilon \quad .$$



- (3) Let  $\phi \in K_s(\mathcal{B}^\infty)$ ,  $\psi, \varphi \in K(\mathcal{B})$ , and  $s' < \mathbb{S}(\psi, \varphi)$ ,  $s'_M < \mathbb{S}_M(\psi^\infty, \phi)$ . Then there is a  $\gamma \in \Gamma_\mu$  such that
- $$s' \leq \mathbb{S}(\psi \circ \gamma, \varphi \circ \gamma) \leq \mathbb{S}(\psi, \varphi) \quad \text{and} \quad s'_M \leq \mathbb{S}_M((\varphi \circ \gamma)^\infty, \phi \circ \gamma^\infty) \leq \mathbb{S}_M(\psi^\infty, \phi) \quad .$$
- (4) The above three requirements can be met simultaneously by a suitable  $\gamma \in \Gamma_\mu$ .

**Proof :** (1) We first prove this statement for  $n = 1$  and  $\mathcal{A} = \mathbb{C}$ , that is for  $\mathcal{C}(X)$ . Any collection of  $r$  functions in  $\mathcal{C}(X)$  determines a continuous map  $\vec{B} : X \rightarrow \mathbb{C}^r$ . We may then pick finitely many continuous functions  $\hat{g}_i : \vec{B}(X) \rightarrow \mathbb{R}^+$ , each of which is supported by a subset of the compact set  $\vec{B}(X)$  with diameter less than  $\varepsilon/2$ , and such that  $\sum_i \hat{g}_i = 1$ . Put  $g_i = \hat{g}_i \circ \vec{B}$ . For those  $i$ , with  $\mu(g_i) > 0$ , set  $\nu_i(\cdot) := \mu(g_i)^{-1} \mu(g_i \cdot)$ ; otherwise, let  $\nu_i$  be any state of  $\mathcal{C}(X)$  such that the corresponding measure has support contained in  $\text{supp}(g_i)$ . Then the  $(g_i, \nu_i)$  satisfy the conditions of III.3, and the corresponding coarse-graining  $\gamma$  satisfies

$$\begin{aligned} \|\gamma(B_k) - B_k\| &= \sup_X \left| \sum_i g_i(x) (\nu_i(B_k) - B_k(x)) \right| \\ &\leq \sup_X \sum_i g_i(x) |\nu_i(B_k) - B_k(x)| \\ &\leq \max_i \sup \{ |\nu_i(B_k) - B_k(x)| \mid x \in \text{supp}(g_i) \} \quad . \end{aligned}$$

By definition of  $g_i$ ,  $x \in \text{supp}(g_i)$  iff  $\vec{B}(x) \in \text{supp}(\hat{g}_i)$ . Thus, since  $\text{supp}(\nu_i) \subset \text{supp}(g_i)$ ,  $|\nu_i(B_k) - B_k(x)| \leq \varepsilon$  for  $x \in \text{supp}(g_i)$ , which establishes the claim.

Now every element of  $\mathcal{B}^n = \mathcal{C}(X)^n \otimes \mathcal{A}^n$  can be approximated in norm by finite linear combinations of elements of the form  $B = f_1 \otimes \cdots \otimes f_n \otimes A$  with  $f \in \mathcal{C}(X)$  and  $A \in \mathcal{A}^n$ . (If  $n = \infty$ , this is valid for a suitable finite  $n$ ). Then  $\gamma^n(B) = (\gamma f_1) \otimes \cdots \otimes (\gamma f_n) \otimes A$ . Only a finite set of functions  $f \in \mathcal{C}(X)$  is needed in the uniform approximation of the given  $B_1, \dots, B_r$ , and for all of these functions we can simultaneously make  $\|\gamma f - f\|$  as small as we please.

(2) Given  $\varepsilon$ , we can find  $m$  such that  $\|H_n - \text{sym}_n(H_m)\| \leq \varepsilon/3$ . Applying (1) to the single element  $H_m$ , and using  $\text{sym}_n \circ \gamma^n = \gamma^n \circ \text{sym}_n$ , the result follows.

(3,4) The inequality  $\mathbb{S}(\psi \circ \gamma, \varphi \circ \gamma) \leq \mathbb{S}(\psi, \varphi)$  holds for arbitrary Schwarz-positive unit-preserving maps [22], and the corresponding relation for  $\mathbb{S}_M$  follows herefrom by going to the limit which defines  $\mathbb{S}_M$ . We may assume that the relative entropy in question is finite, and pass to the von Neumann algebra  $\hat{\mathcal{B}} = \pi_\psi(\mathcal{B})''$  generated by the GNS-representation associated with  $\psi$ . We then have the variational formula [22]

$$\mathbb{S}(\psi, \varphi) = \sup_{n \in \mathbb{N}} \sup_b K(n; b) \quad ,$$

where the second supremum is over step functions  $b : [1/n, \infty) \rightarrow \hat{\mathcal{B}}$  with finite range, and such that  $b_t = \mathbb{I}$  for large  $t$ , and where

$$K(n; b) = \log(n) - \int_{1/n}^{\infty} dt (t^{-1} \varphi((\mathbb{I} - b_t)^*(\mathbb{I} - b_t)) + t^{-2} \psi(b_t b_t^*)) .$$

Now for  $s' \leq s' + \varepsilon < \mathbb{S}(\psi, \varphi)$ , we can find  $K(n; b)$  lying between  $s' + \varepsilon$  and  $\mathbb{S}(\psi, \varphi)$ . Since  $b$  has finite range, there is  $\gamma \in \Gamma_\mu$  making both

$$\|\gamma(b_t b_t^*) - b_t b_t^*\| \quad \text{and} \quad \|\gamma((\mathbb{I} - b_t^*)(\mathbb{I} - b_t)) - (\mathbb{I} - b_t^*)(\mathbb{I} - b_t)\|$$

sufficiently small, so that the lower bound  $K(n; \gamma(b))$  on  $\mathbb{S}(\psi \circ \gamma, \varphi \circ \gamma)$  will still be above  $s'$ . This proves the existence of  $\gamma$ , and it is clear that the same argument works for the entropies on  $\mathcal{B}^n$  and for  $\mathbb{S}_M$ , which is a supremum of such entropies. Moreover, it is clear from this proof that (1), (2), and (3) can be satisfied by the same  $\gamma$ . (Remark that (3) without (4) could have been proven directly by invoking  $w^*$ -lower semicontinuity). ■

The following proposition solves the problem of the “divergence of the conditional entropy  $n^{-1} \mathbb{S}(\mu^n, \hat{\mu}_n)$ ” discussed previously in this section. The estimate given should be compared with  $\liminf_{n \rightarrow \nu} n^{-1} \mathbb{S}(\mu^n, \varphi_n) \geq \mathbb{S}_M(\mu^\infty, \varphi)$ , which will follow from III.6 below.

**III.5 Proposition.** *Let  $\gamma$  be a continuous coarse-graining with respect to  $\mu$ . Suppose that  $\varphi_n \in K_s(\mathcal{C}(X)^n)$  is a sequence converging to  $\varphi \in K_s(\mathcal{C}(X)^\infty)$  along a subnet  $\nu$ . Then*

$$\limsup_{n \rightarrow \nu} n^{-1} \mathbb{S}(\mu^n, \varphi_n \circ \gamma^n) \leq \mathbb{S}_M(\mu^\infty, \varphi) .$$

**Proof :** We first prove the claim in the case where  $X$  is a finite set and  $\gamma$  is the identity operator on  $\mathcal{C}(X)$ . This is done in three steps.

**Step 1:** By Størmer’s theorem [35] (Proposition IV.5 of [31]) the symmetric states on  $\mathcal{C}(X)^\infty$  are in one-to-one correspondence with the measures on the simplex  $\Delta := K(\mathcal{C}(X))$ . It will be convenient to represent states of  $\mathcal{C}(X)^n$  in the same way; to do this we use the fact that  $\text{sym}_n(\mathcal{C}(X)^n)$  is isomorphic to  $\mathcal{C}(X^n / \sim)$ , where  $X^n / \sim$  denotes the space of orbits in  $X^n$  under the action of the permutation group of  $n$  elements. Each such orbit is characterized uniquely by the number of times each of the elements of  $X$  appears in it. Thus, an orbit corresponds to an “occupation number function”  $\omega : X \rightarrow \mathbb{N}$ , satisfying the constraint  $\sum_{x \in X} \omega(x) = n$ . To each orbit we can associate a point  $\sigma_\omega = n^{-1} \sum_{x \in X} \omega(x) \delta(x)$  in  $\Delta$ , where  $\delta(x)$  denotes the point-measure at  $x \in X$ . Since  $X$  is finite, every symmetric

state  $\psi \in K_s(\mathcal{C}(X)^n) \equiv K(\mathcal{C}(X^n / \sim))$  is a finite convex combination  $\psi = \sum_{\omega} \lambda(\omega) \delta(\omega)$ . We associate with  $\psi$  a measure  $\hat{\psi}$  on  $\Delta$  given by

$$\hat{\psi} = \sum_{\omega} \lambda(\omega) \delta(\sigma_{\omega}) \quad ,$$

and a symmetric state  $\tilde{\psi}$  of  $\mathcal{C}(X)^{\infty}$  defined by

$$\tilde{\psi} = \int_{\Delta} \hat{\psi}(d\chi) \chi^{\infty} = \sum_{\omega} \lambda(\omega) (\sigma_{\omega})^{\infty} \quad .$$

We will show that

$$\|\psi - \tilde{\psi}|_{\mathcal{C}(X)^n}\| \leq 2(1 - n^{-n}n!) \quad . \quad (*)$$

This then implies that the sequence  $(\tilde{\varphi}_n)$  associated with  $(\varphi_n)$  is also  $w^*$ -convergent to  $\varphi$  and - due to Størmer's Theorem - the sequence  $(\hat{\varphi}_n)$  is  $w^*$ -convergent to  $\hat{\varphi}$ , along the same subnet.

To prove (\*), it suffices to show that

$$|(\delta(\omega) - (\sigma_{\omega})^n)(A)| \leq 2(1 - n^{-n}n!) \|A\| \quad , \quad (**)$$

for every  $A \in \mathcal{C}(X)^n$  and every orbit  $\omega$ . We have, on the one hand,

$$\delta(\omega)(A) = (n!)^{-1} \sum_{\pi} A(\xi_{\pi 1}, \xi_{\pi 2}, \dots, \xi_{\pi n}) \quad ,$$

where the sum is over the permutations of  $\{1, 2, \dots, n\}$ , and  $(\xi_1, \xi_2, \dots, \xi_n)$  is any point of the orbit  $\omega$ . On the other hand,

$$(\sigma_{\omega})^n(A) = n^{-n} \sum_{j=1}^n \sum_{x_j \in X} A(x_1, x_2, \dots, x_n) \omega(x_1) \omega(x_2) \cdots \omega(x_n) \quad .$$

This last sum can be rewritten as a sum over the  $n^n$  mappings  $\eta$  from  $\{1, 2, \dots, n\}$  into itself:

$$(\sigma_{\omega})^n(A) = n^{-n} \sum_{\eta} A(\xi_{\eta 1}, \xi_{\eta 2}, \dots, \xi_{\eta n}) \quad ,$$

due to  $\omega(x) = \{i \mid \xi_i = x\}$ . Since the permutations of  $\{1, 2, \dots, n\}$  are just the  $n!$  injective maps, we have

$$\begin{aligned} (\delta(\omega) - (\sigma_{\omega})^n)(A) &= (n^{-n} - (n!)^{-1}) \sum_{\pi} A(\xi_{\pi 1}, \xi_{\pi 2}, \dots, \xi_{\pi n}) \\ &\quad + n^{-n} \sum_{\eta} A(\xi_{\eta 1}, \xi_{\eta 2}, \dots, \xi_{\eta n}) \quad , \end{aligned}$$

where the second sum is over the  $(n^n - n!)$   $\eta$ 's which are not injective. The modulus of each sum is bounded by  $(1 - n^{-n}n!) \|A\|$ , and (\*\*) follows.

**Step 2:** For every orbit  $\omega$  we compute  $n^{-1} \mathbb{S}(\mu^n, \delta(\omega))$  and relate this to  $\mathbb{S}(\mu, \sigma_{\omega}) = \sum_{x \in X} (\omega(x)/n) (\log(\omega(x)/n) - \log(\mu(x)))$ . Viewed as a symmetric probability measure on  $X^n$ ,  $\delta(\omega)$  is the equidistribution on the orbit  $\omega$ , which consists of  $p_{\omega}^{-1} = n! / (\prod_{x \in X} \omega(x)!)$

points of  $X^n$ :

$$\delta(\omega) = p_\omega \sum_{z \in \omega} \delta(z) \quad .$$

To every point  $z$  in the orbit  $\omega \subset X^n$ , the measure  $\mu^n$  assigns the same probability  $\mu^n(\{z\}) = \prod_{x \in X} \mu(\{x\})^{\omega(x)}$ . Thus,

$$\begin{aligned} \mathbb{S}(\mu^n, \delta(\omega)) &= \sum_{z \in \omega} p_\omega \log(p_\omega / \mu^n(z)) \\ &= \sum_{x \in X} \left( \log(\omega(x)!) - \omega(x) \log(\mu(x)) \right) - \log(n!) \quad . \end{aligned}$$

Using the following precise form of Stirling's formula

$$(12n+1)^{-1} < \log(n!) - \left\{ \frac{1}{2} \log(2\pi) + \left(n + \frac{1}{2}\right) \log(n) - n \right\} < (12n)^{-1} \quad ,$$

and the inequality  $1 \leq \omega(x) \leq n$ , we arrive at

$$\begin{aligned} (2n)^{-1}(|X| - 1) \log(2\pi) - (2n)^{-1} \log(n) + |X|(12n^2 + n)^{-1} - (12n^2)^{-1} \\ < n^{-1} \mathbb{S}(\mu^n, \delta(\omega)) - \mathbb{S}(\mu, \sigma_\omega) < \\ < (2n)^{-1}(|X| - 1) \log(2\pi n) + (12n)^{-1}|X| - (12n^2 + n)^{-1} \quad . \end{aligned}$$

**Step 3:** By convexity of  $\mathbb{S}$ , and the previous steps, we have for  $\varphi_n = \sum_\omega \lambda_n(\omega) \delta(\omega)$ :

$$\begin{aligned} n^{-1} \mathbb{S}(\mu^n, \varphi_n) &\leq \sum_\omega \lambda_n(\omega) n^{-1} \mathbb{S}(\mu^n, \delta(\omega)) \\ &\leq \sum_\omega \lambda_n(\omega) \mathbb{S}(\mu, \sigma_\omega) + \mathbf{O}(\log(n)/n) \\ &= \int_\Delta \hat{\varphi}_n(d\sigma) \mathbb{S}(\mu, \sigma) + \mathbf{O}(\log(n)/n) \quad . \end{aligned}$$

But for finite  $X$ ,  $\mathbb{S}(\mu, \cdot)$  is a continuous function, hence  $w^*$ -convergence of  $(\hat{\varphi}_n)$  to  $\hat{\varphi}$  implies that  $\limsup_n n^{-1} \mathbb{S}(\mu^n, \varphi_n) \leq \int_\Delta \hat{\varphi}(d\sigma) \mathbb{S}(\mu, \sigma) = \mathbb{S}_M(\mu^\infty, \varphi)$ . This completes the proof of the proposition for finite  $X$ .

We now prove the full statement. Let  $(\gamma f)(x) = \sum_{i \in I} g_i(x) \nu_i(f)$  be a continuous coarse-graining with respect to  $\mu$ . Then we can write  $\gamma = \gamma_1 \circ \gamma_2$  with  $\gamma_2 : \mathcal{C}(X) \rightarrow \mathcal{C}(I)$  and  $\gamma_1 : \mathcal{C}(I) \rightarrow \mathcal{C}(X)$  given by  $(\gamma_2 f)(i) = \nu_i(f)$  and  $(\gamma_1 f)(x) = \sum_{i \in I} g_i(x) f(i)$ . Then

$$\begin{aligned} \limsup_n n^{-1} \mathbb{S}(\mu^n, \varphi_n) &= \limsup_n n^{-1} \mathbb{S}(\mu^n \circ \gamma_1^n \circ \gamma_2^n, \varphi_n \circ \gamma_1^n \circ \gamma_2^n) \\ &\leq \limsup_n n^{-1} \mathbb{S}((\mu \circ \gamma_1)^n, \varphi_n \circ \gamma_1^n) \\ &\leq \mathbb{S}_M((\mu \circ \gamma_1)^\infty, \varphi \circ \gamma^\infty) \leq \mathbb{S}_M(\mu^\infty, \varphi) \quad , \end{aligned}$$

where at the first and last inequality we have used the monotonicity of  $\mathbb{S}$  under Schwarz-positive unital maps [22], and the middle inequality is an application of the special case (proved above) to: the finite set  $I$ , the product state built with  $\mu \circ \gamma_1 \in K(\mathcal{C}(I))$ , and the sequence  $\varphi_n \circ \gamma_1^n \in K_s(\mathcal{C}(I)^n)$ , which converges along the given subnet to  $\varphi \circ \gamma_1^\infty$ .

The following proposition is the key entropy estimate for the lower bound; its homogeneous version goes back to Proposition III.4. of [31].

**III.6 Proposition.** *If (LD) holds, the measures  $\hat{\mu}_n \in K(\mathcal{C}(X)^n)$  with  $\hat{\mu}_n(f) = (\text{sym}_n f)(\xi_n)$  are  $w^*$ -convergent to  $\mu^\infty$ . Let  $\phi_n \in K(\mathcal{A}^n)$ , and suppose that  $\lim_{n \rightarrow \nu} \phi_n \circ \Xi_n = \phi$  along some subnet  $\nu$ . Then  $\phi \in K_s^\mu$ , and*

$$\liminf_{n \rightarrow \nu} n^{-1} \mathbb{S}(\rho^n, \phi_n) \geq \mathbb{S}_M((\mu \otimes \rho)^\infty, \phi) \quad .$$

**Proof :** We first show that  $\phi \in K_s^\mu$ . The statement  $\lim_n \hat{\mu}_n = \mu^\infty$  is the special case  $\mathcal{A} = \mathbb{C}$ . Let  $f \in \mathcal{C}(X)$ , and consider for each  $n$  the function  $F_n \in \mathcal{B}^n$  given by

$$F_n(x_1, \dots, x_n) = \mathbb{I}_{\mathcal{A}} \left( n^{-1} \sum_{i=1}^n f(x_i) - \int \mu(dx) f(x) \right)^2 \quad .$$

This is an approximately symmetric sequence as the square of a strictly symmetric sequence [31]. By Proposition II.2 of [31],  $jF(\psi) = (\psi(f \otimes \mathbb{I}) - \mu(f))^2$ . Since  $F_n$  is symmetric,  $\Xi_n(F_n) = F_n(\xi_{n,1}, \dots, \xi_{n,n})$ , which goes to zero by (LD). Hence  $\lim_n (\phi_n \circ \Xi_n)(F_n) = 0$ . On the other hand, for the subnet  $\nu$  along which  $(\phi_n \circ \Xi_n)$  converges to  $\phi = \int m(d\psi) \psi^\infty$ , and Proposition II.2 of [31] implies

$$\lim_{n \rightarrow \nu} (\phi_n \circ \Xi_n)(F_n) = \int m(d\psi) (jF)(\psi) = \int m(d\psi) (\psi(f \otimes \mathbb{I}) - \mu(f))^2 = 0 \quad .$$

Since this equation holds for all  $f \in \mathcal{C}(X)$ , we conclude that  $m$  must be supported by the closed set  $\{\psi \in K(\mathcal{B}) \mid \psi|_{\mathcal{C}(X)} = \mu\}$ .

To prove the entropy estimate, consider a continuous coarse-graining  $\gamma$  with respect to  $\mu$ . By the monotonicity of  $\mathbb{S}$  with respect to Schwarz-positive identity-preserving maps, we have  $n^{-1} \mathbb{S}(\rho^n, \phi_n) \geq n^{-1} \mathbb{S}(\rho^n \circ \Xi_n \circ \gamma^n, \phi_n \circ \Xi_n \circ \gamma^n)$ . Noting that  $(\phi_n \circ \Xi_n \circ \gamma^n)|_{\mathcal{C}(X)^n} = \hat{\mu}_n \circ \gamma^n$ , independently of  $\phi_n \in K(\mathcal{A}^n)$ , and that  $\rho^n \circ \Xi_n \circ \gamma^n = (\hat{\mu}_n \circ \gamma^n) \otimes \rho^n$ , we apply III.2.(3) to  $\mathcal{C}(X^n, \mathcal{A}^n)$  and find that

$$\begin{aligned} \liminf_{n \rightarrow \nu} n^{-1} \mathbb{S}(\rho^n, \phi_n) &\geq \liminf_{n \rightarrow \nu} n^{-1} \mathbb{S}((\hat{\mu}_n \circ \gamma^n) \otimes \rho^n, \phi_n \circ \Xi_n \circ \gamma^n) \\ &= \liminf_{n \rightarrow \nu} (n^{-1} \mathbb{S}(\mu^n \otimes \rho^n, \phi_n \circ \Xi_n \circ \gamma^n) - n^{-1} \mathbb{S}(\mu^n, \hat{\mu}_n \circ \gamma^n)) \\ &\geq \liminf_{n \rightarrow \nu} n^{-1} \mathbb{S}(\mu^n \otimes \rho^n, \phi_n \circ \Xi_n \circ \gamma^n) - \limsup_{n \rightarrow \nu} n^{-1} \mathbb{S}(\mu^n, \hat{\mu}_n \circ \gamma^n) \quad . \end{aligned}$$

Since  $(\hat{\mu}_n)$  is  $w^*$ -convergent to  $\mu^\infty$ , III.5 implies that  $\limsup_{n \rightarrow \nu} n^{-1} \mathbb{S}(\mu^n, \hat{\mu}_n \circ \gamma^n) \leq \mathbb{S}_M(\mu^\infty, \mu^\infty) = 0$ , so the last term above vanishes. The other term is bounded below by  $\mathbb{S}_M((\mu \otimes \rho)^\infty, \phi \circ \gamma^\infty)$  due to Proposition III.4 of [31]. The result follows by taking the supremum over  $\gamma \in \Gamma_\mu$  and III.4.(3). ■

The following proposition summarizes the properties of the trial states  $\chi_n$  used in the proof of the upper bound.

**III.7 Proposition.** *Let  $\psi \in K(\mathcal{B})$  be a state of the form  $\psi = \varphi \circ \gamma$  with  $\gamma \in \Gamma_\mu$ ,  $\varphi \in K(\mathcal{B})$ , and satisfying  $\varphi|_{\mathcal{C}(X)} = \mu$ . Then  $\psi(f \otimes A) = \int \mu(dx) f(x) \psi(x, A)$ , where  $x \in X \mapsto \psi(x) \equiv \psi(x, \cdot) \in K(\mathcal{A})$  is continuous and has finite dimensional range. Let  $\chi_n \in K(\mathcal{A}^n)$  denote the state given by  $\chi_n = \psi(\xi_{n,1}) \otimes \cdots \otimes \psi(\xi_{n,n})$ . Then  $\lim_n \chi_n \circ \Xi_n = \psi^\infty$ . Moreover, if  $\mathbb{S}(\mu \otimes \rho, \varphi) < \infty$ , then  $\mathbb{S}(\rho, \psi(\cdot))$  is bounded and continuous, and*

$$\lim_{n \rightarrow \infty} n^{-1} \mathbb{S}(\rho^n, \chi_n) = \int \mu(dx) \mathbb{S}(\rho, \psi(x)) = \mathbb{S}(\mu \otimes \rho, \psi) \quad .$$

**Proof :** Let  $(\gamma f)(x) = \sum_{i \in I} g_i(x) \nu_i(f)$ . It follows that  $\psi(x, A) = \sum_{i \in J} h_i(x) \varphi(g_i \otimes A)$ , where  $J$  is the set of  $i \in I$  with  $\mu(g_i) \neq 0$ , and  $h_i$  is the continuous Radon-Nikodym derivative of  $\nu_i$  w.r.t.  $\mu$ . Thus  $\psi(x) = \sum_{i \in J} h'_i(x) \psi_i$  with  $h'_i = \mu(g_i) h_i$ , and states  $\psi_i \in K(\mathcal{A})$  given by

$$\psi_i(A) = \mu(g_i)^{-1} \varphi(g_i \otimes A) \quad , \quad i \in J \quad .$$

The statements about  $\psi(\cdot)$  are then obvious.

To prove the first limit formula we use only the  $w^*$ -continuity of  $\psi(\cdot)$ . Define a map  $\eta : \mathcal{B}' \rightarrow \mathcal{C}(X)$  by  $\eta(F) = \psi(x, F(x))$ . Indeed,  $\eta(F)$  is a continuous function since  $(\psi, A) \mapsto \psi(A)$  is jointly continuous on bounded sets for the  $(w^* \times \text{Norm})$ -topology. Clearly,  $\eta$  is completely positive and unit-preserving, and  $\mu \circ \eta = \varphi \circ \gamma = \psi$ . For  $F = B_1 \otimes \cdots \otimes B_n \in \mathcal{B}^n$  we have with  $\eta^n : \mathcal{B}^n \rightarrow \mathcal{C}(X)^n$ :

$$\chi_n(F(\xi_n)) = \prod_{i=1}^n \psi(\xi_{n,i}, B_i(\xi_{n,i})) = \eta^n(F)(\xi_n) \quad .$$

By continuous linear extension this relation carries over to all  $F \in \mathcal{B}^n$ . Now fix some  $k \in \mathbb{N}$ , and  $F \in \mathcal{B}^k$ . Then  $F$  is identified with  $F \otimes \mathbb{I}_{n-k} \in \mathcal{B}^n$  for all  $n \geq k$ , and  $\eta^n(F \otimes \mathbb{I}_{n-k}) = (\eta^k F) \otimes \mathbb{I}_{n-k}$  because  $\eta$  maps the unit of  $\mathcal{B}$  into the unit of  $\mathcal{C}(X)$ . Then

$$\begin{aligned} (\chi_n \circ \Xi_n)(F) &= \chi_n(\text{sym}_n(F \otimes \mathbb{I}_{n-k})(\xi_n)) = (\eta^n(\text{sym}_n(F \otimes \mathbb{I}_{n-k})))(\xi_n) \\ &= (\text{sym}_n(\eta^k F \otimes \mathbb{I}_{n-k}))(\xi_n) = \hat{\mu}_n(\eta^k F \otimes \mathbb{I}_{n-k}) \quad . \end{aligned}$$

Then, as remarked in the proof of III.6,  $(\hat{\mu}_n)$  is  $w^*$ -convergent to  $\mu^\infty$ , and thus  $\lim_n (\chi_n \circ \Xi_n)(F) = \mu^\infty(\eta^k F) = (\mu \circ \eta)^\infty(F) = \psi^\infty(F)$ .

Suppose now that  $\mathbb{S}(\mu \otimes \rho, \varphi) < \infty$ . Since  $\mathbb{S}(\rho, \cdot)$  is convex on the finite dimensional simplex spanned by  $\{\psi_i | i \in J\}$ , the continuity of  $\mathbb{S}(\rho, \psi(\cdot))$  follows if we show that  $\mathbb{S}(\rho, \psi_i) < \infty$

for all  $i \in J$ . Since  $\psi = \varphi \circ \gamma = \sum_{i \in J} \mu(g_i) \nu_i \otimes \psi_i$  is a convex combination of product states, we have

$$\begin{aligned} \infty > \mathbb{S}(\mu \otimes \rho, \varphi) &\geq \mathbb{S}((\mu \otimes \rho) \circ \gamma, \varphi \circ \gamma) = \mathbb{S}(\mu \otimes \rho, \psi) \\ &\geq \sum_{i \in J} \mu(g_i) \mathbb{S}(\mu \otimes \rho, \nu_i \otimes \psi_i) + \sum_{i \in J} \mu(g_i) \log \mu(g_i) \\ &\geq \sum_{i \in J} \mu(g_i) (\mathbb{S}(\mu, \nu_i) + \mathbb{S}(\rho, \psi_i)) - \log |I| \quad . \end{aligned}$$

For  $i \in J$ ,  $\mathbb{S}(\mu, \nu_i) \leq \sup_{x \in X} |h_i(x) \log(h_i(x))| < \infty$ , so  $\mathbb{S}(\rho, \psi_i)$  must also be finite.

The first equality for  $\lim_n n^{-1} \mathbb{S}(\rho^n, \chi_n)$  follows from (LD) and  $n^{-1} \mathbb{S}(\rho^n, \chi_n) = n^{-1} \sum_{i=1}^n \mathbb{S}(\rho, \psi(\xi_{n,i}))$ .

It remains to be shown that  $\int \mu(dx) \mathbb{S}(\rho, \psi(x)) = \mathbb{S}(\mu \otimes \rho, \psi)$ . By III.1 and III.2.(1):

$$\mathbb{S}(\mu \otimes \rho, \psi) = \sup \int \mu(dx) \left\{ \psi(x, k(x) + \mathbb{I}) - \rho^{k(x)}(\mathbb{I}) \right\} \quad ,$$

the supremum being taken over all  $k \in \mathcal{B}$ . Again by III.1. the integrand is bounded above by  $\mathbb{S}(\rho, \psi(x))$ , which proves the inequality " $\leq$ ". To prove " $\geq$ " it suffices to exhibit for every  $\varepsilon > 0$  a  $k \in \mathcal{B}$  such that  $\mathbb{S}(\rho, \psi(x)) \leq \varepsilon + \psi(x, k(x)) - \log \rho^{k(x)}(\mathbb{I})$ . By III.1, we can find for every  $x$  some  $k_0(x) \in \mathcal{A}$  such that  $\mathbb{S}(\rho, \psi(x)) \leq \varepsilon/2 + \psi(x, k_0(x) + \mathbb{I}) - \rho^{k_0(x)}(\mathbb{I})$ . Since  $\mathbb{S}(\rho, \psi(\cdot))$  is continuous and  $\psi(\cdot)$  is  $w^*$ -continuous, the set  $U_z \subset X$  consisting of those  $y \in X$  satisfying

$$\mathbb{S}(\rho, \psi(y)) < \varepsilon + \psi(y, k_0(z) + \mathbb{I}) - \rho^{k_0(z)}(\mathbb{I}) \quad . \quad (*)$$

is open and contains  $z$ . Hence there is a finite subset  $Z \subset X$  such that  $\{U_z \mid z \in Z\}$  covers  $X$ . For each  $z \in Z$  we can pick a function  $\zeta_z \in \mathcal{C}(X)$  such that  $\zeta_z \geq 0$ ,  $\zeta_z$  vanishes outside  $U_z$ , and  $\sum_{z \in Z} \zeta_z = 1$ . We define  $k$  by  $k(y) = \sum_{z \in Z} \zeta_z(y) k_0(z)$ . Then since  $(*)$  holds whenever  $\zeta_z(y) \neq 0$ , and  $k \mapsto \log \rho^k(\mathbb{I})$  is convex we find

$$\begin{aligned} \mathbb{S}(\rho, \psi(y)) &= \sum_{z \in Z} \zeta_z(y) \mathbb{S}(\rho, \psi(y)) < \sum_{z \in Z} \zeta_z(y) [\varepsilon + \psi(y, k(y) + \mathbb{I}) - \rho^{k_0(z)}(\mathbb{I})] \\ &\leq \varepsilon + \psi(y, k(y) + \mathbb{I}) - \sum_{z \in Z} \zeta_z(y) \rho^{k_0(z)}(\mathbb{I}) \leq \varepsilon + \psi(y, k(y) + \mathbb{I}) - \rho^{k(y)}(\mathbb{I}) \quad . \end{aligned}$$

■

### Proof of the main theorem:

**Step 1:** The equality of  $(*)$  and  $(**)$  follows as in [31], since

$$\lim_{n \rightarrow \infty} \phi(H_n) - \mathbb{S}_M((\mu \otimes \rho)^\infty, \phi) = \int m(d\varphi) \{j(H)(\varphi) - \mathbb{S}(\mu \otimes \rho, \varphi)\} \quad ,$$



where  $m$  is the probability measure on  $K(\mathcal{B})$  in the Størmer decomposition  $\phi = \int m(d\varphi)\varphi^\infty$  of the symmetric state  $\phi \in K_s(\mathcal{B}^\infty)$ . The constraint  $\phi \in K_s^\mu$  is equivalent to  $m$  being supported by  $\{\varphi \in K(\mathcal{B}) \mid \varphi|_{\mathcal{C}(X)} = \mu\}$ .

By the Petz Duality Theorem III.1 we have

$$\begin{aligned} a_n &:= n^{-1} \mathbb{F}(\rho^n, nH_n(\xi_n)) := -n^{-1} \log(\rho^n)^{-nH_n(\xi_n)}(\mathbb{I}) \\ &= \inf \{ \varphi(H_n(\xi_n)) + n^{-1} \mathbb{S}(\rho^n, \varphi) \mid \varphi \in K(\mathcal{A}^n) \} \end{aligned} \quad (PD)$$

**Step 2: (Upper bound):** By the first step we may suppose that  $\phi$  is a symmetric product state, i.e.  $\phi = \varphi^\infty$  with  $\varphi|_{\mathcal{C}(X)} = \mu$ , and we may suppose that  $\mathbb{S}(\mu \otimes \rho, \varphi) < \infty$ . Now let  $\gamma \in \Gamma_\mu$  and define  $\chi_n$  as in III.7. Then applying III.7, and Proposition III.3 of [31], we get from (PD):

$$\begin{aligned} \limsup_n a_n &\leq \limsup_n (\chi_n(H_n(\xi_n)) + n^{-1} \mathbb{S}(\rho^n, \chi_n)) \\ &= \lim_n (\chi_n \circ \Xi_n)(H_n) + \lim_n n^{-1} \mathbb{S}(\rho^n, \chi_n) \\ &= j(H)(\varphi \circ \gamma) - \mathbb{S}(\mu \otimes \rho, \varphi \circ \gamma) . \end{aligned}$$

By III.4 we may choose  $\gamma$  such that the right-hand side is arbitrarily close to  $j(H)(\varphi) - \mathbb{S}(\mu \otimes \rho, \varphi)$ .

**Step 3: (Lower bound) :** The state  $\Psi_n = \text{Norm}^{-1}(\rho^n)^{-nH_n(\xi_n)}$  attains the infimum in (PD). Let  $\nu$  be a subnet, along which the sequence  $(\Psi_n \circ \Xi_n)$  is  $w^*$ -convergent to  $\phi \in K_s(\mathcal{B}^\infty)$ . Then we have

$$\begin{aligned} \liminf_{n \rightarrow \nu} a_n &= \liminf_{n \rightarrow \nu} (\Psi_n(\Xi_n(H_n)) + n^{-1} \mathbb{S}(\rho^n, \Psi_n)) \\ &\geq \lim_{n \rightarrow \nu} (\Psi_n \circ \Xi_n)(H_n) + \liminf_{n \rightarrow \nu} n^{-1} \mathbb{S}(\rho^n, \Psi_n) \\ &\geq \lim_{n \rightarrow \infty} \phi(H_n) + \mathbb{S}_M((\mu \otimes \rho)^\infty, \phi) , \end{aligned}$$

where for the last inequality we have used Proposition III.3 of [31] for the first summand and III.6 for the second. Thus any cluster point of  $(\Psi_n \circ \Xi_n)$  maximizes (\*). Since the subnet along which  $a_n$  converges to  $\liminf_{n \rightarrow \infty} a_n$  contains a subnet  $\nu$  along which  $(\Psi_n \circ \Xi_n)$  is  $w^*$ -convergent, the above estimate shows that  $\liminf_n a_n = \lim_{n \rightarrow \nu} a_n \geq (*) \geq \limsup_n a_n$ .

■

## IV. Applications

We consider three applications. The first one is the completion of the discussion of the quasi-spin version of the BCS-model which we used as an example in section II. The second, is to a class of “paired-fermion” models inspired by [14]. The third application concerns random mean-field models.

### IV.1 Quasi-spin BCS model

Consider the BCS-model in its quasi-spin version as introduced in section II. Let  $X$  be the compact subset of  $\mathbb{R}^d$  which is the range of the momenta. For any state  $\varphi \in \mathcal{C}(X, \mathcal{A})$  decomposed as  $\varphi = \int^\oplus d\mu_\varphi(k) \varphi_k$ , we get from (2.1)

$$\begin{aligned} j(H)(\varphi) &= (\varphi \otimes \varphi)(H_2) = \frac{1}{2} \int_X \mu_\varphi(dk) \varepsilon(k) \varphi_k(\mathbb{I} - \sigma^z) \\ &\quad - \frac{1}{\lambda} \int_{X \times X} \mu_\varphi(dk) d\mu_\varphi(p) U(k, p) \Re \{ \varphi_k(\sigma^+) \varphi_p(\sigma^-) \} \quad . \end{aligned}$$

The entropy term (recall that the reference state  $\rho$  was chosen to be the tracial state  $\tau$ ) is given by (III.2.2)

$$\mathbb{S}(\mu \otimes \tau, \varphi) = \int_X \mu(dk) \mathbb{S}(\tau, \varphi_k) \quad ,$$

if  $\mu_\varphi = \mu$ . Thus, the limiting free-energy density (at inverse temperature  $\beta$ ) is given by (2.5):

$$\begin{aligned} \inf \left\{ \right. & \frac{1}{2} \int_X \mu(dk) \varepsilon(k) \varphi_k(\mathbb{I} - \sigma^z) \\ & - \frac{1}{\lambda} \int_{X \times X} \mu(dk) \mu(dp) U(k, p) \Re \{ \varphi_k(\sigma^+) \varphi_p(\sigma^-) \} \\ & \left. - \frac{1}{\beta} \int_X \mu(dk) \mathbb{S}(\varphi_k) \right\} \quad . \end{aligned}$$

We have  $\mathbb{S}(\psi) = -I(\kappa)$ , where  $\kappa$  and  $(1 - \kappa)$  are the eigenvalues of the  $(2 \times 2)$ -density matrix associated with  $\psi$ , and

$$I(s) = s \log(s) + (1 - s) \log(1 - s) \quad , \quad 0 \leq s \leq 1 \quad .$$

Using the parametrization

$$\psi = \frac{1}{2} \begin{pmatrix} 1 + r \cos(\theta) & r \sin(\theta) e^{i\phi} \\ r \sin(\theta) e^{-i\phi} & 1 - r \cos(\theta) \end{pmatrix} \quad (4.1)$$

$(0 \leq r \leq 1, 0 \leq \theta \leq \pi, 0 \leq \phi < 2\pi)$  of the state space of the  $(2 \times 2)$ -matrices, we get:

$$\inf \left\{ \begin{aligned} & \frac{1}{2} \int_X \mu(dk) \varepsilon(k) (1 - r_k \cos(\theta_k)) \\ & - \frac{1}{4\lambda} \int_{X \times X} \mu(dk) \mu(dp) U(k, p) r_k r_p \sin(\theta_k) \sin(\theta_p) \cos(\phi_k - \phi_p) \\ & + \frac{1}{\beta} \int_X \mu(dk) I((1 + r_k)/2) \end{aligned} \right\},$$

where the infimum is over the Borel measurable functions  $k \mapsto r_k, \theta_k$ , and  $\phi_k$ , taking values in  $[0, 1]$ ,  $[0, \pi]$ , and  $[0, 2\pi)$  respectively. This result was obtained by a different method in [9], where the solution of the variational problem is also discussed.

The application to any inhomogeneous mean-field model of "spins" (i.e.,  $\mathcal{A}$  is some finite dimensional matrix algebra) follows the above lines.

## IV.2 Models of paired fermions

We consider a family of fermion-models where the Hamiltonian is expressed in terms of creation/annihilation operators appearing in pairs (i.e. the Cooper pairs in the BCS-model).

Let  $\{\psi_j | j = 1, 2, \dots, 2n\}$  be an orthonormal basis of  $\mathbb{C}^{2n}$ , and  $\mathcal{F}$  be the antisymmetric Fock space built upon  $\mathbb{C}^{2n}$ . Denote the annihilation operator  $a(\psi_j)$  on  $\mathcal{F}$  by  $a[j]$ . Let us pair-up the given basis of  $\mathbb{C}^{2n}$ , say as  $\{(j, j+1) | j = 1, 3, \dots, 2n-1\}$ , and consider the even CAR algebras  $\mathcal{A}_j$  generated by  $\{a[j], a[j+1]\}$ . If  $A$  lies in  $\mathcal{A}_j$ , and  $B$  lies in  $\mathcal{A}_k$  with  $j \neq k$ , then  $A$  and  $B$  commute. Thus, the algebra generated by the collection  $\{\mathcal{A}_j | j = 1, 3, \dots, 2n-1\}$  is isomorphic to the  $n$ -fold tensor product of the *even* part of the CAR algebra over  $\mathbb{C}^2$ , for which we will write  $\mathcal{A}$ .  $\mathcal{A}$  is  $*$ -isomorphic to the direct sum of two copies of the  $(2 \times 2)$ -matrices with complex entries (denoted by  $\mathcal{M}_2$ ):  $\mathcal{A} \cong \mathcal{M}_2 \oplus \mathcal{M}_2$ . This isomorphism is explicitly given by the following identifications of the generators:

$$\begin{aligned} a^*(+)a(+) &= e_{22} \oplus e_{22}, & a(+)a^*(+) &= e_{11} \oplus e_{11}, & a^*(-)a(-) &= e_{22} \oplus e_{11}, \\ a(-)a^*(-) &= e_{11} \oplus e_{22}, & a^*(+)a(-) &= 0 \oplus e_{21}, & a(+)a^*(-) &= 0 \oplus (-e_{12}) \\ a^*(+)a^*(-) &= e_{21} \oplus 0, & a(+)a(-) &= -e_{12} \oplus 0, \end{aligned} \quad (4.2)$$

where  $\{e_{ij} | i, j = 1, 2\}$  is the usual basis of  $\mathcal{M}_2$ , and  $\pm$  are the two components of  $\mathbb{C}^2$ . The state space is thus given by

$$K(\mathcal{A}) = \left\{ t\varphi^{(1)} \oplus (1-t)\varphi^{(2)} \mid 0 \leq t \leq 1, \varphi^{(1)}, \varphi^{(2)} \in K(\mathcal{M}_2) \right\}.$$

As this does not restrict the generality, the reference state which specifies the model will be the faithful trace on  $\mathcal{A}$  defined by  $\rho = \frac{1}{2}\tau \oplus \frac{1}{2}\tau$ ,  $\tau$  being the unique normalized trace on  $\mathcal{M}_2$ . Under the further conditions of Theorem II.2, the limiting free-energy density at the inverse temperature  $\beta$  is given by:

$$f(\beta) = \inf \{j(H)(\varphi) + \beta^{-1}(\mathbb{S}(\mu \otimes \rho, \varphi) - \log(4))\} \quad , \quad (4.3)$$

where the infimum is over the states  $\varphi$  of  $\mathcal{C}(X, \mathcal{A})$ , with  $\varphi = \int^\oplus \mu(dx) \varphi_x$ , and the term  $-\beta^{-1} \log(4)$  comes from the reference free-energy of the system in the state  $\rho^n$ .

We mention that if  $\varphi = t\varphi^{(1)} \oplus (1-t)\varphi^{(2)}$  is a state of  $\mathcal{A}$ , then

$$\begin{aligned} \mathbb{S}(\rho, \varphi) &= \mathbb{S}(\tfrac{1}{2}\tau \oplus \tfrac{1}{2}\tau, t\varphi^{(1)} \oplus (1-t)\varphi^{(2)}) \\ &= I(t) - t\mathbb{S}(\varphi^{(1)}) - (1-t)\mathbb{S}(\varphi^{(2)}) + \log(4) \quad . \end{aligned} \quad (4.4)$$

#### IV.2.1. The BCS-model

Let  $\{\Lambda_\alpha \mid \alpha = 1, 2, \dots\}$  be a sequence of regions in  $\mathbb{R}^{\nu}$  with volume  $V_\alpha$ . Associated with each region, there is a set of momenta  $\mathcal{P}_\alpha = \{\mathbf{k}_\alpha(j) \mid j = 1, 2, \dots\}$ , such that if  $\mathbf{k} \in \mathcal{P}_\alpha$  then  $-\mathbf{k} \in \mathcal{P}_\alpha$ . Moreover, to each  $\mathbf{k}_\alpha(j)$  there is associated a pair of orthogonal unit-vectors  $\psi_\alpha(j; \pm)$  in a Hilbert space  $\mathcal{H}_\alpha$  (the one-particle Hilbert space) such that  $\{\psi_\alpha(j; \pm) \mid \mathbf{k}_\alpha(j) \in \mathcal{P}_\alpha\}$  is a complete orthonormal basis of  $\mathcal{H}_\alpha$ . The fermion annihilation operator  $a(\psi_\alpha(j; \pm))$  acting on the antisymmetric Fock space  $\mathcal{F}_\alpha$  built upon  $\mathcal{H}_\alpha$ , is written  $a[\mathbf{k}_\alpha(j); \pm]$ . One considers a fixed ( $\alpha$ -independent) inversion invariant compact subset  $X$  of momentum space. Letting  $N_\alpha = |\{j \mid \mathbf{k}_\alpha(j) \in X\}|$  be the number of momenta in  $X$ , one assumes that

$$V_\alpha/N_\alpha \longrightarrow \lambda \quad , \quad (4.5)$$

and that there is a limiting distribution for the momenta in  $X$ :

$$\frac{1}{N_\alpha} \sum_{j=1}^{N_\alpha} \delta_{\mathbf{k}_\alpha(j)} \longrightarrow \mu \quad (4.6)$$

in the  $w^*$ -topology as  $\alpha \rightarrow \infty$ .

The Hamiltonian for the *full* BCS-model acts on  $\mathcal{F}_\alpha$ , and is given by

$$\begin{aligned} \mathcal{H}_\alpha &= \frac{1}{2} \sum_{j=1}^{N_\alpha} \varepsilon(\mathbf{k}_\alpha(j)) (a^*[\mathbf{k}_\alpha(j); +]a[\mathbf{k}_\alpha(j); +] + a^*[\mathbf{k}_\alpha(j); -]a[\mathbf{k}_\alpha(j); -]) \\ &\quad - \frac{1}{V_\alpha} \sum_{j,i=1}^{N_\alpha} U(\mathbf{k}_\alpha(j), \mathbf{k}_\alpha(i)) a^*[\mathbf{k}_\alpha(j); +]a^*[-\mathbf{k}_\alpha(j); -]a[-\mathbf{k}_\alpha(i); -]a[\mathbf{k}_\alpha(i); +] \quad , \end{aligned}$$

where  $\varepsilon$  is a continuous real-valued even function on  $X$ , and  $U$  is a continuous, symmetric real-valued function on  $X \times X$ . To verify that this model is of the quadratic inhomogeneous mean-field type, we pair-up  $a[\mathbf{k}_\alpha(j); +]$  with  $a[-\mathbf{k}_\alpha(j); -]$  for  $j = 1, 2, \dots, N_\alpha$ , and choose (see section II, (2.2)):

$$\begin{aligned} A_1 &= a^*(+)a(+) , & A_2 &= a^*(-)a(-) , & A_3 &= A_4^* = a(-)a(+) \\ \varepsilon_1 &= \varepsilon_2 = \varepsilon/2 , & \varepsilon_3 &= \varepsilon_4 = 0 , \\ U_{33} &= U_{44} = -\lambda^{-1}U , & \text{all other } U_{ij} &= 0 . \end{aligned}$$

Using (2.3) we then verify that

$$\|\mathcal{H}_\alpha - N_\alpha(\text{sym}_{N_\alpha}(H_2 \otimes \mathbb{I}_{N_\alpha-2}))(\mathbf{k}_\alpha(1), \dots, \mathbf{k}_\alpha(N_\alpha))\| = o(N_\alpha)$$

so that our result applies and the limiting free-energy density is given by (4.3). Upon using the identifications (4.2), and the formulae (2.4) and (4.4), the functional to be minimized in (4.3) is

$$\begin{aligned} \mathcal{J}'(t(\cdot), \varphi_\cdot) &= \frac{1}{2} \int_X \mu(dx) \varepsilon(x) (1 + t(x) \varphi_x^{(1)} (2e_{22} - \mathbb{I})) \\ &\quad - \frac{1}{\lambda} \int_{X \times X} \mu(dx) \mu(dy) U(x, y) t(x) t(y) \Re \left\{ \varphi_x^{(1)}(e_{21}) \varphi_y^{(1)}(e_{12}) \right\} \\ &\quad + \frac{1}{\beta} \int_X \mu(dx) (I(t(x)) - t(x) \mathbb{S}(\varphi_x^{(1)}) - (1 - t(x)) \mathbb{S}(\varphi_x^{(2)})) , \end{aligned}$$

where  $\varphi_x = t(x) \varphi_x^{(1)} \oplus (1 - t(x)) \varphi_x^{(2)}$ ,  $0 \leq t(\cdot) \leq 1$ ,  $\varphi_x^{(j)} \in K(\mathcal{M}_2)$ . The variation over the  $\varphi_x^{(2)}$ -part of the state is trivial; the corresponding minimizer is  $\varphi_x^{(2)} = \tau$  a.e., and we are left with the minimization of

$$\begin{aligned} \mathcal{J}(t(\cdot), \psi_\cdot) &= \frac{1}{2} \int_X \mu(dx) \varepsilon(x) (1 + t(x) \psi_x (2e_{22} - \mathbb{I})) \\ &\quad - \frac{1}{\lambda} \int_{X \times X} \mu(dx) \mu(dy) U(x, y) t(x) t(y) \Re \left\{ \psi_x(e_{21}) \psi_y(e_{12}) \right\} \\ &\quad + \frac{1}{\beta} \int_X \mu(dx) (I(t(x)) - t(x) \mathbb{S}(\psi_x) - (1 - t(x)) \log(2)) , \end{aligned}$$

where  $\psi_x$  is now a state of  $\mathcal{M}_2$ . Using the parametrization (4.1), we get

$$\begin{aligned} \mathcal{J}(t(\cdot), \psi_\cdot) &= \frac{1}{2} \int_X \mu(dx) \varepsilon(x) - \frac{1}{2} \int_X \mu(dx) \varepsilon(x) t(x) r(x) \cos(\theta(x)) \\ &\quad - \frac{1}{4\lambda} \int_{X \times X} \mu(dx) \mu(dy) U(x, y) t(x) t(y) r(x) r(y) \\ &\quad \quad \cdot \sin(\theta(x)) \sin(\theta(y)) \cos(\phi(x) - \phi(y)) \\ &\quad + \frac{1}{\beta} \int_X \mu(dx) (I(t(x)) + t(x) I(\frac{1+r(x)}{2}) - (1 - t(x)) \log(2)) . \end{aligned}$$

Thus our result is:

$$f(\beta) = \lambda^{-1} \inf \{ \mathcal{J}(t(\cdot), r(\cdot), \theta(\cdot), \phi(\cdot)) \} ,$$

reproducing the result of [14], obtained by totally different methods. This also confirms the mysterious finding of [14, **Theorem 10**]: the free-energy density of the full BCS-Model is equal to that of its quasi-spin version at the doubled temperature.

#### IV.2.2. The Overhauser Model

The specification of the model is analogous to that of the BCS-model [14]. The sequence of momenta  $\mathcal{P}_\alpha$  is now unrestricted, and  $X$  need not be inversion invariant. Conditions (4.5) and (4.6) are assumed. The Hamiltonian is

$$\begin{aligned} \mathcal{H}_\alpha = & \sum_{j=1}^{N_\alpha} (\eta_\alpha^+(\mathbf{k}_\alpha(j)) a^*[\mathbf{k}_\alpha(j); +] a[\mathbf{k}_\alpha(j); +] + \eta_\alpha^-(\mathbf{k}_\alpha(j)) a^*[\mathbf{k}_\alpha(j); -] a[\mathbf{k}_\alpha(j); -]) \\ & - \frac{1}{V_\alpha} \sum_{j,i=1}^{N_\alpha} U(\mathbf{k}_\alpha(j), \mathbf{k}_\alpha(i)) a^*[\mathbf{k}_\alpha(j); +] a[\mathbf{k}_\alpha(j); -] a^*[\mathbf{k}_\alpha(i); -] a[\mathbf{k}_\alpha(i); +] , \end{aligned}$$

where  $\eta_\alpha^\pm$  are real-valued functions on  $X$  converging uniformly as  $\alpha \rightarrow \infty$  to continuous functions  $\eta^\pm$ . The further steps and computations are as in the previous example; we only give the results. The pairing is now  $a[\mathbf{k}_\alpha(j); +]$  with  $a[\mathbf{k}_\alpha(j); -]$ , and  $H_2$  is specified by the choice:

$$\begin{aligned} A_1 &= a^*(+)a(+) , & A_2 &= a^*(-)a(-) , & A_3 &= A_4^* = a^*(-)a(+) , \\ \varepsilon_1 &= \eta^+ , & \varepsilon_2 &= \eta^- , & \varepsilon_3 &= \varepsilon_4 = 0 , \\ U_{33} &= U_{44} = -\lambda^{-1}U , & \text{all other } U_{ij} &= 0 . \end{aligned}$$

The model is now over the gauge-invariant subalgebra of  $\mathcal{A}$  which is generated by the first group of elements of (4.2), and isomorphic to  $\mathcal{D}_2 \oplus \mathcal{M}_2$ , where  $\mathcal{D}_2$  is the diagonal subalgebra of  $\mathcal{M}_2$ . The limiting free-energy density is given by (4.3). Putting

$$\eta = \frac{1}{2}(\eta^+ + \eta^-) , \quad \varepsilon = \eta^+ - \eta^- ,$$

the functional to be minimized in (4.3) is

$$\begin{aligned} \mathcal{J}'(t(\cdot), \varphi(\cdot)) = & \int_X \mu(dx) \eta(x) + \frac{1}{2} \int_X \mu(dx) \varepsilon(x) (1 - t(x)) \varphi_x^{(2)} (2e_{22} - \mathbb{I}) \\ & - \frac{1}{\lambda} \int_{X \times X} \mu(dx) \mu(dy) U(x, y) (1 - t(x)) (1 - t(y)) \Re \left\{ \varphi_x^{(2)}(e_{21}) \varphi_y^{(2)}(e_{12}) \right\} \\ & + \frac{1}{\beta} \int_X \mu(dx) (I(t(x)) - (1 - t(x)) \mathbb{S}(\varphi_x^{(2)})) \\ & + \int_X \mu(dx) t(x) (\eta(x) \varphi_x^{(1)} (2e_{22} - \mathbb{I}) - \frac{1}{\beta} \mathbb{S}(\varphi_x^{(1)})) \quad . \end{aligned}$$

The last summand lives on the abelian two-point algebra  $\mathcal{D}_2$ ; the corresponding variation with respect to  $x \mapsto \varphi_x^{(1)} \in K(\mathcal{D}_2)$ , can be done immediately, and contributes  $-\beta^{-1} \int_X \mu(dt) \log(2 \cosh(\beta \eta))$ . This leaves us with the minimization of (interchange  $t$  and  $1 - t$ ):

$$\begin{aligned} \mathcal{J}(t(\cdot), r(\cdot), \theta(\cdot), \phi(\cdot)) = & \int_X \mu(dx) \eta(x) - \frac{1}{\beta} \int_X \mu(dx) (1 - t(x)) \log(2 \cosh(\beta \eta(x))) \\ & - \frac{1}{2} \int_X \mu(dx) \varepsilon(x) t(x) r(x) \cos(\theta(x)) \\ & - \frac{1}{4\lambda} \int_{X \times X} \mu(dx) \mu(dy) U(x, y) t(x) t(y) r(x) r(y) \\ & \quad \cdot \sin(\theta(x)) \sin(\theta(y)) \cos(\phi(x) - \phi(y)) \\ & + \frac{1}{\beta} \int_X \mu(dx) (I(t(x)) + t(x) I(\frac{1 + r(x)}{2})) \quad , \end{aligned}$$

thus recovering the result obtained in [14].



### IV.3 Random Mean-Field Models

Statistical mechanics models, in which the Hamiltonian depends on random parameters have attracted a lot of attention recently. In this section we shall apply Theorem II.2. to such random models. Since the Hamiltonian  $H_n(\xi_n)$  of an inhomogeneous mean-field model depends on the parameters  $\xi_{n,1}, \dots, \xi_{n,n}$  the most straightforward application will be by taking these parameters as random variables. Since we consider the free energy and the equilibrium states separately for each value of  $\xi_n$ , these are called *quenched* random variables. To be specific, we consider a “discrete time” stochastic process, i.e. a sequence  $\{x_i | i = 1, \dots\}$  of random variables defined on a probability space  $(\Omega, \Sigma, \mathbb{P})$  and taking values in a compact space  $X$  (equipped with its Borel  $\sigma$ -algebra  $\mathcal{B}$ ). For each sample  $\omega \in \Omega$  and  $n \in \mathbb{N}$  we make the simplest choice of parameters  $\xi_n$  by setting

$$\xi_{n,i} = \xi_{n,i}(\omega) = x_i(\omega) \quad , \quad i = 1, \dots, n \quad .$$

Since just one random variable per site appears in the Hamiltonian, models of this kind are called [12] *site random* mean-field models as opposed to bond random models like the Sherrington-Kirpatrick model [34].

Theorem II.2. applies to a sample  $\omega \in \Omega$ , whenever the sequence  $\xi_n$  satisfies (LD), i.e. if there is a measure  $\mu$  on  $X$ , for which  $\omega$  belongs to the set

$$\Omega_{LD}^\mu := \left\{ \omega \in \Omega \mid \lim_n n^{-1} \sum_{j=1}^n f(x_j(\omega)) = \int_X \mu(x) f(dx) \text{ for all } f \in \mathcal{C}(X) \right\} \quad .$$

In the theory of quenched random systems one is usually interested in statements which hold with probability one. Theorems II.2. and II.3. become statements of this genre, provided that (LD) holds  $\mathbb{P}$ -almost everywhere, i.e.

$$\mathbb{P}(\Omega_{LD}^\mu) = 1 \quad . \quad (RLD)$$

This random version of the limiting density assumption indeed holds in many cases of interest. For example, if the random variables  $x_i$  are independent, and all have distribution  $\mu$ , then condition (RLD) is merely a restatement of the strong law of large numbers. However, independence is by no means necessary for (RLD) to hold, which is essentially the statement that the stochastic process  $(x_i)$  is ergodic. For example, let  $\{x_z \mid z \in \mathbb{Z}^d\}$  be a stochastic process with sample space  $(\Omega, \Sigma, \mathbb{P})$ , and compact state space  $X$ , indexed by the points in the  $d$ -dimensional integer lattice. If the process is *strongly stationary* [8] the distribution (call it  $\mu$ ) of  $x_z$  does not depend on  $z$ . If, moreover, the process is *ergodic* [8], then

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \sum_{z \in \mathbb{Z}^d} X_z[f]$$

exists  $\mathbb{P}$ -almost surely and is the constant random variable  $\mathbb{E}\{X[f]\} = \int_X \mu(dx)f(x)$ . Given *any* ergodic process, *any* random inhomogeneous mean-field model specified by  $\xi_\Lambda(\omega) = \{X_z(\omega) | z \in \Lambda\}$ ,  $\Lambda \subset \mathbb{Z}^d$ ,  $|\Lambda| < \infty$ , fullfills the (RLD) property.

Through the  $\omega$ -dependence of  $\xi_n$ , the free energy density of the  $n^{\text{th}}$  system becomes a random variable  $f_n(\omega) = n^{-1} \mathbb{F}(\rho^n, nH_n(\xi_n(\omega)))$ . Then Theorem II.2 says that for all  $\omega \in \Omega_{LD}^\mu$ , and in particular almost everywhere,  $f_n(\omega)$  converges to the  $\omega$ -independent quantity defined by the variational formula. Consider the equilibrium states  $\Psi_n(\xi_n(\omega)) \in K(\mathcal{A}^n)$ , with  $\Psi_n(\xi_n) = \text{Norm}^{-1}(\rho^n)^{-nH_n(\xi_n)}$ . Since we have made the choice  $\xi_{n,i}(\omega) = \xi_{m,i}(\omega) = x_i(\omega)$  for  $i \leq n, m$ , we may expect that, at least in the absence of phase transitions, these states may have a limit in  $K(\mathcal{A}^\infty)$ . It is obvious, however, that in contrast to the free energy this limit must depend on  $\omega$  [23]. We used the device of the algebra  $\mathcal{C}(X, \mathcal{A})$  to obtain states that become  $\omega$ -independent in the limit: through its dependence on  $\xi_n$ , the operator  $\Xi_n$  also depends on the sample  $\omega$ , and, in the absence of phase transitions, the states  $\Psi_n(\xi_n(\omega)) \circ \Xi_n^\omega$  converge to the unique  $\omega$ -independent minimizer of the Gibbs variational principle (\*). We can thus recover results obtained in [12,17,19,20,24,25,33].

The algebra  $\mathcal{C}(X, \mathcal{A})$  has been used by Blobel and Messer [4] in a different way to discuss the limit of Gibbs states. They consider the states

$$\Psi_n^{BM} = \int^\oplus \mu(dx_1) \cdots \mu(dx_n) \Psi_n(x_1, \dots, x_n)$$

of  $\mathcal{C}(X^n, \mathcal{A}^n)$ . It is easy to see that if we take the  $x_i$  as independent random variables with distribution  $\mu$ ,  $\Psi_n^{BM}$  is just the  $\mathbb{P}$ -expectation of the  $\omega$ -dependent states discussed above:

$$\Psi_n^{BM} = \int \mathbb{P}(d\omega) \Psi_n(\xi_n(\omega)) \circ \Xi_n^\omega.$$

Since by Theorem II.2. all accumulation points of the sequence  $\Psi_n(\xi_n(\omega)) \circ \Xi_n^\omega$  lie in the compact convex set  $M_*$  of minimizers of the variational principle, the accumulation points of the averages  $\Psi_n^{BM}$  also lie in this set. Similarly, the expectations  $f_n^{BM} = \int \mathbb{P}(d\omega) f_n(\omega)$  converge to the almost sure limit of the  $f_n$ , i.e. the infimum of Theorem II.2. These results were obtained in [4] for the special case of finite dimensional  $\mathcal{A}$ , and quadratic interactions.

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