Correlation Inequalities for Quantum Spin Systems with Quenched Centered Disorder

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It is shown that random quantum spin systems with centered disorder satisfy correlation inequalities previously proved [1] in the classical case. Consequences include monotone approach of pressure and ground state energy to the thermodynamic limit. Signs and bounds on the surface pressures for different boundary conditions are also derived for finite range potentials.

Quantum spin system with quenched randomness are both important and theoretically challenging. They are widely used as models for metallic alloys in condensed matter physics, see [2] for a review. They are also important in combinatorial optimization problems especially in relation to quantum annealing procedures [3] and quantum error correcting codes [4].

One approach to studying such macroscopic systems is via correlation inequalities. These are useful in many areas of statistical mechanics. They have been used to prove that the free energy, correlation functions and surface free energy have well defined thermodynamic limits. They further show that some of these quantities approach their limit monotonically at increasing volumes. They have also proved important for computing bounds on critical temperatures and critical exponents by comparing lattices in different dimensions.

In a previous work [1] we have shown that, despite the presence of competing interactions, a general classical spin glass model with quenched centered disorder has a family of positive correlation functions.This positivity implies a monotone behavior of the pressure with respect to the strength of the random interaction. From the monotonicity one can deduce sub-additivity of the free energy (which implies existence of its thermodynamic limit) and also the sign of and bounds on the surface pressure for different boundary conditions. See also [5] for further applications of the inequalities.

The extension to the quantum case of classical correlation inequalities may not be possible or require further conditions. Examples were found in [8] where some correlations violate the GKS inequality of type II for the isotropic Heisenberg model with ferromagnetic interactions, and in [10] where the GKS inequality of type I is violated for the anisotropic ferromagnetic Heisenberg model. In order to reestablish the validity of the GKS inequalities in quantum systems it is then necessary to impose further conditions on the interaction coefficients beyond positivity (see for instance [10] for conditions to prove GKS I in the anisoptropic Heisenberg model with zero magnetic field and [11] for the conditions to prove GKS II).

Here we show that quantum systems with quenched centered disorder do fulfill the same family of correlation inequalities of the classical case without any further restriction with respect to the classical case. The result is obtained as follows.

For each finite set of points Λ let us consider the quantum spin system with Hamiltonian

$$U := -\sum_{X\subset\Lambda} \lambda_X J_X \Phi_X + U_0 \tag{1}$$

The operators Φ_X are self-adjoint elements of the real algebra generated by the set of *spin operators*, the Pauli matrices, $\sigma_i^{(x)}, \sigma_i^{(y)}, \sigma_i^{(z)}$, $i \in \Lambda$, on the Hilbert space $\mathcal{H}_X := \otimes_{i\in X}\mathcal{H}_i$. U_0 is a non random quantum Hamiltonian acting on the Hilbert space $\mathcal{H}_\Lambda$. The random interactions J_X are centered and mutually independent i.e. $Av(J_X) = 0$ for all X and $Av(J_X J_Y) = \Delta_X^2 \delta_{X,Y}$. The λ's are numbers which tune the magnitude of the random interactions. An example is the anisotropic quantum version of the nearest-neighboor Edwards-Anderson model with transverse field. This is defined in terms of the Pauli matrices:

$$\Phi_i = \sigma_i^z \ , \tag{2}$$

$$\Phi_{i,j} = \alpha_x \sigma_i^x \sigma_j^x + \alpha_y \sigma_i^y \sigma_j^y + \alpha_z \sigma_i^z \sigma_j^z \ , \tag{3}$$

for $|i-j| = 1$ and $\Phi_X = 0$ otherwise.

Our main observation is that the pressure (Gibbs free energy up to a sign) for $\lambda = (\lambda_X, \lambda_Y, ...)$:

$$P_\Lambda(\lambda) = Av \log \mathrm{Tr}\, \exp(-U), \tag{4}$$

is convex with respect to each λ_X. We have set the inverse temperature $\beta = 1$ since our results do not depend on its value. We shall also drop the subscript Λ when it is unambiguous.

The proof of convexity is straightforward. The first derivative gives in fact

$$\frac{\partial P}{\partial \lambda_A} = Av(J_A < \Phi_A >_U) \tag{5}$$

where

$$< C >_U := \frac{\mathrm{Tr}\, C e^{-U}}{\mathrm{Tr}\, e^{-U}} . \tag{6}$$

while, for the second derivative, one has (see [12], Chapter IV, page 357)

$$\frac{\partial^2 P}{\partial \lambda_A^2} = Av(J_A^2[< \Phi_A, \Phi_A >_U - < \Phi_A >_U^2]) \tag{7}$$

where $< \cdot, \cdot >_U$ denotes the Duhamel inner product [13]:

$$< C, D >_U := \frac{\mathrm{Tr}\, \int_0^1 ds\ e^{-sU} C^* e^{-(1-s)U} D}{\mathrm{Tr}\, e^{-U}} . \tag{8}$$

By using the fact that $< 1, D >=< D >$ and $< C, 1 >=< C >$ we see that

$$\frac{\partial^2 P}{\partial \lambda_A^2} = Av(J_A^2[< \Phi_A - < \Phi_A >_U, \Phi_A - < \Phi_A >_U >_U]) \geq 0. \tag{9}$$

This yields the following result:

For systems described by the quantum potential (1) *the following inequality holds: for all* $A \subset \Lambda$ *and for* $\lambda_A \geq 0$

$$Av(J_A < \Phi_A >_U) \geq 0 . \tag{10}$$

Proof. Since the second derivative of the pressure is non negative

$$\frac{\partial^2 P}{\partial \lambda_A^2} \geq 0. \tag{11}$$

we deduce that the first derivative

$$\frac{\partial P}{\partial \lambda_A} = Av(J_A < \Phi_A >_U) \tag{12}$$

is a monotone non decreasing function of λ_A (indipendently of the values of all the other λ's). As a consequence we have that for $\lambda_A \geq 0$

$$\frac{\partial P}{\partial \lambda_A} \geq Av(J_A < \Phi_A >_U)|_{\lambda_A = 0} \tag{13}$$

But for $\lambda_A = 0$ the two random variables J_A and $< \Phi_A >_U$ are independent:

$$Av(J_A < \Phi_A > |_{\lambda_A=0}) = Av(J_A) Av(< \Phi_A > |_{\lambda_A=0}) = 0 \tag{14}$$

where the last equality comes from having chosen distributions with $Av(J_A) = 0$. It also follows that for $\lambda_A \leq 0$ one has $Av(J_A < \Phi_A >_U) \leq 0$.

Although the consequences we are going to derive apply only to the case considered in (1) where U_0 is the sum of one body terms we note that the inequality (10) holds for general U_0. This include the case where $Av(< \Phi_A >_U) \leq 0$, as would happen in the case where the J_X are bounded and U satisfy the conditions necessary for GKS I to hold. A different example where one exploits symmetry and translation invariance would be the anisotropic Heisenberg model

$$U = - \sum_{\alpha = x,y,z} K_\alpha \sum_{i,j} \sigma_i^\alpha \sigma_j^\alpha - \sum_i (h + \lambda_i J_i) \sigma_i^z , \tag{15}$$

with centered J_i and negative field h. It would also include the case $h = 0$, $\Lambda \nearrow \mathbb{Z}^d$, $d \geq 3$ with minus boundary conditions and K_α positive and large.

We now consider the case where U_0 is a sum of one body terms, e.g. $U_0 = -\sum_i \vec{h}_i \cdot \vec{\sigma}_i$. By using the same standard strategies of the classical spin glass case [1] or the standard ferromagnetic interaction [12] one can easily deduce from (10) the super-additivity of the pressure. For a disjoint union of two regions $\Lambda = \Lambda_1 \cup \Lambda_2$ one obtains

$$P_\Lambda \geq P_{\Lambda_1} + P_{\Lambda_2} . \tag{16}$$

It follows from (16) that the pressure is monotonically increasing as the volume increase and hence the existence of the thermodynamic limit (see also [14]). Considering for instance a system on a d-dimensional square lattice $\mathbb{Z}^d$, with translation invariant distributions of the random interactions, one has that by dividing the lattice into cubes the following result holds for free boundary conditions:

$$p \ = \ \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{P_\Lambda}{|\Lambda|} \ = \ \sup_\Lambda \frac{P_\Lambda}{|\Lambda|} , \tag{17}$$

where the supremum is a well defined function (doesn't blow up) provided the stability condition (see [14]):

$$\sum_{X \subset \Lambda} Av(J_X^2) ||\Phi_X||^2 \ \leq \ c|\Lambda| , \tag{18}$$

is verified for some positive constant c. A simple bound shows that when the interactions have a finite range the limit does not depend on boundary conditions.

By introducing the inverse temperature in the definition of the pressure, for instance taking all the lambdas equal to β, we can study the properties of the ground state energy E_Λ by relating it to the free energy. Since by general thermodynamic arguments (see for instance [15])

$$\lim_{\beta \to \infty} - \frac{P_\Lambda(\beta)}{\beta} \searrow E_\Lambda , \tag{19}$$

one obtains

$$E_\Lambda \leq E_{\Lambda_1} + E_{\Lambda_2} , \tag{20}$$

which implies

$$e \ = \ \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{E_\Lambda}{|\Lambda|} \ = \ \inf_\Lambda \frac{E_\Lambda}{|\Lambda|} . \tag{21}$$

The physical significance of a quantum disordered model is related to the fact that the random free energy (using now the potential with all $\lambda_X = 1$)

$$\Pi_\Lambda = \log \mathrm{Tr}\, \exp(-U_\Lambda) \tag{22}$$

and the random ground state energy

$$\mathcal{E}_\Lambda = \lim_{\beta\to\infty} -\frac{\Pi_\Lambda}{\beta} \tag{23}$$

do converge, for large volumes, to the same non random object for almost all the disorder realizations. Following [16] and [17] we can achieve this stronger version of the existence of the thermodynamic limit by observing that the condition (18) entails the exponential version of the law of large numbers for the free and ground state energy:

$$Prob\left(\left|\frac{\Pi_\Lambda}{|\Lambda|\beta} - \frac{P_\Lambda}{|\Lambda|\beta}\right| \geq x\right) \leq e^{-\frac{|\Lambda| x^2}{2c}} \ , \tag{24}$$

$$Prob\left(\left|\frac{\mathcal{E}_\Lambda}{|\Lambda|} - \frac{E_\Lambda}{|\Lambda|}\right| \geq x\right) \leq e^{-\frac{|\Lambda| x^2}{2c}} \ . \tag{25}$$

Standard probability theory (Borel-Cantelli lemma) implies that for *almost all* configurations of the J's:

$$\lim_{\Lambda\nearrow\mathbb{Z}^d} \frac{\Pi_\Lambda}{|\Lambda|} \ = \ \sup_\Lambda \frac{P_\Lambda}{|\Lambda|} = p \ , \tag{26}$$

and

$$\lim_{\Lambda\nearrow\mathbb{Z}^d} \frac{\mathcal{E}_\Lambda}{|\Lambda|} \ = \ \inf_\Lambda \frac{E_\Lambda}{|\Lambda|} = e \ . \tag{27}$$

From inequality (10) we can also deduce, by decomposing a (d+1)-dimensional hypercube Λ into d-dimensional hypercubes, that the pressure in dimension d, $p^{(d)}$ is a non-decreasing function of d and the ground state energy a non increasing one:

$$p^{(d)} \leq p^{(d+1)} \ , \tag{28}$$

$$e^{(d)} \geq e^{(d+1)} \ . \tag{29}$$

In the case of finite range interactions, i.e. $\lambda_X = 0$ for $|X| \geq r$ (e.g. the nearest neighbor case), the inequality (10) leads to an estimate of the size and sign of the surface pressures T_Λ i.e. the first correction to the leading term of the pressure:

$$P_\Lambda = p|\Lambda| + T_\Lambda \ . \tag{30}$$

Using the methods of [1] and [18] a straightforward computation shows that the T_Λ is of surface size and, as it happen for ferromagnets and classical spin glasses, it does depend on boundary conditions. For instance for free (Φ) and periodic (Π) boundary conditions one may show that there are two positive constants $c_{(\Phi)}$ and $c_{(\Pi)}$ such that

$$-\, c_{(\Phi)}|\partial\Lambda| \leq T^{(\Phi)}_\Lambda \leq 0 \ , \tag{31}$$

and

$$T^{(\Phi)}_\Lambda \leq T^{(\Pi)}_\Lambda \leq c_{(\Pi)}|\partial\Lambda| \ , \tag{32}$$

where $|\partial\Lambda|$ is the area of the surface of Λ, i.e. the number of terms in (1) which connect sites inside Λ to sites outside Λ.

We have shown that a disordered quantum systems fulfills a new correlation inequality which entails the same consequences as the first GKS inequality and holds in full generality without any restriction with respect to the classical case. It would be interesting to investigate correlation inequalities of type II (see [19, 20] for the classical case) as well as the validity of similar results on the Nishimori line [21] especially in view of the applications of the correlation inequalities to error correcting codes [22] and their possible extension to the quantum case.

The results we have presented in this letter can of course be extended to quantum Hamiltonian systems with general bounded interaction.

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