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 [P. Contucci and J. Lebowitz, Ann. Henri Poincare **8**, 1461 (2007)] 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. © *2010 American Institute of Physics.*
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Quantum spin system with quenched randomness is experimentally important and theoretically challenging. They are widely used as models for metallic alloys in condensed matter physics (see Ref. 1 for a review). They are also important in combinatorial optimization problems especially in relation to quantum annealing procedures[2] and quantum error correcting codes.[3]

Correlation inequalities are useful in many areas of statistical mechanics. In the case of ferromagnetic interactions, they have been used to prove that the free energy, correlation functions, and surface free energy have well defined thermodynamic limits and 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,[4] 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.

The extension to the quantum case of classical correlation inequalities may not be possible or require further conditions. Examples were found in Refs. 5 and 6, where some correlations for the quantum Heisenberg model with ferromagnetic interactions violate important inequalities known to hold for the classical system.

In order to reestablish the validity of these inequalities in quantum systems, it is then necessary to impose further conditions on the interaction coefficients beyond positivity.[6,7]

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 that. The inequalities imply a monotone behavior of the pressure with respect to the strength of the random interaction. From the monotonicity, one can deduce subadditivity of the free energy and ground state energy, which implies existence of their thermodynamic limit in average and almost surely in the disorder. Moreover, the same property implies the control of the sign of and bounds on the surface pressure for different boundary conditions. See also Ref. 8 for further applications of the inequalities. The result is obtained as follows.

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

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

The operator Φ_X is a self-adjoint element 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 nonrandom quantum Hamiltonian acting on the Hilbert space $\mathcal{H}_\Lambda$. The random interaction J_X is centered and is 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 that tune the magnitude of the random interactions. An example is the anisotropic quantum version of the nearest-neighbor 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. Another example is the random transverse field Ising model

$$U_0 = -\sum_{i,j} K_{i-j}\sigma_i^z\sigma_j^z - h_1\sum_i \sigma_i^x - h_3\sum_i \sigma_i^z \tag{4}$$

to which random fields are added

$$\sum_i \eta_i^x\sigma_i^x + \eta_i^z\sigma_i^z. \tag{5}$$

This system has recently been used to model the behavior of some compounds in a strong magnetic field.[9,10]

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

$$P_\Lambda(\lambda) = Av\ \log\ \mathrm{Tr}\ \exp(-U) \tag{6}$$

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,

$$\frac{\partial P}{\partial\lambda_A} = Av(J_A\langle\Phi_A\rangle_U), \tag{7}$$

where

$$\langle C\rangle_U := \frac{\mathrm{Tr}\ Ce^{-U}}{\mathrm{Tr}\ e^{-U}}. \tag{8}$$

while for the second derivative, one has (see Ref. 11, Chap. IV, p. 357)

$$\frac{\partial^2 P}{\partial\lambda_A^2} = Av(J_A^2[\langle\Phi_A,\Phi_A\rangle_U - \langle\Phi_A\rangle_U^2]), \tag{9}$$

where $\langle\cdot,\cdot\rangle_U$ denotes the Duhamel inner product[12]

$$\langle C,D\rangle_U := \frac{\mathrm{Tr}\int_0^1 \mathrm{d}s e^{-sU}C^* e^{-(1-s)U}D}{\mathrm{Tr}\ e^{-U}}. \tag{10}$$

By using the fact that $\langle 1,D\rangle=\langle D\rangle$ and $\langle C,1\rangle=\overline{\langle C\rangle}$, we see that

$$\frac{\partial^2 P}{\partial \lambda_A^2} = Av(J_A^2[\langle \Phi_A - \langle \Phi_A \rangle_U, \Phi_A - \langle \Phi_A \rangle_U \rangle_U]) \geq 0. \tag{11}$$

The sign of the second derivative of P carries a profound physical meaning, which is the positivity of the specific heat. That is at the base of our main result.

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

$$Av(J_A \langle \Phi_A \rangle_U) \geq 0. \tag{12}$$

Proof: Since the second derivative of the pressure is non-negative

$$\frac{\partial^2 P}{\partial \lambda_A^2} \geq 0, \tag{13}$$

we deduce that the first derivative

$$\frac{\partial P}{\partial \lambda_A} = Av(J_A \langle \Phi_A \rangle_U) \tag{14}$$

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

$$\frac{\partial P}{\partial \lambda_A} \geq Av(J_A \langle \Phi_A \rangle_U)|_{\lambda_A=0}. \tag{15}$$

However, for $\lambda_A = 0$, the two random variables J_A and $\langle \Phi_A \rangle_U$ are independent,

$$Av(J_A \langle \Phi_A \rangle|_{\lambda_A=0}) = Av(J_A) Av(\langle \Phi_A \rangle|_{\lambda_A=0}) = 0, \tag{16}$$

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 $Av(J_A \langle \Phi_A \rangle_U) \leq 0$.

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 (12) holds for general U_0. This include the case where $Av(\langle \Phi_A \rangle_U) \leq 0$, as would happen in the case where the J_X is bounded and U satisfies the conditions necessary for Griffiths–Kelly–Sherman first inequality to hold.[13] A different example where one exploits symmetry and translation invariance would be the anisotropic Heisenberg model,

$$U = -\sum_{\alpha=x,y,z} K_\alpha \sum_{i,j} \sigma_i^\alpha \sigma_j^\alpha - \sum_i (h + \lambda_i J_i) \sigma_i^z, \tag{17}$$

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 term as in, e.g., $U_0 = -\Sigma_i \vec{h}_i \cdot \vec{\sigma}_i$, as in (5). By using the same standard strategies of the classical spin glass case[4] or the standard ferromagnetic interaction,[11] one can easily deduce from (12) the superadditivity of the pressure. For a disjoint union of two regions $\Lambda = \Lambda_1 \cup \Lambda_2$, one obtains

$$P_\Lambda \geq P_{\Lambda_1} + P_{\Lambda_2}. \tag{18}$$

It follows from (18) that the pressure monotonically increases as the volume increases and hence the existence of the thermodynamic limit (see also Ref. 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:

$$p = \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{P_\Lambda}{|\Lambda|} = \sup_\Lambda \frac{P_\Lambda}{|\Lambda|}, \tag{19}$$

where the supremum is a well defined function (does not blow up) provided the stability condition (see Ref. 14)

$$\sum_{X \subset \Lambda} Av(J_X^2) \|\Phi_X\|^2 \le c|\Lambda|, \tag{20}$$

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 the boundary conditions.

By introducing the inverse temperature in the definition of the pressure, for instance, taking all 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, Ref. 15)

$$\lim_{\beta \to \infty} -\frac{P_\Lambda(\beta)}{\beta} \searrow E_\Lambda, \tag{21}$$

one obtains

$$E_\Lambda \le E_{\Lambda_1} + E_{\Lambda_2}, \tag{22}$$

which implies that

$$e = \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{E_\Lambda}{|\Lambda|} = \inf_\Lambda \frac{E_\Lambda}{|\Lambda|}. \tag{23}$$

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

$$\Pi_\Lambda = \log \mathrm{Tr} \exp(-U_\Lambda) \tag{24}$$

and the random ground state energy

$$\mathcal{E}_\Lambda = \lim_{\beta \to \infty} -\frac{\Pi_\Lambda}{\beta} \tag{25}$$

do converge, for large volumes, to the same nonrandom object for almost all the disorder realizations. Following Refs. 16 and 17, we can achieve this stronger version of the existence of the thermodynamic limit by observing that the condition (20) entails the exponential version of the law of large numbers for the free and ground state energy,

$$\mathrm{Prob}\left(\left| \frac{\Pi_\Lambda}{|\Lambda|\beta} - \frac{P_\Lambda}{|\Lambda|\beta} \right| \ge x \right) \le e^{-|\Lambda|x^2/2c}, \tag{26}$$

$$\mathrm{Prob}\left(\left| \frac{\mathcal{E}_\Lambda}{|\Lambda|} - \frac{E_\Lambda}{|\Lambda|} \right| \ge x \right) \le e^{-|\Lambda|x^2/2c}. \tag{27}$$

Standard probability theory (Borel–Cantelli lemma) implies that for *almost all* configurations of J's,

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{\Pi_\Lambda}{|\Lambda|} = \sup_\Lambda \frac{P_\Lambda}{|\Lambda|} = p, \tag{28}$$

and

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{\mathcal{E}_\Lambda}{|\Lambda|} = \inf_\Lambda \frac{E_\Lambda}{|\Lambda|} = e. \tag{29}$$

From inequality (12), 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 nondecreasing function of d and the ground state energy a nonincreasing one,

$$p^{(d)} \leq p^{(d+1)}, \tag{30}$$

$$e^{(d)} \geq e^{(d+1)}. \tag{31}$$

In the case of finite range interactions, i.e., $\lambda_X=0$ for $|X| \geq r$ (e.g., the nearest neighbor case), inequality (12) leads to an estimate of the size and sign of the surface pressure T_Λ, i.e., the first correction to the leading term of the pressure,

$$P_\Lambda = p|\Lambda| + T_\Lambda. \tag{32}$$

Using the methods in Refs. 4 and 18, a straightforward computation shows that T_Λ is of surface size and, as it happens for ferromagnets and classical spin glasses, it does depend on the 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

$$-c_{(\Phi)}|\partial\Lambda| \leq T_\Lambda^{(\Phi)} \leq 0 \tag{33}$$

and

$$T_\Lambda^{(\Phi)} \leq T_\Lambda^{(\Pi)} \leq c_{(\Pi)}|\partial\Lambda|, \tag{34}$$

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 system fulfills a new correlation inequality which holds in full generality without any restriction with respect to the classical case. The result is deduced from the a simple convexity argument based on the positivity of the Duhamel inner product proved in Ref. 12 whose physical content is equivalent to the positivity of the specific heat. It would be interesting to investigate other quantum correlation inequalities (see Refs. 19 and 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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[1] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, 1999).
[2] S. Morita and H. Nishimori, J. Math. Phys. **49**, 125210 (2008).
[3] J.-I. Inoue, *Quantum Annealing and Other Optimization Methods*, Lecture Notes in Physics (Springer, Berlin, 2005).
[4] P. Contucci and J. Lebowitz, Ann. Henri Poincare **8**, 1461 (2007).
[5] C. A. Hurst and S. Sherman, Phys. Rev. Lett. **22**, 1357 (1969).
[6] J. Ginibre, Commun. Math. Phys. **16**, 310 (1970).
[7] G. Gallavotti, Stud. Appl. Math. **50**, 8992 (1971).
[8] P. Contucci and S. Starr, J. Stat. Phys. **135**, 1159 (2009)
[9] M. Schechter, Phys. Rev. B **77**, 020401(R) (2008).
[10] M. Schechter and P. Stamp, Phys. Rev. B **78**, 054438 (2008).

[11] B. Simon, *The Statistical Mechanics of Lattice Gases* (Princeton University Press, Princeton, NJ, 1993).
[12] F. Dyson, E. Lieb, and B. Simon, J. Stat. Phys. **18**, 335 (1978).
[13] R. B. Griffiths, J. Math. Phys. **5**, 1215 (1964); **8**, 478 (1967); D. G. Kelly and S. Sherman, *ibid.* **9**, 466 (1968).
[14] P. Contucci, C. Giardinà, and J. Pulé, Rev. Math. Phys. **16**, 629 (2004).
[15] D. Ruelle, *Statistical Mechanics. Rigorous Results* (World Scientific, Singapore, 1969).
[16] F. Guerra and F. L. Toninelli, Commun. Math. Phys. **230**, 71 (2002).
[17] P. Contucci, C. Giardina, and H. Nishimori, *Spin Glasses: Statics and Dynamics* in Progress in Probability, edited by Boutet de Monvel, A. and Bovier, A., (Birkhäuser, 2009), pp. 103–121.
[18] P. Contucci and S. Graffi, Commun. Math. Phys. **248**, 207 (2004).
[19] P. Contucci, F. Unguendoli, and C. Vernia, J. Phys. A: Math. Theor. **41**, 385001 (2008).
[20] P. Contucci and F. Unguendoli, Atti Accad. Naz. Lincei, Cl. Sci. Fis., Mat. Nat., Rend. Lincei, Mat. Appl. **19**, 141 (2008).
[21] P. Contucci, S. Morita, and H. Nishimori, J. Stat. Phys. **122**, 303 (2006).
[22] N. Macris, IEEE Trans. Inf. Theory **53**, 664 (2007).