Rounding of First Order Transitions in Low-Dimensional Quantum Systems with Quenched Disorder

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We prove that the addition of an arbitrarily small random perturbation to a quantum spin system rounds a first-order phase transition in the conjugate order parameter in $d \leq 2$ dimensions, or for cases involving the breaking of a continuous symmetry in $d \leq 4$. This establishes rigorously for quantum systems the existence of the Imry-Ma phenomenon which for classical systems was proven by Aizenman and Wehr.

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A first-order phase transition, in Ehrenfest's terminology, is one associated with a discontinuity in the density of an extensive quantity. In thermodynamic terms this corresponds to a discontinuity in the derivative of the free energy with respect to one of the parameters in the Hamiltonian, more specifically the one conjugate to the order parameter, e.g., the magnetic field in a ferromagnetic spin system. In what is known as the Imry-Ma phenomenon [1,2], any such discontinuity is rounded off in low dimensions when the Hamiltonian of a homogeneous system is modified through the incorporation of an arbitrarily weak random term, corresponding to quenched local disorder, in the field conjugate to the order parameter.

This phenomenon has been rigorously established for classical systems [3,4], where it occurs in dimensions $d \leq 2$, and $d \leq 4$ when the discontinuity is associated with the breaking of a continuous symmetry. In this Letter we prove analogous results for quantum systems at both positive and zero temperatures (ground states).

The existence of this effect was first argued for random fields by Imry and Ma on the basis of a heuristic analysis of free energy fluctuations. While the sufficiency of Imry and Ma's reasoning was called into question, the predicted phenomenon was established rigorously through a number of works [3–9]. The statement was further extended to different disorder types by Hui and Berker [10,11].

The general existence of the Imry-Ma phenomenon in quantum systems was not addressed by these rigorous analyses, and, in particular, the Aizenman-Wehr [3,4] proof of the rounding effect applies only for classical systems. However, as stressed in [12], establishing whether the Imry-Ma phenomenon extends to first-order quantum phase transitions (QPT_1) is an important open problem. The results presented here answer this question. We find that the critical dimensions for the phenomenon for quantum systems are the same as for classical systems, including at zero temperature.

We consider spin systems on the d-dimensional lattice $\mathbb{Z}^d$, where the configuration at each site is described by a finite-dimensional Hilbert space, with a Hamiltonian of the form

$$\mathcal{H} = \mathcal{H}_0 - \sum_x (h + \epsilon \eta_x) \kappa_x, \tag{1}$$

where $\{\kappa_x\}$ are translates of some local operator κ_0, and h and ϵ are real parameters. The quenched disorder is represented by $\{\eta_x\}$, a family of independent, identically distributed random variables. $\mathcal{H}_0$ may be translation invariant and nonrandom, or it can include additional random terms (although we will not discuss the latter case, our results hold there also). For convenience we will assume that $\|\kappa_x\| = 1$, which can be arranged by rescaling h and ϵ. We will refer to the ηs as random fields, although in general they may also be associated with some other parameters, e.g., random bond strengths.

An example of a system of this type (with $\kappa_x = \sigma_x^{(3)}$) is the ferromagnetic transverse-field Ising model with a random longitudinal field [13] (henceforth QRFIM), with

$$\mathcal{H} = -\sum J_{x-y} \sigma_x^{(3)} \sigma_y^{(3)} - \sum [\lambda \sigma_x^{(1)} + (h + \epsilon \eta_x) \sigma_x^{(3)}], \tag{2}$$

where $\sigma_x^{(i)}$ ($i = 1, 2, 3$) are single-site Pauli matrices, and $J_{x-y} > 0$. The QRFIM has recently been studied as a model for the behavior of $LiHo_xY_{1-x}F_4$ with $x > 0.5$ in a strong transverse magnetic field [14,15].

We will examine phase transitions where the order parameter is the volume average of the expectation value of κ_x with respect to an equilibrium state (that is, a state satisfying the Kubo-Martin-Schwinger condition [16]), and show that this quantity cannot be discontinuous in h for low-dimensional systems. As is well known, this order parameter is related to the directional derivatives ($\pm$) of the *free energy density*,

$$m_{\pm}(T, h, \epsilon) := -\frac{\partial}{\partial h \pm} \mathcal{F}(T, h, \epsilon), \tag{3}$$

where, as usual, at positive temperatures

$$\mathcal{F}(T, h, \epsilon) = \lim_{\Gamma \nearrow \mathbb{Z}^d} \frac{-1}{\beta|\Gamma|} \log \mathrm{Tr} e^{-\beta H_\Gamma} \tag{4}$$

(with $\beta := 1/k_B T$), and $\mathcal{F}(0, h, \epsilon)$ is the corresponding limit of the ground state energy. Here H_Γ is the Hamiltonian of the system restricted to the finite box $\Gamma \subset \mathbb{Z}^d$, and $|\Gamma|$ is the number of sites in that box. It is known under the assumptions enumerated below that for almost all η this limit exists and is given by a nonrandom function of the parameters (see, e.g. [4,17]), which does not depend on the boundary conditions. By general arguments which are valid for both classical and quantum systems, $\mathcal{F}$ is convex in h; therefore the directional derivatives exist, and are equal for all but countably many values of h [16].

For typical realizations of the random field, the interval $[m_-(T, h, \epsilon), m_+(T, h, \epsilon)]$ provides the asymptotic range of values of the order parameter for any sequence of finite volume Gibbs states or ground states (the argument is similar to that found in [4] for classical systems). At a first-order phase transition $m_- < m_+$, and there are then at least two distinct infinite volume equilibrium states [16] with different values of the order parameter. In the QRFIM the m_+ and the m_- states can be obtained through the $+$ or $-$ boundary conditions (i.e., the spins $\sigma_x^{(3)}$ are replaced by ± 1 for all $x \notin \Gamma$). In general, such states are obtained by adding $\pm\delta$ to the uniform field h and letting $\delta \to 0$ *after* taking the infinite volume limit.

Our discussion is restricted to systems satisfying: (A) The interactions are *short range*, in the sense that for any finite box $\Lambda \in \mathbb{Z}^d$ the Hamiltonian may be decomposed as: $\mathcal{H} = H_\Lambda + V_\Lambda + H_{\Lambda^c}$, with H_Λ acting only in Λ, H_{Λ^c} only in the complement Λ^c, and V_Λ of norm bounded by the size of the boundary:

$$\|V_\Lambda\| \leq C|\partial\Lambda|. \tag{5}$$

(B) The variables η_x have an *absolutely continuous* distribution with respect to the Lebesgue measure (i.e., one with a probability density with no delta functions), and a finite rth moment, for some $r > 2$.

Our main results are summarized in the following two statements. The first applies regardless of whether the order parameter is related to any symmetry breaking.

Theorem 1.—In dimensions $d \leq 2$, any system of the form of (1) satisfying the above assumptions has $m_+(T, h, \epsilon) = m_-(T, h, \epsilon)$ for all h, and $T \geq 0$, provided $\epsilon \neq 0$.

The next result is formulated for situations where the first-order phase transition would represent continuous symmetry breaking. An example is the $O(N)$ model with

$$\mathcal{H}_0 = -\sum J_{x-y} \vec{\sigma}_x \cdot \vec{\sigma}_y \tag{6}$$

where $\vec{\sigma}$ are the usual quantum spin operators. More generally, $\mathcal{H}_0$ is assumed to be a sum of finite range terms which are invariant under the global action of the rotation group $SO(N)$, and $\vec{\sigma}_x$ is a collection of operators of norm one which transform as the components of a vector under rotations. With the random terms the Hamiltonian is

$$\mathcal{H} = \mathcal{H}_0 - \sum (\vec{h} + \epsilon \vec{\eta}_x) \cdot \vec{\sigma}_x. \tag{7}$$

Theorem 2.—For the $SO(N)$-symmetric system described above, with the random fields $\vec{\eta}_x$ having a rotation-invariant distribution, the free energy is continuously differentiable in $\vec{h}$ at $\vec{h} = 0$, whenever $\epsilon \neq 0$, $d \leq 4$, and $N \geq 2$.

Before describing the proof, let us comment on the implications of the statements, and their limitations.

(i) While the statements establish uniqueness of the expectation value of the bulk averages of the observables κ_x, or $\vec{\sigma}_x$ (in Theorem 2), they do not rule out the possibility of the coexistence of a number of equilibrium states, which differ from each other in some other way than the mean density of κ, which they share. More can be said for models for which it is known by other means that nonuniqueness of state is possible only if there is long-range order in κ. (Such is the case for QRFIM, through its relation to the classical ferromagnetic Ising model in $d + 1$ dimensions [18]).

(ii) The results address only the discontinuity, or symmetry breaking (as in the QRFIM), but they leave room for other phase transitions, or singular dependence on h. For instance, for the Ashkin-Teller spin chain for which Goswami *et al.* [12] report finding the Imry-Ma phenomenon in some range of the parameters but not elsewhere, the results presented here rule out the persistence of a first-order transition between the paramagnetic and Baxter phases in the full range in the model's parameters. However, they do not rule out the possibility of other phase transitions.

(iii) Randomness which does not couple to the order parameter of the transition need not cause a rounding effect. For example, in the transverse-field Ising model in a random *transverse* field, where the random field η_x couples to $\sigma^{(1)}$, ferromagnetic ordering is known to persist [18,19]. Presumably the same is true for the Baxter phase of the Ashkin-Teller model. It was even suggested that there are systems in which the introduction of randomness of this sort may even induce long-range order which would not otherwise be present [20,21], and our results do not contradict this. In addition we can draw no conclusions about quasi-long-range order, that is power law decay of correlations, including of κ_x.

Other comments, on the technical assumptions under which the statements hold, are found after the proofs.

The proofs of Theorems 1 and 2 are based on the analysis of the differences, between the m_+ and the m_- states, in the free energy (at $T = 0$, ground state energy) which can be ascribed to the random field within a finite region Λ of diameter L. Putting momentarily aside the question of existence of limits, a relevant quantity could be provided by

$$\tilde{G}_\Lambda(\eta_\Lambda) := \lim_{\delta\to 0}\lim_{\Gamma\to\mathbb{Z}^d} \mathrm{Av}[G^\delta_{\Lambda,\Gamma}|\eta_\Lambda] - \mathrm{Av}[G^\delta_{\Lambda,\Gamma}], \quad (8)$$

where $G^\delta_{\Lambda,\Gamma}$ is the difference of free energies

$$G^\delta_{\Lambda,\Gamma}(\eta) := \tfrac{1}{2}(F_\Gamma^{\eta,h+\delta} - F_\Gamma^{\eta^{(\Lambda)},h+\delta} - F_\Gamma^{\eta,h-\delta} + F_\Gamma^{\eta^{(\Lambda)},h-\delta}), \quad (9)$$

with

$$F_\Gamma^{\eta,h} := \frac{-1}{\beta}\log\mathrm{Tr}\exp(-\beta H_\Gamma^{\eta,h}), \quad (10)$$

$\eta^{(\Lambda)}$ is the random field configuration obtained from η by setting it to zero within Λ, and $\mathrm{Av}[\cdot|\eta_\Lambda]$ is a conditional expectation, i.e., an average over the fields outside of Λ. (The modification of the field h by $\pm\delta$ serves to select the desired ($m_\pm$) states).

Somewhat inconveniently, it is not obvious that for all models the limits in (9) exist. Nevertheless, one can prove that for each system of the class considered here there is a sequence of volumes $\Gamma_j \nearrow \mathbb{Z}^d$ for which the limit exists for all Λ, with convergence uniform in η_Λ. The proof of this assertion is by a compactness argument, whose details can be found elsewhere [22].

The essence of the proof of Theorem 1 is the contradiction between two estimates: (i) Under assumption A, Eq. (5):

$$|\tilde{G}_\Lambda(\eta)| \le 4C|\partial\Lambda|. \quad (11)$$

(ii) Whenever $m_- < m_+$, $\tilde{G}_\Lambda/\sqrt{|\Lambda|}$ converges in distribution to a normal random variable with a positive variance (as one would guess by considering the difference in the random field terms between states of different mean magnetizations, neglecting the states' local adjustments to the random fields).

More explicitly, for the upper bound we note that in the absence of the interaction terms V_Λ, the right-hand side of (9) would be zero. Using (5), one gets (11).

To prove the normal distribution for $G^\delta_{\Lambda,\Gamma}$, we apply a theorem of [4], Proposition 6.1 (as corrected in [23], p. 124). It implies that for $\Lambda \nearrow \mathbb{Z}^d$, under assumption B, $\tilde{G}_\Lambda/\sqrt{|\Lambda|}$ converges in distribution to a normal random variable with variance of the order of

$$b = \mathrm{Av}\left[\frac{\partial \tilde{G}_\Lambda}{\partial \eta_x}\right] = \epsilon(m_+ - m_-). \quad (12)$$

The two statements described above contradict the assumption that $m_- < m_+$ in dimensions $d \le 2$. That is so even at the critical dimension, where $L^{d/2} = L^{d-1}$. The reason is that the lower bound implies the existence of arbitrarily large fluctuations on that scale, whereas the upper bound is with a uniform constant. This proves Theorem 1.

The above proof is similar to that of the classical results [3,4] which this work extends. However, the discussion of the free energy fluctuations was based there on the analysis of the Gibbs states, and more specifically of the response to the fluctuating fields of the "metastates" which were specially constructed for that purpose. Except for special cases, such as the QRFIM, that argument was not available for quantum systems, where the equilibrium expectation values are no longer given by integrals over positive measures. The proof of the quantum case is enabled by a more direct analysis of the free energy.

Theorem 2 is proven by establishing that in the presence of continuous symmetry the upper bound (11), for $\Lambda = [-L, L]^d$, can be replaced by

$$|\tilde{G}_\Lambda(\eta_\Lambda)| \le KL^{d-2}. \quad (13)$$

Here $\tilde{G}_\Lambda$ is defined as in (8) and (9), but $\vec{h} = \vec{0}$, and δ is replaced by by $\vec{\delta} := \delta\hat{e}$ with $\hat{e}$ a unit vector. This change in the upper bound raises the critical dimension to $d = 4$.

To obtain (13) we focus on

$$g^\delta_{\Lambda,\Gamma}(\vec{\eta}_\Lambda) := \mathrm{Av}[F_\Gamma^{\vec{\eta},\delta\hat{e}} - F_\Gamma^{\vec{\eta},-\delta\hat{e}}|\vec{\eta}_\Lambda]. \quad (14)$$

Since $\tilde{G}_\Lambda(\eta_\Lambda) = \lim_{\delta\to 0}\lim_{\Gamma\to\mathbb{Z}^d}\frac{1}{2}(g^\delta_{\Lambda,\Gamma}(\vec{\eta}_\Lambda) - g^\delta_{\Lambda,\Gamma}(0))$, any uniform bound on $|g^\delta_{\Lambda,\Gamma}|$ for given Λ implies a similar bound on $|\tilde{G}_\Lambda|$. The claimed bound may be obtained though a soft-mode deformation analysis, which we shall make explicit for the case of pair interaction (the general case can be treated by similar estimates).

The free energy $F_\Gamma^{\vec{\eta},-\delta\hat{e}}$ in (14) may be rewritten by rotating both the spins and the field vectors with respect to an axis perpendicular to $\hat{e}$ at the slowly varying angles

$$\theta_x := \begin{cases} 0, & \|x\| \le L \\ \frac{\|x\|-L}{L}\pi, & L < \|x\| < 2L \\ \pi, & \|x\| \ge 2L \end{cases}. \quad (15)$$

The rotation aligns the external fields in the two terms ($\pm\,\delta\hat{e}$), except in the region $\| x \| < 2L$ where the effect is negligible when $\delta \to 0$. The effect of the rotation on the random fields is absorbed by rotation invariance of the average. In the end, the Hamiltonian of the rotated system differs from the Hamiltonian used to define the other free energy by

$$\Delta H_{\underline{\theta}} := \sum_{\{x,y\}\subset\Gamma} J_{x-y}[\vec{\sigma}_x \cdot \vec{\sigma}_y - \vec{\sigma}_x \cdot (e^{i(\theta_y-\theta_x)\rho_y}\vec{\sigma}_y e^{-i(\theta_y-\theta_x)\rho_y})]. \quad (16)$$

When the resulting expression for $F_\Gamma^{\vec{\eta},-\delta\hat{e}}$ in (14) is expanded in powers of $\theta_x - \theta_y \approx \pi\|x-y\|/L$, the zeroth-order term cancels with $F_\Gamma^{\vec{\eta},-\delta\hat{e}}$, and the second and higher order terms yield the claimed bound. The main difficulty is to eliminate the first-order terms, which amount to a sum of $O(L^d)$ quantities each of order $1/L$. However, the sign of these terms is reversed when the rotation is in the reversed direction. To take advantage of this, we combine two expressions for $g^\delta_{\Lambda,\Gamma}(\vec{\eta}_\Lambda)$ with the rotations applied in opposite directions, yielding

$$g^\delta_{\Lambda,\Gamma}(\vec{\eta}_\Lambda) = \mathrm{Av}[\log\mathrm{Tr}e^{-\beta H} - \tfrac{1}{2}\log\mathrm{Tr}e^{-\beta(H+\Delta H_{\underline{\theta}})} - \tfrac{1}{2}\log\mathrm{Tr}e^{-\beta(H+\Delta H_{-\underline{\theta}})}|\vec{\eta}_\Lambda] \quad (17)$$

(where $H \equiv H_\Gamma^{\vec{\eta},\delta\hat{e}}$.) By known operator inequalities [16]

$$\log\mathrm{Tr}e^{-\beta H} - \tfrac{1}{2}\log\mathrm{Tr}e^{-\beta(H+\Delta H_{\underline{\theta}})} - \tfrac{1}{2}\log\mathrm{Tr}e^{-\beta(H+\Delta H_{-\underline{\theta}})} \le \tfrac{1}{2}\|\Delta H_{\underline{\theta}} + \Delta H_{-\underline{\theta}}\|. \quad (18)$$

The right-hand side is zero to first order, and one is left with an *upper bound* on $g^\delta_{\Lambda,\Gamma}$ of the desired form. Repeating this analysis with the roles of the terms exchanged we obtain an identical *lower bound*, and thus inequality (13) follows.

The above argument is spelled out in detail in [22]. Let us end with few additional comments on the assumptions.

(iv) For Theorem 2, the assumption that the interaction has a strictly finite range can be weakened to a condition somewhat similar to Assumption A. For pair interactions [Eq. (7)] it suffices to assume

$$\sum_{x\in\mathbb{Z}^d} |J_x|\|x\|^2 < \infty. \quad (19)$$

(v) The restriction to absolutely continuous distribution excludes a number of models of interest. Such an assumption is generally necessary at zero temperature, as can be seen by the behavior of the Ising chain in a random field [24] which takes only a finite number of values. For positive temperatures it can be replaced by the requirement that the distribution has a continuous part which extends along the entire range of values. For the QRFIM at finite temperature one need only assume that the random field has more than one possible value, and this may well be the case more generally.

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