Melting transition of an Ising glass driven by magnetic field.

L. Arrachea[1,*], D. Dalidovich[2], V. Dobrosavljević[2] and M. J. Rozenberg[3]
[1] Scuola Internazionale Superiore di Studi Avanzati (SISSA) and Istituto Nazionale per la Fisica della Materia (INFM) (Unitá di Ricerca Trieste-SISSA), Via Beirut n. 4 I-34013 Trieste, Italy.
[2] National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32306, U.S.A.
[3] Departamento de Física, FCEN, Universidad de Buenos Aires, Ciudad Universitaria Pab.I, (1428) Buenos Aires, Argentina.

The quantum critical behavior of the Ising glass in a magnetic field is investigated. We focus on the spin glass to paramagnet transition of the transverse degrees of freedom in the presence of finite longitudinal field. We use two complementary techniques, the Landau theory close to the $T = 0$ transition and the exact diagonalization method for finite systems. This allows us to estimate the size of the critical region and characterize various crossover regimes. An unexpectedly small energy scale on the disordered side of the critical line is found, and its possible relevance to experiments on metallic glasses is briefly discussed.

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Understanding disordered systems is one of the main challenges of condensed matter physics, since the presence of disorder is always unavoidable in experiments. When disorder is strong it can dominate the physics and lead to exotic states of matter such as the glassy phases[2]. The most salient properties observed in glassy systems are the slow dynamical relaxation and history dependence of thermodynamics. Research on quantum spin systems is of primary importance because of potential technological applications. Current work in quantum computing and spintronics, where the understanding of relaxation processes is crucial [3, 4], is boosting a renewed interest in basic models of disordered quantum magnets.

The goal of the present work is to consider the random Ising model that displays a quantum paramagnet to spin glass transition driven by fluctuations introduced by an external magnetic field. We tackle the problem by utilizing two different theoretical approaches. We solve the model using the recently introduced technique of exact diagonalization that includes the averaging over an ensemble of disorder realizations in a finite system. The relevant results are then obtained by extrapolation of the data to the thermodynamic limit[5, 6]. This method allows for a direct investigation of the T=0 behavior in the whole range of parameters, circumventing thus the usual technical difficulties encountered in the replica formalism. On the other hand, to investigate in detail the critical behavior[7], we formulate the Landau theory in the vicinity of the quantum phase transition[8, 9]. The consistency check of results obtained using those two approaches allows us not only to confirm their reliability, but also to identify an unexpectedly narrow subregime near the phase boundary, in which the rapid onset of the glassy ordering occurs. We discuss the significance of our findings for the current experiments on metallic glasses[10].

We consider the random Ising model that is placed in a magnetic field that has both the transverse and longitudinal components,

$$H = -\sum_{<ij>} J_{ij} \mathrm{S}_i^z \mathrm{S}_j^z - \sum_i \mathbf{h} \cdot \mathbf{S}_i. \qquad (1)$$

The random interactions J_{ij} are chosen to be infinite range and Gaussian distributed with variance J, that sets the unit of energy in the model, while $\mathbf{h} = (h^T, 0, h^L)$. This model has an experimental realization in the $\mathrm{LiY}_{1-x}\mathrm{Ho}_x\mathrm{F}_4$ compound that has been the subject of recent experiments [11, 12]. In this insulating compound, the ground state of the magnetically active Ho ions is the low energy Ising doublet. In addition to that, the long-range nature of dipolar interactions between the spins enables us to perform the treatment in the large coordination limit. Disorder in the system arises from the fact that the substitutions of the Y atoms by the Ho ions are positionally random. The strong randomness leads to the clear observation of the spin-glass and ferro-glass phases at low concentration x [13].

To investigate the transition in the system described by the Hamiltonian (1), we employ two methods that complement each other in their scope and range of applicability. The main theoretical tool we use to obtain the detailed analytic behavior is based on the Landau theory approach[8, 9]. Though attractive, this method is rigorously valid only close to the quantum critical point, so that the actual range of applicability of this approach is always difficult to assess. Hence, in addition, we also use the exact diagonalization scheme, in which one has to obtain the solution of H for a number of explicit realizations of disorder (typically several tens of thousands). The procedure is implemented on finite systems of up to 17 spins. The physical observables, such as gaps or spectral functions, are obtained along the lines of Ref.[6]. In this approach, no *a priori* assumptions are made, and its validity is limited by the reliability of the required extrapolations to the large size limit. The main reason for success of the previous applications of the method is that for high connectivity models the numerical extrapolation to the thermodynamic limit is rather well behaved. Nevertheless, as we shall see and discuss later on, in the present study we find a certain range of parameters,where the previous statement does not hold. Remarkably, this circumstance allows us to gain new insight into the problem.

It is useful to characterize the parameter space by h^L and h^T, the longitudinal and transverse components of external magnetic field $\mathbf{h}$ respectively. The pure transverse field case was the subject of previous investigations [5]. At T=0, the existence of the quantum phase transition was established for a value of $h^T \sim O(J)$. At this point the spin-spin dynamical local suceptibility becomes gapless[14, 15]. When the longitudinal field is turned on, the net longitudinal magnetization is immediately generated and the critical point extends into a quantum critical line $h^T_c(h^L_c)$. This line separates the two phases, in which the transverse degrees of freedom of spins are either disordered (large h^T and h^L) or spin-glass ordered (small h^T and h^L). As we shall show, the excitation gap closes at this critical line, becoming very small in some crossover region on the disordered side of the line.

The Landau functional is constructed using the cumulant expansion about the quantum critical point at zero longitudinal field. Both the term with random interactions and the part with longitudinal field in the Hamiltonian (1) are treated as perturbations. This procedure implies that the longitudinal magnetic field h^L is small compared to the primary microscopic energy scale $h^T \sim J$. The derivation is straightforward and leads to the following Ginzburg-Landau action[8]

$$\begin{aligned}\beta\mathcal{F} &= \sum_{a,\omega_n}\left(\frac{r+\omega_n^2}{\kappa}\right)Q^{aa}(\omega_n) + \frac{u}{2\beta}\sum_a\left[\sum_{\omega_n}Q^{aa}(\omega_n)\right]^2 \\ &- \frac{\kappa}{3}\sum_{abc}\sum_{\omega_n}Q^{ab}(\omega_n)Q^{bc}(\omega_n)Q^{ca}(\omega_n) - \frac{\beta h^2}{2}Q^{ab}(\omega_n=0) \\ &- \frac{\beta y}{6}\int\int d\tau_1 d\tau_2\sum_{ab}\left[Q^{ab}(\tau_1-\tau_2)\right]^4. \end{aligned} \tag{2}$$

Here r, being some function of h^T/J, is the parameter that governs the transition, while u and y are taken at the critical point $(h^T/J)_{\rm c} \sim O(1)$. It is important to retain the quartic term, responsible for the RSB instability[9]. We must insert then the mean field ansatz

$$\kappa Q^{ab}(\omega_n) = \begin{cases} D(\omega_n) + \beta q_{\rm EA}\delta_{\omega_n,0}, & a = b, \\ \beta q_{ab}\delta_{\omega_n,0}, & a \neq b. \end{cases}$$

into Eq.(2) and vary subsequently the free energy with respect to $D(\omega_n)$, q_{EA} and q_{ab}. The parametrization of q_{ab} depends, however, on the phase under consideration. In the disordered paramagnetic phase (PM) we must use the replica-symmetric ansatz $q_{ab} = q_{EA}$, while in the spin glass phase (SG) the solution with a broken symmetry should be used[9, 16]. The variational procedure is lengthy albeit identical to that performed in the previous works. As a result, we obtain that the equation determining $D(\omega_n)$ is the same in both PM and SG phases and reads

$$\begin{aligned} &r + \omega_n^2 + u\left[\frac{1}{\beta}\sum_{\omega_n}D(\omega_n) + q_{\rm EA}\right] - D^2(\omega_n) \\ &- \frac{2y}{\kappa^2}q_{\rm EA}^2 D(-\omega_n) - \frac{2y}{\kappa^2}\frac{q_{\rm EA}}{\beta}\sum_{\omega_1}D(\omega_1)D(-\omega_1-\omega_n) \\ &- \frac{2y}{3\kappa^2}\frac{1}{\beta^2}\sum_{\omega_1,\omega_2}D(\omega_1)D(\omega_2)D(-\omega_1-\omega_2-\omega_n) = 0. \end{aligned} \tag{3}$$

This equation must be supplemented by

$$2D(0)q_{\rm EA} + \frac{2y}{3\kappa^2}q_{\rm EA}^3 + \frac{h^2\kappa}{2} = 0 \tag{4}$$

in the PM phase and

$$q_{\rm EA}^2 = -[D(0)\kappa^2]/y \tag{5}$$

in the SG phase, to comprise the full system to be solved self-consistently. Though the exact treatment of this system is not possible, we can obtain the leading order of the correct solution close to the quantum critical point. We consider here only the case of $T = 0$, so that all the sums over Matsubara frequencies are substituted by the corresponding integrals.

We notice first that, if $y = 0$, the complete solution is easily derived to be [8] $D(\omega_n) = -\sqrt{\omega_n^2 + \Delta^2}$. The gap Δ^2, that turns to zero right at the critical point, is determined using the following identity

$$\int\frac{d\omega}{2\pi}(\omega^2+\Delta^2)^{1/2} = \frac{\Lambda_\omega^2}{2\pi} + \frac{\Delta^2}{2\pi}\ln(c_1\Lambda_\omega/\Delta) \tag{6}$$

In Eq.(6) Λ_ω is the upper frequency cutoff and c_1 is some constant of order unity. Let's assume that for $y \neq 0$ the leading approximation of $D(\omega_n)$ contains the same square root singularity as for $y = 0$, and analyze how the last two terms in Eq.(3) affect the solution in the leading approximation. Simple inspection reveals that in the prelast term it is sufficient to put $\omega_n = 0$, $\Delta = 0$ while calculating the integral over ω_1. This contributes only to the renormalization of the coefficient u before $q_{\rm EA}$, so that $uq_{\rm EA} \to u_1 q_{\rm EA}$.

The last term requires, however, the calculation of the integral

$$\begin{aligned} K(\Delta,\omega_n) &= \int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}\sqrt{\omega_1^2+\Delta^2}\sqrt{\omega_2^2+\Delta^2} \\ &\times\sqrt{(\omega_1+\omega_2+\omega_n)^2+\Delta^2}, \end{aligned} \tag{7}$$

that is difficult to perform exactly for arbitrary ω_n and Δ^2. We need, however, only the leading behavior of this integral provided $\omega_n, \Delta \ll 1$. A simple estimate yields:

$$K(\Delta,\omega_n) = A + B\omega_n^2 + C_1\Delta^2\ln(C_2/\Delta), \tag{8}$$

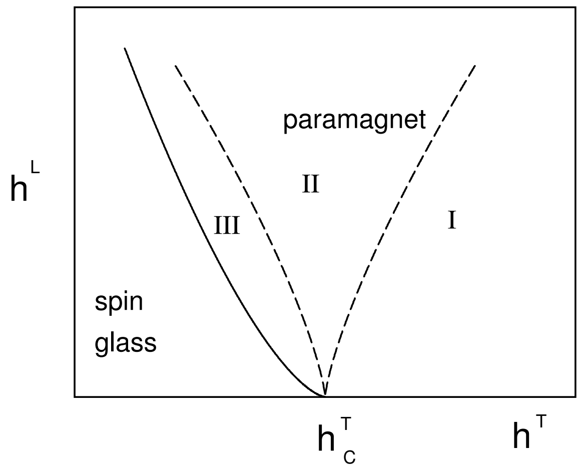

FIG. 1: Schematic phase diagram predicted by the Landau theory. The dashed lines denote crossovers while the full line is a critical line.

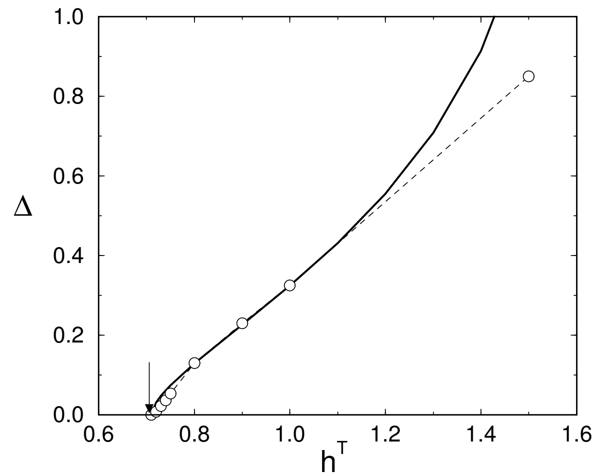

FIG. 2: Gap vs. transverse field h^T at $h^L = 0$ (open circles). The fitting function from Eq.(9) with $q_{\rm EA}$=0 is plotted in the solid line. The arrow indicates the critical field.

where the constants A, B, C_1 and C_2 are some cut-off Λ_ω dependent functions. We see that the first term in the above expression renormalizes the critical value r_c (equal to $u\Lambda_\omega^2/2\pi$ for $y = 0$), while the contribution from the second one can be simply absorbed by the appropriate rescaling of temperature T in ω_n^2. The third term in Eq.(8) leads to the renormalization of the coefficient before the Δ-dependent part of Eq.(6).

Similarly as in Ref.[9], we obtain that in the PM phase

$$D(\omega_n) = -yq_{\rm EA}^2/\kappa^2 - \sqrt{\omega_n^2 + \Delta^2},$$
$$\Delta^2 = \frac{r - r_c + u_1 q_{\rm EA}}{u_2 \ln[Cu_2/(r - r_c + u_1 q_{\rm EA})]}, \tag{9}$$

where C, u_1 and u_2 are again some Λ_ω dependent functions of the order unity. As a result of solution of Eqs.(3) and (4), one can distinguish the following regimes on a $(r - r_c,\, h)$ plane (see Fig.1).

(I) In this regime, in which $h \ll (r - r_c)^{3/4}$, $q_{\rm EA}$ is the smallest parameter and can be treated as a perturbation. As a result, we obtain with the logarithmic accuracy, that $q_{\rm EA} = (\kappa h^2)/4\Delta$, $\Delta \approx \{(r - r_c)/u_2 \ln(1/(r - r_c)\}^{1/2}$. This equation shows that when h^L becomes non zero, $q_{\rm EA}$ also becomes finite even in the PM phase due to the finite magnetization along the longitudinal axis.

The expression for the gap was first obtained in Ref.[14] and [17] that considered the h^L=0 case. To answer the question of the region of validity of the Landau approach, we use the exact diagonalization method to obtain the gap as a function of h^T at h^L=0. The results are shown in Fig.2. The agreement at small values of Δ demonstrates the reliability of our methods and gives an indication of the size of the critical region.

(II) This region is characterized by the condition $|r - r_c|^{3/4} \ll h$. In the leading approximation $\Delta \approx \{(u_1\kappa h^2)/4u_2 \ln(1/h^{4/3})\}^{1/3}$, while $q_{\rm EA} \approx \{(\kappa h^2/4)\sqrt{(u_2/u_1)\ln(1/h^{4/3})}\}^{2/3}$.

(III) This regime, in which $(r_c - r)^{3/4} \gg h$, is the closest to the $T = 0$ critical boundary. The EA order parameter, that crosses over to its value in the glassy phase, is given by $q_{\rm EA} = [(r_c - r)/u_1] + (u_2\Delta^2/u_1)\ln\left[1/\Delta^2\right]$, with $\Delta \approx [\kappa u_1 h^2/4(r_c - r)] - [2y(r_c - r)^2/3u_1^2\kappa^2]$. From this expression it is easily seen that Δ vanishes at the critical line given by $h = (8y/3)[(r_c - r)/u_1\kappa]^{3/2}$.

Finally, in the SG phase:

$$D(\omega_n) = -yq_{\rm EA}^2/\kappa^2 - |\omega_n|, \quad q_{\rm EA} = (r_c - r)/u_1, \tag{10}$$

resulting in a gapless form of the spectral density ${\rm Im}\chi(\omega) \propto \omega$.

We would like now to discuss the nature of the crossover between subregimes II and III in more detail. A rather surprising result, one obtains from the exact diagonalization method, is that in fact the freezing transition of the transverse degrees of freedom takes place at the critical boundary line given by $h_{c{\rm ED}}^T \propto |h^L - h_c^L|^{3/4}$ (see Fig. 3). This result was verified by two different criteria: (i) the divergence of the spin-glass susceptibility given by $J^2\langle[\chi_{loc}^{zz}]^2\rangle = 1$, and (ii) the vanishing of the excitation energy gap of the regular part of the dynamical spin susceptibility, that corresponds to the so called "replicon" mode[16]. It is notable that the infinite system size extrapolations for these two different freezing transition criteria do agree well. However, these results seem paradoxical since the Landau theory predicts a phase transition boundary with a different functional form, namely, $h_c^T \propto |h^L - h_c^L|^{3/2}$ (and different curvature, see Fig. 2).

This paradox is resolved upon further scrutiny of the results from the Landau theory. To this end, it is important to note that, in the presence of the non-zero longitudinal field, the critical behavior of the gap is dif-

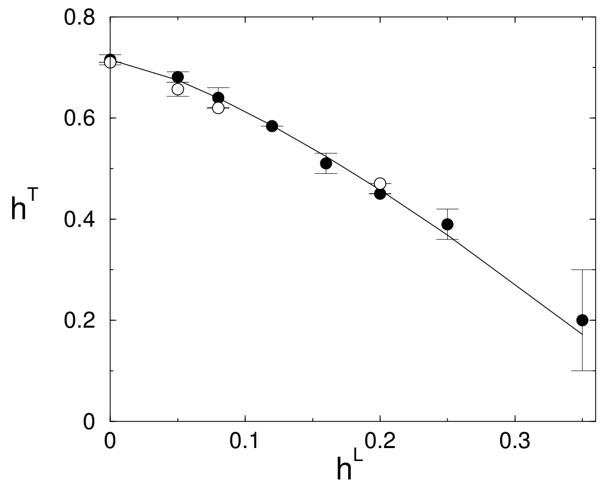

FIG. 3: SG-PM phase boundary obtained with exact diagonalization. Filled and open circles correspond to the two different criteria (i) and (ii), respectively (see text). The solid line corresponds to the fitting function $h^T = h_c^T - 2.2(h^L)^{3/4}$.

ferent than at $h^L = 0$. It takes a much slower, linear form $\Delta(\delta r) \sim \delta r$ (δr is the distance to the critical line), becoming the new effective small energy scale that characterizes the region III. This linear regime of $\Delta(\delta r)$ crosses over to the regime II, at values of $r_c - r \approx (\kappa u_1 h^2/4)^{2/3} u_2^{1/3} \ln^{1/3}(1/h^{4/3})$. Remarkably, this is precisely the functional form obtained for the critical line (and gap closure) from the numerical calculation.

The key point is that for systems of the size that one can diagonalize, the physics of the small gap is masked by the finite size effects, affecting thus the validity of extrapolations. This is a well known limitation of exact diagonalization studies that occurs in systems in which the small energy scales emerge[18]. Interestingly, similar discrepancies are found in the prediction of the de Almeida - Thouless (AT) line in the classical Sherrington-Kirkpatrik (SK) model (with $h^T = 0$) in a longitudinal field. Numerical calculations suggest that the critical temperature is $T_c \propto |h^L - h_c^L|^{3/4}$, instead of the correct result $T_c \propto |h^L - h_c^L|^{3/2}$. In the classical case, this can be an indication that the free energies of the ordered and paramagnetic phases are actually very close within a crossover region in the $T - h^L$ diagram, equivalent to the region III of Fig. 1. The large finite-size effects were found also in the recent numerical simulations of the classical model [19], and are possibly relevant to the anomalous behavior observed in experimental studies of the AT line [20]. For the quantum systems, such small gaps may be also difficult to observe in experiments as well as in numerical calculations. In contrast, in regions I and II, the r-dependence of Δ assumes a form similar to the zero field limit (see Eq.(9), except that r is shifted by the quantity $u_1 q_{\rm EA}$). Since in region II (dropping logarithmic corrections) $q_{\rm EA} \sim h^{4/3}$, we conclude that the crossover line separating regions II and III may play a role of an *apparent* critical line, below which the gap, although finite, may assume unobservable small values.

This outstanding feature, which was overlooked in previous works, may have important consequences. For instance, it may be responsible for the peculiar observation of the quenching of the nonlinear susceptibility at the quantum critical point of the $\mathrm{LiY}_{1-x}\mathrm{Ho}_x\mathrm{F}_4$ series [21]. Another example is the electron glass model that was recently described in Ref. [9] and for which essentially identical arguments apply. In this case the dynamical exponent is $z = 1$, and we find that the crossover energy scale (corresponding to the gap in the Ising case) behaves as $\Delta \sim \delta r^2$ and corresponds to a crossover temperature separating the Fermi liquid regime (at low T) from the quantum critical regime (at high T). The second power in δr indicates an even broader quantum critical regime than in the Ising case. Such an extended quantum critical region may result in enhanced dissipation at low temperatures, a possibility which may bear relevance for the puzzling absence of weak localization (interference) corrections in certain two-dimensional electron gases in the low density regime.

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[1] *Permanent address: Departamento de Física, Universidad de Buenos Aires, Ciudad Universitaria Pabellón I, (1428) Buenos Aires, Argentina.

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