RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 39, NUMBER 16 1 JUNE 1989

Instabilities in the quantum Sherrington-Kirkpatrick Ising spin glass in transverse and longitudinal fields

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(Received 24 October 1988)

The infinite-range quantum Ising spin glass in transverse (Γ) and longitudinal (h) fields is studied by means of thermo-field-dynamics as a substitute for the n-replica trick. With the use of a one-loop approximation for the dynamic self-interaction the stability of the mean-field-type solution against the action of fluctuations is investigated in the parameter space (k_BT,Γ,h).

There is currently great experimental and theoretical interest in the quantum version of the Sherrington-Kirkpatrick (SK) (Ref. 1) Ising spin-glass in a transverse field motivated by the discovery of characteristic spin-glass properties in nonmagnetic cases such as the mixed-hydrogen-bonded ferroelectrics—the so-called proton glasses.[2-5] In these systems ferroelectric glass ordering can be regarded as the freezing of random projections of electric dipole moments at the paraelectric-ferroelectric glass-phase transition.[5]

The model under consideration contains N interacting pseudospins described by the following Hamiltonian:

$$H=-\sum_{(ij)}J_{ij}\sigma_{iz}\sigma_{jz}-\Gamma\sum_i\sigma_{ix}-h\sum_i\sigma_{iz}\,, \tag{1}$$

where σ_i are the Pauli matrices referred to the ith site of the lattice, while Γ and h denote the transverse and longitudinal field, respectively. The sum in Eq. (1) is performed over all distinct pairs of pseudospins and the exchange interactions J_{ij} are independent random field variables with the symmetric Gaussian probability distribution

$$P(J_{ij})=\left(\frac{N}{2\pi J^2}\right)^{1/2}\exp(-NJ_{ij}^2/2J^2)\,. \tag{2}$$

The long-range nature of the interactions J_{ij} originating from the dipolar character of the interbond forces[3] justifies the use of the formula (2). For a proton-glass system a new mechanism which tends to destroy the glass order is provided by the proton tunneling,[6] an intrinsic quantum effect described by the transverse field Γ representing the tunneling frequency, while the longitudinal field h refers to the energy splitting of a bond in an applied electric field.

The quantum spin-glass problem is far from being a trivial one due to the noncommutativity of operators and different methods have been introduced to handle this problem. Typically, quantum mechanics introduces frequency-dependent self-interactions and order parameters and it is important to understand this frequency dependence as has been emphasized earlier.[7-9]

As is well known the SK solution of the model for $\Gamma=0$ becomes unstable in an applied longitudinal field h below the de Almeida–Thouless (AT) (Ref. 10) line, signaling the apparent breakdown of ergodicity and history dependence. Moreover, for vanishing longitudinal field the spin-glass transition is controlled by the temperature and transverse field and the system is expected to stay in the spin-glass phase below the field-dependent critical line $T_c(\Gamma)$ which extends down to zero temperature[11]—a phenomenon which possesses its classical counterpart in vector spin glasses studied by Gabay and Thouless (GT).[12] However, due to the complexity of quantum spin glasses the exact $T_c(\Gamma)$ dependence has been obtained only very recently for the infinite-range model by employing a perturbative approach[7] and a numerical Trotter-Suzuki method[8] as well as for a short-range model studied in mean-field theory by employing a path-integral approach.[9] There are other theoretical studies of the freezing temperature of the infinite-range model using a static approximation for a frequency-dependent self-interaction,[11,13,14] a phenomenological approach,[6] and a quantum version[15-17] of the Thouless, Anderson, and Palmer (TAP) (Ref. 18) method. The obtained approximate results for $T_c(\Gamma)$ are in qualitative agreement with each other and with the exact $T_c(\Gamma)$ although the exact $T_c(\Gamma)$ is significantly lower at low temperatures due to strong quantum fluctuations.

It is the purpose of the present Rapid Communication to report on the stability analysis of the mean-field theory of the infinite-range quantum transverse Ising-spin system described by the Hamiltonian (1) in the whole parameter space (k_BT,Γ,h).

The method we use to handle both the disorder average and the quantum problem has been proposed earlier by one of us.[19] It is based on thermo-field-dynamics (TFD),[20] a real-time finite-temperature quantum field theory. Apart from the interest in dynamics, which, due to the quantum nature of the problem, becomes an intrinsic theoretical ingredient of the model, this method allows one to circumvent the use of the n-replica trick[21] while performing the quenched average and deals directly with the physical observables like the response and correlation functions. In this context TFD make close connection to the dynamic approach known from the classical spin-glass problem.[22]

In order to incorporate thermal effects in TFD one requires the doubling of degrees of freedom[20] by associating to any operator $A(\equiv A^1)$ a tilde conjugate one $\tilde{A}(\equiv A^2)$. Specifically, the dynamics is generated by the thermal

Hamiltonian $\hat{H}$

$$\hat{H}=H-\tilde{H}\equiv H[\sigma^1]-H[\sigma^2]\,, \tag{3}$$

where H is the conventional Hamiltonian of the system (1) whereas $\tilde{H}$ refers to the copy of the original system moving backwards in time in the "mirror space."[23] The temperature enters the theory through the thermal vacuum $|O(\beta)>$ constructed in such a way that the quantum expectation value between thermal vacua corresponds to the conventional statistical average

$$\langle O(\beta)|\cdots|O\beta\rangle=\frac{\mathrm{Tr}\,e^{-\beta H}\cdots}{\mathrm{Tr}\,e^{-\beta H}}\,. \tag{4}$$

To proceed, we start from the disorder-averaged generating functional for the real-time finite-temperature Green's functions in the form[19]

$$\langle Z[\eta]\rangle_J=\int\mathcal{D}\mathbf{Q}\exp(-N\mathcal{L}[\mathbf{Q}]+\Omega[\eta])\,, \tag{5}$$

where the single-site dynamic Lagrangian reads

$$\mathcal{L}[\mathbf{Q}]=\mathrm{Tr}\mathbf{Q}^2-\ln\Phi[\mathbf{Q}]\,, \tag{6}$$

while $\Omega[\eta]$ refers to the source term. Furthermore,

$$\mathrm{Tr}\mathbf{Q}^2=\int_{-\infty}^{+\infty}dt\int_{-\infty}^{+\infty}dt'\sum_{\alpha\beta}Q^{\alpha\beta}(t,t')Q^{\beta\alpha}(t',t)\,, \tag{7}$$

where $Q^{\alpha\beta}(t,t')$ represents a 2×2 matrix field, which is symmetric $[Q^{\alpha\beta}(t,t')=Q^{\beta\alpha}(t',t)]$ and nonlocal in time. Subsequently,

$$\Phi[\mathbf{Q}]=\langle O,\beta|U_Q(-\infty;+\infty)|O,\beta\rangle \tag{8}$$

where $|O,\beta\rangle$ denotes the thermal vacuum corresponding to the single-site Hamiltonian $\mathcal{H}_0=-\Gamma\sigma_x-h\sigma_z$ while

$$U_Q(-\infty;+\infty)=T\exp\left[-i\int_{-\infty}^{+\infty}dt\int_{-\infty}^{+\infty}dt'\hat{H}_Q(t,t')\right] \tag{9}$$

is the time-ordered exponential resulting from the interaction picture. The effective time-dependent single-site Hamiltonian then reads

$$\hat{H}_Q(t,t')=\sum_{\alpha\beta}JQ_\tau^{\alpha\beta}(t,t')\sigma_z^\alpha(t)\sigma_z^\beta(t')\,, \tag{10}$$

where

$$Q_\tau^{\alpha\beta}=(\tau^{1/2}\mathbf{Q}\tau^{1/2})^{\alpha\beta},\quad \tau^{1/2}=\begin{bmatrix}1&0\\0&i\end{bmatrix}. \tag{11}$$

Finally, the pseudospin operators are defined in the interaction picture in the standard way as

$$\sigma_z^\alpha(t)=\exp(i\hat{\mathcal{H}}_0t)\sigma_z^\alpha\exp(-i\hat{\mathcal{H}}_0t)\,. \tag{12}$$

The averaged generating functional (5) bears some formal resemblance to the averaged replicated partition function in statics[1] where the $n\times n$ replica field corresponds to $Q^{\alpha\beta}(t,t')$ in our formalism. However, in the present case the matrix $Q^{\alpha\beta}(t,t')$ has a nontrivial time dependence. In fact, the quantum generalization of the SK spin-glass model shows an interesting new feature. The effective local field acting on a pseudospin has a fluctuating dynamical part which results in an effective dynamic self-interaction $JQ^{\alpha\beta}(t,t')$ in the thermal Hamiltonian (10) which has to be calculated self-consistently. In the $N\to\infty$ limit the saddle-point method can be used, which amounts to finding the Q's stationary point values $Q_0^{\alpha\beta}$ determined from the relation

$$\delta\mathcal{L}[\mathbf{Q}]/\delta Q^{\alpha\beta}=0\,. \tag{13}$$

Consequently, one obtains

$$Q_0^{\alpha\beta}(t,t')=\tfrac{1}{2}JG_\tau^{\alpha\beta}(t,t'),\quad \mathbf{G}_\tau=\tau^{1/2}\mathbf{G}\tau^{1/2}\,, \tag{14}$$

where

$$G^{\alpha\beta}(t,t')=-i\frac{\langle O,\beta|T\sigma_z^\alpha(t)\sigma_z^\beta(t')U_{Q_0}(-\infty;+\infty)O,\beta\rangle}{\langle O,\beta|U_{Q_0}(-\infty;+\infty)|O,\beta\rangle}\,. \tag{15}$$

It turns out that the dynamic self-interaction persists also in the paramagnetic phase making an explicit solution of Eq. (14) a highly nontrivial task. This is in contrast to the classical spin-glass case where the properties of the system in the paramagnetic regime are rather simple.

Below the freezing temperature the general strategy for constructing the mean-field theory of a spin glass is to look for time persistent qualities. Therefore, we factorize the matrix of causal Green's functions (15) into finite time $G_{\mathrm{reg}}^{\alpha\beta}$ and time persistent part $G_{\mathrm{sing}}^{\alpha\beta}$ as follows:

$$G^{\alpha\beta}(t,t')=G_{\mathrm{reg}}^{\alpha\beta}(t,t')+G_{\mathrm{sing}}^{\alpha\beta}(t,t')\,. \tag{16}$$

The TFD causal matrix propagator $G_{\mathrm{reg}}^{\alpha\beta}$ is most convenient for calculations but more direct contact with measurable quantities is established when one decomposes it. Supposing that after a sufficiently long time the system reaches equilibrium one has restored time translational invariance $G_{\mathrm{reg}}^{\alpha\beta}(t,t')=G_{\mathrm{reg}}^{\alpha\beta}(t-t')$. In this case the Fourier transformed matrix $G_{\mathrm{reg}}^{\alpha\beta}(\omega)$ can be presented as follows:

$$\begin{aligned}\mathbf{G}_{\mathrm{reg}}(\omega)&=\mathbf{U}_B(\omega)\tau\bar{\mathbf{G}}(\omega)\mathbf{U}_B(\omega)\\&=\tau\bar{\mathbf{G}}(\omega)-\frac{2iC_{\mathrm{reg}}(\omega)}{e^{\beta\omega}+1}\begin{bmatrix}1&e^{\beta\omega/2}\\e^{\beta\omega/2}&1\end{bmatrix},\end{aligned} \tag{17}$$

where

$$\begin{aligned}\mathbf{U}_B(\omega)&=\begin{bmatrix}\sinh\phi(\omega)&\cosh\phi(\omega)\\\cosh\phi(\omega)&\sinh\phi(\omega)\end{bmatrix},\\\sinh^2\phi(\omega)&=\frac{1}{e^{\beta\omega}-1}\,,\end{aligned} \tag{18}$$

is the thermal transformation matrix,[20] while

$$\bar{\mathbf{G}}(\omega)=\begin{bmatrix}G^R(\omega)&0\\0&G^A(\omega)\end{bmatrix}, \tag{19}$$

with $G^{R(A)}$ being the retarded (advanced) Green's function. Correspondingly, $C_{\mathrm{reg}}(\omega)$ refers to the thermodynamic correlation function being related to the G^R by means of the fluctuation-dissipation theorem

$$C_{\mathrm{reg}}(\omega)=\coth(\beta\omega/2)\mathrm{Im}G^R(\omega)\,. \tag{20}$$

Furthermore, it turns out that the time persistent part

$G^{\alpha\beta}_{\rm sing}(\omega)$ has the form

$$\mathbf{G}_{\rm sing} = -2\pi i q \delta(\omega) \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \tag{21}$$

where q is the Edwards-Anderson (EA) (Ref. 21) spin-glass order parameter. Indeed, by substitution of Eq. (21) into (16) using the relation (17) one obtains for the total correlation function

$$C(\omega) = C_{\rm reg}(\omega) + 2\pi q \delta(\omega), \tag{22}$$

according to the dynamic EA definition of the spin-glass order parameter.

It is convenient to represent the time persistent contribution to the effective thermal Hamiltonian (10) in a form of a static Gaussian noise component, which acts as a random longitudinal field to generate time persistent autocorrelations. Accordingly, the functional (8) becomes

$$\Phi[\mathbf{Q}] = \langle \exp(\ln\Phi_z[\mathbf{Q}]) \rangle, \tag{23}$$

where

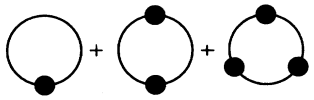
$$\langle \cdots \rangle \equiv \int_{-\infty}^{+\infty} \frac{dz}{(2\pi)^{1/2}} e^{-z^2/2} \cdots, \tag{24}$$

and

$$\Phi_z[\mathbf{Q}] = \langle O(\beta,z) | U_{Q_{\rm reg}}(-\infty;+\infty) | O(\beta,z) \rangle, \tag{25}$$

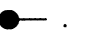
where $|O(\beta,z)\rangle$ is the thermal vacuum associated with the single-site Hamiltonian $\mathcal{H}_0' = \mathcal{H}_0 + Jzq^{1/2}\sigma_z$ with the static noise, while the time-ordered exponential (9) contains only the finite time part of the dynamic self-interaction.

Due to the complicated nature of the interaction it is not possible to work out the explicit form of the functional (23) in the general case. However one can resort on the diagrammatic analysis by noticing that the functional $\ln\Phi_z[\mathbf{Q}]$ expanded in powers of the dynamic self-interaction generates in the usual way the linked-cluster expansion[24] for the thermo-field-Green's functions. Taking into account the action of quantum fluctuations in the one loop order amounts to sum up all ring diagrams according to

$\ln\Phi_z[\mathbf{Q}] =$  (26)

where

$J\mathbf{Q}_\tau =$

$\Sigma(z) =$  .

Here, the line denotes the dynamic self-interaction, while the dot corresponds to the self-energy part. The final result is then

$$\ln\Phi_z[\mathbf{Q}] = -\frac{1}{2}\mathrm{Tr}\ln[1 - 2J\mathbf{Q}_\tau\Sigma(z)], \tag{27}$$

where the trace operation is defined by means of Eq. (7). Now, in order to study the fluctuations around the saddle point (13) we work out, by using Eqs. (6), (23), and (27) the term which is quadratic in the fluctuations $\delta\mathbf{Q}$, yielding

$$\mathcal{L}[\mathbf{Q}_0+\delta\mathbf{Q}] - \mathcal{L}[\mathbf{Q}_0] = \mathrm{Tr}[\delta\mathbf{Q}\delta\mathbf{Q} - J^2\langle \delta\mathbf{Q}\mathbf{G}_\tau(z)\delta\mathbf{Q}\mathbf{G}_\tau(z)\rangle] + o((\delta\mathbf{Q})^3), \tag{28}$$

where

$$\mathbf{G}(\omega,z) = \Sigma(\omega,z)\frac{1}{1 - 2J\mathbf{Q}_\tau(\omega)\Sigma(\omega,z)} \tag{29}$$

is the Dyson equation for the noise-dependent causal Green's function.

For a stable solution a 4×4 matrix defined by the right-hand side of Eq. (28) should have no negative eigenvalues. Applying Eq. (17) in the static approximation[19] that decouples the mixed thermo-field components of the effective Hamiltonian (10) and which gives a satisfying estimate of $T_c(\Gamma)$ except for very low temperatures one finally obtains from (28) the stability condition in the form

$$1 - J^2\langle \chi^2(z) \rangle \geq 0, \tag{30}$$

where $\chi(z) \equiv G^R(\omega=0,z) = G^A(\omega=0,z)$ is the local static longitudinal susceptibility (electric permittivity in the case of ferroelectric glass). Furthermore,

$$\begin{aligned} \chi(z) &= (\Gamma^2/\Theta_z^3)\tanh(\beta\Theta_z) \\ &\quad + \beta((J_q^{1/2}z + h)/\Theta_z)^2 \mathrm{sech}^2(\beta\Theta_z), \\ q &= \langle m^2(z) \rangle, \\ m(z) &= [(J_q^{1/2}z + h)/\Theta_z]\tanh(\beta\Theta_z), \\ \Theta_z &= [(J_q^{1/2}z + h)^2 + \Gamma^2]^{1/2}. \end{aligned} \tag{31}$$

It is easy to see that for $\Gamma = 0$ Eq. (30) reduces to the conventional AT instability line.[6] For $h = 0$ and nonzero transverse field, approaching from the high-temperature phase one has $q = 0$, and from Eqs. (30) and (31) it follows that

$$(J/\Gamma)\tanh(\beta_c\Gamma) = 1 \tag{32}$$

for the critical line describing the transverse freezing,[14,19]

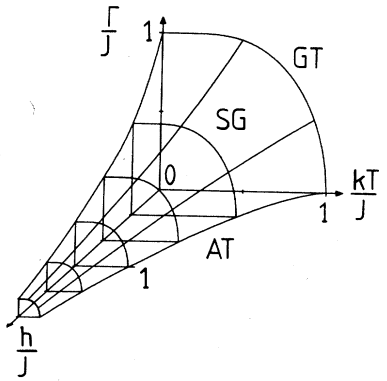


FIG. 1. Phase diagram of the quantum SK Ising spin glass in the transverse (Γ) and longitudinal (h) fields, calculated from Eqs. (30) and (31).

implying that the ergodicity is broken immediately below $T_c(\Gamma)$. For small fields one has

$$1-\frac{T_c(\Gamma)}{T_c(0)}\approx\frac{1}{3}\left[\frac{\Gamma}{J}\right]^2, \tag{33}$$

i.e., the quadratic field dependence characteristic for GT instability line.[12] In the general case one has in the parameter space (k_BT,Γ,h) the instability surface depicted in Fig. 1.

To conclude, in the present Rapid Communication we have calculated for the first time the spin-glass freezing temperature for transverse *and* longitudinal external field and we have performed the stability analysis for the corresponding mean-field-type theory. It is explicitly shown that the mean-field solution appears to be unstable in the whole parameter space bounded by the instability surface, signaling that a simple description of the glassy phase based on a single EA spin-glass order parameter is no longer valid in this region.

In closing we would like to add a further observation. The peculiar feature of the quantum spin-glass problem is that the statics and dynamics of the model are inextricably connected, so their simple decomposition as in the classical case[22] is no longer possible. Even in the static limit the local susceptibility (31) will depend on the details of the dynamic self-interaction. This implies that, e.g., an exact calculation of the critical surface $T_c(\Gamma,h)$ enforces a full solution of the self-consistent Eq. (13). The complexity of the problem, of course, prevents from any nonperturbative approach. An estimate of the exact transverse freezing line for $h=0$ already exists.[8] An extension of this work covering the whole parameter space is currently under investigation on the basis of the theory outlined in this note.

This work was supported by the Deutsche Forschungsgemeinschaft through Sonderforshungsbereich No. 166 Duisburg-Bochum.

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[1]D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **32**, 1792 (1975).
[2]E. Courtens, Phys. Rev. Lett. **52**, 69 (1984).
[3]J. Slak, R. Kind, R. Blinc, E. Courtens, and S. Zumer, Phys. Rev. B **30**, 85 (1984).
[4]E. Courtens, F. Huard, and R. Vacher, Phys. Rev. Lett. **55**, 722 (1985).
[5]I. A. Akheizer and A. I. Spolnik, Fiz. Tverd. Tela **25**, 148 (1983) [Sov. Phys. Solid State **25**, 18 (1983)].
[6]R. Pirc, B. Tadić, and R. Blinc, Z. Phys. **61**, 69 (1985); Phys. Rev. B **36**, 8607 (1987).
[7]T. Yamamoto and H. Ishii, J. Phys. C **20**, 6053 (1987).
[8]K. D. Usadel and B. Schmitz, Solid State Commun. **64**, 975 (1987); K. D. Usadel, Nucl. Phys. **B5**, 91 (1988).
[9]V. Dobroslavljević and R. Stratt, Phys. Rev. B **36**, 8484 (1987).
[10]J. R. L. de Almeida and D. J. Thouless, J. Phys. A **11**, 983 (1978).
[11]K. D. Usadel, Solid State Commun. **58**, 629 (1986).
[12]M. Gabay and G. Toulouse, Phys. Rev. Lett. **47**, 201 (1981).
[13]Ya. V. Fedorov and E. F. Shender, Pis'ma Zh. Eksp. Teor. Fiz. **43**, 526 (1986) [JETP Lett. **43**, 681 (1986)].
[14]K. Walasek and K. Lukierska-Walasek, Phys. Rev. B **34** 4962 (1986).
[15]H. Ishii and T. Yamamoto, J. Phys. C **18**, 6225 (1985).
[16]T. Yokota, Phys. Lett. A **125**, 482 (1987).
[17]K. Walasek and K. Lukierskia-Walasek, Phys. Rev. B **38**, 725 (1988).
[18]D. J. Thouless, P. W. Anderson, and R. G. Palmer, Philos. Mag. **35**, 593 (1977).
[19]T. K. Kopeć, J. Phys. C **21**, 297 (1988); **21**, 6053 (1988).
[20]H. Umezawa, Y. Takahashi, and H. Matsumoto, *Thermo Field Dynamics and Condensed States* (North-Holland, Amsterdam, 1982).
[21]S. F. Edwards and P. W. Anderson, J. Phys. F **5**, 965 (1975).
[22]H. Sompolinsky and A. Zippelius, Phys. Rev. Lett. **47**, 359 (1981).
[23]M. Schmutz, Z. Phys. B **30**, 97 (1978).
[24]H.-J. Sommers and K. D. Usadel, Z. Phys. B **47**, 63 (1982).