Стекольный переход в 3D фрустрированной модели Гейзенберга: Описание в рамках калибровочного подхода

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УНИВЕРСАЛЬНОСТЬ

Стеклование молекулярных систем

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Pablo G. Debenedetti* & Frank H. Stillinger

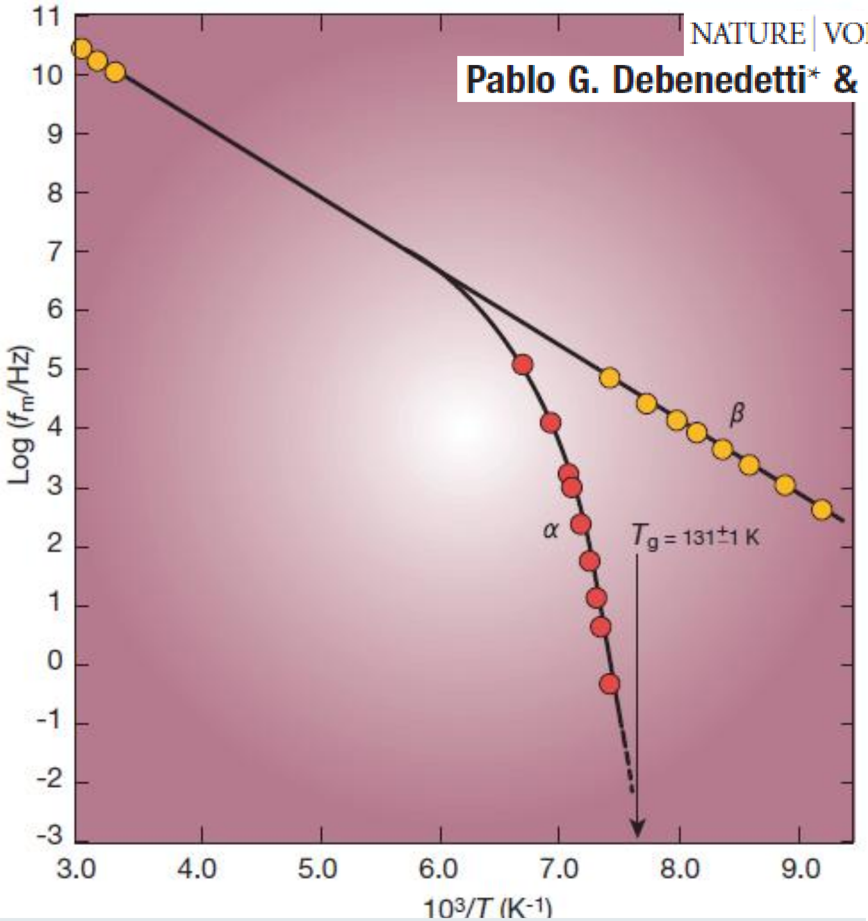


Figure 3 Temperature dependence of the peak dielectric relaxation frequency of the glass-forming mixture chlorobenzene/*cis*-decalin (molar ratio 17.2/82.8%). At high enough temperature there is a single relaxation mechanism. In the moderately supercooled regime the peak splits into slow (α) and fast (β) relaxations, of which α-processes exhibit non-Arrhenius temperature dependence and vanish at T_g. (Adapted from refs 9 and 41.)

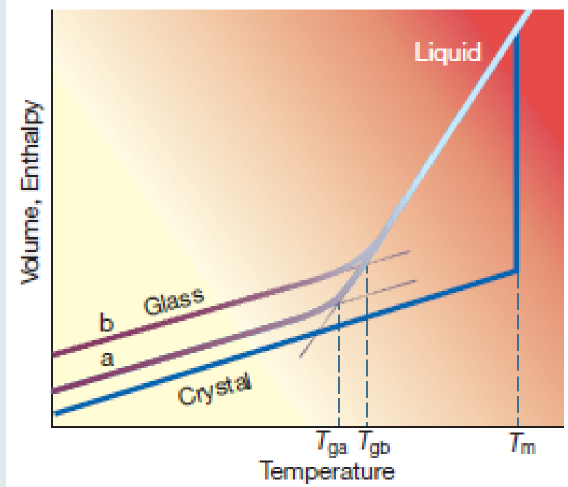


Figure 1 Temperature dependence of a liquid's volume v or enthalpy h at constant pressure. T_m is the melting temperature. A slow cooling rate produces a glass transition at T_{ga}; a faster cooling rate leads to a glass transition at T_{gb}. The thermal expansion coefficient $\alpha_p = (\partial \ln v/\partial T)_p$ and the isobaric heat capacity $c_p = (\partial h/\partial T)_p$ change abruptly but continuously at T_g.

Стеклование спиновых систем

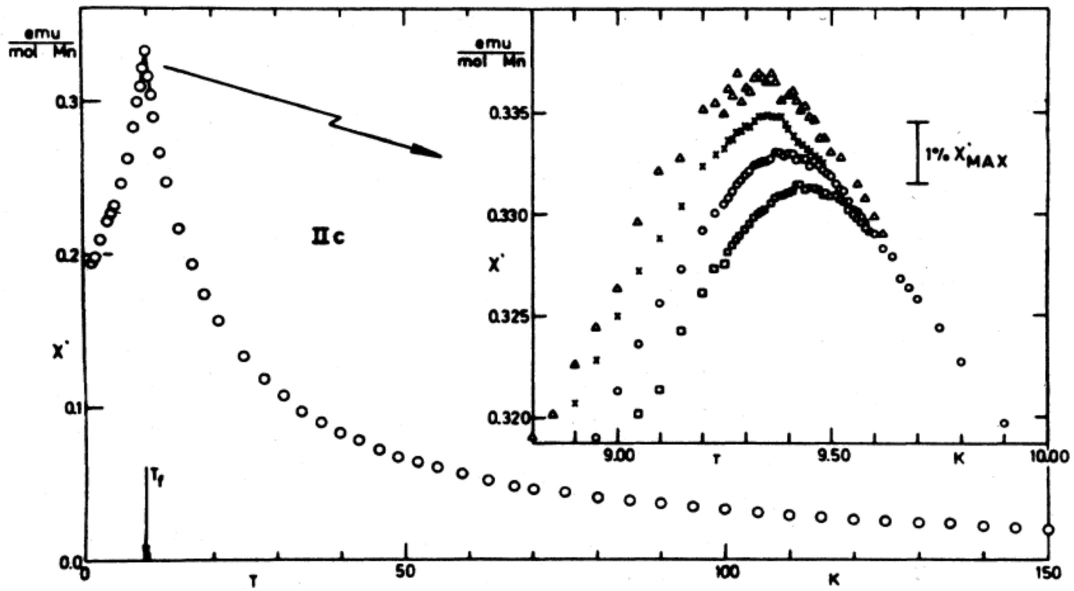


FIG. 1. Real part χ' of the complex susceptibility $\chi(\omega)$ as a function of temperature for sample IIc (*Cu*Mn with 0.94 at. % Mn, powder). Inset reveals frequency dependence and rounding of the cusp by use of strongly expanded coordinate scales. Measuring frequencies: □, 1.33 kHz; ○, 234 Hz; ×, 104 Hz; △, 2.6 Hz. From Mulder *et al.* (1981).

$$\chi_L = \partial\langle\phi\rangle/\partial h \qquad \chi_L\,(T_g) = \mathrm{const}$$

$$\chi_N = \partial^3\langle\phi\rangle/\partial h^3 \qquad \chi_N \propto (T - T_g)^{-\gamma}$$

K. Binder and A. P. Young: Spin glasses Rev. Mod. Phys., Vol. 58, No. 4, October 1986

Стеклование спиновых систем

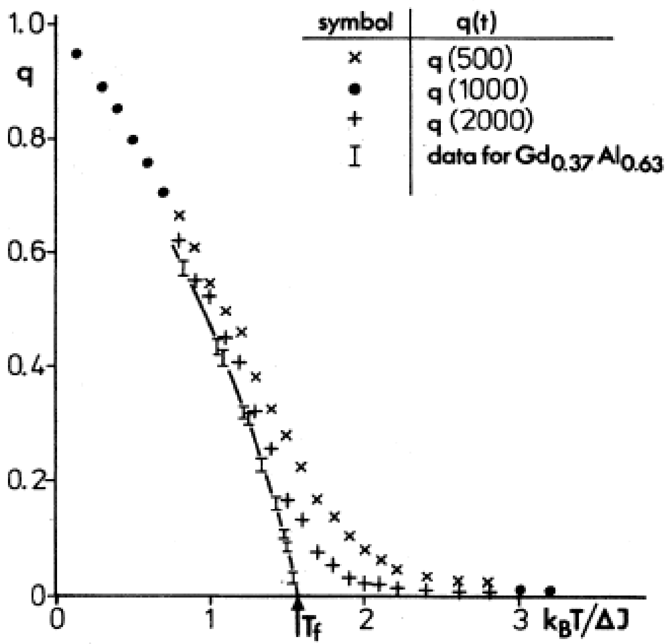


FIG. 8. Spin glass order parameter vs temperature for $Gd_{0.37}Al_{0.63}$ (from Mizoguchi *et al.*, 1977) compared to simulations of a $16\times16\times16$ Ising spin glass at various observation times t, measured in Monte Carlo steps per spin (from Binder, 1977a). ΔJ is the width of the Gaussian distribution of the simulation, and the experimental $k_B T_f/\Delta J$ is chosen arbitrarily.

$$q=[\langle S_i\rangle_T^2]_{\rm av}$$

Vogel–Tammann–Fulcher (VTF)

$$\eta = A\exp[B/(T-T_o)]$$

$$\tau^{\max} \propto \xi^z \propto |1-T/T_c|^{-z\nu}$$

$$\gamma\approx3.2,\quad \beta\approx0.5,\quad \nu=1.4$$

$$z\nu\approx7$$

Bhatt and Young (1985)

K. Binder and A. P. Young: Spin glasses Rev. Mod. Phys., Vol. 58, No. 4, October 1986

Характерные особенности стекольного перехода в спиновой системе:

- **нулевая средняя намагниченность**

- **появление ненулевого параметра Эдвардса-Андерсона**

- **Критическое замедление вблизи** T_g

- **Конечный корреляционный радиус (отсутствие дальнего порядка)**

- **Конечная линейная восприимчивость**

- **Расходящаяся при** T_g **температурная зависимость нелинейной восприимчивости**

План:

- Калибровочная модель спинового стекла Гейзенберга
- Неравновесная динамика стекольного перехода

Калибровочная модель спинового стекла Гейзенберга

Модель Гейзенберга (3D)

$$L = \frac{1}{2}|\partial_i \mathbf{s}|^2 - U(\mathbf{s}),$$

$$U(\mathbf{s}) \;=\; \mu^2 \mathbf{s}^2 \;+\; v\mathbf{s}^4$$

$\mathbf{s}$ - вектор намагниченности

$$\mu^2 = \alpha k_B (T - T_c)$$

T_c - **критическая температура**

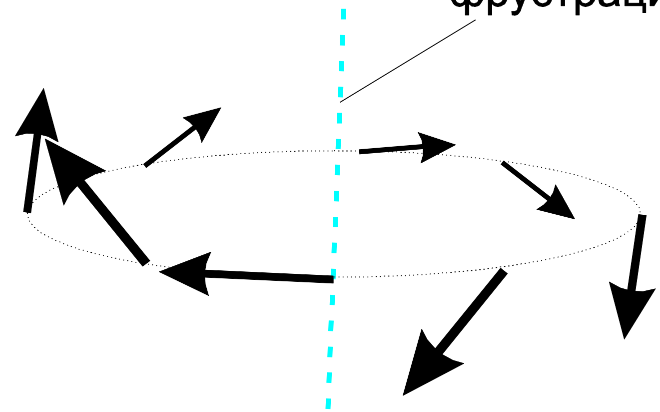
Калибровочная модель спинового стекла

Toulouse, G., 1977, Commun. Phys. 2, 115.

J.A. Hertz, Phys.Rev.B, **18,** 4875–4885 (1978);
G.E. Volovik, I.E. Dzyaloshinskii, Sov. Phys. JETP 48(3), 555-559 (1978);
I. Kanazawa, Journal of Non-Crystalline Solids 293-295, 615–619 (2001);

Калибровочная модель спинового стекла

$$L = \frac{1}{2}|D_i \mathrm{s}|^2 - U(\mathrm{s}) - \frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} + J^\mu_a A^a_\mu,$$



$$D_i s^a = \partial_i s^a + g\varepsilon^{abc}A^b_i s^c,$$

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g\varepsilon^{abc}A^b_\mu A^c_\nu.$$

$$\langle \mathrm{s}\rangle_0 = (0,\, 0,\, i\mu/\sqrt{2v}), \quad \phi = s - i\mu/\sqrt{2v}$$

$$L = \frac{1}{2}(\partial_\mu\phi)^2 - 2\mu^2\phi^2 - \frac{g^2\mu^2}{4v}A^\kappa_\mu A^{\kappa\mu} - \frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} -$$
$$- v\phi^4 + \frac{g^2}{2}\phi^2 A^a_\mu A^{a\mu} + J^{a\mu}A^a_\mu.$$

$$L = \frac{1}{2}(\partial_\mu \phi)^2 - 2\mu^2\phi^2 - \frac{g^2\mu^2}{4v} A^\kappa_\mu A^{\kappa\mu} - \frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} -$$
$$- v\phi^4 + \frac{g^2}{2}\phi^2 A^a_\mu A^{a\mu} + J^{a\mu} A^a_\mu.$$

$$\langle \mathbf{JJ} \rangle_k = I_0,$$

$$M^2 = I_0 + M_0^2 = I_0 - \mu^2 g^2/4v.$$

$$M_0 = ig\mu/\sqrt{2v},$$

$$\mu^2 = \alpha k_B (T - T_c)$$

Переход происходит не при T_c, а при $T_g > T_c$.

$$M^2 = 0$$

$$T_g = T_c + 4I_0 v/\alpha g^2 \quad (M^2 = \alpha k_B (T - T_g))$$

Неравновесная динамика

M.G. Vasin, N.M. Shchelkachev, and V.M. Vinokur, Theoretical and Mathematical Physics, 163(1): 537–548 (2010);

Функциональные методы (метод динамического производящего функционала, метод Келдыша)

$$\vec{\phi} = \{\bar{\phi}, \phi\}, \ \vec{A}^a_\mu = \{\bar{A}^a_\mu, A^a_\mu\}$$

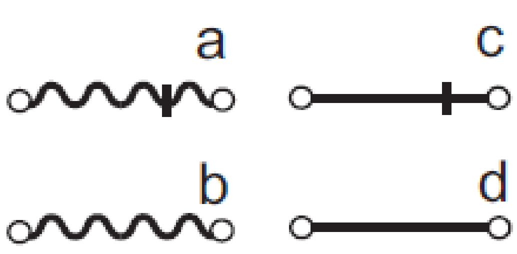
$$\hat{G} = \begin{pmatrix} G^K & G^A \\ G^R & 0 \end{pmatrix}, \quad \hat{\Delta}_{\mu\nu} = \begin{pmatrix} \Delta^K_{\mu\nu} & \Delta^A_{\mu\nu} \\ \Delta^R_{\mu\nu} & 0 \end{pmatrix}.$$

$$i\Delta^{R(A)}_{\mu\nu}(k, \omega) = \frac{-i\delta_{\mu\nu}}{k^2 + M^2 \pm i\Gamma_A \omega},$$

$$iG^{R(A)}(k, \omega) = \frac{i}{k^2 + \mu^2 \pm i\Gamma_\phi \omega},$$

$$i\Delta^K_{\mu\nu}(k, \omega) = \frac{-i2\Gamma_A \delta_{\mu\nu}}{(k^2 + M^2)^2 + \Gamma_A^2 \omega^2},$$

$$iG^K(k, \omega) = \frac{i2\Gamma_\phi}{(k^2 + \mu^2)^2 + \Gamma_\phi^2 \omega^2},$$

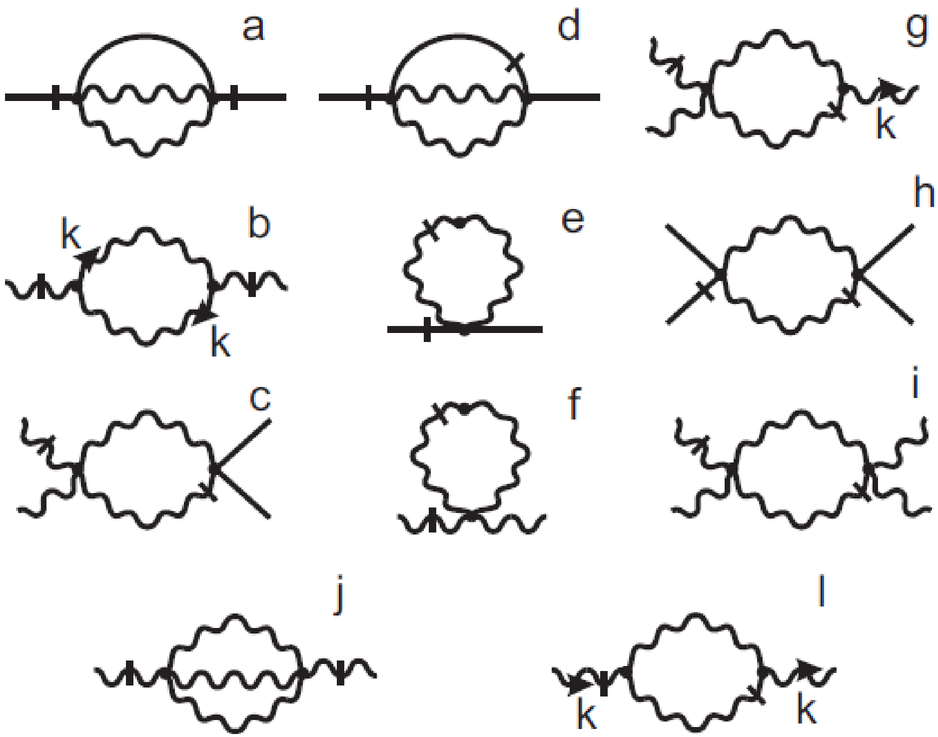


$$\vec{\phi} = \{\bar{\phi}, \phi\}, \ \vec{A}^a_\mu = \{\bar{A}^a_\mu, A^a_\mu\}$$

$$Z = \int D\vec{\phi} D\vec{A}^a_\mu \exp\Big\{ \frac{i}{2}\int_{t,t'} \vec{\phi}(t)\hat{G}^{-1}(t,t')\vec{\phi}(t') +$$
$$\frac{i}{2}\int_{t,t'} \vec{A}^a_\mu(t)\hat{\Delta}^{-1}_{\mu\nu}(t,t')\vec{A}^a_\nu(t') - ig\varepsilon^{abc}\int_t (\partial_\mu \bar{A}^a_\nu) A^b_\mu A^c_\nu -$$
$$ig\varepsilon^{abc}\int_t (\partial_\mu A^a_\nu)\bar{A}^b_\mu A^c_\nu - ig\varepsilon^{abc}\int_t (\partial_\mu A^a_\nu) A^b_\mu \bar{A}^c_\nu -$$
$$ig^2\varepsilon^{abc}\varepsilon^{aij}\int_t \bar{A}^b_\mu A^c_\nu A^i_\mu A^j_\nu -$$
$$ig^2\int_t \bar{A}^a_\mu A^a_\mu \phi^2 - ig^2\int_t (A^a_\mu)^2\bar{\phi}\phi - iv4\int_t \bar{\phi}\phi^3 \Big\},$$

$$M^2 = 0$$
$$\mu^2 = 4I_0 v/g^2$$

Перенормировка



$$\Sigma \approx \Gamma_\phi \frac{g^4 \ln(1/\Lambda)}{\pi^2}\left(1 - e^{-4 I_0 v |t_0| / \Gamma_\phi g^2}\right)$$

Λ - параметр регуляризации

$t_o \gg \Gamma_\phi g^2/4I_0 v$

$$\frac{\partial \ln(\Gamma_\phi)}{\partial \xi} = g^4/\pi^2,$$

$$\frac{\partial \ln(\Gamma_A)}{\partial \xi} = 3g^4/\pi^2 + g^2/2\pi^2,$$

$$\frac{\partial \ln(M^2)}{\partial \xi} = 2 + 3g^2/2\pi^2,$$

$$\frac{\partial \ln(\mu^2)}{\partial \xi} = 2 + \frac{M^2 g^2}{2\mu^2\pi^2} \approx 2,$$

$$\frac{\partial \ln(g^2)}{\partial \xi} = \varepsilon - g^2/\pi^2,$$

$$\frac{\partial \ln v}{\partial \xi} = \varepsilon - g^4/2v\pi^2,$$

ренормгруппа

$t_o \ll \Gamma_\phi g^2/4I_0 v$

$$\frac{\partial \ln(\Gamma_\phi)}{\partial \xi} = 0.$$

$$\frac{\partial \ln(\Gamma_A)}{\partial \xi} = 3g^4/\pi^2 + g^2/2\pi^2,$$

$$\frac{\partial \ln(M^2)}{\partial \xi} = 2 + 3g^2/2\pi^2,$$

$$\frac{\partial \ln(\mu^2)}{\partial \xi} = 2 + \frac{M^2 g^2}{2\mu^2\pi^2} \approx 2,$$

$$\frac{\partial \ln(g^2)}{\partial \xi} = \varepsilon - g^2/\pi^2,$$

$$\frac{\partial \ln v}{\partial \xi} = \varepsilon - g^4/2v\pi^2,$$

$\xi = \ln(1/\Lambda)$

$$\frac{\partial \ln(\Gamma_\phi)}{\partial \xi} = g^4 S(\xi)/\pi^2,$$

$$S(\xi) = 1 - \Lambda^z = 1 - \exp(-z\xi),$$

$z \approx 2$

$$\mu^2 = \alpha k_B(T - T_g) \approx e^{2\dot{\xi}} \qquad g^2 = \pi^2\varepsilon \quad v = g^2/2$$

$$\tau_{rel} = \Gamma_\phi \propto \exp\left(\frac{g^4 T_g}{2\alpha\pi^2(T - T_g)}\right).$$

Vogel–Tammann–Fulcher (VTF)

Флуктуационно-диссипативная теорема (ФДТ)

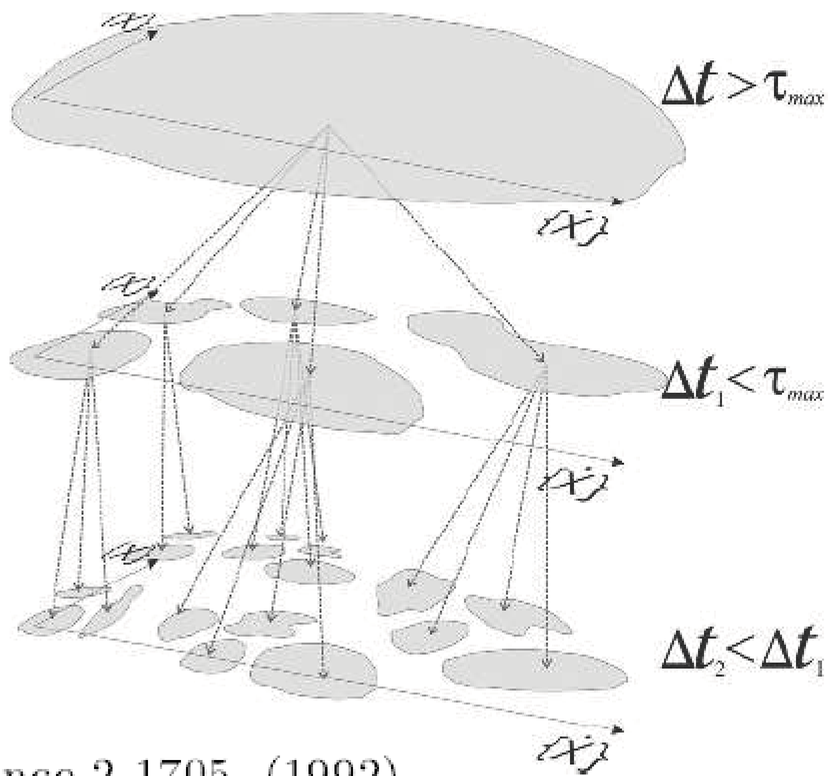
$$G^K(\omega) = \frac{2T}{\omega}\left\{G^R(\omega) - G^A(\omega)\right\}$$

$t_o \gg \Gamma_\phi g^2/4I_0 v$

$t_o \ll \Gamma_\phi g^2/4I_0 v$

ФДТ не нарушена

ФДТ нарушена



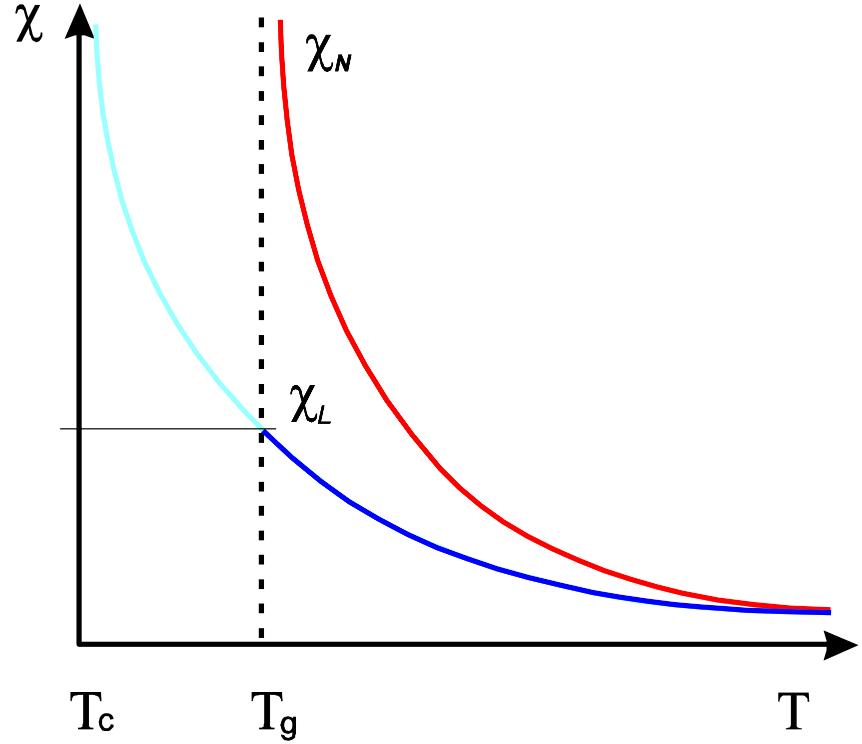
scenario of weak ergodicity breaking

J.-P. Bouchaud, J. Phys. France 2 1705, (1992).

$$r_{cor} \sim \sqrt{g^2/4I_0 v}$$

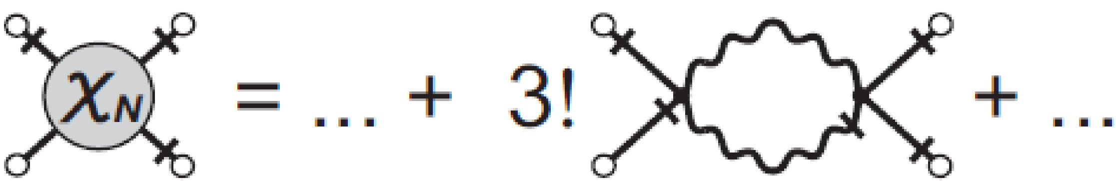
$$\chi_L = \partial\langle\phi\rangle/\partial h \sim \mu^{-2} = g^2/4I_0 v$$

Не расходятся в T_g



$$\chi_N = \partial^3\langle\phi\rangle/\partial h^3$$

$$\chi_N = \langle\phi\bar{\phi}\bar{\phi}\bar{\phi}\rangle_{k=0} \qquad (e^{\xi})^{-3!/(2+3\varepsilon/2)}$$



$$\chi_N \propto (T - T_g)^{-\gamma} \text{ for } T \to T_g^+$$

$$12/7 < \gamma < 3$$

Обсуждение

``frustration-limited domain theory''

D. Kivelson, G. Tarjus, Phyl.Mag.B, **77**, 245–256 (1998);

Спасибо за внимание