Pressure induced orientational glass phase in molecular para-hydrogen.

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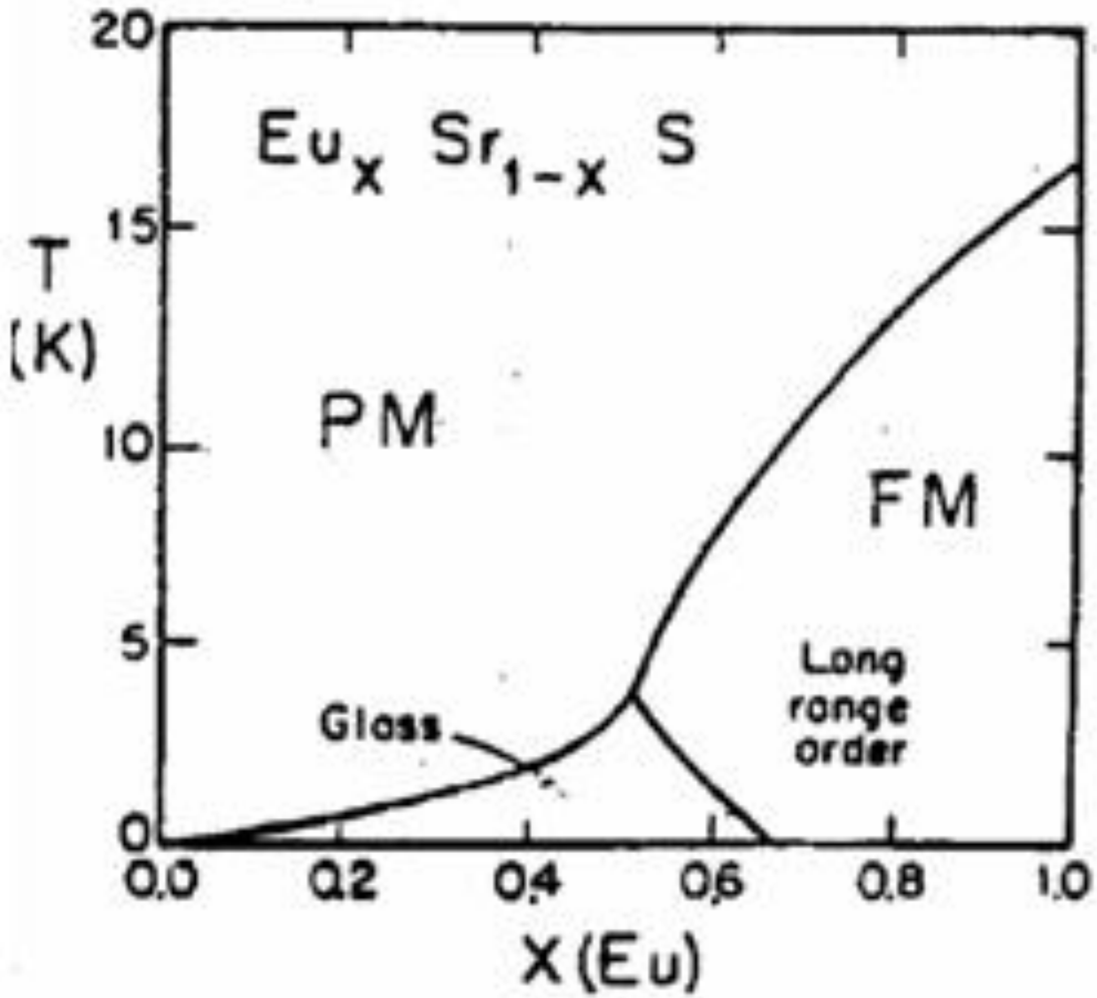
- INTRODUCTION
  - Sherrington–Kirkpatrick model and RSB (replica symmetry breaking) à la Parisi.
  - p-spin spherical model, 1RSB, scenario of real glass transition.
- SPIN-GLASS-LIKE PHASE IN COMPLEX SYSTEMS
  - Reflection symmetry and ∞-RSB.
  - Quadrupole glasses with J=1 and with J=2.
  - Orientational glass in C_{60}.
  - Cluster model of liquid-glass transition.
  - RSB in the absence of reflection symmetry.
- CONCLUSION

- Sherrington–Kirkpatrick model and RSB (replica symmetry breaking) à la Parisi.



H.Maletta, W.Felsh. Phys.Rev.B 20,1245 (1979)

SK, EA

$$H = -\frac{1}{2}\sum_{i\neq j} J_{ij}S_iS_j, \;\; S = \pm 1$$

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi J}} \exp\left[-\frac{(J_{ij}-J_0)^2}{2J^2}\right]$$

$$J = \tilde{J}/\sqrt{N}, \;\; J_0 = \tilde{J}_0/N$$

$$x = << S >_T >_J; \;\; q_{EA} = << S_i(t_1) >_T < S_i(t_2) >_T >_J$$

Replica method

$$-\beta F = \overline{lnZ} = \lim_{n\to 0}\frac{1}{n}(\overline{Z^n} - 1) = \lim_{n\to 0}\frac{1}{n}(\overline{\prod_{\alpha=1}^{n} Z_\alpha} - 1)$$

$$F = F(x^\alpha, q^{\alpha\beta})$$

Order parameters:

$$x^\alpha = \frac{1}{N}\sum_{i=1}^{N} S_i^\alpha \qquad\qquad q^{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} S_i^\alpha S_i^\beta$$

$\Downarrow$ magnetization

$\Downarrow$ spin-glass order

$$\rho_{\alpha\beta} = 1 - q^{\alpha\beta}$$

1RSB

$$n \Rightarrow \frac{n}{m} \times m$$

$$q^{\alpha\beta} \Rightarrow q, q + v$$

$$\text{1RSB stability} \Rightarrow \lambda_{1RSB} > 0$$

PARISI

RS $\Rightarrow$ 1RSB $\Rightarrow$ ∞RSB (FRSB)

$\Downarrow$

$$
Q_{\alpha,\beta} = \left|\begin{array}{cc}
\begin{array}{cccc} 0 & q_0 & q_1 & q_1 \\ q_0 & 0 & q_1 & q_1 \\ q_1 & q_1 & 0 & q_0 \\ q_1 & q_1 & q_0 & 0 \end{array} & q_2 \\
q_2 & \begin{array}{cccc} 0 & q_0 & q_1 & q_1 \\ q_0 & 0 & q_1 & q_1 \\ q_1 & q_1 & 0 & q_0 \\ q_1 & q_1 & q_0 & 0 \end{array}
\end{array}\right| .
$$

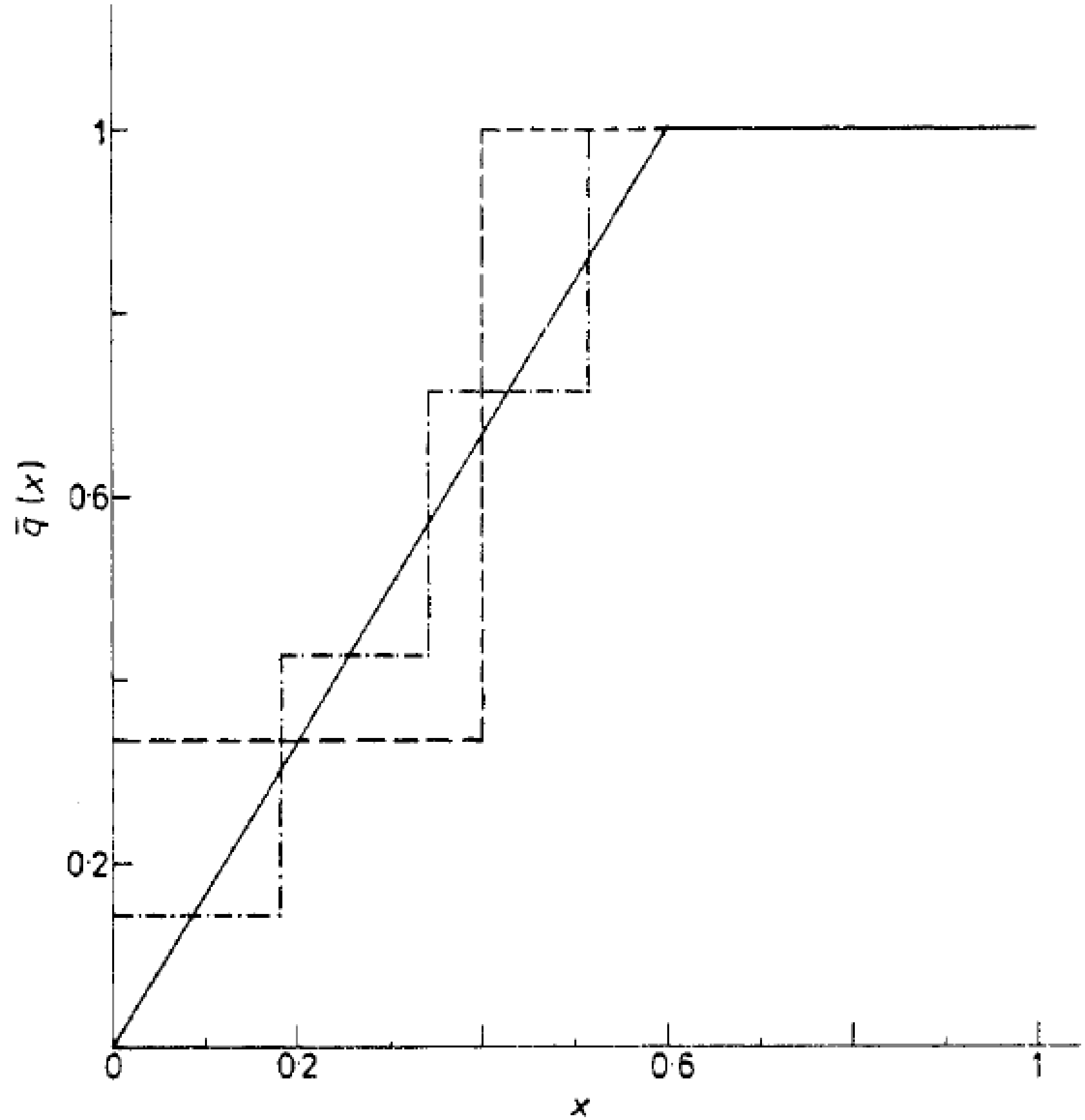


Figure 1. The broken curve, chain curve and full curve are, respectively, the function $q^{(K)}(x)$ for $K = 1$, 4 and ∞ in units of τ.

$$H = -\frac{1}{2}\sum_{i\neq j} J_{ij}\hat{U}_i\hat{U}_j$$

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi J}}\exp\left[-\frac{(J_{ij})^2}{2J^2}\right]$$

$$\mathrm{Tr}\left[\hat{U}^{(2k+1)}\right] = 0$$

$$J = \tilde{J}/\sqrt{N}$$

$$\tau = 1 - \frac{T}{T_c}, \qquad \frac{kT_c}{\tilde{J}} = p(T_c).$$

$$q(x) = \begin{cases} cx, & 0 \le x \le \frac{\tau}{ct_c}; \\ q(x) = \frac{\tau}{t_c}, & \frac{\tau}{ct_c} \le x \le 1. \end{cases}$$

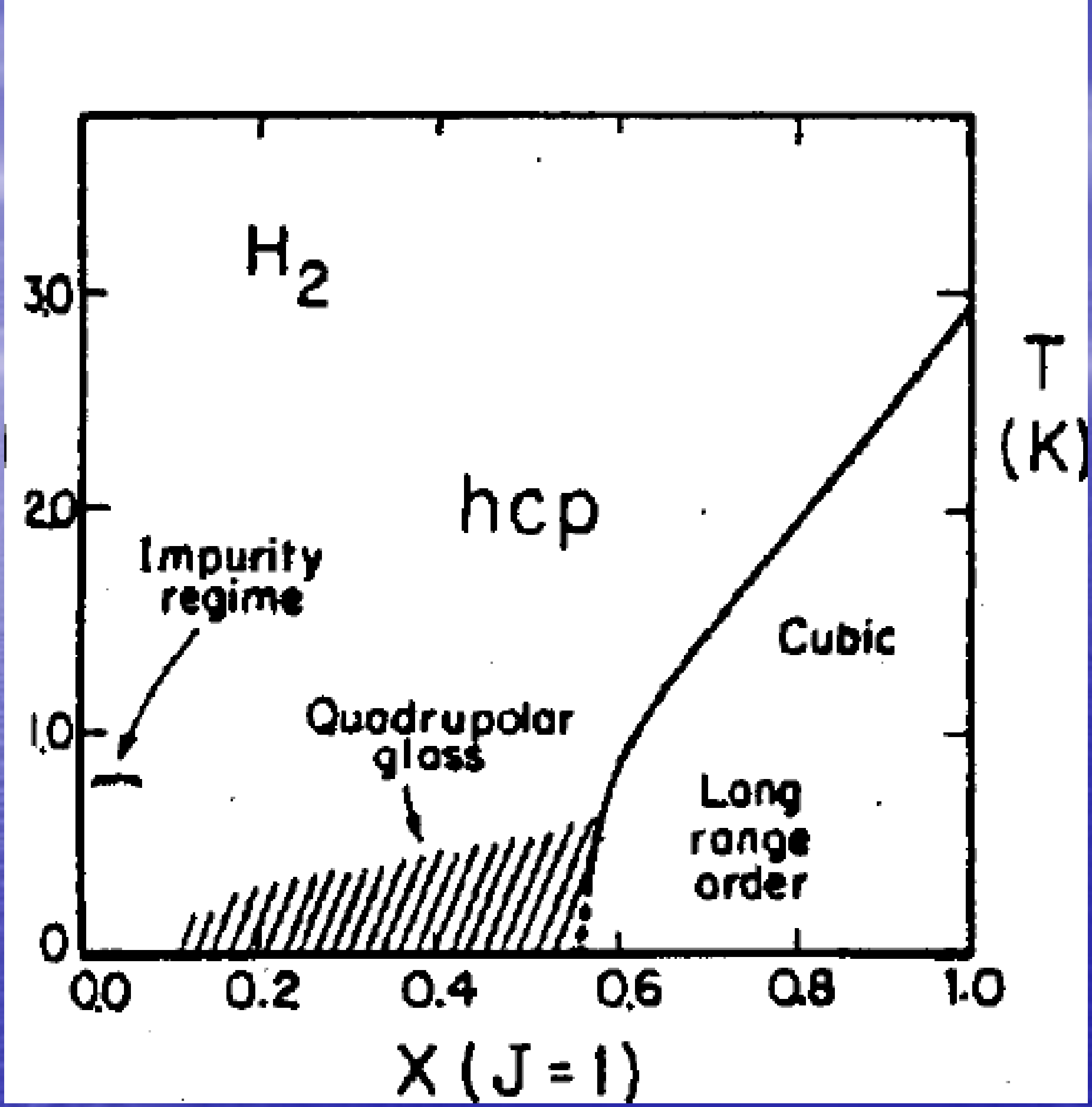
$$c = \frac{2\langle [U^2] \rangle^5}{\left[3\langle [U^2] \rangle^2 - \langle [U^4] \rangle\right]^2}$$

- p-spin spherical model, 1RSB, real glasses

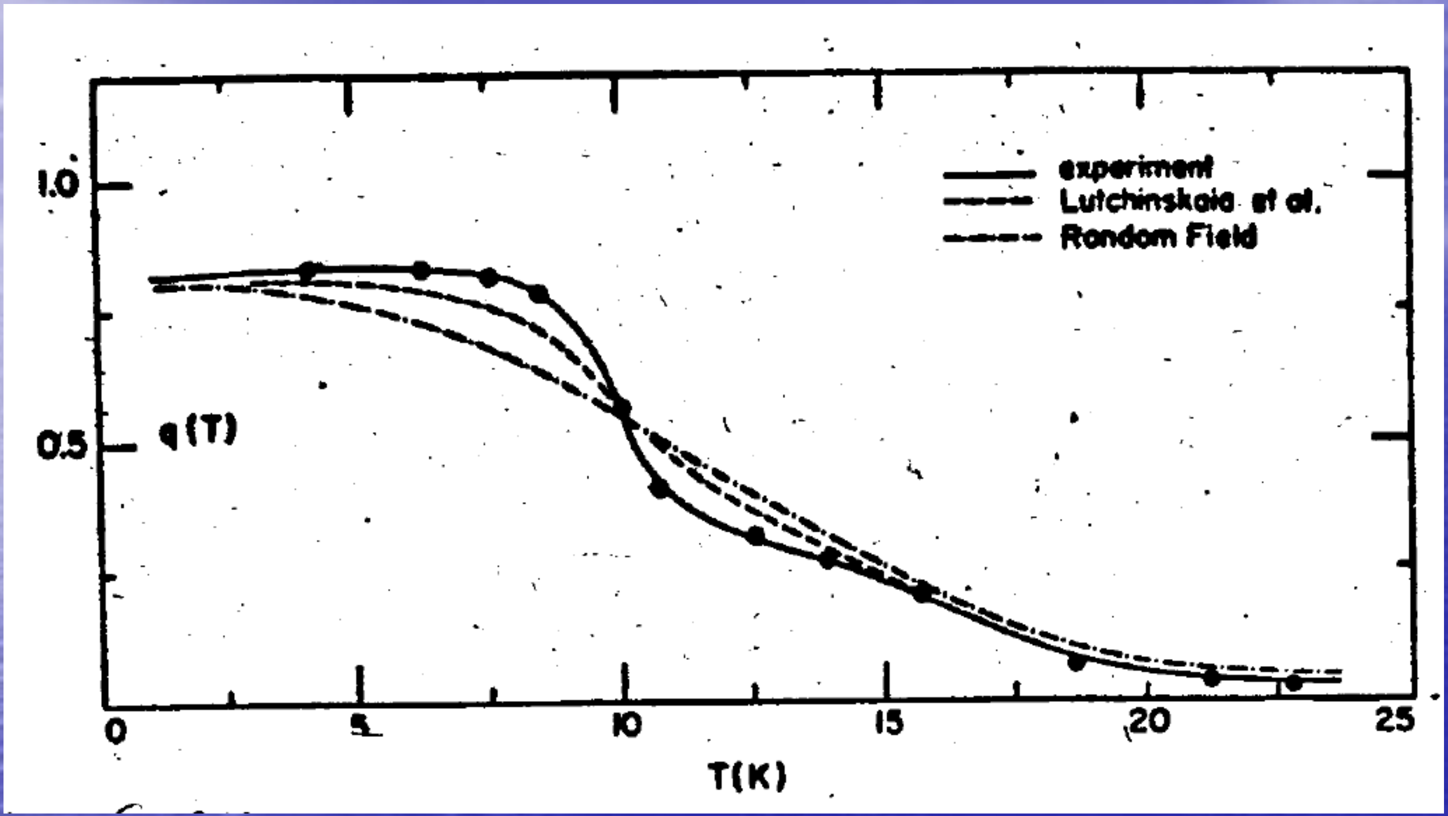
E.Gardner, A.Crisanti, H.-J.Sommers, D.Thirumalai, T.R.Kirkpatrick

- QUADRUPOLE GLASSES

$$ortho - para \text{ mixtures } (H_2, D_2),$$
$$Ar - N_2 \text{ mixture (J=1)}$$
$$para - H_2 \text{ under pressure (J=2)}$$

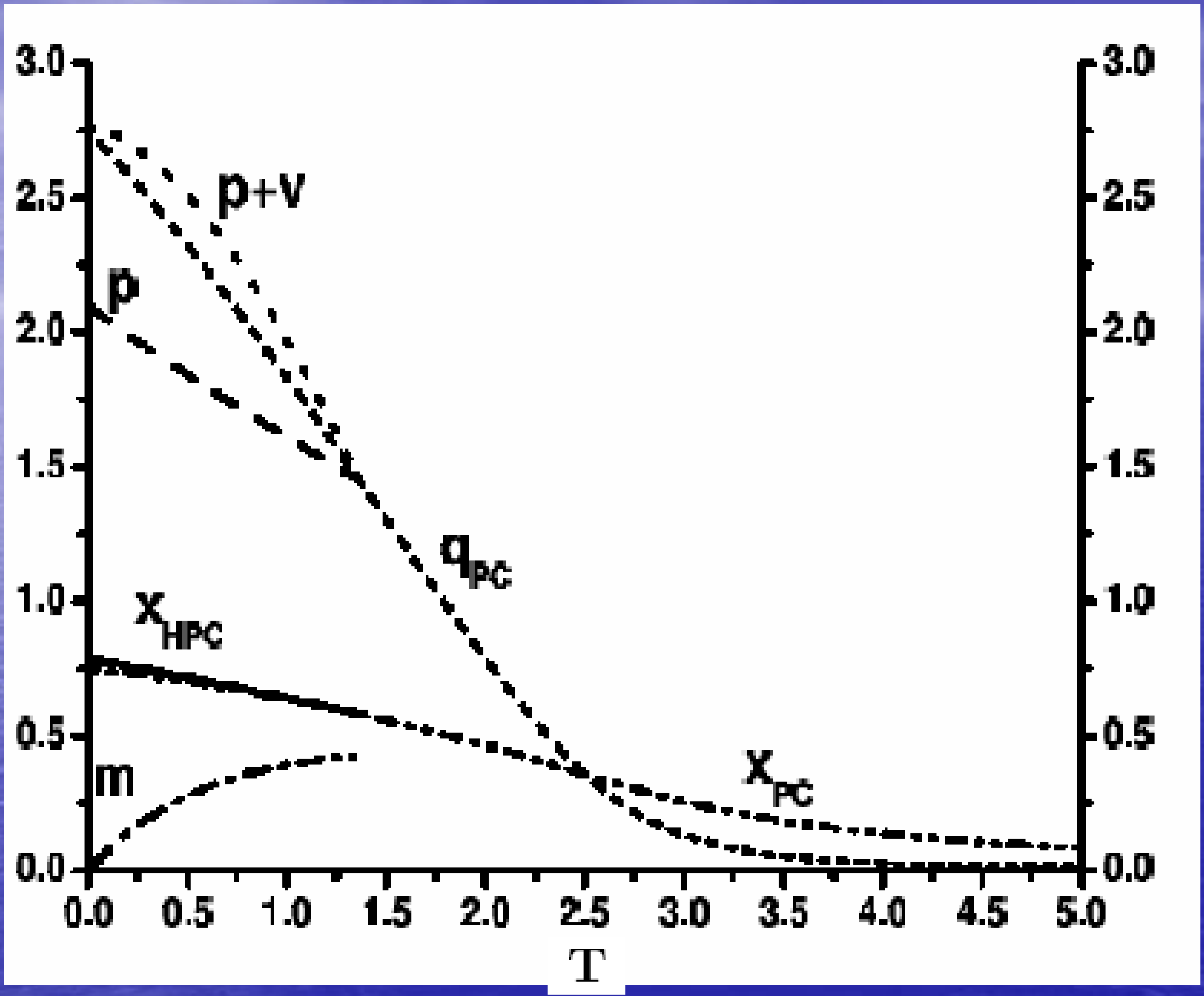


N.S.Sullivan et all. Phys.Rev.B 17, 5016 (1978).



N.S. Sullivan, C.M. Edwards and J.R. Brookeman,

Mol. Cryst. Liq. Cryst. **139**, 385(1986).



$$H = -\frac{1}{2}\sum_{i\neq j} J_{ij} Q_i Q_j,$$

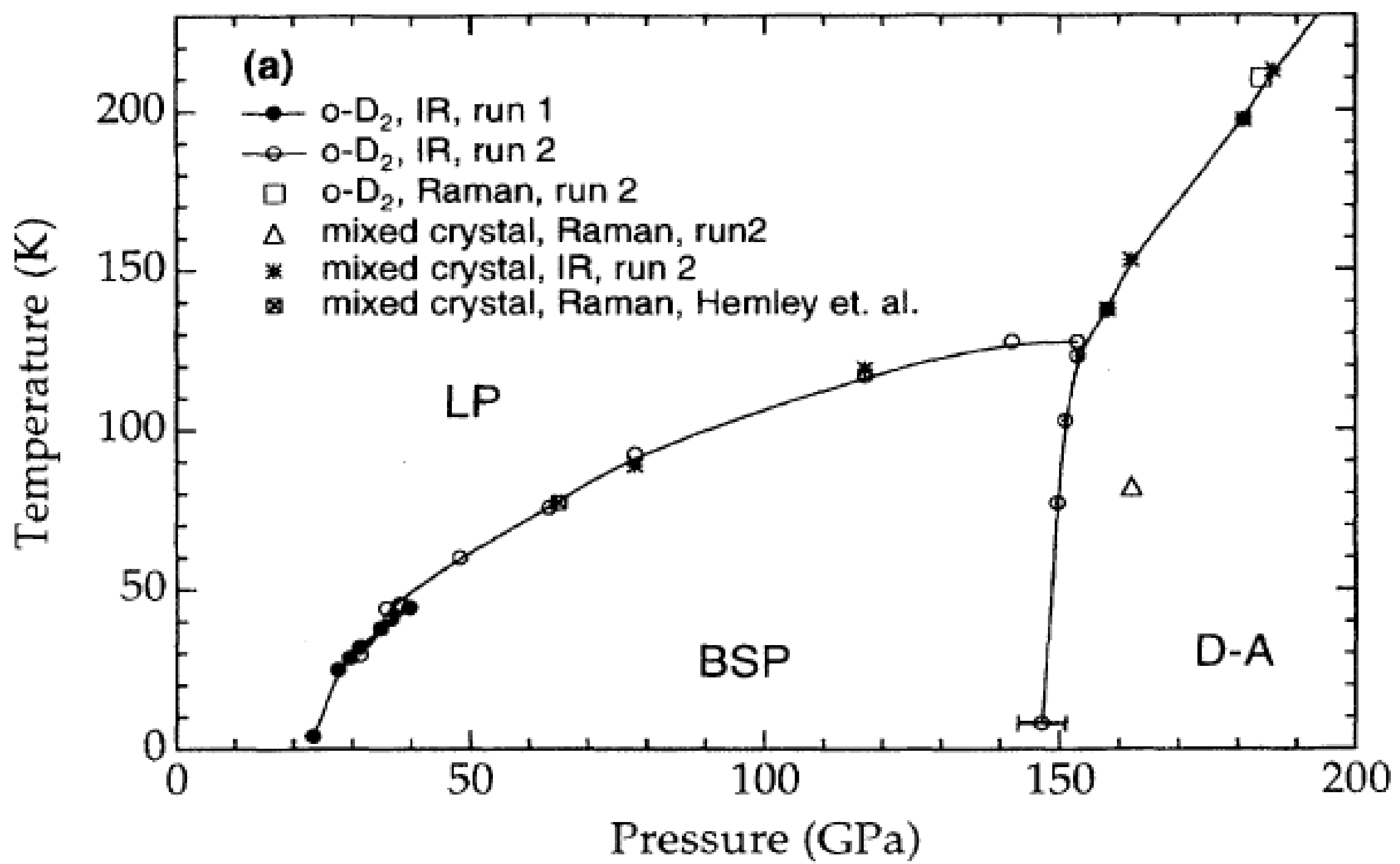
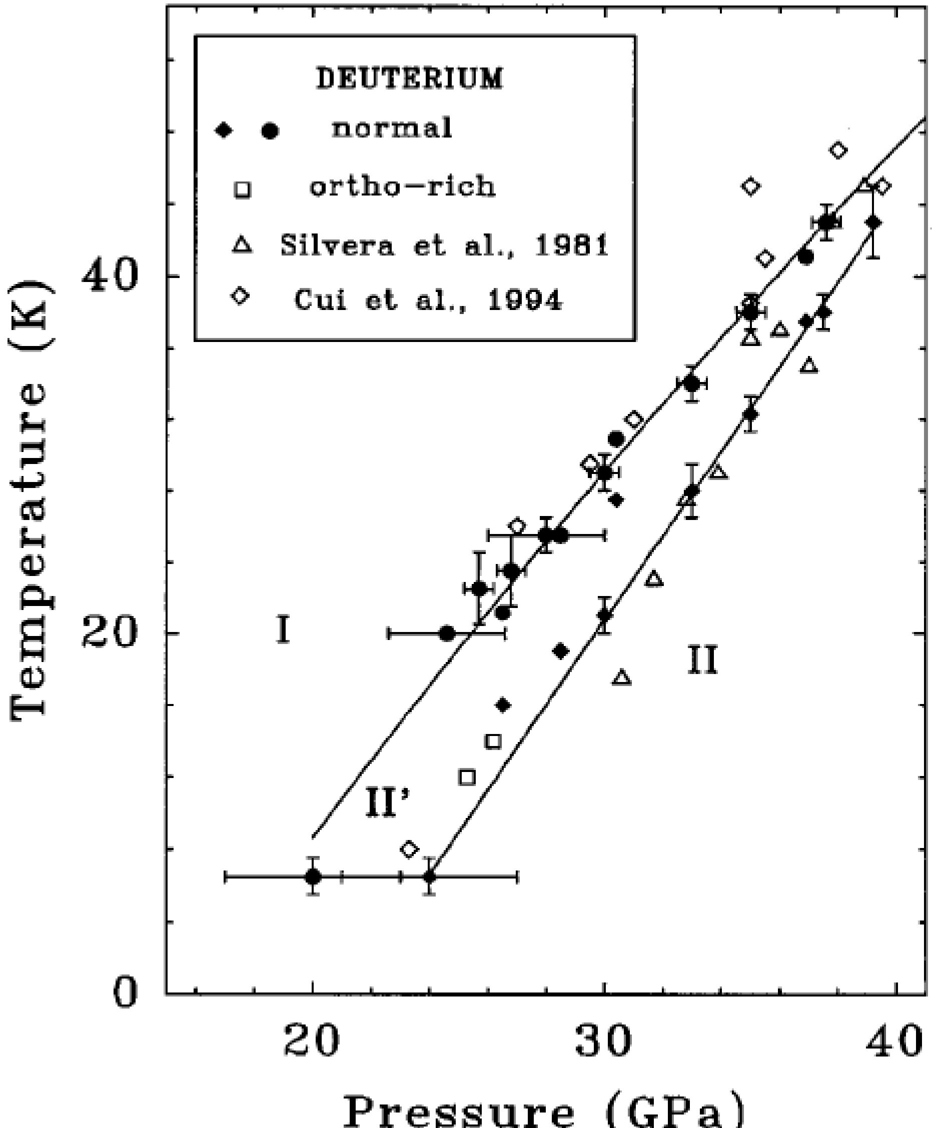


FIG. 1. (a) Various phases of high-pressure solid deuterium identified by IR absorption in this work.

L. Cui *et al.*, Phys. Rev. B **51**, 14 987 (1995).



A.F. Goncharov, J.H. Eggert, I.I. Mazin, R.J. Hemley, and H.K. Mao, Phys. Rev. B **54**, R15590 (1996).

$$\alpha(J = 0 -> J = 2) = \frac{\eta}{(1+\eta)}$$

$$\eta = 3.8\left(\frac{25}{26}\frac{\Gamma}{12B}\right)\left(\frac{R_0}{R}\right)^{10}$$

$$\Gamma/B = 0.011(H_2);\ \Gamma/B = 0.028(D_2)$$

$\alpha = 0.1$ при 40 Gpa в $o - D_2$

I.

J=2

$$H = -\frac{1}{2}\sum_{i\neq j} J_{ij}\hat{Q}_i\hat{Q}_j, \qquad \hat{Q} = \frac{1}{3}\left[3{J_z}^2 - 6\right]$$

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi J}}\exp\left[-\frac{(J_{ij})^2}{2J^2}\right]$$

$$\langle F\rangle_J/NkT = \lim_{n\to 0}\frac{1}{n}\max\left\{\frac{t^2}{4}\sum_{\alpha}(p^\alpha)^2 + \frac{t^2}{2}\sum_{\alpha>\beta}(q^{\alpha\beta})^2 - \ln \mathrm{Tr}_{\{U^\alpha\}}\exp\hat{\theta}\right\}$$

$$\hat{\theta} = t^2\sum_{\alpha>\beta}(q^{\alpha\beta})\hat{Q}^\alpha\hat{Q}^\beta + \frac{t^2}{2}\sum_{\alpha}(p^\alpha)(\hat{Q}^\alpha)^2$$

$$q^{\alpha\beta} = \frac{\mathrm{Tr}\left[\hat{U}^{\alpha}\hat{U}^{\beta}\exp\left(\hat{\theta}\right)\right]}{\mathrm{Tr}\left[\exp\left(\hat{\theta}\right)\right]}$$

$$p^{\alpha} = \frac{\mathrm{Tr}\left[(\hat{U}^{\alpha})^2\exp\left(\hat{\theta}\right)\right]}{\mathrm{Tr}\left[\exp\left(\hat{\theta}\right)\right]}$$

$$\hat{\theta} = \frac{t^2}{2}\sum_{\alpha} p^{\alpha}(\hat{U}^{\alpha})^2 + t^2\sum_{\alpha>\beta} q^{\alpha\beta}\hat{U}^{\alpha}\hat{U}^{\beta}.$$

1RSB

$$n \Rightarrow \frac{n}{m} \times m$$

$$q^{\alpha\beta} \Rightarrow q, q+v$$

$$\text{1RSB stability} \Rightarrow \lambda_{1RSB} > 0$$

$$\lambda_{repl(1RSB)} = 1-$$

$$t^2 \int dz^G \frac{1}{\int dx^G \left(\mathrm{Tr}[\exp\hat{\theta}_{1RSB}(z,x)]\right)^m} \int dy^G \left(\mathrm{Tr}[\exp\hat{\theta}_{1RSB}(z,y)]\right)^m$$

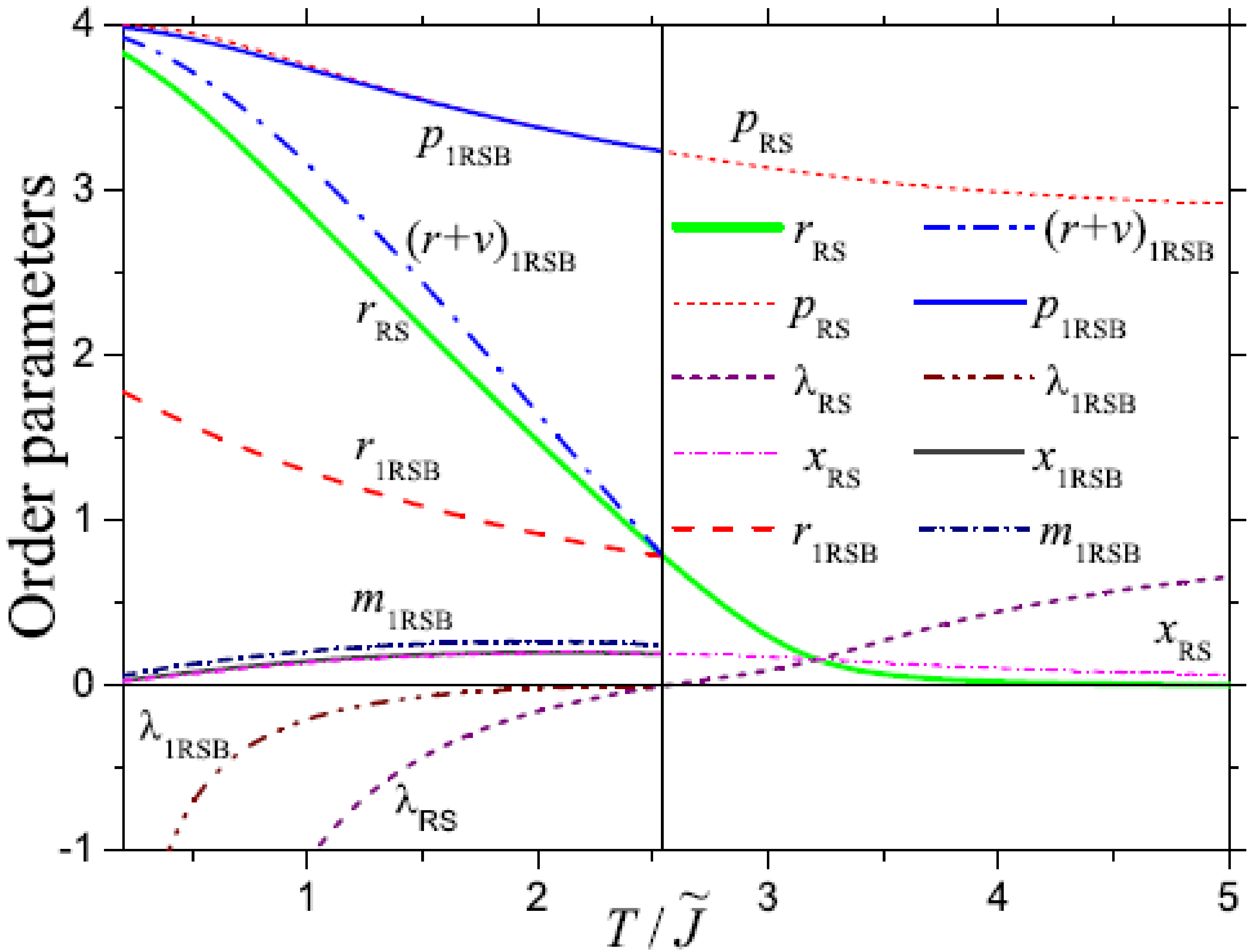
$$\left\{\frac{\mathrm{Tr}\left[\hat{U}^2 \exp\hat{\theta}_{1RSB}(z,y)\right]}{\mathrm{Tr}\left[\exp\hat{\theta}_{1RSB}(z,y)\right]} - \left[\frac{\mathrm{Tr}\left[\hat{U} \exp\hat{\theta}_{1RSB}(z,y)\right]}{\mathrm{Tr}\left[\exp\hat{\theta}_{1RSB}(z,y)\right]}\right]^2\right\}^2 . \qquad (13)$$

Here

$$\hat{\theta}_{1RSB}(z,x) = (\sqrt{r}tz + \sqrt{v}tx)\hat{U} + \frac{t^2}{2}(p-r-v)\hat{U}^2.$$

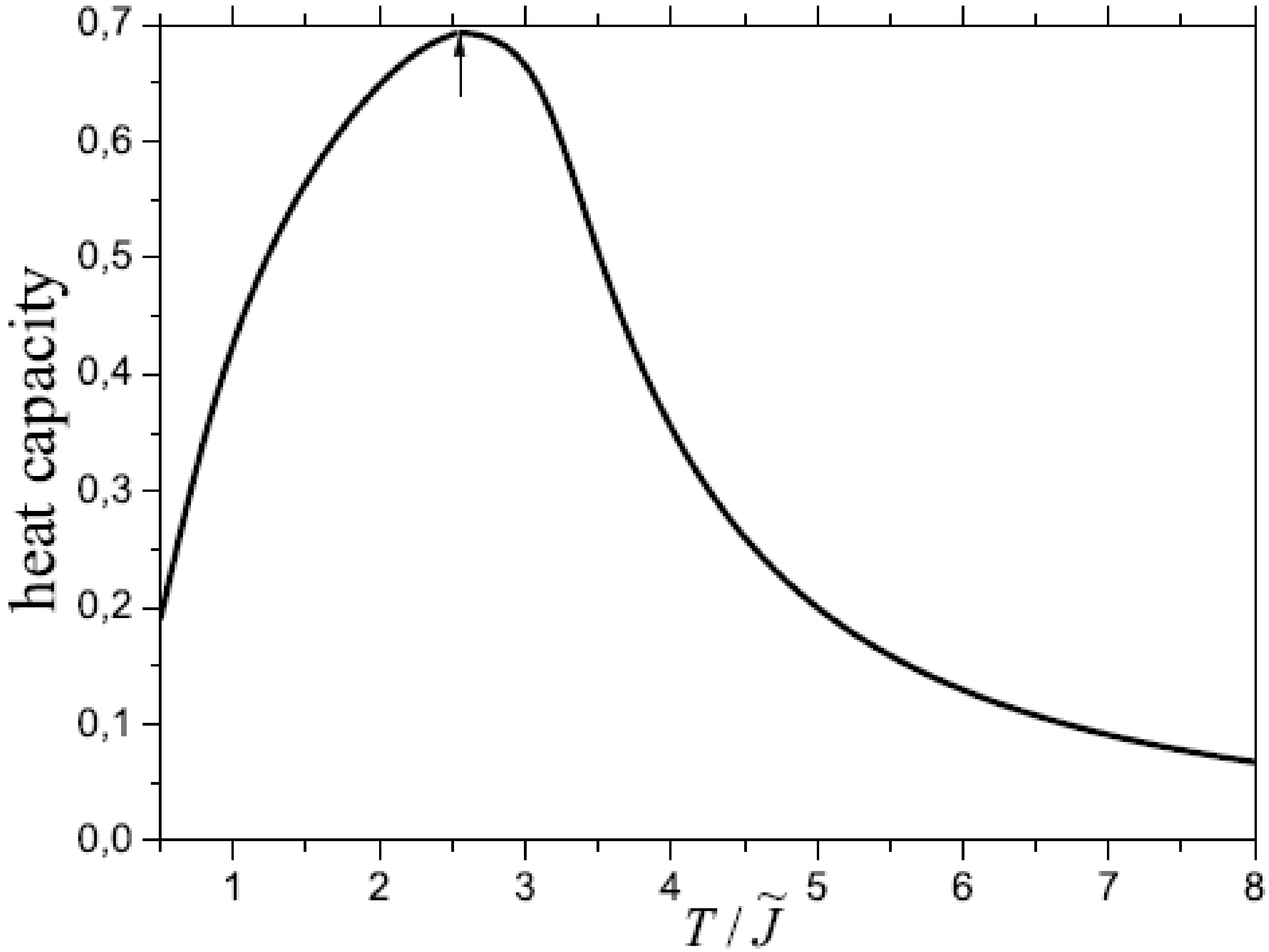
The 1RSB solution is characterized by m and two values r and $r+v$ of $q^{\alpha\beta}$. For $r=0$ and $v=0$ the equation (13) reduces to Eq. (11).

I.



Order parameters
$T/\tilde{J}$
p_{1RSB}
p_{RS}
$(r+v)_{1RSB}$
r_{RS}
r_{1RSB}
m_{1RSB}
x_{RS}
λ_{1RSB}
λ_{RS}
r_{RS} $(r+v)_{1RSB}$
p_{RS} p_{1RSB}
λ_{RS} λ_{1RSB}
x_{RS} x_{1RSB}
r_{1RSB} m_{1RSB}

I.



II.

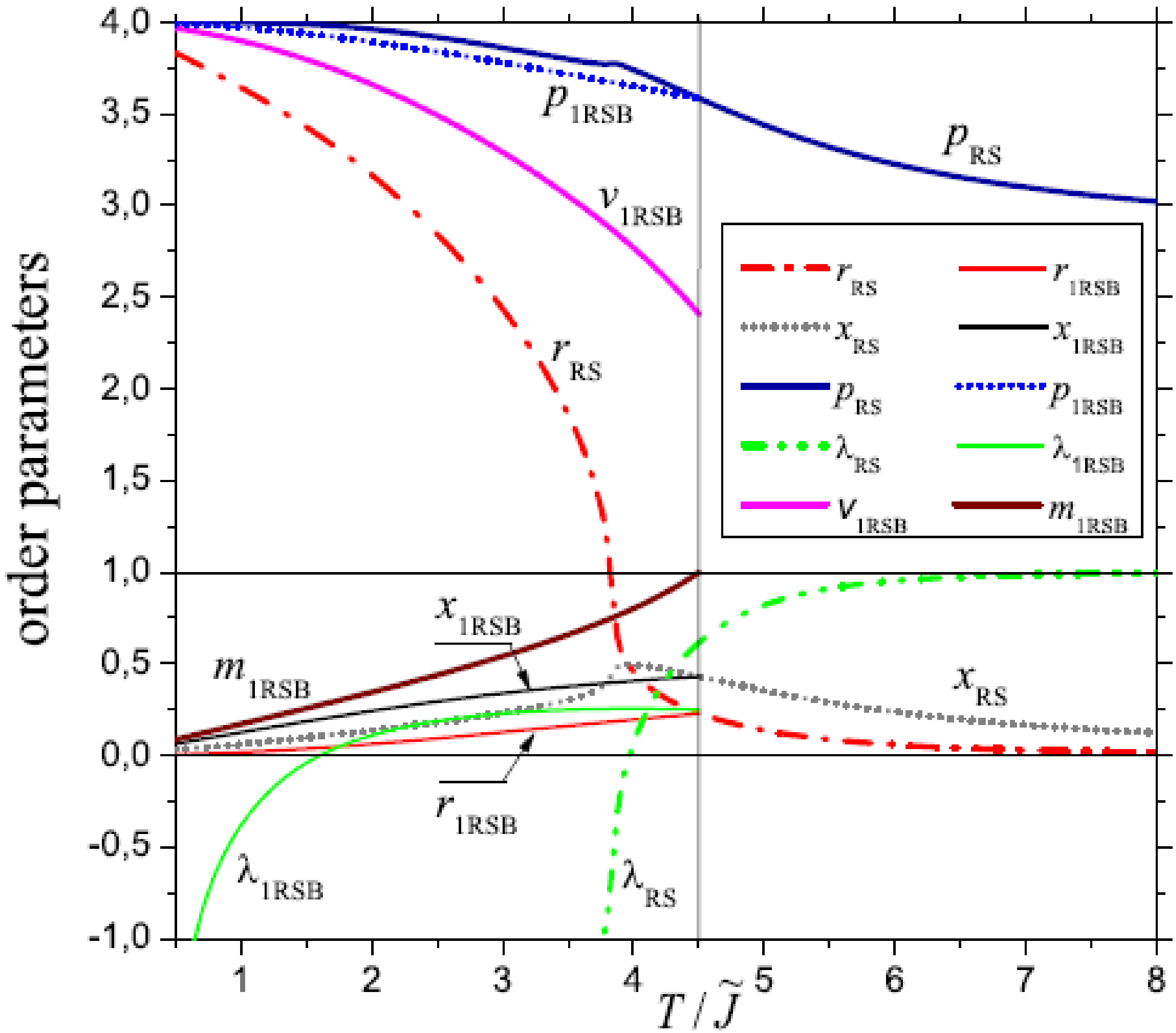
$$H = -\sum_{i_1 \le i_2 \dots \le i_l} J_{i_1 \dots i_l} \hat{Q}_{i_1} \hat{Q}_{i_2} \dots \hat{Q}_{i_l}$$

$$P(J_{i_1 \dots i_l}) = \frac{\sqrt{N^{(l-1)}}}{\sqrt{l! \pi} J} \exp\left[-\frac{(J_{i_1 \dots i_l})^2 N^{(l-1)}}{l! J^2}\right]$$

$$\langle F \rangle_J / NT = \lim_{n \to 0} \frac{1}{n} \max \left\{ -\frac{t^2}{4} \sum_{\alpha} (p^\alpha)^l + \sum_{\alpha} \mu^\alpha (p^\alpha) + \right.$$

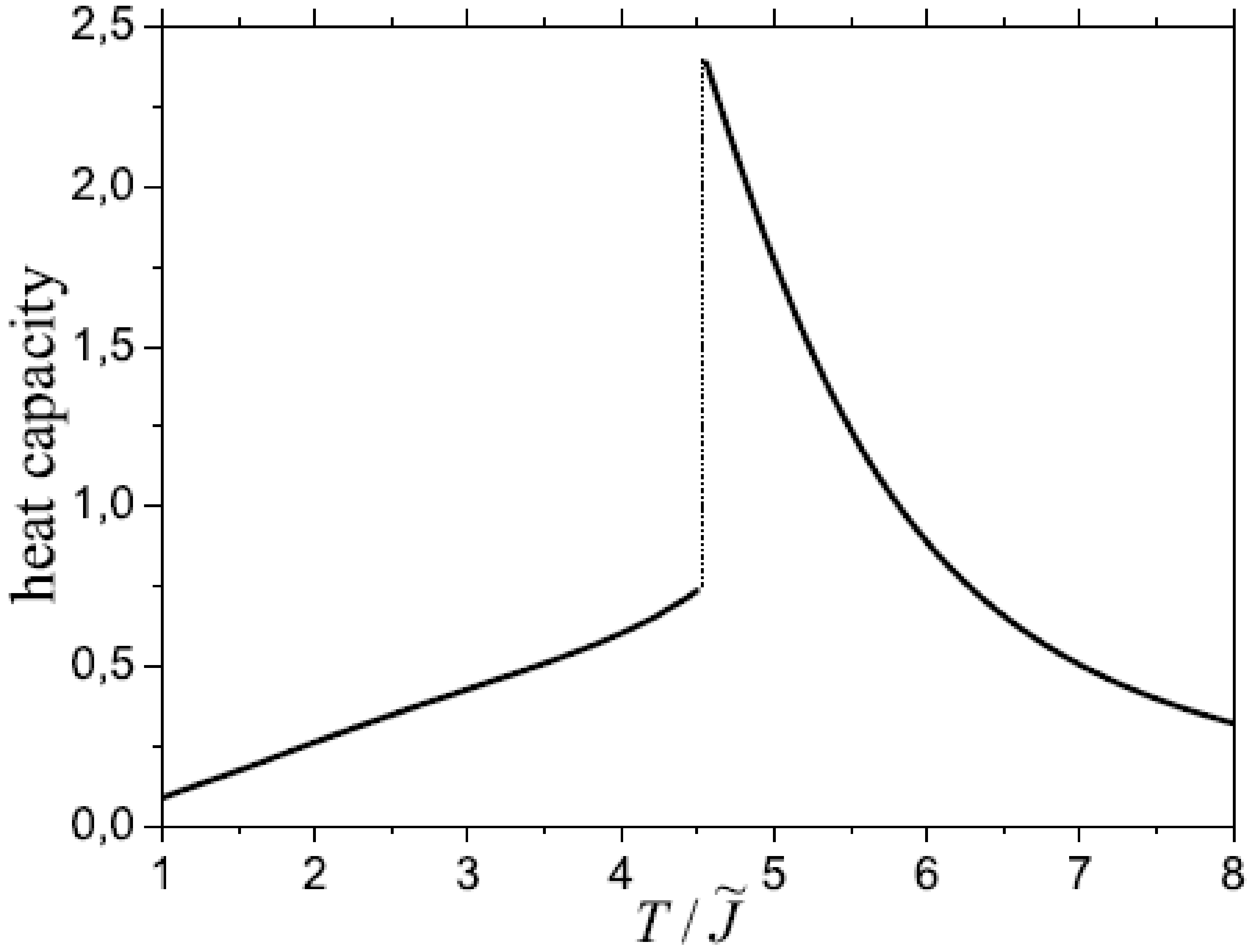
$$\left. -\frac{t^2}{4} \sum_{\alpha \neq \beta} (q^{\alpha\beta})^l + \sum_{\alpha \neq \beta} \lambda^{\alpha\beta} q^{\alpha\beta} - \ln \mathrm{Tr}_{\{Q^\alpha\}} \exp \hat{\theta} \right\}$$

II.



order parameters
$T/\tilde{J}$
p_{1RSB}
p_{RS}
v_{1RSB}
r_{RS}
x_{1RSB}
m_{1RSB}
x_{RS}
r_{1RSB}
λ_{1RSB}
λ_{RS}
r_{RS} r_{1RSB}
x_{RS} x_{1RSB}
p_{RS} p_{1RSB}
λ_{RS} λ_{1RSB}
v_{1RSB} m_{1RSB}
4,0
3,5
3,0
2,5
2,0
1,5
1,0
0,5
0,0
-0,5
-1,0
1
2
3
4
5
6
7
8

II.



• CONCLUSION

•REAL PHYSICAL SYSTEMS

•REFLECTION SYMMETRY

Disordered systems

$$\frac{\Delta F^{s}}{NkT} = \lim_{n\to 0}\frac{1}{n}\sum\left[\ldots + a_3\delta q^{\alpha\beta}\delta q^{\beta\gamma}\delta q^{\gamma\alpha} + a_4'(\delta q^{\alpha\beta})^4 + a_4\delta q^{\alpha\beta}\delta q^{\beta\gamma}\delta q^{\gamma\delta}\delta q^{\delta\alpha}\ldots\right]$$

∞-RSB ? YES (a theorem)

$$\frac{\Delta F^{ns}}{NkT} = \lim_{n\to 0}\frac{1}{n}\sum\left[\ldots + b_3(\delta q^{\alpha\beta})^3 + \ldots + b_4\delta q^{\alpha\beta}\delta q^{\beta\gamma}\delta q^{\gamma\alpha}\delta q^{\delta\alpha}\ldots\right]$$

1RSB ? NO (3 counterexamples)