# MODEL OF GLASS

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A model of glass is presented, based on the introduction of quenched random disorder in a model of defect melting.

While spin glasses have found a satisfactory model formulation [1–8], ordinary glasses are still in a pre-Edwards–Anderson state [9]. The reason used to be the absence of a satisfactory model of defect melting, comparable to the spin model of ferromagnetism, which would permit the introduction of quenched random disorder. With the finding of such a model [10,11], this obstacle has been removed. It is now possible to study ensembles of dislocations and disclinations with their proper long-range elastic forces. Above a certain temperature, they proliferate in a first order transition [12], which can be identified with crystal melting, in agreement with experiment [12,13].

The new model is a simple extension of a spin model and is closely related [11] to lattice gauge theories [14]. Its partition function reads:

$$Z = \prod_{x,i} \int_{-\pi}^{\pi} \frac{dA_i(x)}{2\pi} \exp\left\{ \mathrm{Re}\left[ \beta \left( \sum_{x,i>j} U_i(x) U_j^\dagger(x+i) U_i^\dagger(x+j) U_j(x) + 2 \sum_{x,i} U_i(x) U_i^\dagger(x+i) \right) \right] \right\}, \tag{1}$$

where $\beta = \mu a^3/T(2\pi)^2$ is a reduced inverse temperature ($\mu$ = shear module, $a$ = lattice spacing) and $U_i(x)$ is a phase $\exp[iA_i(x)]$ with $A_i$ denoting the atomic displacement field $u_i(x)$, renormalized by $2\pi/a$. The exponent involves the "compactified strain"

$$\sum_{x,i>j} \cos(\nabla_i A_j + \nabla_j A_i) + 2 \sum_{x,i} \cos(\nabla_i A_i) ,$$

with the periodicity of the cosine functions giving rise to the proper crystalline defects [10] [just as $\cos(\nabla_i \theta)$ in the $XY$ model gives rise to the vortex lines of superfluid $^4$He].

Because of the similarity of (1) with the classical spin model it is just as easy to introduce quenched random disorder as in ref. [1]. If, for example, $\beta$ is allowed to carry phases, $\beta \to \beta \exp[i\omega_{ij}(x)]$, the cosines become

$$\sum_{x,i>j} \cos(\nabla_i A_j + \nabla_j A_i - \omega_{ij}) + 2 \sum_{x,i} \cos(\nabla_i A_i - \omega_{ii}) ,$$

and the ground state of displacement vectors is no longer given by $A_i(x) \equiv 0$ but by a random set of $A_i(x)$. It is obvious that in such a ground state also the elastic forces will depend on $x$, $ij$. The simplest ansatz which allows for this situation is the free energy.

$$-\beta F = \prod_{x,i>j} \int \frac{d\beta_{ij}(x)}{(2\pi\Delta^2)^{1/2}} \frac{d\beta_{ij}^\dagger(x)}{(2\pi\Delta^2)^{1/2}} \exp[-|\beta_{ij}(x) - \beta|^2/2\Delta^2] \log\left\{ \prod_{x,i} \int_{-\pi}^{\pi} \frac{dA_i(x)}{2\pi} \right.$$

$$\left. \times \exp\left[ \mathrm{Re}\left( \sum_{x,i>j} \beta_{ij}(x) U_i(x) U_j^\dagger(x+i) U_i^\dagger(x+j) U_j(x) + 2 \sum_{x,i} \beta_{ii}(x) U_i(x) U_i^\dagger(x+i) \right) \right] \right\} . \tag{2}$$

Using the replica trick, the $\beta$ integral can be done with the result


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$$-\beta F = \lim_{n\to 0} n^{-1} \prod_{x,i} \int_{-\pi}^{\pi} \frac{\mathrm{d}A_i(x)}{2\pi} \exp\Big[\beta\, \mathrm{Re}\Big(\sum_{x,i>j,\alpha} U_i^\alpha(x) U_j^{\alpha\dagger}(x+i)\, U_i^{\alpha\dagger}(x+j) U_j^\alpha(x) + 2 \sum_{x,i,\alpha} U_i^\alpha(x)\, U_i^{\alpha\dagger}(x+i)\Big)$$

$$+\tfrac{1}{2}\Delta^2\, \mathrm{Re}\Big(\sum_{x,i>j,\alpha,\beta} Q_i^{\alpha\beta}(x) Q_j^{\alpha\beta\dagger}(x+i) Q_j^{\alpha\beta}(x) + 4 \sum_{x,i,\alpha,\beta} Q_i^{\alpha\beta}(x) Q_i^{\alpha\beta\dagger}(x+i)\Big)\Big] , \tag{3}$$

where $Q_i^{\alpha\beta}(x) \equiv U_i^\alpha(x) U_i^{\beta\dagger}(x)$. Separating out the trivial $\alpha = \beta$ terms $Q_i^{\alpha\alpha}(x) = 1$, we can introduce auxiliary integrations and arrive at the free energy:

$$-\beta F = \lim_{n\to 0} n^{-1} \prod_{x,i,\alpha} \iint_{-\infty}^{\infty} \mathrm{d}u_i^\alpha(x)\, \mathrm{d}u_i^{\alpha\dagger}(x) \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \frac{\mathrm{d}\xi_i^\alpha(x)\, \mathrm{d}\xi_i^{\alpha\dagger}(x)}{(2\pi \mathrm{i})^2}$$

$$\times \prod_{x,i,\alpha>\beta} \iint_{-\infty}^{\infty} \mathrm{d}q_i^{\alpha\beta}(x)\, \mathrm{d}q_i^{\alpha\beta\dagger}(x) \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \frac{\mathrm{d}\lambda_i^{\alpha\beta}(x)\, \mathrm{d}\lambda_i^{\alpha\beta\dagger}(x)}{(\pi \mathrm{i})^2} \exp\{S[u, q, \xi, \lambda]\} ,$$

where

$$S = \beta\, \mathrm{Re}\Big(\sum_{x,i>j,\alpha} u_i^\alpha(x) u_j^{\alpha\dagger}(x+i) u_i^{\alpha\dagger}(x+j) u_j^\alpha(x) + 2 \sum_{x,i,\alpha} u_i^\alpha(x) u_i^{\alpha\dagger}(x+i)\Big)$$

$$+ \Delta^2 \mathrm{Re}\Big(\sum_{x,i>j,\alpha>\beta} q_i^{\alpha\beta}(x) q_j^{\alpha\beta\dagger}(x+i) q_i^{\alpha\beta\dagger}(x+j) q_j^{\alpha\beta}(x) + 4 \sum_{x,i,\alpha>\beta} q_i^{\alpha\beta}(x) q_i^{\alpha\beta\dagger}(x+i) + \tfrac{15}{2} n\Big)$$

$$-\frac{1}{2}\Big(\sum_{x,i,\alpha} \xi_i^\alpha(x) u_i^{\alpha\dagger}(x) + \sum_{x,i,\alpha>\beta} \lambda_i^{\alpha\beta}(x) q_i^{\alpha\beta\dagger}(x) + \text{c.c.}\Big) + V[\xi, \lambda] , \tag{5}$$

with a potential

$$V = \log \prod_{x,i} \int_{-\pi}^{\pi} \frac{\mathrm{d}A_i(x)}{2\pi} \exp \frac{1}{2}\Big(\sum_{x,i,\alpha} \xi_i^\alpha(x) U_i^{\alpha\dagger}(x) + \sum_{x,i,\alpha>\beta} \lambda_i^{\alpha\beta}(x) U_i^\alpha(x) U_i^{\beta\dagger}(x) + \text{c.c.}\Big) . \tag{6}$$

The properties of the model (2) or (4) can be studied by using for small $\beta$ a high temperature series [‡1] and for large $\beta$ the mean field approximation plus loop corrections [‡2].

In this note we shall estimate the properties of $F$ at the same level as Edwards and Anderson, namely by looking for an optimal replica symmetric mean field $\xi_i^a \equiv \xi$, $\lambda_i^{\alpha\beta} \equiv \lambda$. In this case, the potential $V$ can be integrated as follows

$$\exp(V/3N) = \int_{-\pi}^{\pi} \frac{\mathrm{d}A_i}{2\pi} \exp[-\tfrac{1}{2}\xi \Sigma_\alpha U_i^\alpha + \text{c.c.} + \tfrac{1}{2}\lambda(\Sigma_\alpha\, U_i^\alpha\, \Sigma_{\alpha'}\, U_i^{\alpha'\dagger} - n)]$$

$$= \exp(-\tfrac{1}{2}\lambda n) \iint \frac{\mathrm{d}x \mathrm{d}x^+}{2\pi\lambda} \exp(-|x|^2/2\lambda) \int_{-\pi}^{\pi} \frac{\mathrm{d}A_i}{2\pi} \exp[-\tfrac{1}{2}(\xi + x)\Sigma_\alpha\, U_i^\alpha + \text{c.c.}]$$

$$= \exp(-\tfrac{1}{2}\lambda n) \iint \frac{\mathrm{d}x \mathrm{d}x^+}{2\pi\lambda} \exp(-|x|^2/2\lambda) I_0^n(|\xi + x|)$$

$$= \exp(-\tfrac{1}{2}\lambda n)\lambda^{-1} \int_0^\infty \mathrm{d}r\, r \exp[-(r^2 + \xi^2)/2\lambda] I_0(r\xi/\lambda) I_0^n(r) , \tag{7}$$

‡1 In spin glasses, see ref. [15].
‡2 For a review see ref. [16].

where $N$ is the number of sites. If we introduce the function

$$v(\xi, \lambda) = \lambda^{-1} \int_0^\infty \mathrm{d}r\, r \exp[-(r-\xi)^2/2\lambda]\, \widetilde{I}_0(r\xi/\lambda) \log I_0(r)\,, \tag{8}$$

with $\widetilde{I}_n(z) \equiv \mathrm{e}^{-z} I_n(z)$, the free energy density $f \equiv F/3N$ becomes

$$-\beta f = \beta(u^4 + 2u^2) - \tfrac{1}{2}\Delta^2(q^4 + 4q^2 - 5) - \xi u + \tfrac{1}{2}\lambda(q-1) + v(\xi, \lambda)\,. \tag{9}$$

This is minimal at

$$4\beta(u^3 + u) = \xi\,, \quad 4\Delta^2(q^3 + 2q) = \lambda\,, \quad u = \lambda^{-1} v_1 - (\xi/\lambda) v\,, \tag{10a,b,c}$$

$$q = 1 + (2/\lambda) v + \lambda^{-2}[-\xi^2 v - v_2 + 2\xi v_1]\,, \tag{10d}$$

where

$$v_1 \equiv \lambda^{-1} \int_0^\infty \mathrm{d}r\, r^2 \exp[-(r-\xi)^2/2\lambda]\, \widetilde{I}_1(r\xi/\lambda) \log I_0(r)\,,$$

$$v_2 \equiv \lambda^{-1} \int_0^\infty \mathrm{d}r\, r^3 \exp[-(r-\xi)^2/2\lambda]\, \widetilde{I}_0(r\xi/\lambda) \log I_0(r)\,.$$

Introducing $\gamma \equiv \Delta/\beta$ as a measure for the glassiness, the solution of (10) gives a behavior of the order parameters and the phase diagram as shown in figs. 1 and 2.

For $T \to 0$, $\beta \to \infty$, $\xi$ and $\lambda$ tend to infinity with $\xi/\sqrt{\lambda} \equiv \kappa$ fixed, such that

$$v(\xi, \lambda) \to \sqrt{2\pi\lambda}\,[(\tfrac{1}{2} + \tfrac{1}{4}\kappa^2)\widetilde{I}_0(\tfrac{1}{4}\kappa^2) + \tfrac{1}{4}\kappa^2 \widetilde{I}_1(\tfrac{1}{4}\kappa^2)]\,, \tag{11}$$

$$u \to \tfrac{1}{2}[i_0(\kappa) + i_1(\kappa)]\,, \quad q \to 1 - \lambda^{-1/2}\kappa^{-1} i_0(\kappa) \to 1\,, \tag{12a,b}$$

$$-f - \sqrt{6\pi}\gamma \to -3u^4 - 2u^2 + 2\sqrt{6\pi}\gamma\{\tfrac{1}{2}[\widetilde{I}_0(\tfrac{1}{4}\kappa^2) - 1] + \tfrac{1}{4}\kappa^2[\widetilde{I}_0(\tfrac{1}{4}\kappa^2) + \widetilde{I}_\pi(\tfrac{1}{4}\kappa^2)]\}\,, \tag{12c}$$

where we have set $i_n(\kappa) \equiv (2\pi\kappa^2/4)^{1/2} \widetilde{I}_n(\tfrac{1}{4}\kappa^2)$. In the same limit, (10a) becomes

$$(2/\sqrt{3}\gamma)(u^3 + u) = \kappa\,, \quad 12\gamma^2\beta^2 = \lambda\,. \tag{13}$$

Together with (12a) this can be solved for $\gamma(\kappa)$ as shown in table 1. If the glassiness exceeds a certain value, $\gamma_0 = 0.8337$, there is a first order transition to the minimal solution $u_0 = 0.845$. For $\gamma > \gamma_0$, the ground state is in the glass phase and its energy is given by

$$-\beta f = -\tfrac{1}{2}\beta^2\gamma^2(q^4 + 4q^2 - 5) + \tfrac{1}{2}\lambda(q-1) + v(0, \lambda)\,, \tag{14}$$

with

$$v(0, \lambda) = \lambda^{-1} \int_0^\infty \mathrm{d}r\, r \exp(-r^2/2\lambda) \log I_0(r) = \int_0^\infty \mathrm{d}r \exp(-r^2/2\lambda) I_1(r)/I_0(r) = \tfrac{1}{2}\lambda - \tfrac{1}{8}\lambda^2 + \tfrac{1}{12}\lambda^3 - \tfrac{11}{64}\lambda^4 + \ldots\,.$$

Then $\beta(\lambda)$ is determined from

$$4\beta^2\gamma^2(q^3 + 2q) = \lambda\,, \quad q = 1 - 2v_\lambda = 1 - \lambda^{-2} \int_0^\infty \mathrm{d}r\, r^2 \exp(-r^2/2\lambda) I_1(r)/I_0(r) \tag{15}$$

and the solution is shown in table 2.

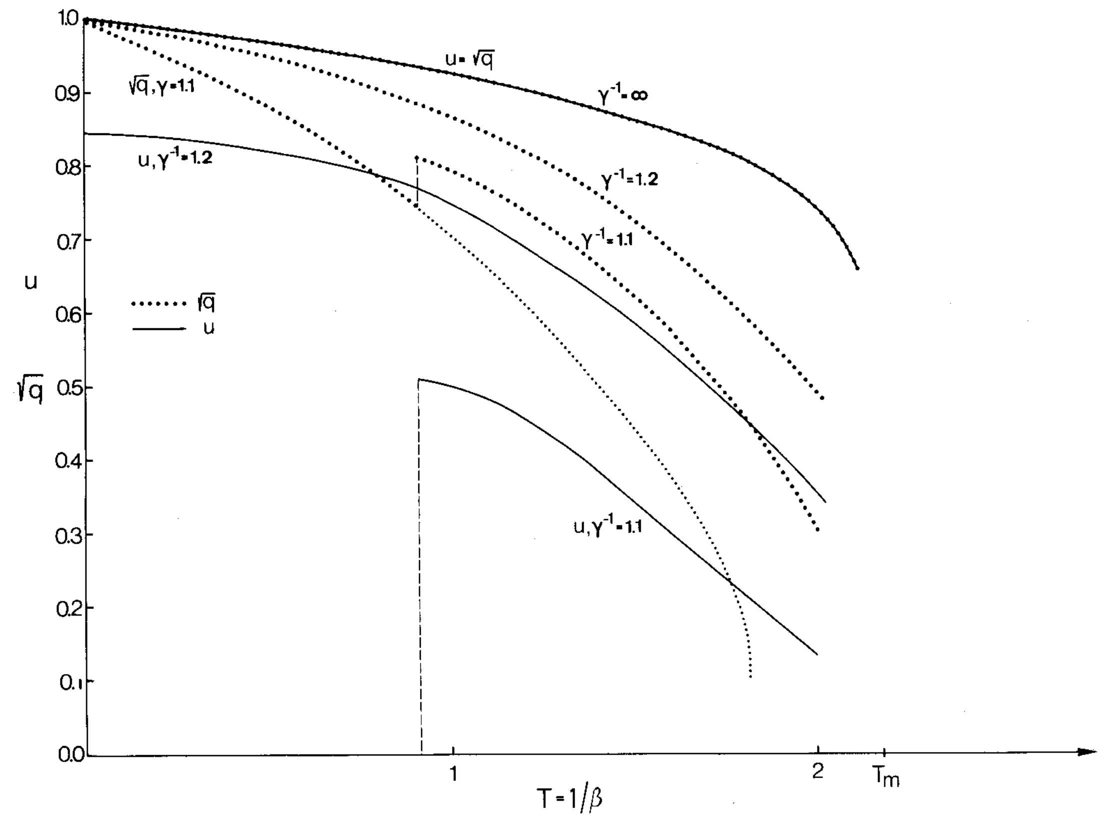


Fig. 1. The order parameters $\sqrt{q}$ and $u$ as a function of $T$. For $\gamma = 0$, $u = \sqrt{q}$ and the ground state is a pure crystal. For $\gamma^{-1} < 1$, $u$ vanishes identically and $\sqrt{q}$ follows a curve which is universal in $T/\gamma$ starting out at $\sqrt{q} = 1$ and going to zero at $T = \gamma^{-1}$. For $\gamma \in (1, \gamma_0^{-1})$, there is a first order phase transition of recrystallization, at which $u$ becomes non-zero and $\sqrt{q}$ jumps upwards after which they both decrease slowly towards the melting point. The example is for $\gamma^{-1} = 1.1$. For $\gamma^{-1} > \gamma_0^{-1}$, the ground state is crystalline and there is only a melting transition. The example is $\gamma^{-1} = 1.2$.

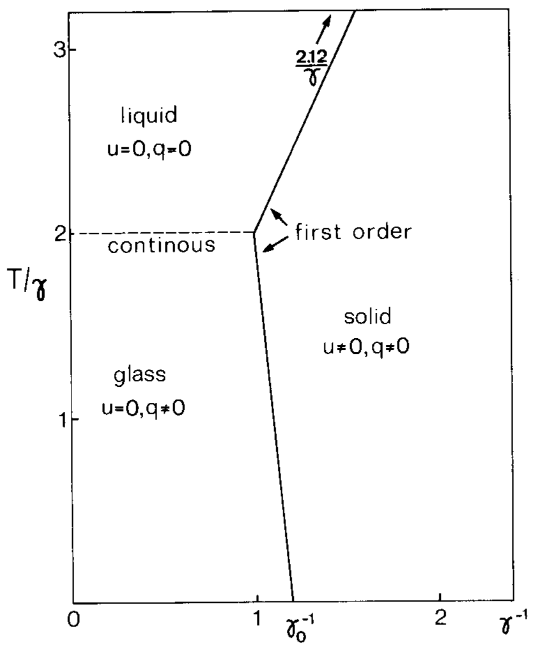


Fig. 2. The phase diagram of the glass model at the mean field level. The parameter $\gamma$ is the glassiness. In the glass phase, $u = 0$ and $\sqrt{q}$ decreases from 1 to zero as $T/\gamma$ runs from zero to 2. On the base line, as $\gamma^{-1}$ exceeds $\gamma_0^{-1}$, the variable $u$ jumps to 0.845 and approaches unity as $\gamma^{-1} \to \infty$ (see table 1).

Table 1
The order parameter $u$ and the free energy for $T = 0$ as a function of glassiness $\gamma$. At $\gamma_0 = 0.8337$ there is a jump from $u = 0$ to $u_0 = 0.845$.

| $\kappa$ | $\gamma$ | $u$ | $-f-\sqrt{6\pi\gamma}$ |
|---|---|---|---|
| 0 | 0.7236 = $\pi/6$ | 0 | 0 |
| 2 | 0.8350 | 0.8443 | −0.0027 |
| 2.2 | 0.8075 | 0.8730 | 0.0641 |
| 2.4 | 0.7763 | 0.8955 | 0.1457 |
| 3 | 0.6779 | 0.9374 | 0.4326 |
| 4 | 0.5401 | 0.9669 | 0.8846 |
| 6 | 0.3741 | 0.9858 | 1.4830 |
| 8 | 0.2841 | 0.9921 | 1.8277 |
| 10 | 0.2286 | 0.9950 | 2.0469 |
| 15 | 0.1533 | 0.9978 | 2.3522 |
| 20 | 0.1152 | 0.9987 | 2.5099 |

Table 2
Order parameter and energy for the glass phase, $\xi \equiv 0, u \equiv 0, \lambda \neq 0, q \neq 0$.

| $\lambda$ | $\sqrt{q}$ | $T/\gamma$ | $-\beta f - \frac{5}{2}\beta^2\gamma^2$ |
|---|---|---|---|
| 0 | 0 | 2 | 0 |
| 0.2 | 0.290 | 1.838 | −0.0013 |
| 0.4 | 0.383 | 1.723 | −0.0023 |
| 0.6 | 0.443 | 1.634 | −0.0040 |
| 0.8 | 0.488 | 1.562 | −0.0077 |
| 1.0 | 0.522 | 1.502 | −0.0127 |
| 2 | 0.625 | 1.297 | −0.0472 |
| 4 | 0.716 | 1.078 | −0.1649 |
| 6 | 0.762 | 0.952 | −0.324 |
| 8 | 0.791 | 0.865 | −0.509 |
| 10 | 0.812 | 0.801 | −0.713 |
| 20 | 0.864 | 0.618 | −1.915 |
| 30 | 0.888 | 0.525 | −3.284 |
| 50 | 0.913 | 0.424 | −6.280 |
| 100 | 0.938 | 0.313 | −14.480 |

Another special case which can be discussed analytically is that of small glassiness, $\gamma \to 0$, for all $\beta$. Then $\lambda$ is small and $v$ can be expanded as

$$v(\xi, \lambda) = \log I_0(\xi) + \tfrac{1}{2}\lambda\{1 - [I_1(\xi)/I_0(\xi)]^2\} + \dots . \tag{16}$$

This gives

$$q = u^2 ,$$

with $u$ satisfying

$$4\beta(u^3 + u) = \xi , \quad u = I_1(\xi)/I_0(\xi) - \lambda[I_1(\xi)/I_0(\xi)][1 - \xi^{-1}I_1/I_0 - (I_1/I_0)^2] ,$$

and the case $\lambda = 0$ reducing to the pure melting model with a transition at $T_m \sim 2.12$ (see table 3). For large $\beta$, $u = \sqrt{q} \sim 1 - 1/8\beta$. Eqs. (15) and (16) show that the order parameter $q$ depends much less on $\gamma$ than $u$. The phase diagram is similar to that of spin glasses [1] only in that the transitions liquid–solid and glass–solid are of first order with the order parameters $u$, $q$ jumping to finite values. It will be interesting to extend the mean field study to Parisi's proper order parameter [5–8] and to include fluctuation corrections. The model can also serve to include quantum effects by adding a kinetic term $[\rho a^5/2(2\pi)^2] \int \mathrm{d}t\, \Sigma_x \dot{A}^2$ and functionally integrating over time dependent $A_i(x, t)$ fields. In this case it becomes possible to calculate the experimentally observable structure functions

$$S(q, \omega) = \int \mathrm{d}^3x\, \mathrm{d}t\, \exp[\mathrm{i}(\boldsymbol{q}\cdot\boldsymbol{x} - \omega t)] \langle \exp[\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{u}(\boldsymbol{x}, t)]\ \exp[-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{u}(0, 0)] \rangle .$$

More details will be published elsewhere.

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