Quasi equilibrium construction for long time glassy dynamics

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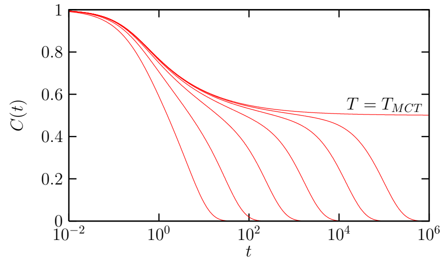
Overview

Overview of the talk

- Dynamics of glassy systems
- Mean Field disordered systems
  - Langevin Dynamics
  - Supersymmetric approach
- The Potential Method
- The Boltzmann Pseudodynamics
- Application to mean field spin glass systems
- Results in the replicated liquid theory
  - Dynamical Ornstein-Zernike equations
  - HNC closure
- Conclusions and perspectives

Dynamics of glassy systems



Two exponents:

$$C(t) \simeq q_{EA} + c_1 t^{-a} + \ldots$$
$$C(t) \simeq q_{EA} + c_2 t^{b} + \ldots$$

The λ exponent is defined by

$$\lambda = \frac{\Gamma^2(1-a)}{\Gamma(1-2a)} = \frac{\Gamma^2(1+b)}{\Gamma(1+2b)} \qquad \tau_\alpha \sim |T - T_d|^{-\gamma} \qquad \gamma = \frac{1}{2a} + \frac{1}{2b} = f(\lambda)$$

Dynamics from statics: first steps

Mean Field models (Caltagirone, Ferrari, Leuzzi, Parisi, Ricci-Tersenghi, Rizzo, 2011) → schematic mode coupling equations:
Ingredients (Kurchan 1992):

- Langevin Dynamics
- Martin-Siggia-Rose functional
- Supersymmetric formalism
- Dynamical action
- Saddle point equations → schematic mode coupling equation
- ultrafast motion limit ("replicas = supertimes")

$$\boxed{\lambda = \frac{w_2}{w_1}}$$

where w_1 and w_2 are two of the cubic coefficient of a replica field theory action that can be written from the statics.

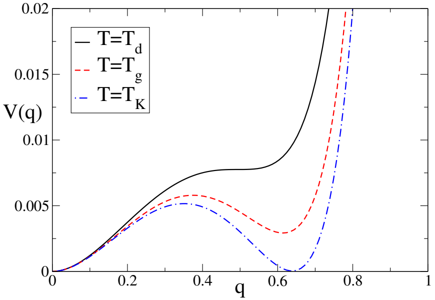
The Potential Method

Consider a system with hamiltonia $H_J(\underline{\sigma})$ where J is an internal quenched disorder and $\underline{\sigma}$ is the configuration of the internal degrees of freedom. Define the potential (Franz Parisi 1995)

$$V(q) = -\lim_{N\to\infty} \frac{1}{N\beta} \mathbf{E_J} \sum_{\underline{\tau}} \frac{\mathrm{e}^{-\beta H_J[\underline{\tau}]}}{Z_J} \log Z_J[q, \underline{\tau}]$$

where

$$Z_J[q, \underline{\tau}] = \sum \mathrm{e}^{-\beta H_J[\underline{\sigma}]} \delta\left(q - q(\underline{\sigma}, \underline{\tau})\right) \qquad Z_J = \int \mathrm{d}q Z_J[q, \underline{\tau}]$$



The Boltzmann Pseudodynamics

Let us consider a generalization of the Franz-Parisi potential.
We define the potential of a *chain of coupled systems* of length L the following way (Franz Parisi, 2012)

$$V\left[\{\beta_k\};\{\tilde{C}(k-1,k)\}\right] = -\lim_{N\to\infty}\frac{1}{N}\mathbf{E}_J\sum_{\underline{\sigma}_1}\dots\sum_{\underline{\sigma}_{L-1}}\frac{1}{Z}\mathrm{e}^{-\beta_1 H_J[\underline{\sigma}_1]}\prod_{k=1}^{L-2}M(\underline{\sigma}_{k+1}|\underline{\sigma}_k)\times$$

$$\times \ln\sum_{\underline{\sigma}_L}\mathrm{e}^{-\beta_L H_J[\underline{\sigma}_L]}\delta\left(\tilde{C}(L-1,L)-q(\underline{\sigma}_{L-1},\underline{\sigma}_L)\right)$$

and

$$M(\sigma_k|\sigma_{k-1}) = \frac{1}{Z(\underline{\sigma}_{k-1})}\mathrm{e}^{-\beta_k H_J[\underline{\sigma}_k]}\delta\left(\tilde{C}(k-1,k)-q(\underline{\sigma}_{k-1},\underline{\sigma}_k)\right)$$

$$Z(\underline{\sigma}_{k-1}) = \sum_{\underline{\sigma}_k}\mathrm{e}^{-\beta_k H_J[\underline{\sigma}_k]}\delta\left(\tilde{C}(k-1,k)-q(\underline{\sigma}_{k-1},\underline{\sigma}_k)\right)\ .$$

We considered the most general case where the temperature of each system is different one from another. The kernel $M(\sigma_k|\sigma_{k-1})$ defines the Boltzmann Pseudodynamics Markov Chain.

Schematic models - p-spin (1)

Let us consider the p-spin spherical model.

The replica method can be employed to treat the logarithm and the factors $Z(\underline{\sigma}_{k-1})^{-1}$.
In this way we have a replicated chain. For each system we have a certain number of replicas that eventually will be sent to zero.
By averaging over the disorder, the potential becomes a function of the overlap

$$Q_{ab}(t,s) = \frac{1}{N}\sum_{i=1}^{N} \sigma_i^{(a)}(t)\sigma_i^{(b)}(s)$$

and the action for the potential becomes

$$S(Q) = \frac{\beta^2}{4}\sum_{t,s=1}^{L}\sum_{a=1}^{n_t}\sum_{b=1}^{n_s} Q_{ab}(t,s)^p + \frac{1}{2}\ln\det Q$$

We must choose a parametrization for the overlap matrix that is compatible with the constraints.

Schematic models - p-spin (2)

Replica symmetric parametrization for the overlap matrix

$$Q_{ab}(t,s) = C(t,s) + \delta_{ab}\delta_{su}\Delta C(s,s) + \Theta_>(s-t)\delta_{a1}\Delta C(t,s) + \\ + \Theta_>(t-s)\delta_{a1}\Delta C(s,t)$$

$$\Delta C(t,s) = \tilde{C}(t,s) - C(t,s)$$

We want to optimize over the free parameter of the overlap matrix. However, as in the standard potential method, we will search for a stationary point of the potential with respect to all the constraints. In this way we will optimize over all the parameters of Q. The saddle point equations are

$$\frac{\beta^2 p}{2}\sum_{z=1}^{L}\sum_{c=1}^{n_z}\left[Q_{ac}(k,z)\right]^{p-1} Q_{cb}(z,j) + \delta_{kj}\delta_{ac} - \nu_k Q_{ab}(k,j) = 0$$

In the limit in which the chain becomes infinitely long we put the crucial ansatz

$$\frac{1}{\beta}R(u,s)\mathrm{d}s = \Theta_>(u-s)\Delta C(s,u)$$

that can be justified by an explicit computation of the response function within the Boltzmann pseudodynamics process.

Schematic models - p-spin (3)

The crucial result is that

$$\lim_{\{n(t)\}\to 0}\sum_{z=1}^{L}\sum_{c=1}^{n_z}\left[Q_{ac}(k,z)\right]^{p-1}Q_{cb}(z,j)=\int \mathrm{d}c\, Q(a,c)^{p-1}Q(c,b)$$

The resulting equations are

$$\nu(t)C(t,u)=\frac{\beta^2 p}{2}\Big[C^{p-1}(t,u)\Delta C(u,u)+\Delta C_{p-1}(t,t)C(t,u)+C^{p-1}(t,0)C(u,0)+$$
$$+\frac{1}{\beta}\int_0^u \mathrm{d}z\, C^{p-1}(t,z)R(u,z)+\frac{p-1}{\beta}\int_0^t \mathrm{d}z\, C^{p-2}(t,z)R(t,z)C(z,u)\Big]$$
$$\frac{1}{\beta}\nu(t)R(t,u)=\frac{\beta^2 p}{2}\Big[\frac{1}{\beta}\Delta C_{p-1}(t,t)R(t,u)+\frac{p-1}{\beta}C^{p-2}(t,u)R(t,u)\Delta C(u,u)+$$
$$\frac{p-1}{\beta^2}\int_u^t \mathrm{d}z\, C^{p-2}(t,z)R(t,z)R(z,u)\Big]$$
$$\nu(t)\Delta C(t,t)=\frac{\beta^2 p}{2}\Delta C_{p-1}(t,t)\Delta C(u,u)+1\,.$$

By imposing $\Delta C(t,t)=1-q_d$ we recover the dynamical equation in the α regime.

The Boltzmann Pseudodynamics for structural glasses-(1)

Consider a replicated system of particles so that we can define the fields

$$\rho_a(x) = \langle \sum_{i=1}^{N} \delta(x - x_i^{(a)}) \rangle \qquad \rho_{ab}(x; y) = \langle \sum_{[ij]} \delta(x - x_i^{(a)}) \delta(y - x_j^{(b)}) \rangle$$

$$h_{ab}(x, y) = \frac{\rho_{ab}(x, y)}{\rho_a(x) \rho_b(y)} - 1$$

And the replicated Ornstein-Zernike equations that defines the direct correlation function

$$c_{ab}(x, y) = h_{ab}(x, y) - \sum_{c=1}^{n} \int \mathrm{d}z \, h_{ac}(x, z) \rho_c(z) c_{cb}(z, y)$$

We will consider solutions such that $\rho_a(x) = \rho$. Note that in the OZ equation there is the product between the matrix h and the matrix c.

The Boltzmann Pseudodynamics for structural glasses-(2)

Put now the pseudodynamics ansatz

$$h_{ab}(x) = h(s,u;x) + \delta_{ab}\delta_{su}\Delta h(s,s;x) + \Theta_>(u-s)\delta_{a1}\Delta h(s,u;x) + \\ + \Theta_>(s-u)\delta_{b1}\Delta h(s,u;x)$$

$$\frac{1}{\beta}R_h(q;u;s)\mathrm{d}s = \Theta_>(u-s)\Delta h(q;s,u)$$

and the analogous expression for the direct correlation function. The OZ equations become

$$h(q;s,u) = c(q;s,u) + \rho\left[h(q;s,0)c(q;0,u) + h(q;s,u)\Delta c(q;u,u) + \right. \\ \left. + \Delta h(q;s,s)c(q;s,u) + \frac{1}{\beta}\int_0^u \mathrm{d}z h(q;s,z)R_c(q;u,z) + \frac{1}{\beta}\int_0^s \mathrm{d}z R_h(q;s,z)c(q;z,u)\right]$$

$$\Delta h(q;s,s) = \Delta c(q;s,s) + \rho\Delta h(q;s,s)\Delta c(q;s,s)$$

$$R_h(q;u,s) = R_c(q;u,s) + \rho\left[R_h(q;u,s)\Delta c(q;u,u) + \Delta h(q;s,s)R_c(q;u,s) + \right. \\ \left. + \frac{1}{\beta}\int_s^u \mathrm{d}z R_h(q;z,s)R_c(q;u,z)\right].$$

The Boltzmann Pseudodynamics for structural glasses-(3)

We have to choose a closure for the OZ equations. We choose HNC.

$$\ln[h_{ab}(x,y)+1]+\beta\phi_{ab}(x,y)=h_{ab}(x,y)-c_{ab}(x,y)$$

Putting the BPD ansatz in the equation we get

$$\ln[h(x;s,u)+1]=h(x;,s,u)-c(x;s,u)$$
$$R_c(x;s,u)=R_h(x;s,u)\frac{h(x;s,u)}{1+h(x;s,u)}\,.$$

and moreover that $\Delta h(q,s,s)$ and $\Delta c(q,s,s)$ are actually s independent. We can now analyze the full set of equations. First we go to the equilibrium regime and we see that the equations admits a solution that satisfies TTI + FDT

$$-\beta\frac{\mathrm{d}h(x;s-u)}{\mathrm{d}s}=R_h(x;s-u)$$

The Boltzmann Pseudodynamics for structural glasses-(4)

The final equation is

$$0 = W_q[h] - \rho \int_0^s \dot{h}(q,z)[c(q,s-z) - c(q;s)]$$

$$W_q[h] = c(q;s) - h(q;s) + \rho\left[h(q;s)\Delta c_0(q) + c(q;s)\Delta h_0(q) + c(q;0)h(q;s) - \right.$$
$$\left. -(h(q,s) - h(q,0))c(q,s)\right]$$

where

$$\ln[h(x;s,u)+1] = h(x;s,u) - c(x;s,u)$$

This is a particular MCT equation where the kernel is defined through the direct correlation function A non trivial solution exist if

$$\det\left[(2\pi)^D\delta(q-k)(2\rho\Delta c(q) - \rho^2\Delta c^2(q)) - \mathrm{T.F.}\left(\frac{1}{\tilde{g}(x)}\right)(q-k)\right] = 0$$

This operator is the equivalent of the replicon eigenvalue for the schematic models. Moreover using this MCT equation we can compute the exponent parameter λ

$$\lambda = \frac{\int \mathrm{d}^D x \frac{k_0^3(x)}{\tilde{g}^2(x)}}{2\rho\int_q k_0^3(q)(1-\rho\Delta c(q))^3}$$

that is in agreement we the static calculation based on the relation $\lambda = w_2/w_1$ obtained in Franz Jaquin Parisi Urbani Zamponi 2012

The Boltzmann Pseudodynamics for structural glasses-(5)

Moreover we can study the aging regime.

$$
\begin{aligned}
h(q;s,u) = c(q;s,u) + \rho\,[h(q;s,u)\Delta c(q) + \Delta h(q)c(q;s,u)+ \\
+\frac{1}{\beta}\int_0^u \mathrm{d}z R_c(q;u,z)h(q;s,z) + \frac{1}{\beta}\int_0^s \mathrm{d}z R_h(q;s,z)c(q;z,u)\Big] \\
R_h(q,s,u) = R_c(q;s,u) + \rho\,[R_h(q;s,u)\Delta c(q) + \Delta h(q)R_c(q;s,u)+ \\
+\frac{1}{\beta}\int_u^s \mathrm{d}z R_h(q;z,u)R_c(q;s,z)\Big]\ .
\end{aligned}
$$

Following (Cugliandolo Kurchan 1993) we search for a solution of the type

$$
h(q;s,u) = \underline{h}\left(q;\frac{u}{s}\right) \qquad R_h(q;s,u) = \frac{1}{s}\mathcal{R}_h\left(q;\frac{u}{s}\right)
$$

and that satisfies Quasi-FDT

$$
\mathcal{R}_h(q;\lambda) = \beta x \frac{\mathrm{d}}{\mathrm{d}\lambda}\underline{h}(q;\lambda)
$$

Here the FDT ratio is independent on q in agreement with (Latz 2001).

The Boltzmann Pseudodynamics for structural glasses-(6)

The value of FDT ratio x can be computed by looking at the equations in the limit $\lambda \to 1$.

What can be easily seen by inspections is that in that limit the aging equations reduce to the standard replicated HNC equations within a replica symmetric ansatz but with a number of replicas $m = x$.

The value of x is fixed by the equation for the response function in the limit $\lambda \to 1$ that gives rise to the marginal stability condition

$$\det \left[(2\pi)^D \delta(q-k)(2\rho \Delta c(q) - \rho^2 \Delta c^2(q)) - \mathrm{T.F.} \left(\frac{1}{\tilde{g}(x)} \right)(q-k) \right] = 0$$

This is equivalent to replicon instability in mean field schematic models and as in the p-spin spherical model the marginal stability condition does not depend on m.

All the picture follows the Cugliandolo-Kurchan theory of aging.

Conclusions and perspectives

We have discussed a static construction for the whole dynamics of glassy systems in the α regime. The new insight and advantages from this construction are

- It gives an interpretation of glassy dynamics in terms of quasi-equilibrium exploration of phase space.
- It is a static construction so that approximation methods and techniques can be employed
- Standard MCT and the Szamel's closure scheme (Szamel 2010)

The future work to do is

- Use different (possibly better) approximation schemes than HNC
- Understand how to incorporate the full-RSB effects in the quasi-equilibrium construction
- Study dynamical fluctuations in the α regime. In the β regime it has been discovered that the fluctuations can be described by a cubic field theory in a random field. Is it true also in the long time regime?