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Aging and effective temperatures in the low temperature mode-coupling equations.

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The low-temperature generalization of the mode-coupling equations corresponds to the dynamics of mean-field disordered models in the glassy phase. The system never achieves equilibrium, preserving the memory of the time elapsed after the quench throughout its evolution.

A concept of effective temperature can be made quite rigorous in this context by considering readings of thermometers in different time-scales and the thermalization of weakly coupled subsystems.

In the past few years progress has been made in the analytical understanding of glassy dynamics. On the one hand, it was realized that the out of equilibrium dynamics of mean-field disordered models was solvable for long times, and that the solution showed aging phenomena qualitatively close to the ones of real systems.

On the other hand, it became clear that, at least at the mean-field level, the important distinction is not between models with and without quenched randomness but rather between different kinds of nonequilibrium dynamics. This became particularly evident when it was noticed that the mode-coupling equations for supercooled liquids could be obtained as the dynamical equations for mean-field disordered models in the high-temperature phase. By considering the low-temperature dynamics of these spin-glass models, a low-temperature extension of the mode-coupling equations was immediately obtained.

Indeed, except for the crucial (for structural glasses) question of the behaviour near the glass transition, and the related problem of cooling-rate dependence, the models described above yield a rather realistic picture of glassy dynamics well below $T_g$.

Let us consider $n$ modes $O_1, ..., O_n$, their correlations $C_{ab}(t, t_w) = \langle O_a(t)O_b(t_w) \rangle$ and their responses to perturbations $h_a$ conjugate to $O_a$:

$$R_{ab}(t, t_w) = \frac{\delta O_a(t)}{\delta h_b(t_w)} \bigg|_{h=0}, \quad \chi_{ab}(t, t_w) = \int_{t_w}^{t} dt' R_{ab}(t, t').$$ (1)

One can write, in general, Schwinger-Dyson equations for their correlations.
\[ C = (C_{ab}) \text{ and responses } R = (R_{ab}): \]

\[
\frac{\partial C_{ab}(t,t_w)}{\partial t} = 2TR_{ab}(t_w,t) + \sum_c \left( -\mu_{ac}(t)C_{cb}(t,t_w) + \int_0^{t_w} dt'^n D_{ac}(t,t')R_{cb}(t_w,t') \right) + \sum_c \int_0^t dt'^n \Sigma_{ac}(t,t')C_{cb}(t',t_w),
\]

(2)

\[
\frac{\partial R_{ab}(t,t_w)}{\partial t} = \delta(t-t_w)\delta_{ab} + \sum_c \left( -\mu_{ac}(t)R_{cb}(t,t_w) + \int_0^{t_w} dt'^n \Sigma_{ac}(t,t')R_{cb}(t',t_w) \right).
\]

(3)

In mean-field models one can close the Schwinger-Dyson equations into a set of dynamical equations involving only the correlation and response functions:

\[
D_{ab}(t,t') = F_{ab}(C(t,t')), \quad \Sigma_{ab}(t,t') = \sum_{c,d} F_{ab,cd}(C(t,t'))R_{cd},
\]

(4)

\[
F_{ab}(q) = \frac{\partial F}{\partial q_{ab}}, \quad F_{ab,cd}(q) = \frac{\partial^2 F}{\partial q_{ab} \partial q_{cd}},
\]

(5)

where \( F \) is a given function determined by the model.

If the system equilibrates, 1) the two-time functions become time-translational invariant (TTI), 2) there is reciprocity \( C_{ab}(t-t_w) = C_{ba}(t-t_w) \), and 3) we have the fluctuation-dissipation theorem (FDT):

\[
R_{ab}(t-t_w) = \frac{1}{T} \frac{\partial C_{ab}}{\partial t_w}(t-t_w), \quad \chi_{12}(t-t_w) = \frac{1}{T} (C_{12}(0) - C_{12}(t-t_w)).
\]

(6)

Putting this information in Eqs. (2) and (3) one obtains a single equation for the correlations:

\[
\frac{\partial C_{ab}(t-t_w)}{\partial t} = -\sum_c \mu_{ac} C_{cb}(t-t_w) + \frac{1}{T} \sum_c [D_{ac}(0) C_{cb}(t_w-t_w) - D_{ac}^\infty C_{cb}^\infty] + \frac{1}{T} \sum_c \int_0^t dt'^n D_{ac}(t-t') \frac{\partial C_{cb}(t'^n-t_w)}{\partial t'^n},
\]

(7)

where \( D_{ac}^\infty, C_{cb}^\infty \) stand for \( \lim_{t\to\infty} C_{ac}(t) \) and \( D_{ac}^{\infty} \equiv \lim_{t\to\infty} D_{ac}(t) \), respectively. Equation (7) is the usual equilibrium MCT equation for liquids. It would be quite difficult to guess (2) and (3) from (7)!

As an example, consider the single-mode case

\[ F(q) = q^0. \]

(8)

The mass \( \mu(t) \) is chosen so as to impose normalization at equal times of the auto-correlation \( C(t,t) = 1 \). With these choices Eq. (7) is the simplest Mode-Coupling equation proposed by Leutheusser and Bengtzelius, Götte and Sjölander. The two-time dynamical equations correspond to the low temperature dynamics of a spin-glass model introduced by Crisanti and Sommers.
The correlation decay in the high-temperature phase is obtained by solving (7) where one sees the familiar $\alpha$ and $\beta$ decay (see Fig. 1).

As one approaches the transition temperature from above the plateau in $q_{EA}$ becomes larger and larger, but at the same time something else happens: going back to the original out of equilibrium equations (2) and (3) and solving them starting from a random initial condition we discover that the time needed to equilibrate diverges at the transition. Hence, for temperatures at or below $T_g$ we no longer can assume TTI or FDT, and Eq. (7) becomes irrelevant.

In fact, the two-step process in the correlation decay becomes a waiting-time dependent two-step process: the correlations fall below $q_{EA}$ ever more slowly as one considers an older system (see Fig. 2). Non-trivial $T$-dependent exponents $\alpha$ and $\beta$ characterize the relaxation around $q_{EA}$.

We thus see that one of the equilibrium conditions (TTI) is violated: we might expect that also the FDT will be violated. Indeed, this is so: a parametric plot of $\chi(t, t_w)$ vs. $C(t, t_w)$ does not yield a straight line with gradient $-1/T$ as in equilibrium (cfr. Eq. (6)), but a family of curves as in Fig. 3. As one considers larger $t_w$ the curves approach two straight lines, one with gradient $-1/T$, corresponding to large and similar times and another with gradient $-X/T$ ($X < 1$), corresponding to large and widely separated times (i.e. the aging regime).

The fact that $T/X$ — the fluctuation-dissipation ratio — might be related to an effective temperature $T_{\text{eff}} = T/X$ was noted several times, in particular by Hohenberg and Shraiman in the context of spatiotemporal chaos and weak turbulence. Recently, it was argued that indeed $T_{\text{eff}}$ deserves the name temperature in that 1) it is related to the reading of a thermometer that is brought in contact with
Fig. 2. Decay of the auto-correlation function in the low temperature phase. $C(\tau + t_w, t_w)$ vs. $\tau$ for different waiting times, $t_w$. The plateau is larger the larger $t_w$.

with the glass, 2) it decides the direction of heat-flow and 3) it is a criterion for equilibration.

Let us first consider a very simple thermometer consisting of a harmonic oscillator that is weakly coupled to an observable $O$ of the glass. For example, in Fig. 4 we show how this can be done if $O$ is the magnetization.

In the absence of coupling $O(t)$ has fluctuations with, we assume, zero mean $\langle O(t) \rangle = 0$ and correlations $\langle O(t)O(t_w) \rangle = C_O(t, t_w) = O(N)$. The response of the system to a field $h$ conjugate to $O$ is $R_O(t, t_w) = \delta(O(t))/\delta h(t_w)|_{h=0}$.

The oscillator takes up energy from the fluctuations of $O$, and dissipates it through the response of the system until a stationary regime is achieved. If the system is in equilibrium, equipartition of energy implies that $T = \langle E_{osc} \rangle$ (we have set Boltzmann constant to one). If we now take $T_O(\omega, t_w) = \langle E_{osc} \rangle$ as the natural definition of frequency and time dependent temperature of $O$, a simple calculation yields:

$$
T_O(\omega, t_w) \equiv \langle E_{osc} \rangle_{t_w} = \frac{\omega_0 \tilde{C}_O'(\omega_0, t_w)}{\chi''_O(\omega_0, t_w)},
$$

where we have used the waiting-time dependent susceptibility and correlations defined from:

$$
[\chi'(\omega, t) + i\chi''(\omega, t)] \exp(i\omega t) \equiv \int_0^t dt' R(t, t') \exp(i\omega t'),
$$

$$
[\tilde{C}'(\omega, t) + i\tilde{C}''(\omega, t)] \exp(i\omega t) \equiv \int_0^t dt' C(t, t') \exp(i\omega t').
$$

If a system is in equilibrium, FDT holds and $T_O(\omega, t_w)$ is independent of the observable $O$, the waiting time $t_w$ and the frequency $\omega$, and is equal to the temperature
Fig. 3. The susceptibility $\chi(t, t_w)$ vs. the auto-correlation function $C(t, t_w)$ at $T < T_g$. The full curves correspond to different total times $t$, from bottom to top, $t = 12.5, 25, 37.5, 50, 75$. The dots represent the analytical solution when $t_w \to \infty$.

Fig. 4. An effective temperature measurement for a magnetic system. The coil is wound around the sample, which is in contact with the bath. Th ‘thermometer’ is the $L - C$ circuit.
of the bath.

In the system defined above, we obtain for large frequencies $T_O(\omega, t_w) = T$ as $\omega \to \infty$. If instead we consider a frequency-waiting time domain such that $C(t_w + \frac{1}{\omega}, t_w) < q_{EA}$ (i.e. we are probing the aging scale), then: $T_O(\omega, t_w) = T/X > T$.

Consider now an experiment in which we connect the oscillator to an observable $O_1$ and let it equilibrate at the temperature $T_{O_1}(\omega, t_w)$, after that we disconnect it and connect it to another observable $O_2$ and let it equilibrate at the temperature $T_{O_2}(\omega, t_w)$. The net result is that an amount of energy $T_{O_1}(\omega, t_w) - T_{O_2}(\omega, t_w)$ was transferred from the degrees of freedom associated with $O_1$ to those associated with $O_2$: the flow goes from high to low temperatures.

This is somewhat like touching two points of a glass that has been thermalizing for a long time with a copper wire. Even if the glass is still out of equilibrium we would be surprised if one could obtain an energy flow through the wire this way. Proposing that this cannot happen is equivalent to saying that for an ‘old’ glass, different observables should have in the same frequency range the same temperature.

In order to test this idea, we enlarge the model we have been discussing by considering two modes, with $F$ given by:

$$F(q) = q_{11}^p + K^2 q_{22}^p .$$

We impose normalization at equal times of the autocorrelation of both modes:

$$C_{11}(t, t) = C_{22}(t, t) = 1 .$$

through two Lagrange multipliers $\mu_{11}(t), \mu_{22}(t)$. We couple both modes through $\mu_{12} = \mu_{21} = \epsilon$ (cfr. Eqs. (2) and (3)). The constant $K \sim 0.7$ was introduced in order to break the symmetry between the modes.

Remarkably, it turns out that one can close the equations with two ansatze for the long-time aging behaviour. In terms of the effective temperatures their meaning is:

1. **Thermalized aging regime.** The effective temperatures associated with the observables $O_1, O_2$ are equal to each other for frequencies and waiting times in the aging regime differ from the temperature of the bath. At higher frequencies, their temperatures coincide with the one of the bath:

$$T_1(\omega, t_w) = T_2(\omega, t_w) = T , \quad t_w \to \infty , \quad C_{ab} > q_{ab}^{EA} , \quad \text{quasieq} .$$

$$T_1(\omega, t_w) = T_2(\omega, t_w) \neq T , \quad \omega \to 0 , \quad t_w \to \infty , \quad C_{ab} < q_{ab}^{EA} , \quad \text{aging} .$$

Not surprisingly, in this case we find that $O_1$ and $O_2$ are strongly coupled (also in the aging regime) in the sense that the cross responses in the aging regime

$$R_{12}(t, t_w) = \frac{X}{T} \partial C_{12} / \partial t_w , \quad R_{21}(t, t_w) = \frac{X}{T} \partial C_{21} / \partial t_w ,$$

are of the the same order of the self response functions ($X > 0$).
2. *Unthermalized aging regime*. The effective temperatures associated with the observables $O_1$, $O_2$ for combinations of frequencies and waiting times corresponding to the aging regime are neither equal to each other nor to that of the bath, while for higher frequencies they both coincide with the one of the bath.

\[
T_1(\omega, t_w) = T_2(\omega, t_w) = T, \quad t_w \to \infty, \quad C_{ab} > C_{ab}^{\text{EA}}, \quad \text{quasieq.}
\]

\[
T_1(\omega, t_w) \neq T_2(\omega, t_w) \neq T, \quad \omega \to 0, \quad t_w \to \infty, \quad C_{ab} < C_{ab}^{\text{EA}}, \quad \text{aging}.
\]

In this case, $O_1$ and $O_2$ are effectively uncoupled (in the aging regime):

\[
R_{12}(t, t_w) = \frac{X_{12}}{T} \frac{\partial C_{12}}{\partial t_w}; \quad R_{21}(t, t_w) = \frac{X_{21}}{T} \frac{\partial C_{21}}{\partial t_w}; \quad (14)
\]

with $X_{12} \to 0$ and $X_{21} \to 0$.

In Fig. 5 we plot $\chi(C)$ for the two uncoupled systems ($\epsilon = 0$) evolving from the initial condition $C_{11}(0, 0) = C_{22}(0, 0) = 1$ and $C_{12}(0, 0) = C_{21}(0, 0) = 0$. We see that $X_{11} \neq X_{22}$ while $X_{12} = X_{21} = 0$ (unthermalized case). In Fig. 6 we consider the same two systems, this time coupled weakly ($\epsilon = 0.7$) Clearly, after a short transient associated to short times, all curves $\chi_{ij}(C_{ij})$ become parallel. The aging-regime temperatures for the two subsystems have become equal (thermalized case).

![Fig. 5](image_url)

The effective temperature indeed regulates thermalization, and we believe this the reason why it deserves its name. The out of equilibrium dynamics of the model can then be interpreted as having fast scales that are thermalized with the bath, and slow (aging) scales that are at a higher effective temperature. As time passes,
Fig. 6. The susceptibilities \( \chi_{ij}(t, t_w) \) vs. the correlation functions \( C_{ij}(t, t_w) \) for the two weakly coupled subsystems. All the curves become parallel: also the aging regimes have thermalized.

more modes thermalize with the bath, and the frequencies that are in the aging regime become lower and lower. The effective temperature shares some, but not all, properties with the ‘fictive temperature’ of glass phenomenology (see Ref. [14] for a discussion).

References

[1] L. F. Cugliandolo and J. Kurchan; Phys. Rev. Lett. 71 (1993) 173; Phil. Magaz. B71 (1995) 50.
[2] L. Lundgren, P. Svedlindh, P. Nordblad and O. Beckman; Phys. Rev. Lett. 51 911 (1983). E. Vincent, J. Hammann and M. Ocio; in Recent Progress in Random Magnets p.297-236, editor D.H. Ryan, World Scient. Pub. Co. Pte. Ltd., Singapore 1992.
[3] L. C. E. Struik; Physical Aging in Amorphous Polymers and Other Materials, Elsevier, Houston (1978).
[4] J.P. Bouchaud and M. Mézard; J. Phys. I (France) 4 (1994) 1109. E. Marinari, G. Parisi and F. Ritort; J. Phys. A27 (1994) 7615; J. Phys. A27 (1994) 7647.
[5] L. F. Cugliandolo, J. Kurchan, G. Parisi and F.Ritort; Phys. Rev. Lett. 74 (1995) 1012. P. Chandra, M. V. Feigel’man and L. Ioffe; Phys. Rev. Lett. 76, 4805 (1996).
[6] W. Götze, L. Sjögren, Rep. Prog. Phys. 55 241 (1992).
[7] T. R. Kirkpatrick and D. Thirumalai; Phys. Rev. 36, 5388 (1987).
[8] S. Franz and J. Hertz; Phys. Rev. Lett. 74, 2114 (1995).
[9] J-P Bouchaud, L. F. Cugliandolo, J. Kurchan and M. Mézard; Physica A226, 243 (1996).
[10] L. F. Cugliandolo and P. Le Doussal, Phys. Rev. E53, 1525 (1996).
[11] E. Leutheusser, Phys. Rev. A29. 2765 (1984); U. Bengtzelius, W Götze and A. Sjölander; J. Phys. C17, 5915 (1984); W Götze and L. Sjögren; J. Phys. C17, 5759 (1984).
[12] A. Crisanti and H-J Sommers, Z. Phys. B87, 341 (1992).
[13] A. Crisanti, H. Horner and H-J Sommers; Z. Phys. B92, 257 (1993).
[14] P. C. Hohenberg and B. I. Shraiman; Physica D37, 109 (1989).
[15] M. C. Cross and P. C. Hohenberg; Rev. Mod. Phys. 65, 851 (1993).
[16] M. S. Bourzutschky and M. C. Cross; Chaos, 2, 173 (1992).
M. Caponeri and S. Ciliberto; Physica D58, 365 (1992).

[14] L.F.Cugliandolo, J. Kurchan and L. Peliti; Energy flows, partial equilibration and effective temperatures in systems with slow dynamics, cond-mat/9611044.

[15] A. Q. Tool; J. Am. Ceram. Soc., 29, 240 (1946). I. Hodge; J. Non Cryst. Solids 169, 211 (1994).