Clustering and machine learning for many body problems (orignal title- not to be discussed

arXiv:1101.0008, 1102.1519

Detecting structures in complex physical (classical or quantum) systems by multiresolution network clustering. Test cases are provided by general images where the results can be vividly seen. Ideas applied to computer vision- arXiv:1106.5793 A Replica Inference Approach to Unsupervised Multi-Scale Image Segmentation



The pictures above are challenging images to be segmented via a general unsupervised machine learning algorithm



Right panelts: results obtained via a statistical mechanical image recognition approach



(a)The variation of information V as a function of length ℓ at $\gamma = 0.1$



(b)The normalized mutual information I_N as a function of length ℓ at $\gamma = 0.1$



l=0.63



(d) The variation of information V as a function of length ℓ at $\gamma=0.05$



(e)The normalized mutual information I_N as a function of length ℓ at $\gamma = 0.05$



l = 1

l = 1.29

Do not hesitate to ask me for more





Glassy dynamics as a quantum corollary of the liquid to solid transition

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The "glass transition" problem

ZN, "A one parameter fit for glassy dynamics as a quantum corollary of the liquid to solid transition", arXiv:1510.03875

N. B. Weingartner, C. Pueblo, F. S. Nogueira, K. F. Kelton, ZN, "A quantum theory of the glass transition suggests universality amongst glass formers, arXiv:1512.04565





Possible quantum effects in standard (non supercooled) "classical" fluids

ZN, F. Nogueira, M. Blodgett, K. F. Kelton,"Thermalization and possible quantum relaxation times in "classical" fluids", arXiv:1409.1915





The "glass transition" problem

Supercooled liquids may exhibit a phenomenal increase in relaxation times without any sizable thermodynamic signatures. If it is a "transition", it is not of the standard thermodynamic type.





An eigenstate approach suggests universality in glassy dynamics













Simple theoretical arguments suggest that at high temperatures, extrapolated transport functions may saturate to quantized values.

Experimentally, the "ensemble average" of the extrapolated high temperature viscosity of 23 measured metallic fluids is quite close (0.6%) to a quantized value.





Possible minimal time scale fortransitions exactly equal to

 $\frac{h}{k_B T}$

No pre-factors of "order unity".





Supercooled liquid Viscosity





Ubiquitous glassy dynamics

Silicate, organic, metallic, ..., and electronic liquids

<u>All</u> disorder free liquids transform into a glass on sufficient supercooling.

A universal phenomenon





Numerous theories:

Adam-Gibbs (1965) Free volume (1979) Random First Order Transitions (1989) Mode Coupling (1990) Avoided Critical Transition (1995) Dynamic Facilitation (2002) and countless others

All known forms for relaxation times contain multiple



parameters



A vexing problem:

A plethora of degenerate/nearly degenerate metastable states.





Basic experimental fact:

The relaxation times rise dramatically. No agreement even on the function describing their increase as temperature is lowered!



A. Angell (1995)



The VFTH fit and the ideal glass

Most prominent fit (1921,1925,1926):

$$\eta = \eta_0 \ e^{DT_0/(T-T_0)}$$

implies an essential singularity at $T_{
m O}$

Most prevalent theories suggest such a form





A quantum approach (microscopic details irrelevant):

The system is governed by a disorder free Hamiltonian

$$H = -\sum_{i} \frac{\hbar^{2}}{2M_{i}} \nabla_{R_{i}}^{2} - \sum_{j} \frac{\hbar^{2}}{2m_{e}} \nabla_{r_{j}}^{2} - \sum_{i,j} \frac{Z_{i}e^{2}}{|R_{i} - r_{j}|} + \frac{1}{2} \sum_{i \neq i'} \frac{Z_{i}Z_{i'}e^{2}}{|R_{i} - R_{j}|} + \frac{1}{2} \sum_{j \neq j'} \frac{e^{2}}{|r_{j} - r_{j'}|} + \cdots$$





System spectrum:



 $H|\phi_n\rangle = E_n|\phi_n\rangle$





General results from equilibrium statistical -mechanics:

Although it is impossible to solve the spectral problem, we may infer general properties knowing that the system forms an equilibrated solid at low T and an equilibrated liquid at high T





The character of the eigenstates as a function of energy

As the system may equilibrate, the micro-canonical averages connect eigenstate expectation values to ensemble averages:

$$\langle \mathcal{O}(E) \rangle_{mc} \equiv \frac{1}{\mathcal{N}[E, E + \Delta E]} \sum_{E \leq E_n \leq E + \Delta E} \langle \phi_n | \mathcal{O} | \phi_n \rangle.$$

This constitutes a "dictionary" between measured values and expectation values in eigenstates.

A simple corollary:



(On average) eigenstates $|\phi_n\rangle$ of an energy density $\frac{E_n}{V} > \frac{U(T_{melt})}{V}$ (with $U(T_{melt})$ the internal energy at the melting temperature) are liquid-like





Localization at low energies:

(On average) eigenstates $|\phi_n\rangle$ of an energy density $\frac{E_n}{V} < \frac{U(T_{melt})}{V}$ (with $U(T_{melt})$ the internal energy at the melting temperature) are localized solid-like eigenstates





Supercooling as an evolution operator

An equilibrated liquid in an initial state $|\psi(t_{initial})\rangle$ is supercooled to a final state $|\psi\rangle$ at time $t = t_{final}$ via $|\psi\rangle = U(t_{final}, t_{initial})|\psi(t_{initial})\rangle$; $U(t_{final}, t_{initial}) = \mathcal{T}e^{-\frac{i}{\hbar}\int_{t_{initial}}^{t_{final}} dt'\tilde{H}(t')}$.

 $[\tilde{H}(t), H] \neq 0$

Regardless of the cooling protocol, we may expand the supercooled state in the complete eigenbasis of H:

$$|\psi\rangle = \sum c_n |\phi_n\rangle.$$

n



Broad probability density

As the supercooled liquid is out of equilibrium, a broad range of energy densities must appear. The probability density $p_T(E) = \sum_n |c_n|^2 \delta(E - E_n)$

may, simultaneously have its support from both (i) low energy solid-like states $(E_n < U_{melt})$ and (ii) higher energy fluid-type eigenstates $(E_n > U_{melt})$.





Eigenvector prob. distribution:







Thermodynamic observables

The internal energy

$$U(T) = \langle \psi | H | \psi \rangle = \int dE \ p_T(E) E \equiv \langle E \rangle$$

From this all thermodynamic observables (e.g., specific heats) may be computed





Long time averages:

$$\begin{split} \overline{\mathcal{O}}_{l.t.a.} &= \lim_{\tilde{\mathcal{T}} \to \infty} \frac{1}{\tilde{\mathcal{T}}} \int_{t_{final}}^{t_{final} + \tilde{\mathcal{T}}} dt' \; \langle \psi(t') | \mathcal{O} | \psi(t') \rangle \\ &= \lim_{\tilde{\mathcal{T}} \to \infty} \frac{1}{\tilde{\mathcal{T}}} \sum_{n,m} c_n^* c_m \langle \phi_n | \mathcal{O} | \phi_m \rangle \int_{t_{final}}^{t_{final} + \tilde{\mathcal{T}}} dt' \; e^{i(E_n - E_m)t'/\hbar}. \end{split}$$
Typically, matrix elements of local operators between degenerate global eigenstates vanishes. Phases further cancel at long times.





Long time averages in supercooled state:



$$\sum_{n} |c_{n}|^{2} \langle \phi_{n} | \mathcal{O} | \phi_{n} \rangle = \int_{E_{g.s.}}^{\infty} dE \ p_{T}(E) \ \mathcal{O}(E)$$
$$= \int_{0}^{\infty} dT' \ \mathcal{O}(T') \ p_{T}(E(T')) \ C_{V}(T')$$
$$+ \int_{\mathcal{P}TE\mathcal{I}} dE \ p_{T}(E) \ \mathcal{O}(E)$$





Terminal velocity:

$$v_{\infty} = \sum_{n} |c_{n}|^{2} \langle \phi_{n} | v | \phi_{n} \rangle = \int_{E_{g.s.}} dE \ p_{T}(E) \ v(E)$$

$$dT' v(T') p_T(E(T')) C_V(T')$$

$$+ \int_{\mathcal{PT}E\mathcal{I}} dE p_T(E) v(E)$$

Experimentally, the Stokes law is used to determine the viscosity from the measured terminal velocity of a sphere:

$$v_{\infty} = \frac{2}{9} \frac{\rho_{sphere} - \rho_{fluid}}{\eta} g R^2$$



Relaxation rate:

Similarly, if off-diagonal terms vanish due to phase cancellations then regardless of the strength of a time dependent perturbation, the relaxation rate

$$r_{s.c.} = \frac{d}{dt} \sum_{m} |\langle \phi_m | U_{pert.}(t) | \psi \rangle|^2 = \sum_{n} |c_n|^2 \frac{d}{dt} \sum_{m} |\langle \phi_m | U_{pert.}(t) | \phi_n \rangle|^2$$
$$\equiv \sum_{n} |c_n|^2 r_n = \int_0^\infty dT' \ r(T') \ p_T (E(T')) \ C_V(T')$$
$$+ \int_{\mathcal{PT}E\mathcal{I}} dE \ p_T(E) \ r(E).$$

Equilibrium relaxation rate:

$$r(T') = r(T_{melt}) \frac{T}{T_{melt}} \exp\left[\left(\frac{\Delta G(T_{melt})}{k_B T_{melt}} - \frac{\Delta G(T')}{k_B T'}\right)\right]$$





Prediction for the viscosity:

The viscosity may be computed form the terminal velocity or relaxation rate to obtain an identical form:

$$r_{s.c.}^{hydro}(T) \simeq r^{hydro}(T_{melt}) \int_{E_{melt}}^{\infty} p_T(E') \ dE',$$

$$\eta \propto 1/r, \ r^{hydro}(T' < T_{melt}) = 0,$$

$$\eta_{s.c.}(T) \simeq \frac{\eta(T_{melt}^+)}{\int_{E_{melt}}^{\infty} p_T(E') \ dE'}.$$





Average of probability dist.:

The distribution (assumed normal) has an average

$$U(T) = \langle \psi | H | \psi \rangle = \int dE \ p_T(E) E \equiv \langle E \rangle$$

The width of the Gaussian for the energy density has units of energy. The natural energy density parameter in the problem for a system at a temperature T is (CT). Width must tend to zero at low T.





Prediction for the viscosity:

$$\eta_{s.c.}(T) \simeq \frac{\eta(T_{melt}^+)}{\int_{E_{melt}}^{\infty} p_T(E') \, dE'} = \frac{\eta_{s.c.}(T_{melt})}{erfc\left(\frac{E_{melt} - \langle E \rangle)}{\sigma_E \sqrt{2}}\right)} = \frac{\eta_{s.c.}(T_{melt})}{erfc\left(\frac{T_{melt} - T}{\overline{\sigma}}\right)}$$

This simple form is expected to break down when the specific heat is no longer T independent (and thus the simple widths of the effective Gaussians in the energy density will not translate simply into temperature). By fiat, our simple single parameter form cannot capture details changes in the specific heat.





Comparison to experiment:



Data collapse:

The single parameter form predicts a data collapse (with that para.)















Viable physical content of width

The single parameter in our minimalist form was the Gaussian width for the energy density. Across all liquids examined, this width scales as T*(5%-10%). This relative value is nearly identical to the difference in the cohesive energies between locally preferred structures and global minima.





The glass "transition" is a consequence of a mobility edge for the eigenstates of the clean system.

No transition at the VFTH temperature. Using the micro-canonical ensemble, we see that the eigenstates of the Hamiltonian have a singularity only near the melting energy.

Predictions: The probability density determines both dynamical response and thermodynamic observables. These may be computed for various applied external fields.





Planck's const at very high T

$$\mathcal{Z} = h^{-DN} \int d^{DN} x \ d^{DN} p \ \exp(-\beta H)$$

Classsicaly, h is introduced as a "fudge" factor





A possible deeper origin:

$$J_n \equiv \oint_{n-th \ state} p \ dx = h(n+C)$$

$$\tau(E) = \frac{\partial J(E)}{\partial E} = \sqrt{\frac{m}{2}} \oint \frac{|dx|}{\sqrt{E - V(x)}}$$





Entropy and dynamics:

$$H_{MB} = \sum_{i} \frac{\mathbf{p}_i^2}{2m_i} + V(\{\mathbf{r}_i\}),$$

$$H_{MB}^{\text{arc}} = \frac{1}{2}m \sum_{i=1}^{N} \left(\frac{d\mathbf{r}_{i}^{\text{ rescaled}}}{dt}\right)^{2} + V_{\text{ rescaled}}\left(\{\mathbf{r}_{i}^{\text{ rescaled}}\}_{i=1}^{N}\right)$$
$$= \frac{1}{2}m\left(\frac{dx}{dt}\right)^{2} + V_{\text{arc}}(x) \equiv \frac{p^{2}}{2m} + V_{\text{arc}}(x),$$
$$J_{n} = \oint_{n-th \ state} \sum_{i=1}^{N} \mathbf{p}_{i} \cdot \mathbf{dr}_{i}$$
$$Z = \sum_{\mathbf{r}} Z_{\text{ec}}.$$





Historically, nearly always worked out for "soft" simple harmonic potentials (or none at all- "particle in a box" describing translations)













A simple generalization to arbitrary potentials



$$\sum_{E_n > E_{\text{escape}}} (2\nu_n) \langle \mathsf{n}_n^{class.} \rangle \Theta(\langle p_n \rangle)$$

$$\frac{1}{h} \int dJ \frac{\partial H^{\text{transition}}}{\partial J} e^{-\beta(H^{\text{transition}} - \mu)}$$

$$\int_{E_{\text{escape}}}^{\infty} dH^{\text{transition}} e^{-\beta(H^{\text{transition}} - \mu)}$$

$$\frac{k_B T}{h} e^{\beta(\mu - E_{\text{escape}})}$$



Transition state theory:

A simple generalization to arbitrary potentials

$$r(T) = \frac{k_B T}{h} \int D\phi \, \exp(-\beta \Delta E_{\phi})$$

Eescape

 $E_{\rm final}$

E_{initial}



Transition state theory:

A simple generalization to arbitrary potentials



Kinetic theory of viscosity:A simple generalization of usual kinetic theory
$$f(\vec{r},\vec{v},t) = \int_0^\infty f^{(0)}(\vec{r_0},\vec{v_0},t-t')e^{-t'/\tau} \frac{dt'}{\tau},$$

$$f^{(0)}(v_x - u_x(z), u_y, u_z) \equiv g(U_x, U_y, U_z)$$















The constant A_a is set by the ratio of various lengths

If all lengths are equal to each other (and further set equal to the inter-particle distance) then $A_a=1$.







Kinetic theory of viscosity:

Our trivial extension of kinetic theory to the high T quantum limit

Effectively, A = 1 in Eyring's theory No need to assume that multiple lengths are identical nor posit "holes" in a liquid.





Simple theoretical arguments suggest that at high temperatures, general extrapolated transport functions may saturate to quantized values.

Experimentally, the "ensemble average" of the extrapolated high temperature viscosity of 23 measured metallic fluids is quite close (0.6%) to the quantized





Possible minimal time scale for microscopic transitions that is exactly equal to $\frac{h}{k_B T}$

No pre-factors of "order unity".





Viscosity experiments:



Modulations of a liquid droplet. The viscosity is measured from the dynamics.





Viscosity experiments:



The fraction of liquids in the ensemble of 23 liquids studied, i.e., the probability Prob(s<S), as a function of the extrapolated high temperature viscosity assuming the single exponent form with s = (A-1) (black square symbols associated with the 23 data points). The red curve corresponds to the cumulative function associated with the normal distribution,

 $\frac{1}{2}[1 + Erf(S - \langle s \rangle)/(\sigma_s \sqrt{2})]$

