History of RSB Interview: Jean-Pierre Hansen

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PC: From a prior interview[1], we have a good idea of how you came to work on liquids. How did you first hear and get interested in the glass problem more specifically?

JPH: My PhD thesis under the direction of Loup Verlet[2], in 1969[3], dealt with the full phase diagram of the classical Lennard-Jones model based on extensive Monte Carlo simulations. Although my interests then bifurcated to molecular dynamics (MD) simulations of strongly coupled Coulombic systems, in particular the "one-component plasma"[4], I kept an eye on the

[1] D. Guthleben and B. Rotenberg, "Chapitres clefs de la vie d'un physicien : Jean-Pierre HANSEN", *Histoire de la recherche contemporaine* (2023). http://journals.openedition.org/hrc/8089 (Accessed December 12, 2023.)

[2] Loup Verlet: https://en.wikipedia.org/wiki/Loup_Verlet

[3] Jean-Pierre Hansen, "
Contribution à l'étude des systèmes de Lennard-Jones classiques et quantiques," Thèse de 3e cycle, Université Paris-Sud (1969). https://catalog.crl.edu/Record/bd08228d-7a51-516f-be54-90098253c52b (Accessed December 11, 2023.)

[4] See, *e.g.*, J.-P. Hansen, "Statistical mechanics of dense ionized matter. I. Equilibrium properties of the classical one-component plasma," *Phys. Rev. A* **8**, 3096 (1973). https://doi.org/10.1103/PhysRevA.8.3096; E. L. Pollock and J.-P. Hansen, "Statistical mechanics of dense ionized matter. II. Equilibrium properties and melting transition of the crystallized one-component plasma," *Phys. Rev. A* **8**, 3110 (1973). https://doi.org/10.1103/PhysRevA.8.3110; J.-P. Hansen, I. R. McDonald and E. L. Pollock, "Statistical mechanics of dense ionized matter. III. Dynamical properties of the classical one-component plasma," *Phys. Rev. A* **11**, 1025 (1975). https://doi.org/10.1103/PhysRevA.11.1025; J.-P. Hansen and I. R. McDonald, "Statistical mechanics of dense ionized matter. IV. Density and charge fluctuations in a simple molten salt," *Phys. Rev. A* **11**, 2111 (1975). https://doi.org/10.1103/PhysRevA.11.2111; P. Vieillefosse and J.-P. Hansen, "Statistical mechanics of dense ionized matter. V. Hydrodynamic limit and transport coefficients of the classical one-component plasma," *Phys. Rev. A* **12**, 1106 (1975). https://doi.org/10.1103/PhysRevA.12.1106; S. Galam and J.-P. Hansen, "Statistical mechanics of dense ionized matter. VI. Electron screening corrections to the thermodynamic properties of the one-component plasma," *Phys. Rev. A* **14**, 816 (1976). https://doi.org/10.1103/PhysRevA.14.816; J.-P. Hansen,

stat mech of the full phase diagram of increasingly complex systems. This led me naturally to the problem of the glass transition (GT).

PC: What initially led you to collaborate with Bernard Bernu and Yasuaki Hiwatari on studying a model of glasses with molecular simulations?[5]

JPH: The first step in that direction resulted in the 1985 MD study of the GT of a binary mixture with B. Bernu[6] and Y. Hiwatari during a visit of the latter to Paris. We were later joined by [Giorgio] Pastore in the extensive 1987 MD study of the GT in a similar soft sphere model[7].

PC: You quickly became interested in the mode-coupling theory description of supercooled liquids. In a 1988 publication with Pastore and coworkers[8], you refer to stimulating conversations you had with Prof. Götze on that topic. How did you become acquainted with this theory and why was the description particularly compelling to you?

JPH: In 1987, I moved to the newly created Ecole Normale Supérieure de Lyon (of which I had been appointed Deputy Director in charge of Research). I was joined by J.-L. Barrat[9] and J.-N. Roux[10]. We became rapidly aware of Götze's mode-coupling theory[11]. A key event was the 1989 four-week summer school on "Liquids, Freezing and Glass Transition" which I organized with [Dominique] Lévesque and J. Zinn-Justin[12] (later published by North Holland[13]). The invited lecturers included several of the leading

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G. M. Torrie and P. Vieillefosse, "Statistical mechanics of dense ionized matter. VII. Equation of state and phase separation of ionic mixtures in a uniform background," *Phys. Rev. A* **16**, 2153 (1977). https://doi.org/10.1103/PhysRevA.16.2153; J.-P. Hansen, I. R. McDonald and P. Vieillefosse, "Statistical mechanics of dense ionized matter. VIII. Dynamical properties of binary ionic mixtures," *Phys. Rev. A* **20**, 2590 (1979). https://doi.org/10.1103/PhysRevA.20.2590

[5] B. Bernu, Y. Hiwatari, and J.-P. Hansen, "A molecular dynamics study of the glass transition in binary mixtures of soft spheres," *J. Phys. C* **18**, L371 (1985). https://doi.org/10.1088/0022-3719/18/14/004

[6] **PC:** Bernu had been a graduate student with Hansen. See, *e.g.*, Bernard Bernu, *Dynamique microscopique et transport dans les fluides coulombiens fortement corrélés,* thèse d'état, Université Pierre et Marie Curie (1984). https://www.sudoc.fr/174586523

[7] B. Bernu, J.-P. Hansen, Y. Hiwatari and G. Pastore, "Soft-sphere model for the glass transition in binary alloys: Pair structure and self-diffusion," *Phys. Rev. A* **36**, 4891 (1987). https://doi.org/10.1103/PhysRevA.36.4891

[8] G. Pastore, B. Bernu, J.-P. Hansen and Y Hiwatari, "Soft-sphere model for the glass transition in binary alloys. II. Relaxation of the incoherent density-density correlation functions," *Phys. Rev. A* **38**, 454 (1988). https://doi.org/10.1103/PhysRevA.38.454

[9] Jean-Louis Barrat: https://de.wikipedia.org/wiki/Jean-Louis_Barrat

[10] Jean-Noël Roux, *La dynamique des liquides simples à l'approche de la transition vitreuse*, thèse de doctorat, Université Claude Bernard (1991). https://www.sudoc.fr/185644554

[11] Wolfgang Götze: https://en.wikipedia.org/wiki/Wolfgang_G%C3%B6tze

[12] Jean Zinn-Justin: https://en.wikipedia.org/wiki/Jean_Zinn-Justin

[13] *Les Houches, session LI: Liquides, cristallisation et transition vitreuse = Liquids, freezing and glass transition*, J.-P. Hansen, D. Lévesque and J. Zinn-Justin, Les Houches, France, 3-28 juillet 1989.

figures in the broad field of stat mech of complex systems, in particular W. Götze who lectured precisely on replica symmetry breaking and the structural glass transition.

PC: Can you describe the structure of the community doing numerical simulations of glasses at that time? Was CECAM[14] ever a hub for their discussions? If not, where and how were these exchanges mostly taking place?

JPH: CECAM indeed played an important role in the discussions on the GT when it moved from Paris to Lyon in 1990, under the directorship of Giovanni Ciccotti[15]. J.-L. Barrat and J.-N. Roux, who had followed me to Lyon, wished to have a fresh look at the individual and collective dynamical behaviour in supercooled liquids; this was mostly their successful initiative and resulted in a couple of useful papers in 1989 and 1990[16].

PC: In a 1991 piece for *Physics World*, you mentioned that "the resulting competition between local and global packing, typical of structural glasses, is reminiscent of frustration in intrinsically disordered systems such as spin-glasses"[17]. By that point, were you paying any attention to the proposal of Profs. Kirkpatrick, Thirumalai and Wolynes to integrate the mode coupling theory description within the broader theoretical context of spin glasses[18]?

JPH: In 1991, I became aware of the work by Kirkpatrick, Thirumalai and Wolynes on spin-glass theory. In fact, I returned to this approach, much later, after my return from Cambridge; I will come back to that aspect at the end of the interview.

PC: In the mid-'90s, you largely left the field of glasses. What drew you away?

Proceedings: *Liquids, freezing and glass transition*, J.-P. Hansen, D. Lévesque and J. Zinn-Justin, eds. (Amsterdam: North Holland, 1991).

[14] Centre Européen de Calcul Atomique et Moléculaire: https://en.wikipedia.org/wiki/Centre_Europ%C3%A9en_de_Calcul_Atomique_et_Mol%C3%A9culaire

[15] Giovanni Ciccotti: https://en.wikipedia.org/wiki/Giovanni_Ciccotti

[16] J.-N. Roux, J.-L. Barrat and J-P. Hansen, "Dynamical diagnostics for the glass transition in soft-sphere alloys," *J. Phys.: Condens. Matter* **1**, 7171 (1989). https://doi.org/10.1088/0953-8984/1/39/028;

[17] J.-P. Hansen, "Clarifying the kinetic glass transition," *Physics World* **4**, 32 (1991). https://doi.org/10.1088/2058-7058/4/12/29; J.-L. Barrat, J.-N. Roux and J.-P. Hansen, "Diffusion, viscosity and structural slowing down in soft sphere alloys near the kinetic glass transition," *Chem. Phys.* **149**, 197-208 (1990). https://doi.org/10.1016/0301-0104(90)80139-O

[18] See, *e.g.*, P. Charbonneau, *History of RSB Interview: Devarajan Thirumalai*, transcript of an oral history conducted 2022 by Patrick Charbonneau and Francesco Zamponi, History of RSB Project, CAPHÉS, École normale supérieure, Paris, 2022, 19 p. https://doi.org/10.34847/nkl.a03aux8z

JPH: Concerning my apparent "loss of interest" in glasses, I switched to other fields in stat mech, particularly upon my move to Cambridge in 1997 on the Lennard-Jones Chair[19], a great privilege which allowed me to enter new fields of interest under exceptional conditions. I had the privilege of supervising outstanding students, which opened new perspectives.

PC: Your book, Theory of Simple Liquids, played a major role in structuring and diffusing ideas about the field of liquids. Can you expand a bit about your decision not to include glass-related material in the second edition of the work, and to discuss mode coupling theory in the third?

JPH: Concerning the four editions of *Theory of Simple Liquids*[20], the choice of fields to be covered by Ian McDonald[21] or myself changed between editions. It is plausible that mode-coupling theory was considered to be of lesser importance by Ian when he was in charge of the discussion of phase transitions in the second edition. Remember that the field of liquids evolved dramatically between the first and the fourth editions. In any case, mode coupling theory is well described in the third edition!

PC: You gave lectures about simulation methods in glasses, notably at a NATO Advanced Study Institute on Computer Simulation in Materials Science in Aussois, in 1991[22]. Did you do so elsewhere? Did you ever teach about the theory of glasses? If yes, can you detail?

JPH: I vaguely remember the Aussois NATO Conference. In view of my limited competence, I would not consider teaching the theory of glasses beyond a presentation of the simulation aspects.

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[19] "The Professorship of Chemistry (1968) was one of the first Professorships in theoretical chemistry to be established in the UK and prior to 1968 two distinguished professors of theoretical chemistry held Plummer Professorships in the Department: Sir John Lennard-Jones FRS (1932-1953), and H Christopher Longuet-Higgins FRS (1954-1967). The first holder of the 1968 Professorship was A David Buckingham CBE FRS, succeeded in 1997 by Jean-Pierre Hansen FRS", and in 2007 by Daan Frenkel ForMemRS who occupied it until his retirement in 2017. See, *e.g.*, "Professorship of Chemistry (1968)," *University of Cambridge Human Resources* (2019). https://www.hr.admin.cam.ac.uk/files/chemistrytheo.pdf (Accessed December 12, 2023.)

[20] J.-P. Hansen and I. R. McDonald, *Theory of Simple Liquids* (New York: Academic Press, 1976); *Theory of Simple Liquids, 2nd Edition* (New York: Academic Press, 1986); *Theory of Simple Liquids, 3rd Edition* (New York: Academic Press, 2005); *Theory of Simple Liquids: With Applications to Soft Matter* (New York: Academic Press, 2013)

[21] See, *e.g.*, G. Jackson, "Ian R. McDonald (1938–2020)," *Mol. Phys.* **118**, e1857534 (2020). https://doi.org/10.1080/00268976.2020.1857534

[22] *NATO Advanced Study Institute on Computer Simulation in Materials Science: Interatomic Potentials, Simulation Techniques and Applications*, Aussois, France, 25 March - 5 April 1991. J.-P. Hansen, "An introduction to molecular dynamics, with applications to the glass transition," In: *Computer Simulation in Materials Science: Interatomic Potentials, Simulation Techniques and Applications* (Dordrecht: Springer Netherlands, 1991): 3-20.

PC: Is there anything else you would like to share with us about this era that we may have missed?

JPH: Upon my return from Cambridge to Paris in 2008, I gained interest in integral equation approaches to the equilibrium liquid-ideal glass transition, in collaboration with J.-M. Bomont (Université de Lorraine) and G. Pastore (University of Trieste), under the influence of the spin-glass theory of Giorgio Parisi and co-workers. We published a series of papers from 2014 to 2019[23]. The last paper "Revisiting the replica theory of the liquid-to ideal glass transition" appeared in 2019[24]. To conclude, the glass transition remained of genuine interest throughout much of my scientific career!

[23] See, *e.g.*, J.-M. Bomont, J.-P. Hansen and G. Pastore, "An investigation of the liquid to glass transition using integral equations for the pair structure of coupled replicae," *J. Chem. Phys.* **141**, 174505 (2014). https://doi.org/10.1063/1.4900774; "Hypernetted-chain investigation of the random first-order transition of a Lennard-Jones liquid to an ideal glass," *Phys. Rev. E* **92**, 042316 (2015). https://doi.org/10.1103/PhysRevE.92.042316; "Reflections on the glass transition" In: *Advances in the Computational Sciences: Symposium in Honor of Dr Berni Alder's 90th Birthday* (Singapore: World Scientific, 2017): 108-130. https://doi.org/10.1142/9789813209428_0007

[24] J.-M. Bomont, J.-P. Hansen and G. Pastore, "Revisiting the replica theory of the liquid to ideal glass transition," *J. Chem. Phys.* **150**, 154504 (2019). https://doi.org/10.1063/1.5088811