History of RSB Interview: John Finney

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Over Zoom, from Prof. Finney's home near Gloucester, United Kingdom.
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PC: Good morning, Professor Finney. Thank you very much for joining me. As we discussed ahead of time, the general theme of this series of interviews is the history of spin glasses and replica symmetry breaking. In your case, however, we will be talking about ideas that were in the air mostly before or parallel to the advent of these in the world of structural glasses, which are intimately related to spin glasses. To learn a bit more first about your own background, can you tell us a bit more about your family and your studies before starting university?

JF: [0:00:37] I was brought up in Stockport, a town just south of Manchester. I went to a grammar school at age 11. That, I suppose, is where I got into physics, largely through (a) inspirational teachers, and (b) realizing that if I specialized in something that wasn't a science subject, then the science would probably be a closed book to me for the rest of my life, whereas if I studied science, I could still do other things. Really, it was actually inspirational teachers. I was challenged by the subject. I wanted to know how the world works, and that was a good enough incentive.

PC: What brought you to Cambridge to do physics?

JF: [0:01:38] Again, same reason. I sat a physics, chemistry, and mathematics examination. I think I got in through the chemistry, but immediately dropped it because it was rather boring, and just basically focused on physics, with a bit of metallurgy and crystallography thrown in, which was probably quite useful for the rest of the stuff I ended up doing.

PC: You worked during your undergraduate days with Helen Megaw[1], who was crystallographer. Can you tell us a bit more about that experience?

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[1] Helen Megaw: https://en.wikipedia.org/wiki/Helen_Megaw

JF: [0:02:12] She was one of the crystallography lecturers, and a bit dry. I didn't realize at the time how famous a person she was, just like a lot of the lecturers we had. If I'd known then what I know now, I would have been asking all sorts of things about the building of the atomic bomb, for example. Some of my lecturers were actually involved in the physics of it, and the discovery of fission. A missed opportunity, I must say. The crystallography at that point was what was called a half subject. I had to choose a number of courses, one of which, the main course, was physics and then I had to choose others. I was offered geology, but my Director of Studies advised me not to as he saw no future in it! So, I didn't do any geology, but I did crystallography, which I think served me in good stead later on.

PC: Did you do research as well with her, or was this only a single class interaction?

JF: [0:03:21] No. She was just one of the lecturers. I did a crystallography practical, which was really just taking data on a powder and getting cell dimensions and things from it. That introduced me to the problems of computing. (This was in the very early days of computing.) We processed the data on the old EDSAC 2[2] computer, which required five-hole perforated tape input. I think it took me far longer to correct all the parity errors on the tape than it did to do the rest of the project.

PC: Was that your first interactions with computers?

JF: [0:04:05] It was indeed, yes.

PC: What then drew you to pursue a PhD in crystallography with J. D. Bernal[3], in particular.

JF: That goes back to my school days. I remember one of the classes we were doing with one of the schoolteachers called Roger Stone, who was head of physics. We were doing a class on solids and gases, which was all very straightforward. We learnt all about crystalline solids, and we learnt all about gases. Muggins[4] here thought there was something missing here. So, I said: “Please sir, what about liquids?” To which he replied to the effect that liquids were very difficult, but that there was a guy at Birkbeck College[5], who was trying to do something about it. So, that just somehow

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[2] EDSAC 2: https://en.wikipedia.org/wiki/EDSAC_2

[3] J. D. Bernal: https://en.wikipedia.org/wiki/J._D._Bernal

[4] Muggins: a title used humorously to refer to oneself. See, *e.g.*, https://en.wiktionary.org/wiki/muggins

[5] Birkbeck College: https://en.wikipedia.org/wiki/Birkbeck,_University_of_London

got parked in the back of my mind somewhere. When it came—many years later—for me to think of what I'd like to do, whether I'd want to do any research in physics… Because after I finished my BA, I went on to train for teaching through a post-graduate education course at the University of Leicester. Partly because of (a) idealism, I wanted to actually teach; (b) I wanted a break from what was a highly intensive undergraduate course. But after the teaching one-year course, I thought: "Well, let's see about the research, and approach this guy at Birkbeck." I just wrote a letter, and I got invited down to talk to him. Then things moved from there.

PC: So, there was no relationship between your undergraduate crystallography experience and your PhD.

JF: [0:05:44] No. None whatsoever. Apart from the fact that when I registered to do the MSc in crystallography at Birkbeck, Jim Jeffery, who ran the course, found out I'd done the Cambridge crystallography module and told me not to bother. So, I didn't bother.

PC: Your thesis work with Bernal was on disordered packings of hard spheres.[6] If I understand correctly that thesis involved using particle positions obtained from physical hard sphere models and analyzing them with computational tools for geometrical analysis. Why weren't there direct simulations of hard spheres being crunched? Why weren't you using synthetic hard sphere positions at that point?

JF: [0:05:30] If you look at what Bernal was saying in the early '60s…. He was aware of the work that was going on at Los Alamos[7], for example, but he said that even with the computational power they had, they were limited to small numbers. He really wanted to get away from problems of boundary effects and to be able to try to squash the thing into a maximum density possible, in order to actually see what the geometry was like. In a sense, I was asked—at least in the early stages—to build on the work he'd done on the small models and to build a large model[8], where I could more or less guarantee—because of the way we did it—there were no significant

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[6] John Leslie Finney, *Random packings and the structure of the liquid state*, PhD Thesis, Birkbeck College (1968). http://vufind.lib.bbk.ac.uk/vufind/Record/467729 (Accessed July 11, 2023.)

[7] William Wayne Wood (1924-2005), in Los Alamos, simulated up to 48 hard spheres during that period. See, *e.g.*, W. W. Wood and. J. D. Jacobson, "Preliminary results from a recalculation of the Monte Carlo equation of state of hard spheres," *J. Chem. Phys.* **27**, 1207-1208 (1957). *J. Chem. Phys.* **27**, 1207–1208 (1957). https://doi.org/10.1063/1.1743956; W. W. Wood, *Monte Carlo Calculations of the Equation of State of Systems of 12 and 48 Hard Circles*, LA-2827 (Los Alamos: Los Alamos Scientific Laboratory, 1963). https://books.google.com/books?id=Mi1wmQr4TQkC

[8] For additional background, see, *e.g.*, J. L. Finney, "Bernal's road to random packing and the structure of liquids," *Philo. Mag.* **93**, 3940-3969 (2013). https://doi.org/10.1080/14786435.2013.770179

boundary effects, and to try to achieve the maximum possible density without any crystallization. That was far too big a challenge for computational abilities at the time. Looking at things now, it's a totally different matter, of course. I could get all the computing that I did for my thesis in probably about half an hour on my phone. Things then were of a very different type. It was a question of taking in tapes to the central university computer in the evening where it was run overnight when there was nothing else going on, and then poring over results the day after. It was a very different world in terms of computing. Bernal did actually, in his earlier days, try computing approaches[9]. When he set up his lab at Birkbeck, he was aware of the possibilities of computing, particularly in terms of crystallographic structure solutions. In fact, he set up a computing section in the department under Donald Booth[10], which in the end sort of amalgamated with the university computing service[11]. He did try several ways of building densely packed models by computer but found in fact it was far too computationally difficult and he couldn't see any way of getting over the limitations of the computational power at the time. After the thesis, I suppose I did some… Well, during the thesis work, I did some simulations with soft spheres, where in fact things are somewhat easier to deal with than in hard spheres. As you see if you look at the work I published in 1970[12], you can see how the hard sphere packing, when you soften it, actually went quite close to what you get for something like liquid argon, liquid inert gases etc.

PC: For your thesis proper, where did these two configurations you were working with come from? How were they obtained?

JF: [0:09:24] The main one I used, the dense packing, was made by taking a load of steel balls, ¼" steel balls (or ball bearings) and compressing those in a football bladder, which would… Not a football bladder, but a balloon, if you like, on the inside of which was glued hard spheres, steel balls of

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[9] See, *e.g.*, J. D. Bernal, "Geometry of the structure of monatomic liquids," *Nature* **185**, 68-70 (1960). https://doi.org/10.1038/185068a0; J. D. Bernal, "The structure of liquids," *Sci. Am.* **203**, 124-137 (1960). https://www.jstor.org/stable/24940581

[10] Andrew Donald Booth: https://en.wikipedia.org/wiki/Andrew_Donald_Booth

[11] See, *e.g.*, Roger Johnson, *School of Computer Science & Information Systems: A Short History* (London: Birkbeck University of London, 2008). https://www.dcs.bbk.ac.uk/site/assets/files/1029/50yearsofcomputing.pdf (Accessed July 11, 2023.); R. Johnson, "A short history of Computer Science at Birkbeck," *Birkbeck Perspectives* (25 August 2020). http://blogs.bbk.ac.uk/bbkcomments/2020/08/25/a-short-history-of-computer-science-at-birkbeck/ (Accessed July 11, 2023.); R. Palmer, "Crystallography at Birkbeck," *Crystallography News* 164 (March 2023). https://www.crystallography.org.uk/assets/pdf/crystallography-news/2023-03.pdf (Accessed July 11, 2023.)

[12] J. L. Finney, "Random packings and the structure of simple liquids II. The molecular geometry of simple liquids," *Proc. Roy. Soc. Lond. A* **319**, 495-507 (1970). https://doi.org/10.1098/rspa.1970.0190

different sizes, to try to give a non-regular outer surface to try to prevent crystallization. That was then essentially sealed up. We "worked" it, kneaded it [as] if you're making bread, kneaded it as much as we possibly could, and then hoped we'd got to a stage where it was at the maximum density. Then, we poured liquid wax into the system, and let it solidify. Then, we peeled off the outer layers and measured the coordinates optically, peeling the spheres off layer-by-layer and melting the surrounding wax. So, it was fairly lengthy task – we measured the coordinates of just under 8,000 spheres, which took a bit of time to measure. Then, of course, you can work on the data.

That was the hard sphere data. The loose data packing I worked on was that from David Scott[13]. I didn't do any other of the loose packing stuff at all in terms of constructing models.

PC: How did you obtain the coordinates from Prof. Scott? Did you have a relationship?

JF: [0:11:05] Bernal had gotten a hold of those beforehand.

PC: So, you never were in touch with Professor Scott yourself?

JF: [0:11:12] Yes. In discussions. He was interested in the results that were coming out. There were letters going backwards and forwards every now and then. And I did drop in to see him when I was in Pittsburgh for that year. By that time, of course, most of this work was finished.

PC: What was the immediate reception to your work on these packings?

JF: [0:11:42] It depends on the audience. It was generally positive, but there was a marked resistance from the what I'll call died-in-the-wool theoreticians, who were working on models which were either compressed gases, using assumptions which were not valid at the density of a liquid, or working on disordered crystals, which of course was totally inconsistent with the ideas that we were developing. So, some theoreticians found the concept rather difficult to accept, though the importance of excluded volume in controlling the structure did appear to be realized by some. For example, there was a Faraday Discussion in '67,

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[13] George David Scott (1918-1985). See, *e.g.*, G. D. Scott, "Packing of Spheres: Packing of Equal Spheres," *Nature* **188**, 908–909 (1960). https://doi.org/10.1038/188908a0; G. D. Scott, "Radial Distribution of the Random Close Packing of Equal Spheres," *Nature* **194**, 956–957 (1962). https://doi.org/10.1038/194956a0

on liquids[14], and John Rowlinson[15], whom you may have heard about—a major theoretician in liquids—did actually come out and say: "This is demonstrating the importance of repulsive forces in controlling structure", which is quite obvious, I suppose, to a crystallographer, but I certainly, being a young scientist without much experience of the scientific world, was saying at that time: "Well, these guys aren't actually thinking about structure; they're just playing around with equations and they can't actually see what the reality of those equations is." That might have been an attitude which had been encouraged, or implied if you like, by the way Bernal looked at these things. Because he had similar views. Theoreticians thought this was a crazy way to work. You play with equations. There were some exceptions. John Ziman[16] was extremely positive about our work and was very complementary about it. I was very grateful for that encouragement. Also, soon after the work was finished, I was phoned by Peter Eggelstaff[17], who you may or may not have come across, again another theoretician, who I got to know a lot better later on, who was just about to move from Harwell[18] to the University of Guelph[19], in Canada. I went over to Harwell to talk to him, and he was very interested in trying to use the data that we got to calculate some triplet correlations in the liquid model, which I played around with a bit. But then he popped off to Guelph and that sort of ground to a halt. So, there was quite a lot of positive response, but quite a lot of the theoreticians weren't thinking in this sort of way. Bernal was a crystallographer as well as a polymath and he wanted to try to envisage the liquid structure. I think that some of the things he said in his Bakerian lecture in this respect are worth looking at[20]. Atoms can't approach closer than a certain distance and that is actually going to be a relevant control on structure. For more complex systems, covalent and directional forces will come in, which of course makes a difference to the liquid structure, for example, in water.

PC: You mentioned that Bernal was in touch with the Los Alamos group early on about their simulation work. Were you at all involved or in discussions with them?

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[14] A General Discussion on the Structure and Properties of Liquids, 11-13 April 1967, University of Exeter, Exeter, UK. See, *e.g.*, J. D. Bernal and J. L. Finney, "Random close-packed hard-sphere model. II. Geometry of random packing of hard spheres," *Discuss. Faraday Soc.* **43**, 62-69 (1967). https://doi.org/10.1039/DF9674300062

[15] John S. Rowlinson: https://en.wikipedia.org/wiki/John_Shipley_Rowlinson

[16] John M. Ziman: https://en.wikipedia.org/wiki/John_Ziman

[17] See, *e.g.*, P. Schofield, "Peter Egelstaff in Memoriam (1925–2015)," *Neutron News* **26**(2), 47-48 (2015). https://10.1080/10448632.2015.1028284

[18] AERE Harwell: https://en.wikipedia.org/wiki/Atomic_Energy_Research_Establishment

[19] University of Guelph: https://en.wikipedia.org/wiki/University_of_Guelph

[20] J. D. Bernal, "The Bakerian lecture, 1962. The structure of liquids." *Proc. Roy Soc. Lond. Ser. A* **280**, 299-322 (1964). https://www.jstor.org/stable/241587

JF: [0:15:33] I can't say he was in contact with them. He was aware of the work, and he mentioned it in the Bakerian lecture[21], and said that, in essence, he didn't see that computing was far enough advanced to be able to do the job computationally. I wasn't in touch with them, apart from I had one interaction with Wood, but it wasn't very positive. I can't remember how it came about. I probably have a letter somewhere in the loft, but it would take me several weeks probably to find it. You'll be aware of that sort of problem with archives!

PC: So, you were not comparing results with their simulations, for instance.

JF: [0:16:20] I did later on. I don't know if you've seen the paper I wrote in *Phil. Mag.* in 2013[22], which was the result from a meeting in Dublin[23], which Denis Weaire[24] organized, where I looked at some of their results. Their packings were all at significantly lower density than the limits that we were working at, which perhaps justifies in fact Bernal's position on that, that computations weren't, at that time, sufficiently capable of getting to the high density conditions that he wished to get to.

PC: After your thesis, you obtained a lectureship at Birkbeck, but you went on a sabbatical leave at Pittsburgh for a year, in 1971, with George Jeffrey[25]. What drew you to work with him and go to the US at that point?

JF: [0:17:26] I went to the to the Triannual international crystallography meeting in '69 in Stony Brook[26]. I didn't give a paper, but I was at a session there, where there was paper given by an eminent German scientist on a disordered crystalline model of a liquid, which I had looked at and thought: "This is actually bonkers. This is crazy." Of course, I had data in my back pocket to show, and joining the discussion I showed this data. Jeffrey was

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[21] **PC:** In that lecture, Bernal only mentions the work of Berni J. Alder, citing some work he did while in Caltech, but who as then at Lawrence Livermore National Laboratory. See, *e.g.*, B. J. Alder, S. P. Frankel, V. A. Lewinson, "Radial Distribution Function Calculated by the Monte-Carlo Method for a Hard Sphere Fluid," *J. Chem. Phys.* **23**, 417–419 (1955). https://doi.org/10.1063/1.1742004

[22] See Ref. 8.

[23] *International Workshop on Packing Problems*, S. Hutzler and A. Mughal, Trinity College Dublin, Ireland, 2-5 September 2012. Proceedings: S. Hutzler, "Preface," *Philo. Mag.* **93**(31–33). http://dx.doi.org/10.1080/14786435.2013.854101

[24] Denis Weaire: https://en.wikipedia.org/wiki/Denis_Weaire

[25] See, *e.g.*, Bryan Craven, "George A. Jeffrey (1915–2000)," *Acta Cryst. B* **56**, 545-546 (2000). https://doi.org/10.1107/S0108768100008181

[26] Eighth Congress and General Assembly of the International Union of Crystallography, 13-21 August 1969, Stony Brook, New York, USA. See, *e.g.*, "Eighth General Assembly and International Congress of Crystallography," *Acta Cryst.* **A27**, 497-506 (1971). https://doi.org/10.1107/S0567739471001098

in the audience. I didn't know at the time, but he came to me at breakfast the day after and was quite amused by the way I'd actually treated this eminent German scientists and said: “Come to Pittsburgh for a year.” So, I thought: “Well, why not? I'd like to spend a year in the States in another department and get some wider experience, and it will be giving me a great opportunity to meet a whole lot of other scientists that I may not otherwise have chance to meet.” In fact, it was very helpful, because by that time I was moving further away into aqueous solutions and water-biomolecule systems, and I was able to make a lot of contacts by being over the States. For example, I was invited by Fred Richards[27] to Yale to give a talk. That was all very helpful for my future work. So, it was good. I didn't do much work on the simple liquids then. I worked and did some straightforward crystallography on an organic compound with a horrendous name and a bit more computing on more powerful computers that I had been used to using[28]. It was all very good. I'm very grateful to have had that opportunity. But it did come about in a rather strange way, I thought. You insult a German scientist, and you get invited to work in the States on whatever you want to. I should say that the gentleman concerned, there were no hard feelings, and we had some good sake sessions when we met at a meeting in Japan in 1972.

It also actually resulted in my seeing again how certain aspects of science were working. Bear in mind, I was under 30 at this point. As a result of that Stony Brook session, I got invited to MIT and to Harvard to visit Dave Turnbull's group[29]. He had one of his co-workers there, Slade Cargill[30]**,** who was presenting structural data on an amorphous metal alloy. He showed its experimental pair distribution function. Instead of looking like a simple radial distribution function of a simple liquid, where you have a first sharp peak and a smooth second peak, his second peak was split. That was exactly the behavior that we had been finding in the hard sphere packing. So, as a result of my showing a slide of the pair distribution function of these dense hard sphere packing, I got invited to have a talk with Dave and his group, which again was very good. I enjoyed that interaction. It was very helpful to me. But I was a bit taken aback a year or so later when I

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[27] Frederic M. Richards: https://en.wikipedia.org/wiki/Frederic_M._Richards

[28] P. Carr, J. L. Finney, P. F. Lindley and G. T. De Titta, "The crystal and molecular structure of cis-1,2-dimethyoxy-carbonyl-1,2-bis(4-nitrophenyl)cyclobutane," *Acta Cryst. B* **33**, 1022-1026 (1977). https://doi.org/10.1107/S0567740877005299

[29] David Turnbull: https://en.wikipedia.org/wiki/David_Turnbull_(materials_scientist)

[30] George Slade Cargill III, *Non-crystalline metallic solids: structural models and an investigation of nickel-phosphorus alloys*, PhD Thesis, Harvard University (1970). https://id.lib.harvard.edu/alma/990037772700203941/catalog

found a paper in the *Journal of Applied Physics*[31], reproducing my data and claiming this as a model of structure of an amorphous metal, without any suggestions that I might be involved in the paper. So, it was not a very pleasant experience from that point of view. Perhaps underlining the fact that one ought to be careful about how you use other people's data and what ethics should be operating within the scientific community.

PC: Was that first trip to Cambridge, in Massachusetts, at the same time as the conference?

JF: [0:22:11] It was just after the conference, yes. I was staying over. At the time, my then-wife had a brother who was at Yale, and we planned to spend some time after the conference with him and his wife. So, it was simple enough then to just jump up to Boston. Also, another crystallographic colleague, who was at Birkbeck at the time but who was American, was over visiting his parents in Kingston, Rhode Island. So, we had an invitation to spend a day or two with them. So, we said: "OK! We'll go and see the people in Cambridge and then we'll come back and spend a couple of nights with you in Kingston on the way back."

PC: Coming back to Birkbeck. You started using these packing models for a variety of contexts, including structural glasses. Did your interest in glasses arise from that interaction with the Turnbull group?

JF: [0:23:22] No. It was before. It was when I was working on the model, I'd seen a paper in Nature, I think, somewhere, where there was a radial distribution function presented of, I think, 80/20 palladium-silicon. There was some suggestion in the paper of a split second peak in the reported radial distribution function. So, in one of my discussions with Bernal, I suggested we look at the hard sphere packing as a structural model of a glass. He didn't seem to be interested, and more less I was given free rein to go and develop that line of things if I wished to. In fact, there was probably far more interest in the packing work amongst the metallic glass community than there was amongst the liquid community at the time. So, we began to look at some of the problems involving binary systems. We did some preliminary model building (and later explored computations) on building binary systems, but there was no interaction before the 1969 Stony Book meeting with the metallic glass community. After I'd finished my PhD, I had quite a lot of interactions with the metglass community. As

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[31] G. S. Cargill III, "Structural Investigation of Noncrystalline Nickel-Phosphorus Alloys," *J. Appl. Phys.* **41**, 12-29 (1970). https://doi.org/10.1063/1.1658310; G. S. Cargill III, "Dense Random Packing of Hard Spheres as a Structural Model for Noncrystalline Metallic Solids," *J. Appl. Phys.* **41**, 2248–2250 (1970). https://doi.org/10.1063/1.1659198

well as Dave Turnbull's group, there was work in Japan and Germany, while Robert Cahn's[32] group in Sussex were a particular focus for the work in the UK. There were several meetings I went to where much of the discussion was on the problems problems of measuring and characterizing structures.

PC: You got in touch, eventually, with Charles Bennett,[33] who was working on computational algorithms to generate disordered packings, side-stepping in a sense the compression[34]. How did that interaction come about?

JF: [0:25:28] It came about during the visit to Dave Turnbull, except Charles wasn't around the day I turned up. He was out somewhere else, but he got in touch somehow with me. It must have been a message I got via a phone call or something, I can't remember how. He was getting back in Boston about late afternoon on the day we were leaving, at about six o'clock on the train to Kingston, Rhode Island, to stay with my American colleague and his family as I mentioned earlier. So, I said that the only way we could get together was if he came down to the station where we could talk. So, we started talking at the station and carried on talking – so, he got on the train and came all the way to Kingston, Rhode Island, on the train, stayed for dinner, and caught the last train back to Boston. So, that's how it started.

PC: Then, you kept in touch?

JF: [0:26:24] Yes, we did, and we published a joint paper, which is probably worth forgetting[35]. We kept in touch. He went off to Argonne at some point, working with Aneesur Rahman[36]. We made some contact there, when we were working on computer simulation of water and such like. Charles convinced me on the train from Boston that the coordination number in the random packing should be six, exactly, which we examined later on in some of the models, and we came to the same conclusion[37]. Charles dropped by in London about two to three years ago, so we met up again, which is good because I hadn't seen him for decades. He's not working on this stuff anymore. In the early computing days, he had lovely story of when he was trying computationally to show a sphere packing on

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[32] Robert W. Cahn: https://en.wikipedia.org/wiki/Robert_W._Cahn

[33] Charles Bennett: https://en.wikipedia.org/wiki/Charles_H._Bennett_(physicist)

[34] See, *e.g.*, C. H. Bennett, "Serially deposited amorphous aggregates of hard spheres. Journal of applied physics," **43**, 2727-2734 (1972). https://doi.org/10.1063/1.1661585

[35] J. L. Finney and C. H. Bennett, "Structural changes at the Lennard-Jones glass transition", In: *Rapidly quenched metals,* N. J. Grant and B C. Giessen, eds. (Cambridge: MIT Press, 1976): 231-236.

[36] Aneesur Rahman: https://en.wikipedia.org/wiki/Aneesur_Rahman

[37] K. Gotoh and J. L. Finney, "Statistical geometrical approach to random packing density of equal spheres," *Nature* **252**(5480), 202-205 (1974). https://doi.org/10.1038/252202a0

the screen, computationally, writing the code to exhibit the packing on the screen. He said the most difficult thing to do was to code in hidden line removal. You look at computer games these days and it's a different world.

PC: In the early 1970s, some physicists were suggesting an analogy between low-temperature properties of structural glasses and of spin glasses. There was the work notably of Phil Anderson, Bert Halperin and Chandra Varma[38]. Given that you were working on disordered packings which are essentially zero-temperature versions of liquids, were you paying attention to this proposal? Was this on your radar, or part of discussions?

JF: [0:28:19] Not really. As I said at that point, I was moving much more into non-spherical systems and water. It was in the periphery, but it wasn't something that I felt I should be putting a lot of effort into I'm afraid.

PC: You nevertheless wrote a review, a few years later, in 1977, for *Nature* on "Modelling of amorphous metals and alloys"[39], in which you reiterated your assessment that the quenched rates achieved by molecular dynamics were far too high to compare with what is relevant experimentally. Were you nevertheless paying attention to the work being done at that point, a few future generations of computers later by, say, Leslie Woodcock[40] and Julian Gibbs[41], who were looking at denser supercooled liquids? If yes, what was your impression of the work at that point?

JF: [0:29:24] Earlier when I said I was doing my thesis work on soft sphere systems, I was using Les's software[42]. So, we made contact during that time when he was at Royal Holloway. We came across each other, from time to time since then. I knew he was actually trying to get a high-density packing, which is fine. When he got it, I was delighted because he got exactly the same as we did for the maximum density. So, we've crossed paths every now and then since. We did some collaborative work on trying to identify crystallization from a randomly packed structure. There is a joint paper on this in the literature[43]. Essentially, he and Neil Cape did the computer simulations, and I did the structure analysis, and it went quite well.

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[38] P. W. Anderson, B. I. Halperin and C. M. Varma, "Anomalous low-temperature thermal properties of glasses and spin glasses," *Philo. Mag.* **25**, 1-9 (1972). https://doi.org/10.1080/14786437208229210

[39] J. L. Finney, "Modelling the structures of amorphous metals and alloys," *Nature* **266**(5600), 309-314 (1977). https://doi.org/10.1038/266309a0

[40] L. V. Woodcock, "Glass transition in the hard-sphere model," *J. Chem. Soc., Farad Trans. 2* **72**, 1667-1672 (1976). https://doi.org/10.1039/F29767201667

[41] J. M. Gordon, J. H. Gibbs and P. D. Fleming, "The hard sphere 'glass transition'," *J. Chem. Phys.* **65**, 2771-2778 (1976). https://doi.org/10.1063/1.433422

[42] Leslie V. Woodcock: https://en.wikipedia.org/wiki/Leslie_V._Woodcock

[43] N. J. Cape, J. L. Finney and L. V. Woodcock, "An analysis of crystallization by homogeneous nucleation in a 4000-atom soft-sphere model," *J. Chem. Phys.* **75**, 2366-2373 (1981). https://doi.org/10.1063/1.442299

PC: What about the group Julian Gibbs[44], who was contemporary to Les's work there?

JF: [0:30:39] They worked together. I didn't do any work with Julian. I examined one of his PhD students. I was aware of what they were doing and that was fine. It was good to see the results that came out of it.

PC: Can you give us a feeling of what was the community people interested in hard spheres and packing at that point? Were there any dedicated meetings? Were there collaborations? Or was this just independent groups with loose communication pathways?

JF: [0:31:15] I'm not sure I can answer that, because then I was moving on to other things. There were groups that were working and interacting. I went from time to time to meetings where different groups got together and they talked about some of the problems they had. I remember one in particular in Manchester, when Les was there. I got the impression that there were a few groups around the country that were working, collaborating, and interacting with one another. I suspect they all knew what each group was doing, and they were working in a collaborative fashion, as far as I can tell. That was the British community. In terms of international community, then I think we talked about that before with the metallic glasses people. There was Robert Cahn over here. I did some work on multicomponent packings with D. S. Boudreaux and Harold Frost, but this got no further than a presentation at an APS meeting in 1979[45]. And I was in touch from time to time with Frans Spaepen[46] to talk about things.

PC: As you mentioned a number of times, you were leaving the study of glasses already in my the mid-'70s. Beyond that review, did you stay abreast of the advances that were being made? Or was it only though these odd meetings where you were invited and hearing talks?

JF: [0:32:50] I didn't really remain involved at all, I think. Things would pass by me from time to time. By about that time I was getting funding to develop other things. Since that '77 paper, I don't think I have published much since then on the hard sphere system. A bit on soft sphere relaxation and such like with the group that was then at Bedford College[47], but that really came

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[44] Julian Gibbs: https://en.wikipedia.org/wiki/Julian_Gibbs

[45] D. S. Boudreaux, H. Frost and J. L. Finney, "Short-range order in metallic glass alloys," *Bulletin of the American Physical Society* **24**(3), 331 (1979).

[46] See, *e.g.*, "Frans A. Spaepen," *Physics Tree* (n.d.). https://academictree.org/physics/peopleinfo.php?pid=73949 (Accessed July 11, 2023.)

[47] Bedford College: https://en.wikipedia.org/wiki/Bedford_College,_London

out of bumping into them at a meeting, and we decided we ought to actually see what a hard sphere system would relax to under a Lennard-Jones and other potentials[48]. By that time, I was getting funding for aqueous systems and the group was focused on that. Perhaps I should say that at the time the crystallography department—from mid-'70s onwards—was shifting very much to increase its emphasis on structural molecular biology. In a way, I suppose, because of the work I was doing on water and on water-protein interactions, it was a natural way for me to work and collaborate with others in the department. I suppose, the move towards the more complex systems was lubricated by the changes in the scientific direction of the department under a new Head of Department.

PC: About a decade ago, you nevertheless co-authored a piece with Les Woodcock that reviewed Bernal's sphere packing approach to understand liquids and glasses[49]. How did this article come together?

JF: [0:35:08] Les drove it. It is probably obvious from the paper. When I formally retired—whatever that word means—my colleagues insisted on having a little meeting and, of course, asked me who I would like to talk. Because Les had been quite helpful and he had done all this work on packing, it seemed to me that he would be somebody from whom it would be good to hear what he thought about things at that much later stage. So, I asked him to give a talk at this do. This was in 2009. He was very gung-ho, as Les can be, about the Bernal model and presented data which were quite good. He suggested that perhaps we should try and think of writing something together related to this. So, we followed that up from time to time later. Following a completely unrelated conference in Bradford, I stayed with him a couple of days – he was living nearby up in the Yorkshire Dales. We decided to go ahead and try to do it. I basically did the hard sphere stuff, and he wrote the rest of it. It's probably quite clear who wrote which bit. Have you read it?

PC: I have perused it. During your time in London or elsewhere, did you ever teach about glasses or dense packings in general? If yes, can you detail?

JF: [0:36:56] Not in any detail, no. I was at Birkbeck until '88, and there was no real place for it in the MSc in crystallography or in the biomolecular organization class. My teaching there was essentially diffraction theory etc. and structural chemistry. When I moved to UCL in '93, then it just

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[48] See, *e.g.*, J. A. Barker, M. R. Hoare and J. L. Finney, "Relaxation of the Bernal model," *Nature* **257**(5522), 120-122 (1975). https://doi.org/10.1038/257120a0

[49] J. L. Finney and L. V. Woodcock, "Renaissance of Bernal's random close packing and hypercritical line in the theory of liquids," *J. Phys.: Condens. Matter* **26**, 463102 (2014). https://doi.org/10.1088/0953-8984/26/46/463102

would come in a bit as part of the general condensed matter course, but nothing beyond the very basic.

PC: We are approaching the end of this discussion. Is there anything else you would like to share with us about this era that we may have skipped or overlooked?

JF: [0:38:04] I'm not sure there's much more than I've said. I think there was a clear difference in approach of the scientists who look at structure in three dimensions and the theoreticians, if you like. I've been infected by crystallography in a way, and it seems to me that if you want to understand something which is made up of things in space, then having some idea of how they are organized is actually quite useful. As I said earlier, in the '60s, structure models didn't seem to be a way of looking at things. I think Bernal tried to cut through that. I think he summarizes the situation in his 1962 Bakerian lecture. He said something like: "From all the theories fundamental and satisfying for the crystallographer, however they may appeal to the physical chemist of the mathematician, I wanted to know a more concrete picture of the structure and one making use of Occam razor, not to multiply entities beyond necessity. I wanted some kind theory of liquids that was somehow homologous to a crystalline solid, but rather different in kind, and have a general quality of inhomogeneity without the assumption of any special groups.[50]" I liked that attitude. It seemed to me a good way of looking at things. Though I think it was then a minority of view.

You're working in the glass field now, you will know whether that still is a minority view, or whether you think there is some sensible mileage in looking at these things from a structural viewpoint. Things may have moved on, I don't know. In terms of the work on more complex liquids, then we're still looking there in terms of structures and microphase separation etc., which I still take a structural view on. Or the neutron scattering work that I've been doing in collaboration with various people, we're always ending up looking at detailed real space (three-dimensional), structures, not just two-dimensional partial pair distribution functions. In fact, one of the things I'm really pleased about—this is going away from glasses…

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[50] From Ref. 20, p. 301: "Throughout this period I found all these theories fundamentally unsatisfying to a crystallographer, however much they might appeal to a physical chemist or a mathematician. I wanted a more concrete picture of the structure and one making more use of Ockham's razor 'Not to multiply entities beyond necessity'. I wished to get some kind of theory of liquids that would be homologous to that of the crystalline solid as well as radically different in kind, and have a general quality of homogeneity without the assumption of any special groups, although, as will be seen later, such groups may arise spontaneously and out of necessity."

I remember when I was going to the ‘72 crystallography congress in Japan[51]. Because I was visiting a colleague in the States just beforehand, I tagged on to a chartered flight which the American crystallographers were organizing. On that flight—in these chartered flights in those daysthe bar was free, which may have helped—or perhaps hindered—the conversation on board. I got into talking to a crystallographer called David Harker[52], who did some of the early work on protein crystals and some of the early theoretical work on crystal structure solution. I tried to tell him what I was hoping to do. I said something to the effect of: “You crystallographers, you can find the structure of an assembly of molecules in crystals. What I would like to do is find a way of extracting the structure of a liquid in the same sort of way.” He said at the time that that was impossible. It couldn’t be done.

Well, we actually now can by making use of what is possible with neutron scattering with isotope substitution allied to advanced computational techniques. I’m quite pleased about that! In the early days of the atomic glass work, all people were producing then were total pair distribution functions with no way of separating out the partials. It was though the advent of isotope substitution in neutron diffraction that the Holy Grail at the time could be actually achieved. In those developments, people like John Enderby[53] who was instrumental in getting that sort of work going, were very important and were very constructive in interactions with me. So, I like to look at structures, as looking at structures in real space helps me to understand things. They may not help other people, but they certainly do help me.

PC: In closing, do you still have notes, papers, and correspondence from that epoch? If yes, to have a plan to deposit them in an academic archive at some point?

JF: [0:43:34] The answer is yes, a loft full. It will need a lot of sorting. And who would be interested? Can you answer that question?

PC: We can discuss it afterwards. There are possibilities.

JF: [0:43:52] I’m a bit of a hoarder, so there are all sorts of stuff up there. When I moved to Rutherford in ’88, for about five years, at the neutron

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[51] *Ninth General Assembly and International Congress of Crystallography*, 26 August-7 September 1972, Kyoto, Japan.

[52] David Harker: https://en.wikipedia.org/wiki/David_Harker

[53] John Enderby: https://en.wikipedia.org/wiki/John_Enderby

source, I packed a lot of papers in boxes, and they are still in those boxes, so there is a lot of sorting to do sometime.

PC: Thank you very much for this conversation.