History of RSB Interview: Ulf Bengtzelius

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Interviewer:
Patrick Charbonneau, Duke University, patrick.charbonneau@duke.edu
Location:
Over Zoom, from Dr. Bentzelius's office in Värmdö, Sweden.
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PC: Hello, Dr. Bengtzelius. Thank you very much for joining us. As we discussed ahead of time, the goal of this series of interviews is to go over the history of replica symmetry breaking and its sources of inspiration. That's the context in which we're discussing with you today. But before we get to that, I'd like to ask you a few questions on your background. First, can you tell us a bit about your family and your studies before getting to university.

UB: [0:00:40] I came directly. After high school, I did my military service[1], and then I started at Chalmers, studying engineering physics.

PC: Did you know all along that you wanted to become a scientist or when did this interest arise?

UB: [0:01:00] That was since I was thirteen years [old] or something like that.

PC: When you chose Chalmers, why Chalmers and why engineering physics? What drew you to this particular field?

UB: [0:01:19] Chalmers was the closest to where I was brought up, so it was quite natural. And Chalmers had a good reputation. I wanted to study something that was a bit more theoretical when it comes to mathematics, physics, and chemistry. It's an engineering education. It was a master's program.

I became interested in doing a PhD. My first goal was to do it in experimental physics, but the professor that I was interested to work with, he got a professorship in Lund University, in Sweden. So, I went out to work in industry for one year to see what else I could do. But then I decided to

[1] Conscription in Sweden: https://en.wikipedia.org/wiki/Conscription_in_Sweden

go to one department, Theoretical Physics at Chalmers, when I started my PhD studies.

PC: What led you to join Alf Sjölangren[2]'s group, more specifically, in Theoretical Physics?

UB: [0:02:43] I had taken courses that he gave in thermodynamics and was interested in statistical physics. So, that was the natural choice for me.

PC: Can you tell us more about how the group and how your joining the group functioned? You had completed a master's, you went industry, then you applied to the Theoretical Physics PhD program. Were you directly going to work with him, or did you take classes?

UB: [0:03:17] The first year was mostly classes.

PC: So, you didn't join his group right away?

UB: [0:03:25] I did.

PC: I understand. You knew him from undergraduate or master's level classes you had taken with him. Can you tell us a bit how the group functioned in general? How big was it? Did you have regular meetings?

UB: [0:03:42] No, it was a very small group. Alf Sjölander had a history of only having one PhD student at the time. Now, when I started, we were actually two, so it was a special occasion. We were two: me[3] and Göran Wahnström[4], who after his PhD continued to work. He went for a postdoc and got a professorship at Chalmers.

PC: What was the original research project you started working on when you joined the group?

UB: [0:04:23] That was the glass transition.

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[2] Alf Sjölander: https://sv.wikipedia.org/wiki/Alf_Sj%C3%B6lander

[3] Ulf Bengtzelius, *Dynamics of supercooled liquids and of liquid-glass transitions*, Doctoral Thesis, Chalmers tekniska högskola (1986).

[4] Göran Wahnström, *Theoretical investigation of the motion of an adsorbed atom*, Doctoral Thesis, Chalmers tekniska högskola (1985). https://search.ebscohost.com/login.aspx?direct=true&db=cat09075a&AN=clpc.oai.edge.chalmers.folio.ebsco.com.fs00001000.bf2bc164.8adf.4c88.b0c3.34bed4a1156e&site=eds-live&scope=site&authtype=guest&custid=s3911979&groupid=main&profile=eds (Consulted July 16, 2023.)

PC: From the start?

UB: [0:04:28] Yes, from the start. Alf Sjölander had the idea that some relaxation modes take longer and longer and that ought to be formulated in mathematics. We actually started out with the density-density correlation function. We started out with formally exact equations for the density-density correlation function but that couples to higher-order correlation functions. So, you get this this BBGKY hierarchy of equations[5]. Since we had experience in the group [with] the mode-coupling approach to break this hierarchy[6], we put out the equations with the Mori approach[7] of mode coupling. I was working also with Lennart Sjögren, who was a researcher in the group. At that point, one thing that comes into the mode-coupling approaches is the static structure factor. So, I just took that from the Wertheim and Thiele expression for hard spheres[8], but still though we needed some computation to calculate. So, I came up with the idea of replacing the structure factor with a constant and then a peak, only taking into account the first peak in the static structure constant. So, we came up with a very compact equation that one can easily solve. When we got this far, we were joined by Wolfgang Götze from Munich[9]. His contribution was that we found that diffusivity was scaling with a constant that diverged as a power factor. We calculated [the exponent to be] 1.76[10] or whatever it was. That was a basis for the first paper[11].

PC: Can you tell us a bit more about how that collaboration came about? I think that Götze was then a visitor for a year in the group. Is that right?

UB: [0:07:47] It could have been for more than one year. I don't remember now.

PC: And immediately, you started working with him? You had written equations, and then what happened?

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[5] BBGKY hierarchy: https://en.wikipedia.org/wiki/BBGKY_hierarchy

[6] See, *e.g.*, P. Charbonneau, *History of RSB Interview: Lennart Sjögren*, transcript of an oral history conducted 2021 by Patrick Charbonneau, History of RSB Project, CAPHÉS, École normale supérieure, Paris, 2021, 19 p. https://doi.org/10.34847/nkl.382d6bmv

[7] More-Zwanzig: https://en.wikipedia.org/wiki/Mori-Zwanzig_formalism

[8] "Exact solution of the Percus Yevick integral equation for hard spheres," *SklogWiki* (2018). http://www.sklogwiki.org/SklogWiki/index.php/Exact_solution_of_the_Percus_Yevick_integral_equation_for_hard_spheres (Consulted July 16, 2023.)

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

[10] This exponent is now commonly known as gamma in the glass literature.

[11] U. Bengtzelius, W. Götze and A. Sjölander, "Dynamics of supercooled liquids and the glass transition." *J. Physics C* 17.33 (1984): 5915.

UB: [0:08:03] He was very interested, and he came up with the idea that probably the simplified equation [should] scale with [a power law]. That was his contribution.

PC: As you mentioned, this led to your first paper, which is quite well recognized to this day. Can you walk us through what led to the writing of the paper so you when did you decide that the result deserved to be published and how to publish it?

UB: [0:08:48] We did some comparison with experimental results and found that we were up to something. So, it was quite natural that we wrote an article. That was published in the *Journal of Physics C*, a European journal.

PC: What was the initial reception to that work?

UB: [0:09:23] I don't know that I actually remember. Shortly after, about the same time, Leutheusser[12], a former student of Götze published another paper, and Götze was quite upset about this. I didn't care so much about this because I thought our approach was more solid.

You know, Götze passed away a little more than a year ago. I was contacted by a former colleague of his, Joachim Wuttke, who was writing an obituary[13]. He knew Wolfgang quite well, and what he revealed to me was that during the work we did with the first article, Götze had a seminar in Jülich and Leutheusser was there. According to Götze, that's why Leutheusser had the idea to rush and write an article about the glass transition. He was quite upset about that.

PC: When did you become aware of Leutheusser's manuscript?

UB: [0:10:56] That was after we submitted our article.

PC: So, you got a preprint of his at that point?

UB: [0:11:07] I don't know. It was published at about the same time as ours. I think it was a bit later than ours was first published.

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[12] E. Leutheusser, "Dynamical model of the liquid-glass transition," *Phys. Rev. A* **29**, 2765 (1984). https://doi.org/10.1103/PhysRevA.29.2765. **PC:** Dr Leutheusser's paper was received on 5 December 1983 and published 1 May 1984. Bentzelius et al. submitted their manuscript on 29 March 1984, and it appeared in the November 1984 issue of the journal.

[13] J. Wuttke, "Wolfgang Götze (1936–2021)," *Neutron News* **33**(3), 29 (2022). https://doi.org/10.1080/10448632.2022.2093088

PC: Did you give talks about this? Did you go to conferences where you presented that work yourself?

UB: [0:11:23] No, I didn't.

PC: So, you don't have a perspective on how the other people received these ideas.

UB: [0:11:33] No.

PC: In subsequent papers you studied the thermodynamic implications of this ergodic-non-ergodic transition as well as the specific heat behavior of the Lennard-Jones model.

UB: [0:11:48] Before that, Alf Sjölander went on a sabbatical to the US, and I started discussing with Lennart Sjögren about… The transition looks a lot like a second-order transition. [It has] the same characteristics as a second-order phase transition. So, we wrote an article about how the thermodynamic quantities change at the glass transition point: changes in specific heat, compressibility and so on[14]. We also derived an expression for the Prigogine-Defay ratio[15]. What goes into the Prigogine-Defay ratio is the change in specific heat, compressibility, and heat expansion. For a first order transition, this would be 1, and there had been a lot of papers published by chemists showing that this was larger than 1, but these experiments were done on polymers. We did the calculations for a hard sphere system, but the expression we got—a quite simplified expression—fitted quite well to experimental data. So, we published that in the *Journal of Chemical Physics*. After that, I wrote two papers in *Physical Review A*[16], where we did the calculations on Lennard-Jones liquids.

PC: I presume that the interest in the Lennard-Jones model was because the model was heavily simulated. Were you at all in touch with people who were doing the simulations, such as Les Woodcock[17] and Sidney Yip[18]?

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[14] U. Bengtzelius and L. Sjögren, "Changes of thermodynamic quantities at the glass transition," *J. Chem. Phys.* **84**, 1744–1751 (1986). https://doi.org/10.1063/1.450473

[15] "Prigogine-Defay ratio," *SklogWiki* (2012). http://www.sklogwiki.org/SklogWiki/index.php/Prigogine-Defay_ratio (Consulted July 16, 2023.)

[16] U. Bengtzelius, "Theoretical calculations on liquid-glass transitions in Lennard-Jones systems," *Phys. Rev. A* **33**, 3433 (1986). https://doi.org/10.1103/PhysRevA.33.3433; "Dynamics of a Lennard-Jones system close to the glass transition," *Phys. Rev. A* **34**, 5059 (1986). https://doi.org/10.1103/PhysRevA.34.5059

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

[18] See, *e.g.*, P. Charbonneau, *History of RSB Interview: Sidney Yip*, transcript of an oral history conducted 2022 by Patrick Charbonneau, History of RSB Project, CAPHÉS, École normale supérieure, Paris, 2023, 13 p. https://doi.org/10.34847/nkl.7740w7ht

UB: [0:14:23] I was in contact then with Sidney Yip, because during my dissertation he was the opponent.

PC: But you were not talking about simulations. Were you just taking results that we already published?

UB: [0:14:38] Yeah.

PC: I noticed that none of these follow-up papers list Prof. Götze as a collaborator. Was your collaboration then just for that first paper? Did you not keep in touch with him afterwards?

UB: [0:15:01] No. He was looking at the manuscripts. He was reading the manuscript before I sent it for publishing.

PC: So, he was in touch, you were still exchanging, but he was not contributing.

UB: [0:15:22] No, we didn't do the paper together, but he was reviewing and commenting it.

PC: After your thesis you left academia to industry. You had a pretty successful PhD thesis; did you have any interest in pursuing a postdoc?

UB: [0:15:52] Actually, I got funding in Chalmers, but to me it was a bit lonely. No one else was working in the area, and no one really understood what we were working on. The mathematics was a bit complicated as well. So, I felt it was a bit of a lonely pursuit to continue on this travel. I am an engineer in the background. My first interest was in doing something in experimental physics. So, I decided I'll go work in the industry instead.

PC: Although you left, did you nevertheless keep abreast of list of the evolution of the mode-coupling theory you first formulated, or did you lose contact?

UB: [0:16:48] No, not much. But I started taking up contact with the institution later on. They reorganized. We had one big department. It was the Physics Department, and it was more experimental physics. I was doing my PhD in the Department of Theoretical Physics. These two departments were joined into the Applied Physics Department. I was asked to be a member of a council. That was years ago. Then I participated in… We actually merged the old Physics Department with Theoretical [Physics]. That was already joined, but then we had a bit of leftover. That was Fundamental Physics, people working string theory and that kind of stuff. We merged these two into a new department called Physics Department. This was in 2006. Then, I became the head of this advisory council, which I'm still active

on. I meet with the Head of Physics Department regularly. there are regular meetings with them and this council, following the strategies for long-term research, recruitment; not so much about education, but a bit of that also. So, I'm following a bit the research being done Chalmers.

PC: If I understand correctly, you didn't keep a particular interest in this subfield, but you have remained deeply invested the institution and the Physics Department throughout almost four decades now.

UB: [0:19:45] Yes.

PC: We're getting toward the end of the questions I have. Is there anything else you would like to share with us about the era surrounding your PhD?

UB: [0:20:04] At the time of my dissertation, we had no hope really that the minute details of the elastic peak would ever be observed in experiments. But there were neutron-scattering experiments utilizing a technique called neutron spin-echo, where they could confirm our results from this elastic peak. It was a two-peak structure, [in fact]. Then, I heard that people working with chaos theory classified the simple equation we had according to some classification they have in in chaos theory also. So, it had caught interest[19], but that was after I left Chalmers.

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

UB: [0:21:55] No, I have no communications that I can archive. As I said, the reason I left was that it was quite lonely work because no one else was working in the area. There were a lot of chemists to were doing experiments, but they didn't understand the mathematics behind it. But I know that a lot the chemists who wrote papers also were checking the results from our theories.

PC: Yes, they have. Thank you very much for this discussion.

[19] See, *e.g.*, Wolfgang Götze, *Complex Dynamics of Glass-Forming Liquids: A Mode-Coupling Theory* (Oxford: Oxford University Press, 2009).