History of RSB Interview: Sidney Yip

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PC: Good morning, Professor Yip. Thank you very much for joining us. As we were just discussing, the theme of this series of interviews is the idea of replica symmetry breaking in spin glasses and beyond. But before we get to that, I have a few questions on background to try to situate your contributions to this topic. First, can you tell us a few things about your youth and how you became interested in engineering, in particular?

SY: [0:00:28] Good morning, Patrick. It will be my pleasure to set the context. I was born in China and grew up in Shanghai. At age 14, I immigrated to the US with my parents and two brothers. 1949 was a tumultuous time, the country was changing hands from the Nationalist to the Communists party[1]. That the whole family was able to get out was one of the most fortunate events in my life. We arrived in San Francisco. My education was interrupted during this time. Anyway, I got through high school and went off to college in 1953. For reasons I chose to go to the University Michigan, spending 10 years at Ann Arbor to get three degrees plus a year of postdoctoral research, B.S. in mechanical engineering, M.S. and PhD in nuclear engineering. So, I started off as a mechanical engineer and ended up becoming a nuclear engineer[2]. I had a favorite advisor, who was such a good role model that I stayed on another year to write a book with him, the title of which is *The Foundations of neutron transport theory*[3]. The work turned out to be basically a second quantization derivation of the neutron transport equation, which is essentially the Boltzmann equation for neutrons. My thesis research was about neutron scattering in water. The problem of the dynamics of water molecules was of interest in nuclear engineering at the time because nuclear power reactors being built used

[1] Chinese Communist Revolution: https://en.wikipedia.org/wiki/Chinese_Communist_Revolution
[2] Sidney Yip, *The Scattering of Slow Neutrons by Polar Liquids*, PhD thesis, University of Michigan (1963). https://search.lib.umich.edu/catalog/record/990021459510106381 (Accessed January 18, 2023.)
[3] Richard K. Osborn and Sidney Yip, *The Foundations of Neutron Transport Theory* (New York: Gordon and Breach, 1966).

water as both moderator and coolant. Let me now move to the next stage where I went further into kinetic theory and transport phenomena. Traditional transport theory, like the Boltzmann equation, was well-known to be only valid at low fluid density. The problem of dense fluids, simple liquids, was already a longstanding challenge in kinetic theory.

After Ann Abor I went to Cornell for two years as a research associate in Applied Physics with Mark Nelkin[4]. Nelkin was well-known in nuclear reactor physics and had just moved to Cornell from General Atomics[5]. Through him, I got to know some of the Cornell faculty, people like David Mermin[6] in physics and Ben Widom[7] in chemistry.

PC: You went to work with Nelkin at Cornell, but was your objective to learn more about the kinetic theory of gases and kinetic theory in general?

SY: [0:06:53]. It was a research associate position that allowed me to expand my interest in time correlation functions and statistical mechanics.

PC: So, it was to work with Nelkin mostly, not for the particular topic.

SY: [0:07:13] Yes. Nelkin was interested to see how much of his background in neutron transport could be applied to more general problems in statistical physics. Working with him made me aware of the challenge to extend the Boltzmann equation to the liquid state. If you ask what is the bottleneck, the answer is how should one deal with the many-body dynamics associated with discrete particle collisions in a liquid. When you go through a range of densities from dilute fluid (gases) to intermediate density (liquids at their critical points) and high-density (liquids at their triple points), it is to be expected the dynamics of particle collisions becomes correspondingly more difficult to treat from a first-principles approach. Over time ingenious though heuristic models have been proposed with parameters that require fitting to experiments.

PC: Were these all conversations you were having during your time at Cornell already, or are you anticipating a bit?

SY: [0:14:50] It's a bit of both. When I was at Cornell it was already appreciated particle collisions in low-density gases could be adequately treated as uncorrelated binary collisions as in the Boltzmann equation. But this

[4] Mark Nelkin: https://en.wikipedia.org/wiki/Mark_Nelkin
[5] General Atomics: https://en.wikipedia.org/wiki/General_Atomics
[6] David Mermin: https://en.wikipedia.org/wiki/N._David_Mermin
[7] Benjamin Widom: https://en.wikipedia.org/wiki/Benjamin_Widom

description is expected to break down when the inter-particle distance becomes comparable to the collision mean free path. As for me it was not until I went to MIT in 1965 that I decided to focus on the kinetic regime where details of the collision dynamics need to be treated explicitly.

PC: We'll get to glasses eventually, but I'd like to take you back on your own trajectory. After your time at Cornell, you didn't work much on the kinetic theory up until your collaboration with Gene Mazenko[8], in the early to mid-70s. That's when there was this idea of resummation, or fully renormalized kinetic theory[9]. Can you describe how this collaboration came about and what led you to pursue this work?

SY: [0:17:23] It was my good fortune that after my arrival Gene Mazenko was finishing his thesis at MIT[10]. While looking for a postdoctoral position, he was outside of my office one day wondering how he could just drop in to introduce himself. Unbeknownst to [him], I was looking for someone who could join me in trying to understand the high-density correlated collisions. So, it was serendipitous we got together as soon as he finished his Ph.D.

At about the same time, I should also mention [that] I got to talk to Paul Martin[11], at Harvard. Let me take you back to my second year at Cornell, I got a call from MIT. The nuclear engineering department head at the time remembered meeting me when I was a student at Ann Arbor, Michigan. He said: "We have a position, a faculty opening here. Would you be interested?" I said: "Yes! Of course!" So, I went over for an interview and was offered a position before I left. After I had accepted at MIT but before leaving Ithca, I went to a Gordon conference, and met Paul Martin while shaving together one morning. I told him I was going to start a faculty position at MIT. We hit it off pretty well during that encounter, and he ended up saying "Why don't you come up the street to talk over lunch once

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[8] "Gene F. Mazenko," *Academic Tree* (n.d.). https://academictree.org/physics/peopleinfo.php?pid=165055 (Accessed January 18, 2023.)

[9] See, *e.g.*, G. F. Mazenko, "Fully renormalized kinetic theory. I. Self-diffusion," *Phys. Rev. A* **7**, 209 (1973). https://doi.org/10.1103/PhysRevA.7.209; "Fully renormalized kinetic theory. II. Velocity autocorrelation," *Phys. Rev. A* **7**, 222 (1973). https://doi.org/10.1103/PhysRevA.7.222; "Fully renormalized kinetic theory. III. Density fluctuations," *Phys. Rev. A* **9**, 360 (1974). https://doi.org/10.1103/PhysRevA.9.360

[10] Gene Mazenko, *Quantum Statistical Analysis of Sound and Related Processes in a Gas*, PhD thesis, Massachusetts Institute of Technology (1971). https://mit.primo.exlibrisgroup.com/permalink/01MIT_INST/ejdckj/alma990006005460106761 (Accessed January 18, 2023.)

[11] Paul C. Martin: https://de.wikipedia.org/wiki/Paul_C._Martin_(Wirtschaftswissenschaftler); "Paul Cecil Martin," *AIP Physics History Network* (n.d.). https://history.aip.org/phn/11606015.html (Accessed January 18, 2023.)

in a while." What a stroke of luck! For the next three years I was able to see him every now and then. We ended up with Dieter Forster joining us[12].

Now back to my working with Mazenko. Gene also was very interested in talking to Martin because he had studied the Martin-Schwinger formalism[13]. Looking back Gene and I were both really lucky to be able to interact with Paul Martin while working with each other.

Gene later moved to Chicago and had collaborations with Sid Nagel[14]. Before leaving MIT, he started developing what he later called renormalized kinetic theory [15]. This was around the same time that Ken Wilson[16] at Cornell, did his renormalization group work[17]. Wilson came out to Harvard to give talks on renormalization group and it was appreciated that many other fields in statistical physics could benefit from this breakthrough.

PC: In 1979, you wrote a review of that approach[18], in which you highlighted the connection between renormalized kinetic theory and mode-coupling theory, in that both approaches "in fact should be viewed as basically belonging to the same theoretical description of fluids." You then predicted that the resulting description could claim to be valid for fluids at all densities. Interestingly, in that review, you don't mention viscous fluids or glasses at all. Was the topic not yet of interest to you at that point, or did you not yet see a plausible way of connecting these dynamical approaches to the glass problem?

SY: [0:23:20] It's more the latter. At that time, we had certain urgent issues we wanted to address, but I was still in an exploratory stage. Initially I was not aware of the glass transition problem, which later on became so dominant.

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[12] P. C. Martin and S. Yip, "Frequency-Dependent Friction Constant Analysis of Diffusion in Simple Liquids," *Phys. Rev.* **170**, 151 (1968). https://doi.org/10.1103/PhysRev.170.151; D. Forster, P. C. Martin and S. Yip, "Moments of the momentum density correlation functions in simple liquids," *Phys. Rev. 170*, 155 (1968). https://doi.org/10.1103/PhysRev.170.155; "Moment method approximation for the viscosity of simple liquids: Application to argon," *Phys. Rev.* **170**, 160 (1968). https://doi.org/10.1103/PhysRev.170.160

[13] KMS state: https://en.wikipedia.org/wiki/KMS_state

[14] See, *e.g.*, B. Kim and G. F. Mazenko, "Mode coupling, universality, and the glass transition," *Phys. Rev. A* **45**, 2393 (1992). https://doi.org/10.1103/PhysRevA.45.2393

[15] See, *e.g.*, G. F. Mazenko, T. Y. Wei and S. Yip, "Thermal fluctuations in a hard-sphere gas," *Phys. Rev. A* **6**, 1981 (1972). https://doi.org/10.1103/PhysRevA.6.1981; P. M. Furtado, G. F. Mazenko and S. Yip, "Effects of correlated collisions on atomic diffusion in a hard-sphere fluid," *Phys. Rev. A* **14**, 869 (1976). https://doi.org/10.1103/PhysRevA.14.869

[16] Kenneth G. Wilson : https://en.wikipedia.org/wiki/Kenneth_G._Wilson

[17] See, *e.g.*, K. G. Wilson, "Renormalization group and critical phenomena. I. Renormalization group and the Kadanoff scaling picture," *Phys. Rev. B* **4**, 3174 (1971). https://doi.org/10.1103/PhysRevB.21.1003

[18] S. Yip, "Renormalized kinetic theory of dense fluids," *Annu. Rev. Phys. Chem.* **30**, 547-577 (1979). https://doi.org/10.1146/annurev.pc.30.100179.002555

Around 1980, a pretty critical year for me, I took a sabbatical in Munich. My purpose was to work with Wolfgang Götze[19]. Back in '79 already, I was aware of what Götze [was doing]. He and a two students, Manfred Lücke[27] and Jürgen Bosse[28], were publishing papers on what would now be called the mode-coupling theory approach to liquids[29], showing quite amazing results. Apparently not many people then fully appreciated the potential insights offered by the mode-coupling theory. Certainly Götze was fully aware. He did not just call it mode-coupling theory right away. If you look at his papers, he called it dynamical theory. Later on, some people may say: "It's a mean-field theory with uncontrolled approximations." People who want to criticize him have held such opinion, but to me, given the kinetic theory community was having a hard time predicting or explaining experimental findings, the approach of mode-coupling was certainly worthy of attention. Besides experiments there was also the advent of molecular dynamics simulations, results from Berni Alder[20] and Aneesur Rahman[21]. It is not just theory for theorists, but also for experimentalists who are doing new experiments like neutron and light scattering in liquids. Rahman at Argonne was publishing his seminal paper on molecular dynamics for continuous potentials, while Berni Alder and Tom Wainright, at Lawrence Livermore, were publishing their hard sphere simulations. Very important questions were being asked about the decay of the velocity autocorrelation function. Why is it not exponential? Why is it $t^{d/2}$, where d is the dimension? When I was asked to write an *Annual Reviews*, I was trying to see intuitively what would make sense. It seemed that we're all dealing with the same beast. The beast is how do you gain control of the dynamical description, which includes the mean field.

PC: So, you went on sabbatical to Munich in '79 or '80. Did you know Professor Götze personally ahead of time, or was it only through his papers?

SY: [0:27:57] Again, it was for me a very fortunate personal circumstance. I knew of his work, but I did not know if he knew me. 1979 was to be the year of my second sabbatical. I wanted to go spend at least part of it in Munich with Götze, because I wanted to learn more about this mode-coupling theory approach. I felt it had great potential for many of the issues confronting the statistical physics community, particularly the study of time correlation functions in liquids. It turned out Wolfgang and Kurt Binder[22], another person with whom I wanted to spend some time, jointly

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

[20] Berni Alder: https://en.wikipedia.org/wiki/Berni_Alder

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

[22] Patrick Charbonneau, *History of RSB Interview: Kurt Binder*, transcript of an oral history conducted 2020 by Patrick Charbonneau and Francesco Zamponi, History of RSB Project, CAPHÉS, École normale supérieure, Paris, 2021, 20 p. https://doi.org/10.34847/nkl.5f2b685y

nominated me for the Humboldt prize for US scientists[23]. That's how I got to spend half a year with Wolfgang and the second half with Kurt in Jülich.

PC: This visit, as you said, was to learn more about the mode-coupling approach. It led to a very important series of papers about the random Lorentz gas, what you called the Lorentz model of overlapping hard spheres[24]. First, did you know about this model ahead of time? Second, how did the collaboration come about?

SY: [0:30:03] At my first meeting with Wolfgang in his office, I also met Eberhard Leutheusser[25], a graduate student with Wolfgang at the time. Wolfgang simply said to me: "You and I can talk about what it is we want to do while you're here. Eberhard has been working with me; he's about ready to finish." It seemed like there was immediate agreement the three of us would work together. Wolfgang and I got along very well, and the same with Eberhard. At the end of my sabbatical, I went off to Jülich, and Wolfgang was happy to let Eberhard come visit and continue our collaboration. My association with Eberhard was uninterrupted after I left Wolfgang, and after my sabbatical Humboldt agreed to send Eberhard on a postdoctoral fellowship to spend a year with me at MIT.

PC: I'd like to talk about the random Lorentz gas first. Where did the idea for that work come about. What were you trying to show? What was the program?

SY: [0:32:06] Again, let me take you w back to when I was at Cornell. During 1963 - 1965, while I was at Cornell, I got to work with Hans van Leeuwen[26], a visitor with Ben Widom in the chemistry department. From Hans I learned about a mathematical model in statistical physics, the so-called Lorentz gas[27]. In one dimension, the model particles are always bound,

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[23] Humboldt Foundation: https://en.wikipedia.org/wiki/Alexander_von_Humboldt_Foundation

[24] W. Götze, E. Leutheusser and S. Yip, "Dynamical theory of diffusion and localization in a random, static field," *Phys. Rev. A* **23**, 2634 (1981). https://doi.org/10.1103/PhysRevA.23.2634; "Correlation functions of the hard-sphere Lorentz model," *Phys. Rev. A* **24**, 1008 (1981). https://doi.org/10.1103/PhysRevA.24.1008; "Diffusion and localization in the two-dimensional Lorentz model," *Phys. Rev. A* **25**, 533 (1982). https://doi.org/10.1103/PhysRevA.25.533

[25] Eberhard Leutheusser, *Die Dynamik von klassischen Flüssigkeiten harter Kugeln*, PhD thesis, Technische Universität München (1979). https://opac.ub.tum.de/TouchPoint/perma.do?q=+1035%3D%22BV002076884%22+IN+%5B2%5D&v=tum&l=de (Accessed January 19, 2023.)

[26] Hans van Leeuwen: https://en.wikipedia.org/wiki/Hans_van_Leeuwen_(physicist)

[27] See, *e.g.*, Ya. G. Sinai, "Ergodic properties of the Lorentz gas," *Funct. Anal. Appl.* **13**, 192–202 (1979). https://doi.org/10.1007/BF01077487; H. A. Lorentz, "The motion of electrons in metallic bodies," *KNAW Proc.* **7**, 438, 585 & 604 (1905). https://dwc.knaw.nl/DL/publications/PU00013989.pdf;

while in two and three dimensions the particles could become trapped. So this was in my background when I met Wolfgang. I don't remember now if he was also aware of the Lorentz model, including the work van Leeuwen and A. Weijland were doing[29], in any case we decided fairly quickly this was a good model system to analyze using the mode-coupling theory. We were careful to explore first only the Lorentz gas. We thought if hard sphere works, then corrections with attractive forces could be added along the lines of Weeks-Chandler-Anderson. It turned out the Lorentz gas problem was quite rich. Of the three papers we published the first was a general formulation where we didn't even call it the Lorentz model. I think calling it simply a static random field is appropriate. The second paper is called *Correlation functions of the hard-sphere Lorentz model*, and then the third one is on the two-dimensional Lorentz model. We looked at the diffusion coefficient and analyzed particle localization. That was how I gained insights into nonlinear feedback mechanism in diffusion and localization. It turned out shortly thereafter, for the glass transition, structural arrest and cage localization were also part of the excitement.

PC: At about the same time, you collaborated with Bernie Alder on molecular simulations for determining neutron scattering functions for hard spheres.[28] (So, hard spheres were there as well.) By any chance did you at a time meet Mary Ann Mansigh[29], who was writing the computer codes?

SY: [0:35:50] Oh, yes! I got to know Mary Ann quite well. I also got to know Ed Alley[30] well. He was a grad student and staff member at Lawrence Livermore lab. Mary Ann was the backbone of Alders' research group. She did all the coding and back-ground feeding of the computers at Livermore. As you may appreciate, Livermore and Los Alamos have access to the state-of-the-art computers, because their mission is nuclear weapons research. At Los Alamos, Bill Woods[31], was also doing many-body problems like equations of state, dynamics of liquids and solids, phase transitions and so on. But Woods was focused on Monte Carlo simulations While Alder and

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https://dwc.knaw.nl/DL/publications/PU00014010.pdf; https://dwc.knaw.nl/DL/publications/PU00014024.pdf (Accessed January 23, 2023.)

[28] S. Yip, W. E. Alley and B. J. Alder, "Evaluation of time correlation functions from a generalized Enskog equation," *J. Stat. Phys.* **27**, 201-217 (1982). https://doi.org/10.1007/BF01011747; W. E. Alley, B. J. Alder and S. Yip, "The neutron scattering function for hard spheres," *Phys. Rev. A* **27**, 3174 (1983). https://doi.org/10.1103/PhysRevA.27.3174; E. Leutheusser, S. Yip, B. J. Alder and W. E. Alley, "Dynamical correlations in a hard-disk fluid: Generalized Enskog theory," *J. Stat. Phys.* **32**, 503-521 (1983). https://doi.org/10.1007/BF01008952

[29] Mary Ann Mansigh: https://en.wikipedia.org/wiki/Mary_Ann_Mansigh

[30] William Edward Alley, *Studies in molecular dynamics of the friction coefficient and the Lorentz gas*, PhD thesis, University of California Davis (1979). https://catalog.hathitrust.org/Record/101830745

[31] J. J. Erpenbeck and J. D. Johnson, "William Wayne Wood," *Physics Today* **59**(5), 73 (2006). https://doi.org/10.1063/1.2216975

Wainwright were studying molecular dynamics of hard spheres. I got to spend a couple of summers at Livermore with Berni Alder. When I went to Munich there were two sources of computer simulations available. There was a student in the Netherlands, Cees Bruin—I never met him—who did a PhD thesis on the Lorentz model[32], and had results on the velocity autocorrelation function, on diffusion coefficients as a function of density. But these were not as extensive as the Livermore results. We ended up using the latter to test the mode-coupling calculations.

PC: Was Mary Ann Mansigh at all involved in these projects?

SY: [0:38:54] She was always involved. She's the one who actually did the calculations, while Berni would make the scientific decision, as you might expect, and Alley was sort of riding shotgun[33] on the research to make sure it all goes well.

PC: Let's get back to your collaboration with Leutheusser. After his time at MIT, he went back to Munich and published a seminal article, "The Dynamical model of the liquid glass transition" [34], which as you said was close in time with that of Götze and collaborators[35]. In Leutheusser's article, he acknowledges conversations with you on this topic. Can you tell us a bit about your involvement in the genesis of that work?

SY: [0:40:18] This may take a few minutes for me to recall the sequence of events. After Munich, I went to Jülich, and Leutheusser visited me there once. After I went back to MIT, Leutheusser came on a Humboldt fellowship and stayed with me for a year. During that time, we continued a collaboration on applying the version of mode-coupling theory he developed in his thesis, published in 1982[36]. We were at the point of saying: "Why don't we apply mode-coupling theory to supercooled liquids?" So, he and I were actually talking about these things that he eventually published. I think what actually happened is a matter of historical circumstances. Unfortunately, I no longer have records of what actually transpired. When Leutheusser went back to Munich, I expected he

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[32] Cornelis Bruin, *A computer experiment on diffusion in the Lorentz gas*, Proefschrift, Delft Technische Hogeschool (1978). https://tudelft.on.worldcat.org/oclc/905504948 (Accessed January 20, 2023.)
[33] Riding shotgun: https://en.wikipedia.org/wiki/Riding_shotgun
[34] E. Leutheusser, "Dynamical model of the liquid-glass transition," *Phys. Rev. A* **29**, 2765 (1984). https://doi.org/10.1103/PhysRevA.29.2765
[35] U. Bengtzelius, W. Götze and A. Sjölander, "Dynamics of supercooled liquids and the glass transition," *J. Phys. C* **17**, 5915 (1984). https://doi.org/10.1088/0022-3719/17/33/005
[36] E. Leutheusser, "Dynamics of a classical hard-sphere gas I. Formal theory," *J. Phys. C* **15**, 2801 (1982). https://doi.org/10.1088/0022-3719/15/13/011; "Dynamics of a classical hard-sphere gas. II. Numerical results," *J. Phys. C* **15**, 2827 (1982). https://doi.org/10.1088/0022-3719/15/13/012

would share the results we had at MIT with Götze. Whether Götze was interested or not, at least they communicated. When Leutheusser was in Cambridge, I gathered later that Wolfgang was visiting Alf Sjölander[37], in Göteborg. How much the professor and his former student collaborated or shared results with each other is not known to me. To this date I still don't know. Apparently, they arrived at essentially similar findings following different paths, and their respective results appeared in independent publications in 1984. Leutheusser's paper in *Phys. Rev.*, was submitted in December '83, while Bengtzelius' paper was March '84. The question I cannot answer why they decided not to publish together. I last saw Wolfgang, who unfortunately passed away last year, in Munich in 2000 at his 60th birthday celebration. He didn'y say anything to me and I didn't bring it up. I am very sorry to say I have lost touch with Leutheusser ever since he went back to Munich.

PC: Were you ever going to be involved in the paper with Eberhard? Or was that also not clear?

SY: [0:44:07] That was not clear to me after his 1984 paper was published. Eberhard and I had written a manuscript, which we had submitted to PRL. I can't remember whether this was before he left MIT or after he went back to Munich. After his return I heard from him that he was in a situation where he needed to submit on his own. Unfortunately, I no longer have the file with our correspondence during that period. I recall him saying, without explaining any detail: "Sid, I need to submit this paper first. Let's see what happens with it." We did circulate a PRL preprint to a few people like Mazenko and Shankar Das[38], and I remember (we got a reply from PRL in which the referee said: "I have also just reviewed and accepted the paper by Leutheusser for PRA. Since these two contents are similar, there is no need for a PRL." So, we did not go any further with the PRL submission. This also was the point at which Eberhard and I lost contact. Looking back, I regret very much I did not do more to make sure we stayed in touch.

PC: You mentioned sharing a draft with Gene Mazenko and Shankar Das. Shortly after, Professor Mazenko did publish a work on mode-coupling

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[37] Alf Sjölander: https://sv.wikipedia.org/wiki/Alf_Sj%C3%B6lander. See also P. Charbonneau, *History of RSB Interview: Lennard 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

[38] Shankar Prasad Das, *Effect of Structure on the Liquid-Glass Transition*, PhD thesis, University of Chicago (1987). https://www.proquest.com/docview/303616152

theory as well[39]. How involved or how much were you in contact or discussion with him about these topics?

SY: [0:46:48] After Gene went to Chicago, we continued to stay in touch, so he was informed of what we were doing for a few years thereafter. I recently spoke to Shankar Das about this period, and he indicated he and Gene had seen a copy of the Leuheusser PRL preprint. Because Gene and Shankar were developing their own field-theory approach to supercooled liquids, they soon published their results basically confirming the mode-coupling theory findings but adding another significant finding, namely, that there is no ergodic to non-ergodic transition[40]. Instead, there is a cut-off associated with barrier hopping. Hopping was the issue that Sjögren, in his conversation with you, also mentioned. With hindsight the community agreed on a mechanism which was not in the original mode-coupling theory formulation, and that's the hopping process.

PC: After this series of papers, you largely left the field of glasses, but I think you followed quite closely the developments of mode-coupling theory. Is that correct? If yes, how did you stay involved?

SY: [0:50:31] After working with Götze and Leutheusser I became interested in molecular simulations of crystals, problems of thermodynamics and kinetics of melting[55], and questions of theoretical limits of strength, with applications to plasticity and fracture.

I went back to the glass transition problem around 2005 when I was asked by John Mauro, then at Corning Glass[41], if one can determine the viscosity of supercooled liquids by molecular simulation. The challenge was how does one evaluate a Green-Kubo integral whose value can span some 16 orders of magnitude.

So, I got a small grant from Corning to see if we can find a way to perform the simulation. At the time, I had two postdocs, Xi Lin and Akihiro Kushima, and two graduate students in my group. We sat around discussing different ways one could approach the calculation of the viscosity of supercooled liquids and ended up applying[62] a method proposed by Laio and Parrinello around 2002[42]. It's called metadynamics. In adapting the

[39] S. P. Das, G. F. Mazenko, S. Ramaswamy and J. J. Toner, "Hydrodynamic theory of the glass transition," *Phys. Rev. Lett.* **54**, 118 (1985). https://doi.org/10.1103/PhysRevLett.54.118. Reference 4 mentions "E. Leutheusser and S. Yip, to be published."

[40] S. P. Das and G. F. Mazenko, "Fluctuating nonlinear hydrodynamics and the liquid-glass transition," *Phys. Rev. A* **34**, 2265 (1986). https://doi.org/10.1103/PhysRevA.34.2265

[41] Corning Inc. was formerly Corning Glass Works: https://en.wikipedia.org/wiki/Corning_Inc.

[42] A. Laio and M. Parrinello, "Escaping free-energy minima," *Proc. Natl. Acad. Sci. U.S.A.* **99**, 12562

Liao-Parinello method we developed an algorithm called ABC, for autonomous basin climbing. In a way I eventually found my way back to mode-coupling theory, and barrier hopping on a potential energy landscape[43].

PC: Getting back to MCT, just before we conclude. You organized a special issue in 1995 about MCT, ten years in[44]. As you were saying, you had left the field at the point to work on simulations of solids. How did the idea of the special issue come about and how did you get to be in charge?

SY: [1:04:30] Again, it was an occasion of serendipity. There was this journal *Transport Theory and Statistical Physics* which had a very broad scope. I happened to know one of the founding editors, Paul Zweifel[45]**.** Around 1995, he mentioned to me they were looking for new themes to make a special issue. I felt it would be appropriate to have a 10-year retrospective on mode-coupling theory and the glass transition. I have never forgotten that in 1984 there were these two remarkable papers. I also wanted to call attention to the impact of mode-coupling theory on the experimental community which was what I wrote in the Preface. For the Special issue I remember asking Wolfgang: “Could you write a lead paper giving a 10-year look at mode-coupling theory.” He agreed and so he wrote it with Sjögren[46]. Then, I asked a number of other people like Mazenko[47], and so on. I thought maybe it's not my business, because I didn't have that much to contribute, but I thought it was time to ask the community to stand up and put words on paper what's good and what's still missing. Even if there were something missing, it means there is room for further work for the younger generation.

(2002). https://doi.org/10.1073/pnas.2024273

[43] See, *e.g.*, S. Yip, "Understanding the viscosity of supercooled liquids and the glass transition through molecular simulations," *Mol. Simu.* **42**, 1330-1342 (2016). https://doi.org/10.1080/08927022.2015.1112008

[44] “Relaxation Kinetics in Supercooled Liquids—Mode Coupling Theory and Its Experimental Tests,” *Trans. Theo. Stat. Phys.* **24**(6-8) (1995). https://www.tandfonline.com/toc/ltty20/24/6-8 (Accessed January 21, 2023.); S. Yip, “Preface,” *Trans. Theo. Stat. Phys.* **24**, xi-xiii (1995). https://doi.org/10.1080/00411459508203933

[45] See, e.g., N. J. McCormick, C. E. Siewert, B. D. Ganapol and A. K. Prinja, “Paul Frederick Zweifel,” *Physics Today* **70**(8), 73 (2017). https://doi.org/10.1063/PT.3.3671; “Finding Aid to the Paul Zweifel Physics Notebooks, 1949-1980,” *AIP Niels Bohr Library & Archives* (2001). https://history.aip.org/ead/20010113.html (Accessed January 21, 2023.)

[46] W. Götze and L. Sjögren “The mode coupling theory of structural relaxations,” *Trans. Theo. Stat. Phys.* **24**, 801-853 (1995). https://doi.org/10.1080/00411459508203936

[47] G. F. Mazenko and J. Yeo, “Mode coupling and metastability,” *Trans. Theo. Stat. Phys.* **24**, 881-901 (1995). https://doi.org/10.1080/00411459508203938

PC: During your time at MIT or elsewhere, did you ever teach about the mode-coupling theory of glasses? If yes, can you detail?

SY: [1:09:06] I learned a lot from mode-coupling theory of glasses by analogy and transferring insights. Being in a nuclear engineering department my primary responsibility was to teach nuclear radiation interactions, neutron transport and nuclear reactor physics. There is something common between these topics and statistical physics, for example, the notion of criticality of systems out of equilibrium. Another would be mechanisms at different scales.

PC: Is there anything else that you'd like to share with us about that era that we may have missed or overlooked?

SY: [1:12:52] There are actually two items I would like to mention briefly. At the 60th celebration of Götze's birthday in Munich[48]. Kyozi Kawasaki[49] made a remark that I would just recite. "Despite various criticisms raised against the MCT of supercooled liquids and glass transitions, we feel that the position of the MCT pioneered by Götze and others is now firmly established in history as a classic in the same sense that the mean-field theories due to van der Waals and Weiss are the classics in the history of phase transition studies." I share the same sentiments. The theory may not be perfect, which is actually okay because the future generations can then work on it. The other viewpoint I will close with is to say that the conceptual framework underlying MCT was not developed just to provide an explanation of the glass transition phenomena, rather the predictions of the ideal glass transition are an outcome of MCT. MCT is not a first-principle theory without ansatz. Such theory, in my opinion, does not presently exist and is not likely to emerge from any of the competing formulations.

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

SY: [1:16:52] I have a manuscript on *Molecular Mechanisms in Materials*, which the MIT Press will publish. It would be nice if there is a way to link it with the Oral History Interview project.

PC: Thank you very much for this conversation.

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[48] Proceedings: "Issue dedicated to W. Götze, on the occasion of his 60th birthday," *Z. Phys. B* **103**(3) (1997). https://link.springer.com/journal/257/volumes-and-issues/103-3 (Accessed January 21, 2023.)
[49] Kyozi Kawasaki: https://en.wikipedia.org/wiki/Kyozi_Kawasaki

SY: [1:18:40] Thank you, again it is my pleasure.