VIGRE APPLICATION PART II · SPRING 2010

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1. Timeline, professional development, and outreach activities

I am in my final year of a five-year PhD program. The period of support (spring 2010) will complete my fifth year. The summer and fall of 2009, which have been on VIGRE support, have seen the following:

- I have continued my research. This is discussed in detail below.
- In June, UA's Bob Sims hosted a workshop on quantum spin systems and applications in quantum computation. I gave a talk on lattice quadrupling for percolation in quantum networks, as described in my summer/fall 2009 VIGRE proposal: I am doing follow-on work to [1] for 3D rectangular lattices. In this talk, I brought my written presentation up to my current level of understanding. The only remaining obstacle to publication of this percolation work is final write-up along with finite-size scaling analysis, which is hand-in-hand with FSS as applied to my dissertation research.
- In July, I delivered a contributed talk at the Conference on Stochastic Processes and Their Applications in Berlin. My aim was to pitch the model to probabilists, downplaying the mathematical-physics background and emphasizing intuition, known results, conjectures, and experimental methods. While in Berlin, I made several contacts and had several productive conversations, including a possible postdoctoral research idea involving minimal-distance matching of Poisson point processes.
- Wednesday through Friday of the week before the Berlin conference, I visited Daniel Ueltschi and his collaborators Daniel Gandolfo and Jean Ruiz in Marseille. I received valuable feedback on my slides for my then-upcoming Berlin talk. Gandolfo and I compared several technical details for simulational methods for the model of random spatial permutations, including size reduction for lookup tables and the irrelevance of Binder fourth-order cumulants for our model.
- Friday August 7 through Tuesday August 11, I participated in the department's integration workshop for incoming graduate students. I wrote a project on the Berlekamp algorithm for factorization of polynomials over finite fields, an old area of expertise from my master's-degree days. None of the eight incoming students chose to work on that project; I assisted Angel Chavez and Kevin Davidsaver on their group-representation project, focusing in particular on presentation skills.
- I have been working with Tom Kennedy's bridge group, which consists of three graduate students, two undergraduates, and himself. I am focusing on mentoring of an undergraduate student (Howard Cheng) and a junior graduate student (Shane Passon) on software implementation of probabilistic concepts.
- I presented the progress of my research to the UA mathematical physics seminar in September. This included most of the content of my 30-minute Berlin talk, as well as recently completed work on sample variance of exponentially correlated Markov processes. (Precisely, this uses integrated autocorrelation time to estimate error bars for output of Markov chain Monte Carlo simulation runs.) I treated this as an early dry run of a job talk; I received several useful feedback points which will positively impact my on-site job talks this coming spring.
- On October 26, I gave a talk to the UA Math Department's Software Interest Group on the use of the Python programming language for numerical methods and presentation graphics. This melded a talk on the Perl language from three years ago with an explanation of how I use Python's `pylab` module to create the figures in my dissertation and associated writings (including figure 1 of this proposal).

Date: November 4, 2009.

- I am completing my final course — Probability and Random Processes in Engineering, in the Electrical Engineering department — satisfying an out-of-department requirement.
- Since the start of summer 2009, I have completed the following chapters of my dissertation: definitions and intuition for the probability model, random variables of interest in the model, correctness of the GKU algorithm, correctness of the worm algorithm and discussion of its remaining stopping-time problem, ΔH computations, and software design. I also completed an appendix on sample variance of exponentially correlated Markov processes.
- At Daniel Ueltschi's request, I am drafting a paper stating my dissertation results. On Tom Kennedy's advice, I have structured this so that it will drop neatly into my dissertation. In particular, it will complete my dissertation chapters on finite-size scaling and quantitative results. I plan to submit this paper by the end of the year for publication: this will enhance my job-application materials.
- Since early September I have been actively job-seeking for academic, governmental/laboratory, and industrial positions. At present (early November), I have been gratified to receive two phone interviews and an on-site interview.

The period of support, spring 2010, will include the following:

- Principally, I will complete my doctoral research. This is discussed in detail below.
- Finite-size scaling analysis, in progress now, is not only a key step for the quantitative results in my dissertation. It is also the missing piece for proper write-up of the percolation results described in my summer/fall 2009 proposal, which I spoke on in June.
- I will continue to work with Tom Kennedy's bridge group.
- I will contribute a talk at the AMS/MAA Joint Meetings in San Francisco in January. Of course, my primary purpose for attending this year's meetings will be the job search.
- I will also attend the 23rd Annual Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics at the end of February at the University of Georgia; I am submitting a request for a contributed talk. There, I hope to make professional contacts; as well, I hope to obtain on advice on the stopping-time problem of my worm algorithm for the model of random spatial permutations.
- The results section of my dissertation will be all but complete by the beginning of the spring semester, thanks to Daniel's draft-paper request as described above; I will drop in final numbers once the requisite high-performance-computing runs have completed. I will also tie up all loose ends in my dissertation.
- Spring job-seeking efforts will include attendance at the Joint Meetings, possible on-site interviews, and (one fervently hopes) selection from among multiple job offers.
- I plan to defend my dissertation at the end of March. This should leave time for any re-work, in time for my graduation in May. In particular, Daniel Ueltschi will be on campus at that time.

VIGRE support will be particularly helpful in permitting me to focus on completing a quality dissertation which will facilitate my success on the job market.

2. Plan of study and research

My research is under Daniel Ueltschi, formerly of the University of Arizona, currently at the University of Warwick. We are studying the effects of interparticle interactions on the critical temperature of Bose-Einstein condensation. Ueltschi spent a sabbatical semester at the UA for spring 2009, during which time we met regularly; at present, I am working largely independently. We will continue to communicate; as well, I am working with my local advisor, Tom Kennedy, to bring my dissertation to completion. Daniel will visit the University of Arizona for a few weeks in March; in particular, I will schedule my dissertation defense around his visit.

2.1. **Background.** The model of random spatial permutations arises in the study of the Bose gas, although it is also of intrinsic probabilistic interest; its history includes Bose-Einstein [2, 3], Feynman[4], Penrose-Onsager, Sütő [5, 6], and Ueltschi-Betz [7, 8, 9, 10]. Random permutations arise physically when one symmetrizes the N-boson Hamiltonian with pair interactions, then applies a multi-particle Feynman-Kac formula and a cluster expansion [9, 10].

The state space is $\Omega_{\Lambda,N} = \Lambda^N \times \mathcal{S}_N$, where $\Lambda = [0, L]^3$ with periodic boundary conditions; point positions are $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$ for $\mathbf{x}_1, \dots, \mathbf{x}_N \in \Lambda$. The Hamiltonian takes one of two forms. In the first, relevant to the Bose gas, we have

$$H_B(\mathbf{X}, \pi) = \frac{T}{4} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{i<j} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}) \tag{1}$$

where $T = 1/\beta$ and the V terms are interactions between permutation jumps. (The temperature scale factor $T/4$, not $\beta/4$, is surprising but correct for the Bose-gas derivation of the Hamiltonian.) In the second form of the Hamiltonian, considered in this paper, we use interactions which are dependent solely on cycle lengths:

$$H(\mathbf{X}, \pi) = \frac{T}{4} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{\ell=1}^{N} \alpha_\ell r_\ell(\pi), \tag{2}$$

where $r_\ell(\pi)$ is the number of ℓ-cycles in π and the α_ℓ's are free parameters, called *cycle weights*. One ultimately hopes to choose the α_ℓ's appropriately for the Bose gas; even if not, the model is well-defined and of its own interest.

Different choices of α_ℓ result in different models: The *non-interacting model* [11] has $\alpha_\ell \equiv 0$. The *two-cycle model* [8, 9], has $\alpha_2 = \alpha$ and other cycle weights equal to zero. The *general-cycle model* has no restrictions on α_ℓ. In [10], the *small cycle-weight case* is considered: the only restriction on α_ℓ is that α_ℓ goes to zero in ℓ faster than $1/\log \ell$. Lastly, the *Ewens model*, treated in my research (see also [12]) has $\alpha_\ell \equiv \alpha$ constant in ℓ.

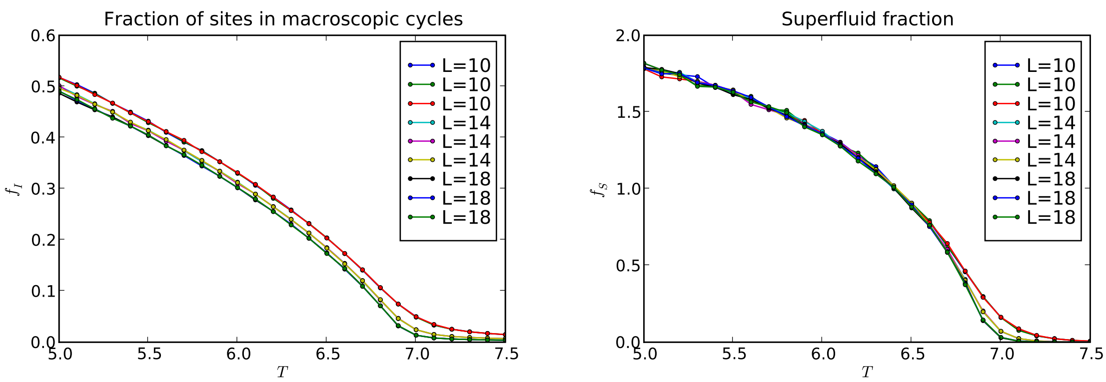

FIGURE 1. Order parameters f_I and f_S for finite systems.

One may hold point positions fixed, e.g. on the unit lattice; this approach has been taken for all simulations done up to the present, including specifically the work described in this paper. One obtains a Gibbs probability distribution on $\mathcal{S}_N$:

$$Y(\Lambda, \mathbf{X}) = \sum_{\sigma \in \mathcal{S}_N} e^{-H(\mathbf{X},\sigma)}, \qquad P_{\Lambda,\mathbf{X}}(\pi) = \frac{e^{-H(\mathbf{X},\pi)}}{Y(\Lambda, \mathbf{X})}. \tag{3}$$

For a random variable $S(\pi)$, we then have

$$\mathbb{E}_{\Lambda,\mathbf{X}}[S] = \frac{1}{Y(\Lambda, \mathbf{X})} \sum_{\pi \in \mathcal{S}_N} S(\pi) e^{-H(\mathbf{X},\pi)}, \qquad \text{i.e.} \qquad \mathbb{E}_\pi[S(\pi)] = \sum_{\pi \in \mathcal{S}_N} P(\pi) S(\pi). \tag{4}$$

An *order parameter* is the expectation over $\mathcal{S}_N$ of a random variable, dependent on T and α, which in the infinite limit is zero to one side of a *critical temperature* T_c and non-zero on the other side, with analyticity at all $T \neq T_c$. See figure 1 for finite-size approximations to two such order parameters, f_I and f_S: the former is the fraction of sites in long cycles, whose specific computation is described in [11]. The latter is a scaled winding number, described in [13]. It quantifies wrapping of long cycles around the 3-torus, which is the three-dimensional L-box with periodic boundary conditions. Yet another order parameter is $\mathbb{E}[\ell_{\max}]/N$, where $\ell_{\max}(\pi)$ is the number of sites in the longest cycle of π.

Shepp and Lloyd [14] showed in 1966 that, for uniformly weighted non-spatial permutations in $\mathcal{S}_N$, $\mathbb{E}[\ell_{\max}]/N \approx 0.6243$; unpublished work of Betz and Ueltschi has found $\mathbb{E}[\ell_{\max}]/Nf_I$ is that same number for the non-interacting case $\alpha_\ell \equiv 0$. That is, if one adds a spatial structure to the permutations, yet restricts consideration to the number Nf_I of points in long cycles, it appears that long cycles are in some sense (as yet to be clearly defined) uniformly distributed with support on the points which participate in long cycles. This issue was also given preliminary experimental treatment in [11]. Thus, we define the *GRU quotient* [11] to be the quantity $\mathbb{E}[\ell_{\max}]/Nf_I$ and ask whether, for fixed α, it is indeed constant in T. (Note that this quotient is only defined for $T < T_c$; for $T > T_c$, f_I is zero.)

A final order parameter is obtained as follows. We define a *correlation length* ξ to be the expected value of the spatial length of cycles. The reciprocal correlation length $1/\xi$ is a right-sided order parameter — a mirror image of the ones shown in figure 1 — permitting bracketing of the critical temperature from the left and from the right.

2.2. **Current work.** Given the ability to correctly determine the finite order parameter $S_L(T, \alpha)$, where S is any of several order parameters, one wishes to take the $L \to \infty$ limit to find $S(T, \alpha)$ and from that find $T_c(\alpha)$. I am employing a finite-size scaling technique adapted from several PIMC studies [15, 13, 16, 17]; see also [PV] for a nice survey. Finite-size scaling takes the form of a hypothesis, or rather a set of hypotheses, which is tested against the data. Namely, define $t = (T - T_c)/T_c$ and examine, say, $0.99 < t < 1.01$.

The first hypothesis is that, in the infinite-volume limit, the correlation length $\xi(T, \alpha)$ and the order parameter $S(T, \alpha)$ follow power laws

$$\xi(T,\alpha) \sim |t|^{-\nu}, \quad T \to T_c \qquad \text{and} \qquad S(T,\alpha) \sim t^{\rho}, (-t)^{\rho}, \quad \text{or} \quad |t|^{\rho}.$$

One moreover hypothesizes that for T near T_c, $S_L(T)$ and $S(T)$ are related by a *universal function* Q which depends only on the ratio L/ξ:

$$S_L(T,\alpha) = L^{-\rho/\nu} Q(L^{1/\nu} t) \sim L^{-\rho/\nu} Q((L/\xi)^{1/\nu}).$$

For my dissertation, testing of the finite-size-scaling hypothesis will be done as follows:

- First, collect MCMC experimental data with error bars (found using the method of integrated autocorrelation time [18]) for a range of L's, T's, and α's.
- Second, estimate the critical exponents: given an order-parameter plot such as 1, vary the trial exponent $\hat{\rho}$. Raise the raw data to the $1/\hat{\rho}$ power. Find the $\hat{\rho}$ with least linear-regression uncertainty. Do the same for $\hat{\nu}$.
- Third, use the *crossing method* [PV] to find T_c: once the exponents are known, plot $L^{\rho/\nu} S_L(T)$ as a function of T. Since at $T = T_c$ we have $t = 0$ and
$$L^{\rho/\nu} S_L(T) = Q(0),$$
regardless of L, these curves will cross (approximately, due to sampling variability) at $T = T_c$. If they do not, the finite-size-scaling hypothesis is not verified.
- Fourth, having estimated ρ, ν, and T_c, plot $L^{\rho/\nu} S_L(T)$ as a function of $L^{1/\nu} t$. This is a plot of the scaling function Q. If the hypothesis is correct, the curves for all L should coincide, or collapse, to within sampling error.

This determination of critical exponents above will allow me to confirm or refute, on a confidence-interval basis, the hypothesis that the GRU quotient $\mathbb{E}[\ell_{\max}]/Nf_I$ is constant in T for $T < T_c$. Namely, if the critical exponents of $\mathbb{E}[\ell_{\max}]/N$ and f_I are equal to within sampling error, one may say that their ratio is constant in T.

My research goals for the spring, in addition to other activities as detailed as the start of this proposal, are quite precise:

- Complete high-performance computing runs.
- Use these to update, with smaller error bars, experimental determination of critical temperature T_c as a function of α which will have been crudely computed by the end of the fall semester.
- Use the estimated critical exponents for $\mathbb{E}[\ell_{\max}]/N$ and f_I to test the hypothesis that the GRU quotient $\mathbb{E}[\ell_{\max}]/Nf_I$ is constant in T for $T < T_c$.
- Complete the results section of my dissertation; tie up all loose ends in my dissertation.
- Off-lattice computations, as well as use of non-Ewens cycle weights, are a postdoctoral research topic.

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