VIGRE APPLICATION PART II · SUMMER AND FALL 2009

JOHN KERL

1. Timeline, professional development, and outreach activities

I am finishing my fourth year of a five-year PhD program. The period of support (summer and fall 2009) will begin my fifth year. The spring of 2009 saw the following:

- I successfully completed my comprehensive examination in January 2009. I exposited a recent paper of Daniel Ueltschi [1], which my dissertation research is extending.
- Ueltschi was present in Tucson on a sabbatical semester; he and I are collaborating closely on my dissertation research. In particular, my funding this semester is from Ueltschi's NSF grant. (In spring of 2008 I was also funded under Ueltschi's grant. The work I did at that time preceded my comprehensive examination, but that work has led seamlessly into my dissertation.)
- I obtained access to the ICE cluster in the University of Arizona's High Performance Computing center. This reduces compute time, relative to my previous use of the math department's chivo cluster, by an order of magnitude.
- The local March 2009 workshop on Entropy and the Quantum, organized by Daniel Ueltschi and Robert Sims, drew several visitors from the international mathematical-physics community. Among these was Volker Betz, Ueltschi's co-worker at Warwick and chief collaborator. During the workshop (as I write this proposal), Betz and I are exploring a question in bulk flow of permutation cycles.
- Also during the workshop, John LaPeyre and I are sketching out a joint paper which follows on work of Perseguers, Wehr, et al. [2]. My portion is an independent study project under Jan Wehr in spring of 2008. I obtained interesting results that spring, and presented them to the UA mathematical physics seminar in October 2008; it would benefit me professionally to write these results up nicely and submit them for publication.
- In the spring of 2009, I am taking Bill Faris' course on Discrete-Time Stochastic Processes, which reinforces my current knowledge of Markov chains. I am also taking Theory of Statistics from Walter Piegorsch. This is a core course in the statistics program; it requires no small amount of effort, but it completes coursework for my PhD minor in statistics.
- For fall 2008 and spring 2009, I am organizing the weekly Graduate Student Colloquium. I am also serving as this year's student representative to the department's graduate committee. In addition to the light committee work per se, I am organizing the weekly grad tea as well as weekly lunches with the departmental colloquium speaker. I also contributed significantly to the department's recruitment workshop in March 2009.

The period of support, summer and fall 2009, will include the following:

- Principally, I will continue my research. This is discussed in detail below.
- I will deliver a contributed talk (already accepted) at the Conference on Stochastic Processes and Their Applications in July in Berlin. I will present my worm algorithm for the random cycle model.
- As time permits, I may visit Daniel Ueltschi in Marseille before that conference.
- Working with John LaPeyre, I will write up the above-described percolation results for publication.

Date: April 6, 2009.

- I have spoken with the department's graduate director about my participation in the department's August integration workshop for incoming graduate students; he was very enthusiastic. I will work side by side with incoming grads throughout the five-day workshop, guiding them through team-based discovery-method projects which help them transition to advanced mathematics.
- Tom Kennedy currently has a group consisting of three graduate students, two undergraduates, and himself making a multi-tiered examination of self-avoiding random walks. I have received his agreement about my participation, which will include regular team meetings and the bridging of computational and theoretical results.
- I will present the progress of my research to the UA mathematical physics seminar in the fall.
- I will complete my final course — Probability and Random Processes in Engineering, in the Electrical Engineering department — in fall 2009, satisfying an out-of-department requirement.

In my final semester at the UA I will continue my dissertation work, with timely graduation in May 2010. I will, of course, be spending much of the year applying for employment. Thus, it is my desire to accomplish as much during the summer and fall as possible. VIGRE support will help me to achieve that goal.

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 is spending a sabbatical semester at the UA for spring 2009; by the time of his return to Warwick, I will be working largely independently. We will continue to communicate; as well, my local advisor, Tom Kennedy, is up to date on my research and I will be working with him to bring the dissertation to completion.

2.1. Historical context.

Bose and Einstein [3, 4] predicted in the 1920s that non-interacting particles with integer spin may collapse into a macroscopic occupation of the ground state of the external potential. Einstein predicted a critical temperature for the phenomenon. Thousands of research papers have investigated BEC theoretically, as well as experimentally following the 1995 Nobel-prize-winning successes of Anderson et al. [5]. Of the many questions that could be asked about BEC, we restrict attention to that of the effects of interbosonic interaction strength a on the condensate's critical temperature $T_c^{(a)}$. Several research groups working over the last three decades have obtained widely varying results; see [6] for a survey. Current consensus within the theoretical physics community [6] is that

$$\Delta T_c = \frac{T_c^{(a)} - T_c^{(0)}}{T_c^{(0)}} \tag{1}$$

is linear in a for small a. The main goal of this project is to determine the constant of linearity with a high degree of certainty, for various interaction models.

2.2. Background.

One begins with a Hamiltonian for particles with two-body interactions. Specifically, consider a system of N bosons in a cube $\Lambda \in \mathbb{R}^d$ of size L and volume L^d. The positions of the particles are either on a unit lattice, so $N = L^d$ with density $\rho = 1$, or continuously distributed according to a point process with variable density $\rho = N/V$. The interparticle potential U is in terms of a scattering length a, where a is nominally the radius of a hard-core potential. The Hamiltonian for pair-interacting particles is

$$H = -\sum_{i=1}^{N} \Delta_i + \sum_{i<j} U(\mathbf{x}_i - \mathbf{x}_j) \tag{2}$$

where Δ_i is the Laplacian and U is a multiplication operator. This operator acts in the space $L^2(\Lambda^N)_{\text{sym}}$ of symmetric, square-summable wavefunctions with periodic boundary conditions.

One may write down the partition function $Z_{\Lambda,N} = \mathrm{Tr}(e^{-\beta H})$ and apply a multi-particle Feynman-Kac formula, involving permutation symmetry of bosonic wave functions, to obtain a Hamiltonian in which permutation jumps rather than particles interact. (The derivation is sketched in [1, 7], and was worked out in full detail in my written comprehensive paper.) A cluster expansion, to first order in the scattering length of the particles, yields a Hamiltonian on $\mathcal{S}_N$ with only jump-pair interactions:

$$H_P(\mathbf{x}_1, \ldots, \mathbf{x}_N, \pi) = \frac{1}{4\beta} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{i<j} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}). \tag{3}$$

The jump-pair interaction $V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)})$ may be interpreted as the collision probability for a pair of Brownian bridges running from $\mathbf{x}_i$ and $\mathbf{x}_j$ to $\mathbf{x}_{\pi(i)}$ and $\mathbf{x}_{\pi(j)}$, respectively, in time 2β.

Equation 3 gives rise to a Gibbs distribution $P(\pi) = e^{-H(\pi)}/Z$ (point positions are either held fixed on the lattice, or integrated out on the continuum) on the $N!$ permutations of the N bosons. Then, one may compute the expectation of various random variables in the finite system. For [1, 7, 8] as well as my computational work in spring 2008, the random variable of interest was the fraction f_I of sites in macroscopic cycles. As suggested by figure 1, one may use f_I as an order parameter namely, a quantity which is zero on one side of a phase transition and non-zero on the other. For finite systems, the $f_I(L,T)$ is smooth in T; as L increases, the graph approaches a non-analyticity at T_c.

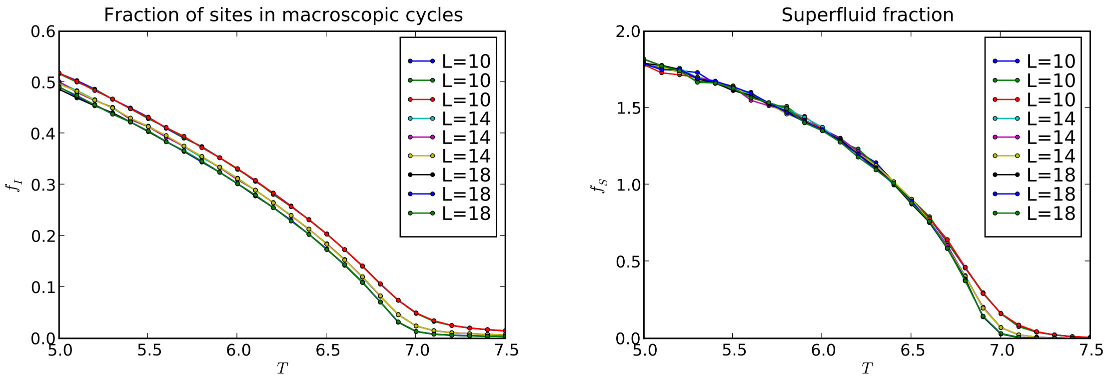


FIGURE 1. Order parameters f_I and f_S for finite systems.

Direct use of the Brownian bridge jump-pair interaction is prohibitive both analytically and numerically. The following approaches have been taken:

- One may drop interactions altogether. This model was examined using Markov chain Monte Carlo methods in [8], with particles distributed on a cubic unit lattice. (To date, [8] is the only work in the literature on the lattice case: my dissertation extends this territory.) One recovers the critical density for the Bose gas in the non-permutation Hamiltonian (equation 2), and finds experimentally that the occurrence of infinite macroscopic cycles corresponds to condensation as predicted by Feynman [9]. An analogous result is proved in [7] for non-interacting particles distributed on a continuum.
- One may drop all jump-pair interactions except the most strongly interacting ones, namely, two-cycles [7]. Letting $N_2(\pi)$ denote the number of two-cycles in the permutation π, one has a simple Hamiltonian of the form

$$H_P(\mathbf{x}_1, \ldots, \mathbf{x}_N, \pi) = \sum_{i=1}^{N} \frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \alpha N_2(\pi). \tag{4}$$

In [10], the N_2 concept is extended to the form

$$H_P(\mathbf{x}_1, \ldots, \mathbf{x}_N, \pi) = \sum_{i=1}^{N} \frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{\ell=2}^{N} \alpha_\ell N_\ell(\pi) \tag{5}$$

where $N_\ell(\pi)$ counts the number of ℓ-cycles in the permutation π. Here, it is not known how to compute the α_ℓ's to match the Brownian-bridge interactions. Nonetheless, one may examine this model for its intrinsic interest — say, with α_ℓ constant in ℓ.

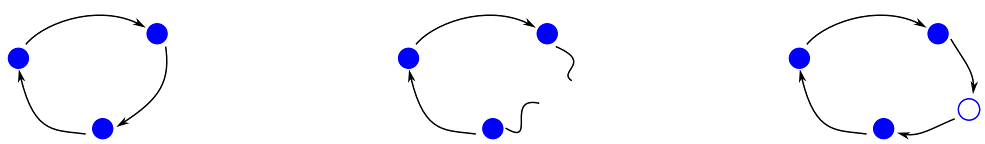
- Recent, unpublished collaboration between Betz and Ueltschi obtains lower and upper bounds on the Brownian-bridge interactions; these can be computed easily. Collision probability for Brownian bridges is increased when paths cross. Thus, Betz expects permutation jumps to be preferentially aligned or anti-aligned.

2.3. **Current work.** I am presently pursuing two threads: (1) re-working individual MCMC simulations, each of which produces an order-parameter data point, and (2) extrapolation and finite-size scaling which permit determination of the critical temperature from order-parameter data.

In spring 2009, Ueltschi and I began to consider the superfluid fraction f_S rather than f_I as an order parameter. As figure 1 suggests, the two order parameters have the same critical temperature but different critical exponents. The choice of f_S as order parameter was motivated by consideration of path-integral Monte Carlo (PIMC) studies [11, 12, 13, 14, 15, 16, 17, 18, 19]. (One may think of PIMC as sampling from Brownian-bridge interactions.) The superfluid fraction is a simple function of the *winding number*: for a given permutation, one counts the number of windings around the 3-torus (with topology emplaced by periodic boundary conditions) in each direction.

We soon discovered that the Metropolis sampling algorithm of [8] suffers from a serious defect: it creates winding cycles only with opposite signs, so that permutations are created with zero winding number. Another concern (as yet unexplained) is that the superfluid fractions we are seeing experimentally on the lattice exceed the unit interval.

To sample permutations with non-zero winding number, I reviewed the above-cited PIMC studies, where the same problem arises, then adapted the PIMC concept of a *worm algorithm* to our random-cycle model. Namely, one opens, rearranges, and closes permutation cycles. The open cycles are free to wrap around the torus before closing. As shown in figure 2, an open cycle on N points may be viewed as a cycle on $N+1$ points. I take the $(N+1)$st point to be *non-spatial*: it lies at no distance from any lattice point. This degree of freedom allows Metropolis udpates to explore the full configuration space of lattice permutations on the 3-torus.



Closed cycle on $N = 3$ points. Open cycle on $N = 3$ points. Open cycle viewed as a permutation on $N + 1 = 4$ points.

FIGURE 2. Open cycles as permutations on $N + 1$ points.

I have proved several results for Metropolis updates on the extended $(N + 1)$-point system, including the aperiodicity and detailed-balance conditions. Full details will be provided in my dissertation.

The second thread of my current efforts, given the ability to correctly determine the finite order parameter $f_S(T,L)$, is to take the $L \to \infty$ limit. One technique, which I am developing ad hoc, is to extrapolate pointwise in T from data such as those in figure 1 to the true f_S curve for $L=\infty$. At this point, it becomes easy, using log-log plots and linear regression, to read off the critical temperature with error bars. In parallel, I am employing a finite-size scaling technique adapted from several PIMC studies [12, 17, 18, 19]. Here one assumes that the finite system's $f_S(T,L)$ is of the form

$$f_S(T,L) = \frac{1}{L}\, Q\left(\left(\frac{T-T_c}{T_c}\right) L^{1/\nu}, \zeta L^{-\delta/\nu}\right) \tag{6}$$

for some analytic function Q and some parameters ν, ζ, and δ. Taylor-expanding to first order in the small arguments, followed by some algebra, permits a two-step regression analysis of the MCMC data resulting in a determination of T_c with error bars.

My research goals for the summer and fall, in addition to other activites as detailed as the start of this proposal, are quite precise:

- Write the worm-algorithm, superfluid-fraction, extrapolation, and finite-size-scaling chapters of my dissertation.
- Quantify ΔT_c for the N_2 model on the lattice; compare to the continuum result in [1].
- Quantify ΔT_c for the N_ℓ model on the lattice with constant N_ℓ. This topic is completely open in the literature.
- Investigate angle correlation and ΔT_c for the Betz-Ueltschi lower-bound and upper-bound interactions. This topic is also completely open in the literature.
- All computations this summer will be done on the lattice. Point-process simulations may be performed in the fall, if we deem that to be of interest for the dissertation. A Poisson point process is a tractable approach; the true point process for the Bose gas is very difficult to obtain.
- Let $\ell_{\max}$ be the length of the longest cycle in a permutation; let Nf_I be the number of cycles in macroscopic cycles. For non-interacting and N_2-interacting spatial permutations, $\langle \ell_{\max}\rangle / Nf_I$ is empirically found to be the same (approximately 63%) as for uniformly distributed permutations. For N_ℓ interactions, this is no longer the case. This phenomenon needs to be characterized.

The above is the current list of priorities, although other questions will certainly suggest themselves through the seven-month period of support.

References

[1] Ueltschi, D. *The model of interaction spatial permutations and its relation to the Bose gas.* `arXiv:0712.2443v3`.
[2] Perseguers, Cirac, Acín, Lewenstein, and Wehr. *Entanglement Distribution in Pure-State Quantum Networks.* Phys. Rev. A, vol. 77, issue 2, 2008. `arXiv:0708.1025v2`.
[3] Bose, S.N. Z. Phys. 26, 178 (1924).
[4] Einstein, A. Sitz. Ber. Preuss. Akad. Wiss. (Berlin) 1, 3 (1925).
[5] Anderson, M.H., Ensher, J.R., Matthews, M.R., Wieman, C.E., and Cornell, E.A. *Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor. Science*, vol. 269, issue 5221 (Jul. 14 1995), 198-201.
[6] Baym, G., Blaizot, J.-P., Holzmann, M., Laloë, F., and Vautherin, D. *Bose-Einstein transition in a dilute interacting gas.* `arXiv:cond-mat/0107129v2`.
[7] Betz, V. and Ueltschi, D. *Spatial random permutations and infinite cycles.* `arXiv:0711.1188`.
[8] Gandolfo, D., Ruiz, J., and Ueltschi, D. *On a model of random cycles.* `arXiv:cond-mat/0703315`. Statist. Phys. 129, 663-676 (2007).
[9] Feynman, R.P. *Atomic theory of the λ transition in Helium.* Phys. Rev. 91, 12911301, (1953).
[10] Betz, V. and Ueltschi, D. *Spatial random permutations with small cycle weights.* `arXiv:0812.0569v1`.
[11] Ceperley, D.M. *Path integrals in the theory of condensed helium.* Rev. Mod. Phys. vol. 67, no. 2, April 1995.
[12] Nho, K. and Landau, D.P. *Bose-Einstein condensation temperature of a homogeneous weakly interacting Bose gas: PIMC study.* `arXiv:cond-mat.stat-mech/0404238v1`.
[13] Boninsegni, M., Prokof'ev, N.V., and Svistunov, B.V. *Worm algorithm and diagrammatic Monte Carlo: A new approach to continuous-space path integral Monte Carlo simulations.* Physical Review E **74**, 036701 (2006).

[14] Prokof'ev, N.V., Svistunov, B.V., and Tupitsyn, I.S. *Exact, complete, and universal continuous-time worldline Monte Carlo approach to the statistics of discrete quantum systems.* Journal of Experimental and Theoretical Physics, vol. 87, no. 2 (1998).

[15] Grüter, P. and Ceperley, D. *Critical temperature of Bose-Einstein condensation of hard-sphere gases.* Physical Review Letters, vol. 79, no. 19 (1997).

[16] Holzmann,M. and Krauth, W. *Transition temperature of the homogeneous, weakly interacting Bose gas.* Physical Review Letters, vol. 83, no. 14 (1999).

[17] Pollock, E.L. and Ceperley, D.M. *Path-integral computation of superfluid densities.* Physical Review B, vol. 36, no. 16 (1987).

[18] Pilati, S., Giorgini, S., and Prokof'ev, N.V. *Critical temperature of interacting Bose gases in two and three dimensions.* Physical Review Letters **100**, 140405 (2008).

[19] Pollock, E.L. and Runge, K.J. *Finite-size-scaling analysis of a simulation of the ^{4}He superfluid transition.* Physical Review B, vol. 46, no. 6 (1992).