VIGRE APPLICATION PART II · FALL 2008

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1. Timeline

I am currently in my third year of a five-year PhD program. The period of support (fall 2008) will begin my fourth year. During that time, I will take two courses, continue my research, and complete my comprehensive examination.

- In fall 2008, I will take Mathematical Physics (Math 541), which will emphasize classical statistical mechanics, and Quantum Mechanics (Physics 570A), which will fulfill half of my out-of-department coursework requirement. Both courses will provide key grounding for my research area (described in detail below).
- I will continue to participate in the mathematical physics seminar. I presented my spring 2008 work this April; this fall I will describe ongoing progress.
- My comprehensive examination will take place in the fall; I will exposit a paper of Volker Betz and Daniel Ueltschi [6] which is the basis for my dissertation research.

The combination of coursework, comprehensive exams, and continued research will be challenging; hence my request for VIGRE support for the fall.

This summer, before the period of support, I will be attending the summer school on Current Topics in Mathematical Physics at the Erwin Schrödinger Institute. I will spend the remainder of the summer preparing for the comprehensive examination.

In the longer term, I will take second-semester Quantum Mechanics (Physics 570B) and Theory of Statistics (Math 566) in spring of 2009. The former will complete my out-of-department requirement; the latter will complete my PhD minor in Statistics. I will then be well prepared for continued research and summer school(s)/conference(s) in summer 2009, followed by research and dissertation in the academic year of 2009-2010 (my fifth year) with timely graduation in May of 2010.

2. Professional development and outreach activities

I will be organizing the departmental weekly Graduate Colloquium for the upcoming year; I have finalized this agreement with Dan Champion, the current coordinator. Duties include scheduling speakers and publicizing the series.

Tom Kennedy has approved my request to serve as super TA for his graduate probability (564) course for fall 2008. I took this course in spring of 2007 and enjoyed it thoroughly. In particular, Tom's pedagogy as well as the course content changed the course of my career. I am excited about probability and equally eager to work with and learn from Tom; I will convey this excitement to the students. Math 564 has for decades been cross-listed with the undergraduate 464 course; now, for the first time, 564 will be convened separately. The course is non-measure-theoretic: it bridges an important gap between the undergraduate curriculum and the fully abstract treatment in Math 563. In particular, the course plays a key role as a core

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course for the new Graduate Interdisciplinary Program in Statistics, and is expected to have high graduate enrollment. Thus, my contributions can positively influence many students as well as the Mathematics and Statistics programs in general.

As a supplementary plan, I have consulted with Dorin Dumitrascu, who has led high-school visitations this year. Since Dorin will not be coordinating these visits next fall, we will be under new leadership. According to Bill Velez, that leadership will not be chosen until the fall. I will be working with that as-yet-unnamed faculty member to help schedule speakers and provide transportation. As well, I will conduct my own presentations.

I had been a bit reluctant to give such talks in the past. Although I am a frequent and avid contributor to the Graduate Colloquium (see Part I of this application), I did not know what I could say to high-school students. About a month ago, though, I realized that I do have an appropriate topic. Before graduate school, when working at Lockheed Martin in an engineering role, I heard that the Cassini probe's newly acquired orbit around Saturn would be circularized by firing reverse thrust at periapsis, rather than apoapsis as my (errant) intuition would have suggested. To help me visualize this, I coded up a Runge-Kutta solver for the two-body problem (and later, I implemented a three-body solver) with graphical controls for thrust: namely, thrust was applied only during the duration of a mouse press, in a specified direction with respect to the velocity vector. As a result of that experiment, it became clear to me why periapsis is the appropriate location for a circularizing burn: it has everything to do with the fact that non-thrusted trajectories in the two-body case are ellipses. The subsequent orbit must pass through the point at which thrust was ceased on the previous orbit; yet, kinetic energy was lost and so the semimajor axis of the orbit must shorten. This topic combines theoretical, computational, and graphical results, in a way that gave me (and will give students) a yes-I-can attitude toward problem solving, mathematics, and the universe beyond our planet.

3. 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.

3.1. **Background.**

Bose-Einstein condensation is the macroscopic occupation of a lowest-energy quantum state by a system of bosons. The effect was theoretically predicted in the mid 1920s, but it occurs at such a low temperature — at the nanokelvin scale! — that it received relatively little attention. Only in 1995 were Bose-Einstein condensates produced in the laboratory by E. Cornell and C. Wiemann, using sophisticated cooling techniques. They, along with W. Ketterle, were awarded the 2001 Nobel Prize for this work. BECs have now enjoyed a resurgence of interest by theorists as well as experimentalists. Their practical applications at this point might be compared to electromagnetism in the mid 1800s: they contain unknown possibilities, but it is certain that there is new physics to be discovered.

The work of S. Bose and A. Einstein [1, 2] predicts a critical temperature T_c for the so-called ideal Bose gas consisting of N non-interacting particles in a domain $\Lambda \subset \mathbb{R}^d$. R. Feynman's approach [3] is as follows. The Hamiltonian for the N-particle system is

$$\mathbf{H} = -\sum_{i=1}^{N} \Delta_i + \sum_{i<j} U(x_i - x_j) \tag{1}$$

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

conditions. Feynman then expands the partition fuction $Z_{\Lambda,N} = \mathrm{Tr}(e^{-\beta \mathbf{H}})$ in the Feynman-Kac representation [4]:

$$Z_{\Lambda,N} = \frac{1}{N!} \int_{\Lambda_N} \mathrm{d}x_1, \cdots \mathrm{d}x_N \sum_{\pi \in \mathcal{S}_N} \int \mathrm{d}W^{2\beta}_{x_1, x_{\pi(1)}}(w_1) \cdots \mathrm{d}W^{2\beta}_{x_N, x_{\pi(N)}}(w_N) \cdot \exp\left\{ -\frac{1}{2} \int_0^{2\beta} \mathrm{d}\tau \sum_{i<j} U(w_i(\tau) - w_j(\tau)) \right\}. \tag{2}$$

Here, $\mathcal{S}_N$ is the group of permutations on N symbols and β is proportional to inverse temperature as usual; $\mathrm{d}W^{2\beta}_{x_i, x_{\pi(i)}}$ is the Wiener measure for trajectories w_i running from x_i to $x_{\pi(i)}$ in time 2β. Feynman then considers the lengths of cycles formed by permutations in $\mathcal{S}_N$, claiming that Bose-Einstein condensation occurs if and only if there are infinite cycles in the thermodynamic limit, namely, $N, |\Lambda| \to \infty$ with fixed density $N/|\Lambda|$.

Ueltschi considers a cube $\Lambda \in \mathbb{R}^d$ of size L and volume L^d. The interparticle potential U is in terms of a scattering length a, where a is nominally the radius of a hard-core potential. The state space of random permutations in the Feynman-Kac representation is $\Omega_{\Lambda,N} = \Lambda^N \times \mathcal{S}_N$. Letting $\ell_x(\pi)$ denote the length of the permutation cycle containing a site x, the density of sites in cycles of specified length — the quantitative setting for Feynman's infinite cycles in the thermodynamic limit — is defined to be

$$\rho_{m,n}(\pi) = \frac{1}{V} \#\{i = 1, \ldots, N : m \leq \ell_{x_i}(\pi) \leq n\}. \tag{3}$$

The expected value of this density is taken with respect to permutation probabilities:

$$E_{\Lambda,N}[\rho_{m,n}] = \frac{1}{Z_{\Lambda,N} N!} \int_{\Lambda^N} \mathrm{d}x_1 \cdots x_N \sum_{\pi \in \mathcal{S}_N} \rho_{m,n}(\pi) e^{-H(x_1, \ldots, x_N, \pi)}. \tag{4}$$

That is, energy (of a permutation) is the logarithm of probability (of a permutation), as is usual in statistical mechanics, and the denominator is a normalizing factor. A thermodynamic limit of this expectation quantifies the probability of the occurrence of infinite cycles. The new H appearing here is a Hamiltonian for positions and permutations. Applying a cluster expansion in the small parameter a to the bosonic Hamliltonian (equation 1), one obtains

$$H = \frac{1}{4\beta} \sum_{i=1}^{N} \|x_i - x_{\pi(i)}\|^2 + \sum_{i<j} V(x_i, x_{\pi(i)}, x_j, x_{\pi(j)}). \tag{5}$$

The central point of Ueltschi's approach is that the energy has been recast in terms of permutations: the new Hamiltonian H is more amenable to analysis than the original Hamiltonian $\mathbf{H}$. Terms in the first sum count lengths of permutation jumps; terms in the second sum count interactions between pairs of permutation jumps. (Higher-order interactions between triples of jumps, etc., are omitted.) For the interjump potential V, one obtains

$$V(x, y, x', y') = \int \left[1 - \mathrm{e}^{-\frac{1}{4\beta} \int_0^{4\beta} U(w(s))\, ds} \right] \mathrm{d}\hat{W}^{4\beta}_{x-x', y-y'}(w) \tag{6}$$

where x jumps to y, x' jumps to y', and $d\hat{W}$ is a unit-normalized Wiener measure on Brownian bridges w running from $x - x'$ to $y - y'$ in time 4β. It can be shown that $V(x, y, x', y')$ is the probability that a Brownian bridge from $x - x'$ to $y - y'$ intersects the ball of radius a.

In the non-interacting case, one has scattering length 0 which corresponds to $V = 0$ in equation 5. This model was treated in [5]. A detailed exposition of the interacting model is in [6], with a summary in [7]. Intermediate between the non-interacting and interacting models is the r_2 model of [6], wherein the only interactions that are retained in equation 5 are those between the jump pairs comprising two-cycles. For technical reasons, the r_2 model is significantly more efficient to simulate than the interacting model, and so merits continued attention.

3.2. **Current results.** I have worked under Daniel Ueltschi in the spring of 2008. To date, the following progress has been obtained.

The non-interacting results of [5] were first reproduced. This gave me confidence in my Monte Carlo simulations. The computational approach is as follows: Given an inverse temperature β and a lattice configuration of $N = L^d$ points, for L ranging from 10 to 50 and $d = 1, 2, 3$, generate a sequence of permutations on the N points. These permutations are generated using the Metropolis-Hastings algorithm (a particular algorithm of Monte Carlo type), sampling from the non-uniform probability distribution which is implicit in the right-hand side of equation 4. Compute the sample means $\rho_{0,k}(\pi)$ over all the permutations π generated. Using this averaged $\rho_{0,k}$, estimate the probability that the origin is in a long-range cycle. Repeat this process, varying β, to find the critical β_c (and thus the critical temperature T_c) at which the transition to long-range cycles occurs.

A key problem at the start of the project was the detection of thermalization. The Metropolis-Hastings algorithm is justified theoretically by an invariant distribution of a particular Markov chain. However, the full Markov matrix is never written down: indeed, for this problem, with a system of 1000 particles, the matrix would have dimensions 1000! by 1000! In practice, it is generally difficult to detect when the Metropolis-Hastings simulation has reached an invariant distribution, or has *thermalized* in statistical-mechanics jargon. The work of Gandolfo and Ruiz [5] used manually detected thermalization. I implemented an automatic thermalization criterion based on counting the number of turning points of a time-smoothed system energy function. The result matches the manual detection results across the full range of parameter values.

The r_2 model was simulated soon thereafter, although I deferred tabulated computations of critical temperature until recently, as Daniel and I were pressing hard toward progress on the fully interacting model. Currently, r_2 simulations are in progress on a departmental minicluster. The computational approach is as outlined at the start of this section, except that now one also varies the scattering length a in order to estimate the critical temperature $T_c(a)$. It is already clear that r_2 interactions do raise the critical temperature; continued simulations will allow me to quantify the interaction dependence of the critical temperature.

The main difficulty in simulating the interacting model has been computation of the interjump potential $V(\cdot)$. The defining equation (equation 6) is in terms of Brownian bridges: for each proposed permutation modification in a step of the Metropolis-Hastings algorithm, one must sum over all affected interactions between pairs of permutation jumps. For each interaction pair, one must generate N_b Brownian bridges, each sampled at N_p points on a time-step mesh from 0 to 4β. For each bridge, one must detect whether the trajectory of the bridge has intersected the ball of radius a centered at the origin. None of these steps is conceptually difficult, yet the product of the number of operations is quite large. Thus, we assessed the parameters N_b and N_p and considered techniques to avoid redundant computation.

It is well known that that the standard deviation of Brownian motion is $\sqrt{\Delta t}$ for a time-step mesh of Δt. Since the time step is $\Delta t = 4\beta/N_p$, one must increase N_p by a factor of 100 in order to reduce the motion's standard deviation by a factor of 10. The standard deviation of a Brownian bridge is different: it scales as $t(T-t)/T$. Nonetheless, the standard deviation of a Brownian bridge is of order $\sqrt{\Delta t}$. Thus, it is perhaps no surprise that the bridge size N_p must be exceedingly large (in experiments, on the order of 500,000) in order for $V(\cdot)$ to stabilize. Interestingly, increasing N_b only decreases the error bars around the stochastic value $V(\cdot)$; bias can only be removed by increasing N_p.

One may reduce the excessive time burden of these computations by precomputing a database of Brownian bridges which run from the origin in $\mathbb{R}^d$ back to the origin in time 1. Then, one may draw from that database to rescale, using a simple change of variable, to an arbitrary bridge.

One may further reduce the computational burden by taking advantage of symmetries of $V(\cdot)$. The potential function $V(\cdot)$ is rotationally invariant; likewise, the probability that a Brownian bridge from $x - x'$ to $y - y'$

intersects the ball of radius a centered at the origin will not change if the bridge is run backward. Thus

$$V(x, y, x', y') = V(x', y', x, y).$$

As well, since only the differences $x - x'$ and $y - y'$ matter, we have, for all real b, c, the double translation invariance

$$V(x + b, y + c, x' + b, y' + c) = V(x, y, x', y').$$

Taking advantage of all these symmetries, we may write the potential in terms of $r_1 = \|x' - x\|$, $r_2 = \|y' - y\|$, and θ being the angle between $x - x'$ and $y - y'$. Then, one may tabulate equation 6 over a range of r_1, r_2, θ, β, and a, and then use interpolation at run time.

Creation of the bridge database, with $N_p = 500,000$ and $N_b = 1000$, is feasible: one needs many hours of compute time and several hundred megabytes of disk space, but the database, once computed, is reusable. Creation of the $V(\cdot)$ database appeared more daunting. Fortunately, Betz and Ueltschi have recently developed a Riemann-integral formula for $V(\cdot)$, which is valid to lowest order in a. Now, the Brownian-bridge database is unnecessary. The V database has been generated and is in computational use at present. (By change-of-variable tricks we may yet be able to obtain a closed-form expression for $V(\cdot)$. If so, we will certainly use it.)

As with the r_2 case, it is clear that the interactions raise the critical temperature as expected from recent consensus within the physics community. Currently-running simulations are providing the data needed to quantify this dependence of critical temperature on scattering length.

3.3. **Future work.** The results obtained up to this point may be extended in theoretical and experimental directions. We will begin pursuing these directions during the period of support.

- The first order of business is to unfreeze particle positions: they were held frozen only as a convenience. The positions follow a point process; however, the process it is not currently known. One may conjecture a Poisson process, but it has been shown [8] that the positions for bosons in a condensate do not satisfy a large-deviation principle which would be expected for Poisson. Thus, one may choose to nonetheless simulate a Poisson process — in terms of initial placement of particles, as well as particle motion during Monte Carlo simulations — and learn whatever lessons are to be had. Also, though, one would like to characterize the true point process at the theoretical level.
- It is known that Bose-Einstein condensation occurs only in dimension $d = 3$. Yet one could replace the $\|x_i - x_{\pi(i)}\|^2$ term in the Hamiltonian by a more general $\xi(x_i, x_{\pi(i)})$ to study effects in dimensions 1 and 2.
- The cluster expansion used to obtain equation 5 is non-rigorous and needs mathematical justification. It is expected to work for a much smaller than interparticle spacing (e.g. on the cubic lattice). For the point process, where interparticle spacing may approach the scattering length a, further work will be required.

References

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