Chapter 12

FUTURE WORK

Macroscopic-cycle quotient: Now that the α -dependence of the macroscopic-cycle quotient's constant upon α has been found empirically, one would next like to explain that dependence analytically.

Non-asymptotic algorithm correctness: The detailed-balance correctness proof of the swap-and-reverse algorithm shows that there is a non-zero transition probability between all pairs of permutations. However, those non-zero transition probabilities can be quite small. As the number of Metropolis steps goes to infinity, asymptotically all permutations can be reached; more interesting is the question of which permutations are actually reachable in reasonable simulation time. One answers this question empirically simply by running simulations; perhaps this suffices. For the system discussed in this paper, as well as for other systems studied using MCMC methods, it would be useful to have a non-asymptotic correctness theory.

Winding numbers of all parities: Ideally, one would have an algorithm to permit odd winding numbers, as discussed in section 5.4.

Bose-gas Hamiltonian: Sampling from the true Bose-gas distribution using the random-cycle model requires three changes. First, one needs to conduct simulations using the Bose-gas interaction (equation (2.1.1)) rather than the cycle-weight interaction (equation (2.1.3)). The interaction term V is a CPU-intensive Brownian-bridge computation [BU07]; unpublished work of Ueltschi and Betz shows that it may be approximated in the weak-interaction case by a simpler Riemann integral. Precomputed tables and interpolation may make use of this integral feasible.

Second, point positions must be allowed to vary on the continuum. This entails a second type of Metropolis step, in addition to that shown in section 5.1. Namely, one picks a point and moves it to a new position nearby, using the detailed-balance condition to choose the acceptance probability.

Third, software efficiency requires a hierarchical partitioning of Λ . The Metropolis step of section 5.1 relies on picking $\pi(\mathbf{y})$ near to $\pi(\mathbf{x})$. For points on the lattice, this is easy: each site has six nearest neighbors. For freely placed points, though, one must remember which sites are close to which. The most naive implementation involves computing the distances between all N(N-1)/2 pairs of points; the $O(N^2)$ computation time is overwhelming. Instead, the lattice may be partitioned into subcubes. Distances need to be computed only between each given point \mathbf{x} and those in \mathbf{x} 's subcube and the 26 nearest-neighbor subcubes.

The second and third points simply require a software effort. Implementing them will be worthwhile only if the interaction terms can be simplified to the point that

they are computationally feasible. This is a mathematical effort.