Chapter 1

Scientific context

1.1 Theory

In 1924, the physicist Satyendra Nath Bose examined the quantum statistics of photons. In 1925, collaborating with Bose, Albert Einstein realized that the same could be done with non-interacting massive particles. He also discovered the condensation phenomenon: a macroscopic occupation of the (single-particle) ground state of the external potential [LSSY]. Moreover, Einstein predicted a critical temperature for the phenomenon. This temperature was so low — at the nanokelvin scale — that Bose-Einstein condensation attracted little interest in the physics community.

Feynman in 1953, along with Penrose and Onsager in 1956 [Feynman, PO], developed the theoretical notion of long permutation cycles in the Feynman-Kac representation of the Bose gas. Feynman claimed that long cycles correspond to Bose-Einstein condensation.

András Sütő referred to the existence of long permutation cycles as cycle percolation. He proved in 1993 that BEC implies cycle percolation in the ideal (non-interacting) gas [Sütő1], and proved the converse in 2002. Sütő moreover proved in the 2002 paper that there are infinitely many macroscopic cycles in the condensation of the non-ideal Bose gas.

For the ideal Bose gas, BEC is defined as the macroscopic occupation of the single-particle ground state of the external potential. For an interacting Bose gas, Hamiltonian eigenfunctions do not factor and thus there are no single-particle ground states. BEC is carefully defined for interacting systems [LSSY] in terms of the largest eigenvalue of a density-matrix operator. The 1983 work of Buffet and Pulè [BP] examines the macroscopic occupation of the zero Fourier mode.

1.2 Experiments

Liquid helium was produced in the laboratory by Kammerlingh Onnes in 1908; Fritz London in 1938 [London] connected superfluidity of liquid helium with Bose-Einstein condensation. Atoms of liquid helium, however, are strongly interacting — they attract only weakly, due to helium being a noble gas, but there are strong repulsive effects due to the high density of the liquid. Thus, Einstein's non-interacting theory could not explain the phenomenon.

Several groups attempted during the 1990s to produce BECs in vapors of spin-polarized hydrogen, but were not able to achieve low enough temperatures. The group of Cornell and Wieman [AEMWC], using hybrid cooling methods, successfully brought rubidium atoms to well below the critical temperature and made numerous measurements on the resulting condensates. (Cornell, Wieman, and Ketterle received the 2001 Nobel prize in physics for this work.)

Interest in BECs was sparked by this experimental success: thousands of papers, both theoretical and experimental, have been published on BECs in the years since. The work of Cornell and Wieman was of interest for several reasons:

- Condensates were directly imaged. Measurements were taken of temperature, density, position, velocity, particle number, and the fraction of the condensate occupying the ground state of the 3D harmonic trapping potential.
- The method was able to vary temperature and density through wide ranges; the condensate fraction was varied from zero to 100 percent.
- The gaseous rubidium condensate was *weakly interacting* — permitting a perturbative analysis which liquid helium, with its strong interactions, did not allow. (Note in particular that recent mathematical studies are weak-interaction theories; they are valid only to first order in the scattering length.)

1.3 Critical temperature

Recall that Einstein predicted a critical temperature T_c for the ideal Bose gas. It is a long-standing question to discover the effects of scattering length a on the critical temperature. Moreover, one may fix the density $\rho_c(a)$ and obtain a critical temperature $T_c(a) = 1/\beta_c(a)$ or vice versa; both of these critical parameters depend on the scattering length a. One expects the critical combination of parameters to be a manifold in (ρ, β, a) space. (See figure 1.1.)

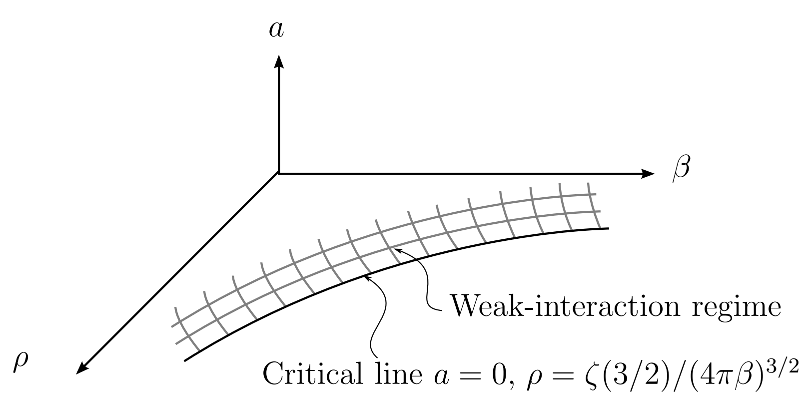

FIGURE 1.1. Critical manifold in (ρ, β, a) for small a.

Much is known about the $a = 0$ line of this critical manifold; off $a = 0$, even the crude shape has been under debate. The following findings are described by [BBHLV]:

The superfluid transition temperature of liquid helium is lower than that of an ideal gas of the same density. Thus, assuming that helium superfluidity is a strongly interacting BEC, one would expect interactions to decrease the critical temperature for the strongly interacting case. Various theoretical work (tabulated below) suggested either an increase or a decrease in critical temperature; path-integral simulations for low density (i.e. weak interactions) suggested that the critical temperature increases with scattering length, for small scattering length. The emerging consensus is that

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

is linear in a for small a, i.e.

$$\Delta T_c(a) = ca + O(a^2).$$

The following summary of the theoretical work on this question is found in [SU09]. (See also [AM, KPS, NL04] for a review on the widely varying analytical and simulational results on $T_c(a)$; see [BBHLV] for a thorough listing of the progress up to 2001 and [SU09] for an up-to-date survey.)

- 1964: *Huang*: $\Delta T_c(a) \sim (a\rho^{1/3})^{3/2}$, increases
- 1971: *Fetter & Walecka*: $\Delta T_c(a)$ decreases
- 1982: *Toyoda*: $\Delta T_c(a)$ decreases
- 1992: *Stoof*: $\Delta T_c(a) = c\, a\rho^{1/3} + o(a\rho^{1/3}), \quad c > 0$
- 1996: *Bijlsma & Stoof*: $c = 4.66$
- 1997: *Grüter, Ceperley, Laloë*: $c = 0.34$
- 1999: *Holzmann, Grüter, Laloë*: $c = 0.7$; *Holzmann, Krauth*: $c = 2.3$;
- 1999: *Baym et. al.*: $c = 2.9$
- 2000: *Reppy et. al.*: $c = 5.1$
- 2001: *Kashurnikov, Prokof'ev, Svistunov*: $c = 1.29$
- 2001: *Arnold, Moore*: $c = 1.32$
- 2004: *Kastening*: $c = 1.27$
- 2004: *Nho, Landau*: $c = 1.32$

1.4 Context of dissertation

The work of Ueltschi and Betz [BU07, U06, U07] extends the permutation point of view originated by Feynman, Penrose, and Onsager, drawing on the work of Sütő, Buffet, and Pulè [Feynman, PO, Sütő1, Sütő2, BP] to develop a model of random spatial permutations. (See chapter 2 for precise definition of the model.) In the permutation representation, this condensate transition manifests itself as the onset of long permutation cycles. The central point of this approach is that the system energy has been recast in terms of permutations, which are amenable to analysis and simulation. This permits a new perspective on an old question: the main goal of Ueltschi and Betz's long-term project is to quantify the shift in critical temperature, as a function of scattering length, for non-ideal Bose gases in the small-scattering-length regime.

The interaction terms for the permutation representation of the Bose gas are difficult to compute. Moreover, it is interesting to consider the model of random spatial permutations (which we sometimes refer to as the random-cycle model) for its own sake. Thus, Ueltschi, Betz, Gandolfo, Ruiz, and the author take various approaches with varying degrees of fidelity to the physical Bose-gas model. In section 2.1, we will see a random-cycle model for N particles which is parameterized by N *cycle weights* $\{\alpha_\ell\} = \alpha_1, \ldots, \alpha_N$ which encourage or discourage permutation cycles of lengths $\ell = 1, \ldots, N$. The remainder of this section involves results that may be obtained, analytically or simulationally, when various constraints are placed on the cycle weights.

In the papers [U07, BU07], Betz and Ueltschi examine the Bose-gas permutation weights with point positions allowed to vary in the continuum; an exact expression for the critical temperature is stated and proved for a simplified interaction model in which only two-cycles interact. The cycle-weight parameter α_2 is expressed in terms of the scattering length a; all other cycle weights are set to zero. In [BU08], this approach is extended to a model in which all the cycle weights α_ℓ may vary, but with the constraint that α_ℓ goes to zero faster than $1/\log(\ell)$. Here, an expression for the shift in critical temperature is found, as a function of all N cycle weights. It is key to note that these α_ℓ's are not computed directly from the physical scattering length a; rather, the result obtained is true for *any* cycle weights $\{\alpha_\ell\}$ satisfying the decaying-cycle-weight hypothesis. In [BU10], Ueltschi and Betz estimate, to first order, cycle weights $\{\alpha_\ell\}$ for the Bose gas.

Betz, Ueltschi, and Velenik [BUV09] examine cycle weights $\{\alpha_\ell\}$ with various hypotheses, including the Ewens [Ewens] case in which cycle weights are constant for all cycle lengths ℓ. These random permutations are non-spatial, i.e. $T = 0$ in the vocabulary of chapter 2. Their work is relevant to section 3.4 of this dissertation.

As is often the case in statistical mechanics, the study of this interacting system necessitates the use of computational methods — specifically, Markov-chain Monte Carlo. In [GRU], a simulational approach is taken for points held fixed on the cubic unit lattice in the non-interacting case ($\alpha_\ell \equiv 0$ in the language of chapter 2).

This dissertation, the only known simulation approach to the interacting model, applies MCMC methods to the case where $N = L^3$ points are held fixed on the fully occupied cubic unit lattice, with small additional probability weights depending on cycle lengths. This extends from[GRU] as well as [BUV09]. We find that even though lattice positions are used, and even though the decaying-cycle-weight hypothesis is invalidated, one nonetheless recovers the shift in critical temperature as predicted in the decaying-cycle-weight model of [BU08].

1.5 Literature review

In addition to the many references made in previous sections of this chapter, we point out the following.

The papers [GCL97], [KPS], [Ceperley], and [NL04] are among path-integral Monte Carlo simulational approaches to Bose-Einstein condensation — perhaps the closest relatives to the numerical work done in [GRU] and in this dissertation.

The doctoral dissertations of Peter Grüter and Markus Holzmann are paradigmatic examples of clear dissertation writing [Grüter, Holzmann]; the latter also provided insight into finite-size scaling.

Mean longest cycle for uniformly distributed (i.e. non-interacting, non-spatial) permutations ($T = 0$ and $\alpha = 0$ in the language of chapter 2) was discussed by [SL], following a question posed by Golomb on the basis of experimental data [Golomb]. See also sections 2.4 and 2.5. Non-uniformly distributed non-spatial permutations with constant cycle weights ($T = 0$ and $\alpha \neq 0$ in the language of chapter 2) arose in mathematical biology [Ewens].

Background in quantum mechanics and statistical mechanics may be found in [Griffiths], [Huang], and [Sakurai].

Worm algorithms for path-integral Monte Carlo, which inspired the random-spatial-permutation worm algorithm of chapter 7, are used throughout simulational physics. See in particular [BPS06] and [PST98].

Finite-size scaling techniques are employed for path-integral Monte Carlo simulations in [GCL97], [HK99], [KPS], [NL04], [PC87], [PGP08], and [PR92]. Citation trails in the above-cited works lead back to [Barber]. Some background information is found in [LB]. An excellent survey, encompassing and explicating all the above methods — truly a blessing for the aspiring learner — is [PV].

Markov chain Monte Carlo methods are discussed in [LB]; this dissertation has been influenced most heavily by [Berg]. Indeed, my appendix B is an elaboration on Berg's discussion of integrated autocorrelation time. The probability background necessary for either Landau and Binder or Berg may be found, with increasing levels of sophistication, in [Lawler], [GS], and [Øksendal]. The standard reference for statistical analysis, including confidence intervals, is [CB]. More practical aspects of the statistical reduction of experimental data are found in [Young].

The Mersenne Twister [MN] is the pseudo-random-number generator used in the this dissertation's computational work. Another good generator is pseudo-DES [NR]. Moreover, any numerical dissertation without a reference to *Numerical Recipes* is incomplete; its inclusion here is as good a point as any to end the literature review.

1.6 Originality of dissertation

Last, we delineate the originality of work presented in this dissertation. Chapters 1-3 are a rephrasing and an elaboration on [BU07, BU08, U07]. Chapter 4 is quite standard; the contribution made here is to present familiar general results in the specific context of random permutations. The essential SO algorithm of chapter 5, with a small modification, was presented in [GRU]; likewise for the SO ΔH computations in chapter 8. The treatment here is the first correctness proof of the SO algorithm. The SAR algorithm of chapter 5 was suggested by Daniel Ueltschi. The band-update algorithm (chapter 6) is due to the author. The worm algorithm and its correctness proof (chapter 7) are due to the author, along with the remaining ΔH computations of chapter 8. The remaining chapters, 9-12, are also original work. Appendix A briefly summarizes part of [BU07, U07]. Appendix B is a new take on an old question; see also [Berg]. The correlated-uniform Markov process is original, as is the explicit comparison of batched and non-batched means for exponentially correlated stationary Markov processes.