Remarks on interacting spatial permutations and the Bose gas

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January 16, 2009

Abstract

I exposit a recent paper of Daniel Ueltschi which connects a random-cycle model for spatial permutations to Bose-Einstein condensation for interacting particles. This work satisfies the requirement for my written comprehensive examination in the University of Arizona Department of Mathematics.

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1 Introduction

My comprehensive examination exposits the paper [U07]. The problem at hand is to determine the effects of interparticle interactions on the critical temperature of Bose-Einstein condensation; a so-called random-cycle model is employed to this end.

A large fraction of this paper is occupied by the appendices. This reflects the fact that much of my work on this project has been in filling the gap between my coursework and the research papers being presented. The experienced reader may wish to skip the appendices entirely.

The plan of this paper is as follows:

- A non-technical discussion of the historical context of the project; a mention of alternative approaches.
- The random-cycle approach to the BEC problem requires a model of spatial permutations. This model is developed mathematically — it is of probabilistic interest on its own — without reference to the Bose gas. (Main results about the latter are summarized in the appendices.)
- The model of spatial permutations is connected to the Bose gas:
  - One begins with a Hamiltonian for particles with two-body interactions.
  - Using a multi-body Feynman-Kac approach involving permutation symmetry of bosonic wave functions, one obtains a Hamiltonian in which permutation jumps rather than particles interact.
  - A cluster expansion, to first order in the scattering length of the particles, yields a Hamiltonian with only jump-pair interactions. At this point, one may employ the random-cycle model of spatial permutations.
- A simplified random-cycle model, called the two-cycle-interaction model, is described. In particular, this simplified model is amenable to Monte Carlo simulation and will play a key role in my dissertation work. Brownian bridges are the theoretical workhorse of this paper, but are computationally expensive to simulate. The two-cycle-interaction model bypasses Brownian bridges entirely.

2 Historical context

2.1 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 non-ideal (interacting) gas [Sütő1], and proved the converse in 2002 for the ideal (non-interacting) gas. 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.

2.2 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. Here, however, atoms of liquid helium 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. (The group received the 2001 Nobel prize in physics for this work.)

Interested 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. Measurments 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 the work of Ueltschi et al. is a weak-interaction theory; it is valid to first order in the interparticle interaction strength.)

2.3 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 interbosonic interaction strength 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; also, both of these critical parameters depend on the interaction strength a. One expects the critical combination of parameters to be a manifold in (ρ, β, a) space. (See figure 1.)

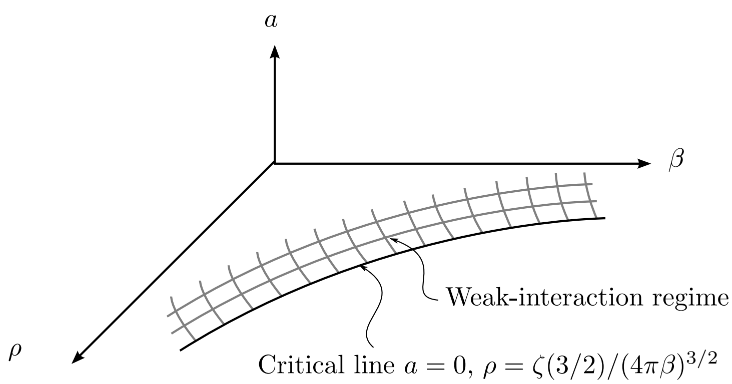

Figure 1: Critical manifold in (ρ, β, a) for small a.

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 expects 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) showed an increase in critical temperature. The emerging consensus is that

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

is linear in a for small a.

Ueltschi makes the following summary of the theoretical work on this question. (See also [AM, KPS, NL] for a review on the widely varying experimental results on $T_c^{(a)}$; see [BBHLV] for a thorough listing of the progress up to 2001.)

- 1964: *Huang*: $\frac{\Delta T}{T_c} \sim (a\rho^{1/3})^{3/2}$, increases
- 1971: *Fetter & Walecka*: $\frac{\Delta T}{T_c}$ decreases
- 1982: *Toyoda*: $\frac{\Delta T}{T_c}$ decreases

- 1992: *Stoof*: $\frac{\Delta T}{T_c} = c\, a\rho^{1/3} + o(a\rho^{1/3}), \quad c > 0$
- 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*: $c = 1.32$

The work of Ueltschi et al. [GRU, 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]. The main goal of the project is to quantify $\Delta T/T_c$ for non-ideal Bose gases in the small-scattering-length regime. As is often the case in statistical mechanics, the study of this interacting system necessitates the use of computational methods. The papers [BU07, U07], which are exposited in my comprehensive examination, develop the theoretical basis for the model which my disseration work will explore computationally and statistically.

3 Models of spatial permutations

Here we define and describe two configuration models of spatial permutations from a mathematical point of view. These models will be related to the physics of the Bose gas in section 4.13. The exposition here follows section 2 of [U07], with additional insights drawn from section 2 of [BU07].

3.1 Definitions

State space: Let $\Lambda \subset \mathbb{R}^d$ be a cube of width L and volume $V = L^d$. Let $N \in \mathbb{Z}^+$ and $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$ for $\mathbf{x}_1, \dots, \mathbf{x}_N \in \Lambda$. The state space of the model of spatial permutations is

$$\Omega_{\Lambda,N} = \Lambda^N \times \mathcal{S}_N$$

where $\mathcal{S}_N$ is the group of permutations of N points. (See figure 2.)

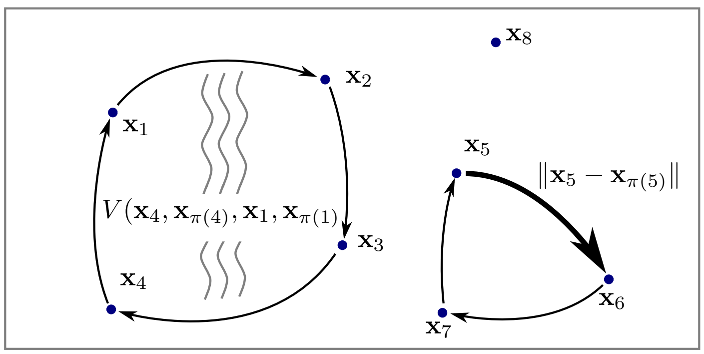

Figure 2: A configuration of $\mathbf{X}$ and π with $N = 8$.

Hamiltonian: The probability measure on this state space will be constructed through a Hamiltonian. The background probability measure is discrete (uniform) in π and continuous (Lebesgue) in $\mathbf{X}$. The Hamiltonian is as follows:

$$H_P(\mathbf{X}, \pi) = \sum_{i=1}^{N} \frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{1 \le i < j \le N} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}). \tag{3.1.1}$$

(The $1/4\beta$ factor is the reciprocal of what is more commonly encountered in statistical mechanics. For now, think of this as an ansatz. In section 4.6, this choice of scale factor will be found to be appropriate.)

The operator H is unbounded, but it is symmetric so we consider its self-adjoint extension. We take its domain to be f in $C^2(\Lambda^N)$ w/ Dirichlet boundary conditions.

There are two contributions to the energy of a configuration $(\mathbf{X}, \pi)$:

- The first[1] contribution to the energy is the sum of squares of permutation jump lengths. (One jump is marked with a heavy arrow in figure 2.) This makes permutations with long jumps disfavored; permutations with many short jumps will be less strongly disfavored.

[1] The papers [BU07] and [U07] generalize from $\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|$ to $\xi(\mathbf{x}_i, \mathbf{x}_{\pi(i)})$ where ξ is a spherically symmetric non-negative-valued function on $\mathbb{R}^d$ having integrable $e^{-\xi}$. This generalization is not of interest in the current paper, nor will it be of interest in my dissertation to follow.

- The second contribution to the energy is the double sum over interactions between permutation jumps. (One such jump-pair interaction is marked with wavy grey lines in figure 2.)

Jump-interaction potentials: The specific form of the jump-pair interaction is left unspecified at present, but we will require the following properties: V is translation-invariant i.e.

$$V(\mathbf{x},\mathbf{y},\mathbf{x}',\mathbf{y}') = V(\mathbf{x}+\mathbf{a},\mathbf{y}+\mathbf{a},\mathbf{x}'+\mathbf{a},\mathbf{y}'+\mathbf{a})$$

for all $\mathbf{a} \in \Lambda$, and

$$V(\mathbf{x},\mathbf{y},\mathbf{x}',\mathbf{y}') = V(\mathbf{x}',\mathbf{y}',\mathbf{x},\mathbf{y})$$

for all $\mathbf{x},\mathbf{y} \in \Lambda$.

We will consider three different jump-interaction potentials:

- One may certainly take the jump interaction V to be zero.
- In section 5, the jump interaction V will involve the probability of the intersection of Feynman paths.
- In section 6, we will treat all jump pairs as non-interacting unless they participate in a two-cycle.

Partition functions: We consider two partition functions, for a fixed point configuration $\mathbf{X}$ and for an average over point configurations, respectively:

$$Y(\Lambda,\mathbf{X}) = \sum_{\sigma\in\mathcal{S}_N} e^{-H_P(\mathbf{X},\sigma)} \quad \text{and} \quad Z(\Lambda,N) = \frac{1}{N!}\int_{\Lambda_N} Y(\Lambda,\mathbf{X})\,d\mathbf{X}.$$

Probability measures: Then we have two corresponding discrete probability measures on the finite set $\mathcal{S}_N$, for a fixed point configuration $\mathbf{X}$ and for an average over point configurations, respectively:

$$P_{\Lambda,\mathbf{X}}(\pi) = \frac{e^{-H_P(\mathbf{X},\pi)}}{\sum_{\sigma\in\mathcal{S}_N} e^{-H_P(\mathbf{X},\sigma)}} \quad \text{and} \quad P_{\Lambda,N}(\pi) = \frac{\frac{1}{N!}\int_{\Lambda^N} d\mathbf{X} e^{-H_P(\mathbf{X},\pi)}}{\frac{1}{N!}\int_{\Lambda^N} d\mathbf{X}\sum_{\sigma\in\mathcal{S}_N} e^{-H_P(\mathbf{X},\sigma)}}.$$

These may also be written in terms of the partition functions as

$$P_{\Lambda,\mathbf{X}}(\pi) = \frac{e^{-H_P(\mathbf{X},\pi)}}{Y(\Lambda,\mathbf{X})} \quad \text{and} \quad P_{\Lambda,N}(\pi) = \frac{\int_{\Lambda^N} d\mathbf{X} e^{-H_P(\mathbf{X},\pi)}}{Z(\Lambda,N)N!}.$$

Note that for the non-interacting $V = 0$ case, we have the following heuristic:

- As $\beta \to 0$, the probability measure becomes supported only on the identity permutation.
- As $\beta \to \infty$, the probability measure approaches the uniform distribution on $\mathcal{S}_N$.

Random variables: Recall from section 2 that Feynman claimed, and Sütő proved for the ideal gas, that Bose-Einstein condensation occurs if and only if there are infinite cycles in an infinite-volume extension of the above probability model. Furthermore, note that cycles depend on the permutation only and not on the geometric placement of $\mathbf{x}_1,\ldots,\mathbf{x}_N$. Thus we will be interested in random variables $\theta(\pi)$ rather than $\theta(\mathbf{X},\pi)$. In this section we confine ourselves to mathematical statements only; the connection with the physics will be made in section 4.13. Yet, we have motivated the choice of the following random variable.

The particular random variable of interest, $\varrho_{m,n}(\pi)$, is as follows. First define

$$\ell_i(\pi)$$

to be the length of the permutation cycle containing the point $\mathbf{x}_i$. For example, for the point configuration $\mathbf{X}$ and the permutation π in figure 2, we have

$$\ell_1(\pi) = \ell_2(\pi) = \ell_3(\pi) = \ell_4(\pi) = 4, \quad \ell_5(\pi) = \ell_6(\pi) = \ell_7(\pi) = 3, \quad \text{and} \quad \ell_8(\pi) = 1.$$

Also let

$$\rho = \frac{N}{V},$$

i.e. ρ is the particle density. For $1 \le m \le n \le N$, define

$$\varrho_{mn}(\pi) = \frac{1}{V} \# \{ i = 1, \ldots, N : m \le \ell_i(\pi) \le n \}$$

This random variable, taking values between 0 and ρ, is the **density of sites** in cycles of specified length.

One may also consider the related random variable

$$f_{m,n} = \frac{1}{N} \# \{ i = 1, \ldots, N : m \le \ell_i(\pi) \le n \}$$

which is $\varrho_{m,n}/\rho$. This runs from 0 to 1 and is the **fraction of sites** in cycles of specified length. For figure 2, we have $f_{2,3}(\pi) = 3/8$.

Expectations: For a random variable $\theta(\pi)$, we have

$$\mathbb{E}_{\Lambda,\mathbf{X}}(\theta) = \frac{1}{Y, \mathbf{X}(\Lambda)} \sum_{\pi \in \mathcal{S}_N} \theta(\pi) e^{-H_P(\mathbf{X},\pi)} \quad \text{and} \quad \mathbb{E}_{\Lambda,N}(\theta) = \frac{1}{Z(\Lambda,N)N!} \int_{\Lambda^N} d\mathbf{X} \sum_{\pi \in \mathcal{S}_N} \theta(\pi) e^{-H_P(\mathbf{X},\pi)}.$$

Models: The probability measure $P_{\Lambda,\mathbf{X}}(\pi)$ and the expectation $\mathbb{E}_{\Lambda,\mathbf{X}}(\rho_{m,n})$ is treated in the paper [GRU] where $\mathbf{X}$ is a cubic unit lattice; $P_{\Lambda,N}(\pi)$ and $\mathbb{E}_{\Lambda,N}(\rho_{m,n})$ are treated in [BU07] and [U07]. The former will be referred to as the **lattice-configuration model**; the latter will be referred to as the **point-process-configuration model**.

3.2 Existence of infinite cycles

Here we describe theorem 1 of [U07], which is proved in section 1 of [BU07]. This applies to the $U \equiv 0$ case.

Thermodynamic limit: We inquire about the fraction of sites participating in short and long cycles (as quantified below) in the infinite-volume limit. Namely, we let $V, N \to \infty$ with fixed ratio $\rho = N/V$, and we ask about the cycle-length distribution as a function of ρ.

One does not need to construct an infinite-volume model, although this is done in section 3, for pure interest: We will examine limits of expectations of random variables, where the limit is taken as the number of points N of the model goes to infinity. The limits then are in $\mathbb{R}$.

Critical density: We define the **critical density**, $\rho_c(0)$, by the following formula. Here, this is simply an ansatz. (See also section 6.4 where the critical density is discussed from a thermodynamic point of view.)

$$\rho_c(0) = \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{e^{4\beta\pi^2\|\mathbf{k}\|^2} - 1}. \tag{3.2.1}$$

Remark 3.2.2. One may compute

$$\rho_c(0) = \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{e^{4\beta\pi^2\|\mathbf{k}\|^2} - 1} = \frac{\zeta(3/2)}{(4\pi\beta)^{3/2}} \tag{3.2.3}$$

where $\zeta(z)$ is the Riemann zeta function.

Statement of the theorem: For any $0 < a < b < 1$ (nominally, a is just above 0 and b is just below 1) and any $s \geq 0$,

$$\begin{aligned}
\lim_{V\to\infty} \mathbb{E}_{\Lambda,N}(\varrho_{1,N^a}) &= \begin{cases} \rho, & \rho \leq \rho_c(0) \\ \rho_c(0), & \rho_c(0) \leq \rho \end{cases} \\
\lim_{V\to\infty} \mathbb{E}_{\Lambda,N}(\varrho_{N^a,N^b}) &= 0 \\
\lim_{V\to\infty} \mathbb{E}_{\Lambda,N}(\varrho_{N^b,sN}) &= \begin{cases} 0, & \rho \leq \rho_c(0) \\ \rho - \rho_c(0), & \rho_c(0) \leq \rho \leq s + \rho_c(0) \\ s, & s + \rho_c(0) \leq \rho. \end{cases}
\end{aligned} \tag{3.2.4}$$

(See figure 3.)

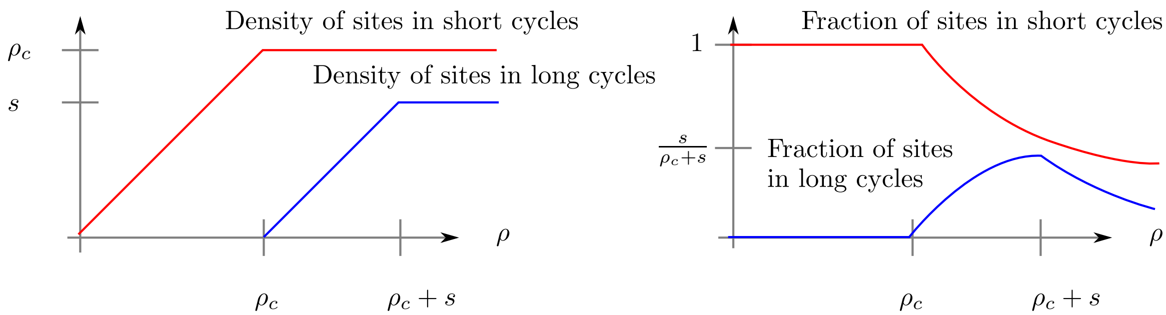

Figure 3: Distribution of cycle lengths as function of density in the infinite-volume limit.

This statement, in terms of the density of sites in cycles of specified lengths, may be more intuitively rephrased in terms of the fraction of sites in cycles of specified length:

$$\begin{aligned}
\lim_{V\to\infty} \mathbb{E}_{\Lambda,N}(f_{1,N^a}) &= \begin{cases} 1, & \rho \leq \rho_c(0) \\ \rho_c(0)/\rho, & \rho_c(0) \leq \rho \end{cases} \\
\lim_{V\to\infty} \mathbb{E}_{\Lambda,N}(f_{N^a,N^b}) &= 0 \\
\lim_{V\to\infty} \mathbb{E}_{\Lambda,N}(f_{N^b,sN}) &= \begin{cases} 0, & \rho \leq \rho_c(0) \\ 1 - \rho_c(0)/\rho, & \rho_c(0) \leq \rho \leq s + \rho_c(0) \\ s/\rho, & s + \rho_c(0) \leq \rho. \end{cases}
\end{aligned}$$

The theorem has the following interpretation:

- At density below $\rho_c(0)$, all sites are in short cycles and no sites are in long cycles.
- As density increases past $\rho_c(0)$ and $\rho_c(0) + s$, fewer sites are in short cycles and more sites are in long cycles. In particular, a strictly positive fraction of sites are in long cycles.

- Asymptotically, all sites are in long cycles.

Late note: The recent paper [BU08] produces an expression for ρ_c, as well as an analogue of the previous theorem, for the weakly interacting ($U \not\equiv 0$) case.

4 Bosonic Feynman-Kac formulas

In this section, the heart of this paper, we recast a familiar Hamiltonian involving **pair-interacting particles** as a new Hamiltonian involving **pair-interacting permutations**. We use the canonical partition function as the vehicle for this transformation:

$$\text{Hamiltonian for particles} \longrightarrow \text{partition function} \longrightarrow \text{Hamiltonian for permuations.}$$

A Feynman-Kac formula for N interacting bosons allows the partition function to be transformed in the middle step.

4.1 Outline

As in section 3.1, we write $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$ for $\mathbf{x}_1, \ldots, \mathbf{x}_N$ in a d-dimensional cube Λ of width L. The Hamiltonian for N pair-interacting particles is

$$H(\mathbf{X}) = -\sum_{i=1}^{N} \nabla_i^2 + \sum_{1 \le i,j \le N} U(\mathbf{x}_i - \mathbf{x}_j). \tag{4.1.1}$$

The U considered in this paper is either identically zero (for the non-interacting case), or a **hard-core potential** with radius a, i.e. $U(\mathbf{x}_i - \mathbf{x}_j)$ is infinite for $|\mathbf{x}_i - \mathbf{x}_j| \le a$ and 0 for $|\mathbf{r}| > a$. (This is an approximation to the true pair potential between helium atoms. See figure 4 [Ceperley].) The hard-core radius a is also known as the **scattering length**.

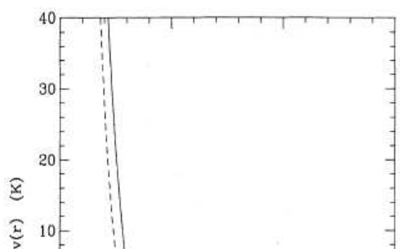

Figure 4: Pair potential between helium atoms (Ceperley, 1995).

As discussed in appendix A.8, the partition function for N distinguishable particles[2] is $\mathrm{Tr}(e^{-\beta H})$. (Section A.8 explains why $\mathrm{Tr}\left(e^{-\beta H}\right)$ is of importance.) Symmetrizing the partitition function, since our particles are bosons, the trace is

$$\mathrm{Tr}_{L^2_{\text{sym}}}(e^{-\beta H}) = \mathrm{Tr}_{L^2}\left(P_+ e^{-\beta H}\right) = \mathrm{Tr}_{L^2}\left(e^{-\beta H} P_+\right)$$

[2]For a particle Hamiltonian, the β factor is in the expected place. This is in contrast to the permutation expression in sections 3.1, where the β factor is, surprisingly, reciprocated. We will see in section 4.6 why the reciprocated β is correct for the permutation Hamiltonian.

where

$$P_+ f(\mathbf{x}_1, \ldots, \mathbf{x}_N) := \frac{1}{N!} \sum_{\pi \in \mathcal{S}_n} M_\pi f(\mathbf{x}_1, \ldots, \mathbf{x}_N)$$

and

$$M_\pi(f\mathbf{x}_1, \ldots, \mathbf{x}_N) := f(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)}).$$

That is,

$$\mathrm{Tr}_{L^2_{\mathrm{sym}}}(e^{-\beta H}) = \frac{1}{N!} \sum_{\pi \in \mathcal{S}_N} \mathrm{Tr}_{L^2}\left(e^{-\beta H} M_\pi\right).$$

(The $e^{-\beta H}$ is bounded and compact, but this fact is not needed.)

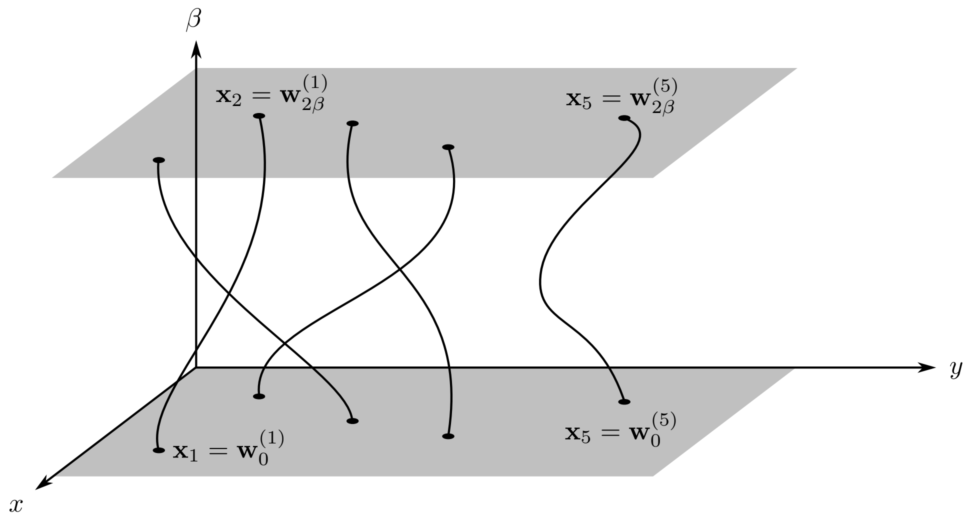

Figure 5: Feynman-Kac representation of a gas of 5 bosons. The horizontal plane represents the d spatial dimensions, and the vertical axis is the imaginary time dimension. The picture shows five particles and two cycles, of respective length 4 and 1.

The following steps remain to develop a bosonic Feynman-Kac formula. The first three steps closely parallel the steps used to construct the familiar single-particle Feynman-Kac formula in appendix E.

- Section 4.2: Interpret $e^{-\beta H} M_\pi$ as an expectation over Brownian motions, as in proposition E.2.1 for the single-particle case.
- Section 4.3: Write $e^{-\beta H} M_\pi$ as an integral operator, and find the kernel.
- Section 4.4: Compute $\mathrm{Tr}(e^{-\beta H} M_\pi)$ in terms of Brownian bridges.
- Section 4.5: Sum over $\pi \in \mathcal{S}_N$ to obtain $Z = \mathrm{Tr}_{L^2_{\mathrm{sym}}}(e^{-\beta H})$. Importantly, we will express Z as sum over permutations π of $e^{-H_P(\mathbf{X},\pi)}$, where this new H_P will be viewed a Hamiltonian for a single permuation π. At this point, the permutation Hamiltonian is found inside $e^{-H_P(\mathbf{X},\pi)}$; we lack an expression for its logarithm.
- Sections 4.6 and 4.7 decouple the non-interacting from the interacting terms in the permutation Hamiltonian, so that we may write $e^{-H_P^{(0)}(\mathbf{X},\pi) - H_P^{(1)}(\mathbf{X},\pi)}$.

- The bosonic Feynman-Kac formula now contains terms for 2-jump interactions, 3-jump interactions, and so on. In section 4.11, we discuss the cluster expansion which allows us to drop all but 2-jump interactions. The cluster expansion furthermore allows us to take the logarithm of $e^{-H_P(\mathbf{X},\pi)}$, with an explicit expression for $H_P(\mathbf{X},\pi)$. We recognize the random-cycle model from section 3, with an explicit 2-jump interaction V.

4.2 $e^{-\beta H} M_\pi$ as expectation

Here we parallel the development for the single-particle case in section E.1.

Proposition 4.2.1. *With H as in equation 4.1.1, we have*

$$e^{-\beta H} f(\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)}) = \mathbb{E}_0^{\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)}}\left[\exp\left\{-\frac{1}{2}\sum_{i<j}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)}-\mathbf{w}_s^{(j)}\right)\,ds\right\} f\left(\mathbf{w}_{2\beta}^{(1)},\ldots,\mathbf{w}_{2\beta}^{(N)}\right)\right].$$

Proof. Using the Trotter product formula (equation E.1.2), namely

$$e^{\beta(A+B)} = \lim_{n\to\infty}\left(e^{\beta A/n}e^{\beta B/n}\right)^n$$

with $A=\sum_{i=1}^N \nabla_i^2$ and $B=-\sum_{i<j} U(\mathbf{x}_i-\mathbf{x}_j)$, we have

$$\begin{aligned}
&e^{-\beta H} f(\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)})\\
&=\lim_{n\to\infty}\left(e^{\frac{\beta}{n}\sum_i\nabla_i^2}e^{-\frac{\beta}{n}\sum_{i<j}U(\mathbf{x}_i-\mathbf{x}_j)}\right)^n f(\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)})\\
&=\lim_{n\to\infty} e^{\frac{\beta}{n}\sum_i\nabla_i^2}e^{-\frac{\beta}{n}\sum_{i<j}U(\mathbf{x}_i-\mathbf{x}_j)}\left(e^{\frac{\beta}{n}\sum_i\nabla_i^2}e^{-\frac{\beta}{n}\sum_{i<j}U(\mathbf{x}_i-\mathbf{x}_j)}\right)^{n-1} f(\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)}).
\end{aligned}$$

Recall that $e^{-\frac{\beta}{n}\sum_{i<j}U(\mathbf{x}_i-\mathbf{x}_j)}$ is simply a scalar. Using the result of section C.2 to write $e^{\frac{\beta}{n}\sum_i\nabla_i^2}$ as an integral operator (since the sum of N Laplacians, each on d dimensions, is a single (Nd)-dimensional Laplacian), and writing

$$\mathbf{Z}^{(k)} = (\mathbf{z}_1^{(k)},\ldots,\mathbf{z}_N^{(k)}),$$

we have

$$\begin{aligned}
e^{-\beta H} f(\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)}) = \lim_{n\to\infty}\int_{\mathbb{R}^{Nd}} & g_{2\beta/n}\left(\mathbf{X}-\mathbf{Z}^{(1)}\right) e^{-\frac{\beta}{n}\sum_{i<j}U(\mathbf{z}_i^{(1)}-\mathbf{z}_j^{(1)})}\\
&\left(e^{\frac{\beta}{n}\sum_i\nabla_i^2}e^{-\frac{\beta}{n}\sum_{i<j}U(\mathbf{x}_i-\mathbf{x}_j)}\right)^{n-1} f(\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)})\,d\mathbf{Z}^{(1)}.
\end{aligned}$$

Repeating $n-1$ more times yields

$$\begin{aligned}
&\lim_{n\to\infty}\underbrace{\int_{\mathbb{R}^{Nd}}\int_{\mathbb{R}^{Nd}}\cdots\int_{\mathbb{R}^{Nd}}}_{n\text{ times}} g_{2\beta/n}\left(\mathbf{X}-\mathbf{Z}^{(1)}\right)\cdots g_{2\beta/n}\left(\mathbf{Z}^{(n-1)}-\mathbf{Z}^{(n)}\right)\\
&\left(\prod_{k=1}^n e^{-\frac{\beta}{n}\sum_{i<j}U(\mathbf{z}_i^{(k)}-\mathbf{z}_j^{(k)})}\right) f(\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)})\,d\mathbf{Z}^{(1)}\cdots d\mathbf{Z}^{(n)}.
\end{aligned}$$

We have an integrand in the form of remark D.3.7, with $\beta_k = 2k\beta/n$, so we can write

$$\lim_{n\to\infty} \underbrace{\int_{\mathbb{R}^{Nd}} \int_{\mathbb{R}^{Nd}} \cdots \int_{\mathbb{R}^{Nd}}}_{n \text{ times}} g_{2\beta/n}\left(\mathbf{X} - \mathbf{Z}^{(1)}\right) \cdots g_{2\beta/n}\left(\mathbf{Z}^{(n-1)} - \mathbf{Z}^{(n)}\right)$$

$$\exp\left\{ \frac{2\beta}{n}\left(-\frac{1}{2}\right) \sum_{i<j} \sum_{k=1}^{n} U\left(\mathbf{z}_i^{(k)} - \mathbf{z}_j^{(k)}\right) \right\} f(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)})\, d\mathbf{Z}^{(1)} \cdots d\mathbf{Z}^{(n)}$$

$$= \mathbb{E}_0^{\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)}} \left[\exp\left\{ -\frac{1}{2} \sum_{i<j} \int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds \right\} f\left(\mathbf{w}_{2\beta}^{(1)}, \ldots, \mathbf{w}_{2\beta}^{(N)}\right) \right].$$

□

4.3 $e^{-\beta H} M_\pi$ as an integral operator

Proposition 4.3.1. *If*

$$H = -\sum_i \nabla_i^2 + \sum_{i<j} U(\mathbf{x}_i - \mathbf{x}_j),$$

then

$$e^{-\beta H} f(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)}) = \int G_{2\beta,U}(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)}, \mathbf{y}_1, \ldots, \mathbf{y}_N)\, f(\mathbf{y}_1, \ldots, \mathbf{y}_N)\, d\mathbf{y}_1 \cdots d\mathbf{y}_N \tag{4.3.2}$$

where

$$G_{2\beta,U}(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)}, \mathbf{y}_1, \ldots, \mathbf{y}_N) = \mathbb{E}_0^{\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)}} \left[\exp\left\{ -\frac{1}{2} \sum_{i<j} \int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds \right\} \prod_{i=1}^{N} \delta\left(\mathbf{w}_\beta^{(i)} - \mathbf{y}^{(i)}\right) \right]. \tag{4.3.3}$$

Proof. Insert equation 4.3.3 into the right-hand side of 4.3.2, interchange expectation and integral, and integrate out the delta function as in proposition E.2.1. □

4.4 $\mathrm{Tr}(e^{-\beta H} M_\pi)$ using Brownian bridges

Proposition 4.4.1. *The trace may be computed using Brownian bridges as follows:*

$$\mathrm{Tr}(e^{-\beta H} M_\pi) = \int d\mathbf{X} \int \left(\prod_{k=1}^{N} d\mathbf{W}_{0,2\beta}^{\mathbf{x}_k, \mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right) \right) \left[\exp\left\{ -\frac{1}{2} \sum_{i<j} \int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds \right\} \right].$$

Proof. Using proposition C.3.1, we have

$$\mathrm{Tr}(e^{-\beta H} M_\pi) = \int G_{2\beta,U}(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)}, \mathbf{x}_1, \ldots, \mathbf{x}_N)\, d\mathbf{X}.$$

Equation 4.3.3 of proposition 4.3.1 gives us an expression for G. Then

$$\mathrm{Tr}(e^{-\beta H} M_\pi) = \int \mathbb{E}_0^{\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)}} \left[\exp\left\{ -\frac{1}{2} \sum_{i<j} \int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds \right\} \prod_{i=1}^{N} \delta\left(\mathbf{w}_{2\beta}^{(i)} - \mathbf{x}^{(i)}\right) \right] d\mathbf{X}.$$

Using proposition D.5.3, we may convert this expectation over Brownian motion into an expectation over Brownian bridges to obtain

$$\mathrm{Tr}(e^{-\beta H}M_\pi) = \prod_{i=1}^{N} g_{2\beta}\left(\mathbf{x}_i - \mathbf{x}_{\pi(i)}\right) \int \mathbb{E}_{0,2\beta}^{\mathbf{x}_1,\mathbf{x}_{\pi(1)};\ldots;\mathbf{x}_N,\mathbf{x}_{\pi(N)}} \left[\exp\left\{-\frac{1}{2}\sum_{i<j}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right)\, ds\right\}\right] d\mathbf{X}.$$

Using definition D.4.5, we may write this using $d\mathbf{W}$ notation:

$$\mathrm{Tr}(e^{-\beta H}M_\pi) = \int d\mathbf{X} \int \left[\prod_{k=1}^{N} d\mathbf{W}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)\right] \exp\left\{-\frac{1}{2}\sum_{i<j}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right)\, ds\right\}.$$

□

4.5 Sum over $\pi \in \mathcal{S}_N$

Applying proposition 4.4.1, we continue the plan laid out in section 4, namely:

$$\begin{aligned}\mathrm{Tr}_{L^2_{\mathrm{sym}}}(e^{-\beta H}) &= \frac{1}{N!}\sum_{\pi\in\mathcal{S}_N} \mathrm{Tr}_{L^2}\left(e^{-\beta H}M_\pi\right)\\ &= \frac{1}{N!}\int d\mathbf{X} \sum_{\pi\in\mathcal{S}_N}\left[\prod_{k=1}^{N}\int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)\right] \exp\left\{-\frac{1}{2}\sum_{i<j}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right)\, ds\right\}.\end{aligned}$$

Notationally, we may split this up as

$$\begin{aligned}\mathrm{Tr}_{L^2_{\mathrm{sym}}}(e^{-\beta H}) &= \frac{1}{N!}\int d\mathbf{X}\sum_{\pi\in\mathcal{S}_N} e^{-H_P(\mathbf{X},\pi)}\\ e^{-H_P(\mathbf{X},\pi)} &= \left[\prod_{k=1}^{N}\int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)\right] \exp\left\{-\frac{1}{2}\sum_{i<j}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right)\, ds\right\}.\end{aligned} \tag{4.5.1}$$

Here is the pivotal point of this paper — the original partition function appears as a sum over π of an $\mathbf{X}$-averaged quantity. That quantity is non-negative so we may write it as the exponential of something which we call H_P. The sum over permutations of e^{-H_P} is precisely what we would want for a partition function involving energies, not of *particles*, but of individual *permutations*. The remaining steps of this section involve separating out the non-interacting terms from the interacting terms in e^{-H_P}, and finding an expression for the logarithm of e^{-H_P}.

4.6 Extraction of the non-interacting terms

In this section we obtain $e^{-H_P^{(0)}(\mathbf{X},\pi)}$ as well as its logarithm.

Let $U \equiv 0$ in equation 4.5.1. Then we have

$$e^{-H_P(\mathbf{X},\pi)} = \left[\prod_{k=1}^{N}\int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)(1)\right].$$

Recall from proposition D.6.3 and definition C.1.1 that

$$\int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)(1) = g_{2\beta}(\mathbf{x}_k - \mathbf{x}_{\pi(k)}) = \frac{1}{(4\pi\beta)^{d/2}} \exp\left\{-\frac{1}{4\beta}\|\mathbf{x}_k - \mathbf{x}_{\pi(k)}\|^2\right\}. \tag{4.6.1}$$

Then

$$\begin{aligned} e^{-H_P(\mathbf{X},\pi)} &= \left[\frac{1}{(4\pi\beta)^{dN/2}} \prod_{k=1}^{N} \exp\left\{-\frac{1}{4\beta}\|\mathbf{x}_k - \mathbf{x}_{\pi(k)}\|^2\right\}\right] \\ &= \left[\frac{1}{(4\pi\beta)^{dN/2}} \exp\left\{-\frac{1}{4\beta}\sum_{k=1}^{N}\|\mathbf{x}_k - \mathbf{x}_{\pi(k)}\|^2\right\}\right]. \end{aligned}$$

We write

$$e^{-H_P(\mathbf{X},\pi)} = \frac{1}{(4\pi\beta)^{dN/2}} e^{-H_P^{(0)}(\mathbf{X},\pi)} \tag{4.6.2}$$

where

$$H_P^{(0)}(\mathbf{X},\pi) = \frac{1}{4\beta}\sum_{k=1}^{N}\|\mathbf{x}_k - \mathbf{x}_{\pi(k)}\|^2. \tag{4.6.3}$$

(We ignore the prefactor in equation 4.6.2 since it cancels out in the computation of expectations of random variables.)

Remark 4.6.4. Here is the key point where we discover that the β in the permutation Hamiltonian is indeed reciprocated — in contrast to our experience with particle Hamiltonians.

4.7 Extraction of the interacting terms

Here we use the result of the previous section to decompose the exponentiated permutation energy as

$$e^{-H_P(\mathbf{X},\pi)} = e^{-H_P^{(0)}(\mathbf{X},\pi)} e^{-H_P^{(1)}(\mathbf{X},\pi)}.$$

Unlike section 4.6 where we found the logarithm of $e^{-H_P^{(0)}}$, though, at this point we have only $e^{-H_P^{(1)}}$. Finding the logarithm of the latter requires the cluster expansion in section 4.11.

Equation 4.5.1 is

$$e^{-H_P(\mathbf{X},\pi)} = \left[\prod_{k=1}^{N}\int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)\right] \exp\left\{-\frac{1}{2}\sum_{i<j}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds\right\}.$$

Recall from definition D.6.1 that

$$d\mathbf{W}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}}\left(\mathbf{w}^{(k)}\right) = g_{2\beta}(\mathbf{x}_i - \mathbf{x}_{\pi(i)})\, d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}}\left(\mathbf{w}^{(k)}\right).$$

Combining the two, we have

$$\begin{aligned} e^{-H_P(\mathbf{X},\pi)} &= \left[\prod_{k=1}^{N}\int g_{2\beta}(\mathbf{x}_i - \mathbf{x}_{\pi(i)})\, d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}}\left(\mathbf{w}^{(k)}\right)\right] \exp\left\{-\frac{1}{2}\sum_{i<j}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds\right\} \\ &= \left[\prod_{k=1}^{N} g_{2\beta}(\mathbf{x}_i - \mathbf{x}_{\pi(i)})\right]\left[\prod_{k=1}^{N}\int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}}\left(\mathbf{w}^{(k)}\right)\right] \exp\left\{-\frac{1}{2}\sum_{i<j}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds\right\}. \end{aligned}$$

Since

$$g_{2\beta}(\mathbf{x}_k - \mathbf{x}_{\pi(k)}) = \frac{1}{(4\pi\beta)^{d/2}} \exp\left\{-\frac{1}{4\beta}\|\mathbf{x}_k - \mathbf{x}_{\pi(k)}\|^2\right\}$$

(equation 4.6.1), we obtain

$$e^{-H_P(\mathbf{X},\pi)} = \frac{1}{(4\pi\beta)^{dN/2}} e^{-H_P^{(0)}(\mathbf{X},\pi)} \left[\prod_{k=1}^{N} \int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}} \left(\mathbf{w}^{(k)}\right)\right] \exp\left\{-\frac{1}{2}\sum_{i<j} \int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds\right\}.$$

Thus we define

$$e^{-H_P^{(1)}(\mathbf{X},\pi)} = \left[\prod_{k=1}^{N} \int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}} (\mathbf{w}^{(k)})\right] \exp\left\{-\frac{1}{2}\sum_{i<j} \int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds\right\}. \tag{4.7.1}$$

This appears very similar to equation 4.5.1; indeed, the only notational difference on the right-hand side is the replacement of $d\mathbf{W}$ by $d\hat{\mathbf{W}}$.

4.8 Expansion of multi-jump interactions

In preparation for the cluster expansion in section 4.11, we reorganize $e^{-H_P^{(1)}}$. We develop a heuristic for multi-jump collision probabilities, then in section 4.9 apply the inclusion/exclusion principle to identify k-jump interactions for increasing values of k.

These manipulations may be done formally, with little intuition. To develop a useful intuition to guide understanding of the manipulations, we first interpret $e^{-H_P^{(1)}}$ in terms of collision probabilities.

Result: The result of this section is that $e^{-H_P^{(1)}}$ (equation 4.7.1) may be interpreted as the probability that all $N(N-1)/2$ jump pairs avoid one another.

The justification for this result is as follows.

- Recall that $U(\mathbf{r}) = \infty$ for $\mathbf{r} \le a$; $U(\mathbf{r}) = 0$ for $\mathbf{r} > a$.
- If the ith and jth Brownian-bridge paths ever come within radius a of one another at any Feynman time between 0 and 2β, for a particular realizations of $\mathbf{w}^{(i)}$ and $\mathbf{w}^{(j)}$, then

  $$\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds$$

  is infinite. If they do not come within radius a of one another, then that integral is 0.
- Thus,

  $$\exp\left\{-\frac{1}{2}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds\right\}$$

  is 0 if the ith and jth bridges collide, and 1 if they avoid one another.
- Recall from definition D.4.5 that

  $$\int \exp\left\{\int_0^{2\beta} f(\mathbf{w}_s)\, ds\right\} d\mathbf{W}_{0,2\beta}^{\mathbf{x},\mathbf{y}}(\mathbf{w}) := \mathbb{E}_{0,2\beta}^{\mathbf{x},\mathbf{y}}\left[\exp\left\{\int_0^{2\beta} f(\mathbf{w}_s)\, ds\right\}\right].$$

  The difference of the Brownian bridges $\mathbf{w}^{(i)}$ and $\mathbf{w}^{(j)}$ is twice another Brownian bridge (proposition D.4.10) so definition D.4.5 applies to $\mathbf{w}^{(i)} - \mathbf{w}^{(j)}$.

- Thus, the expectation

$$\left[\int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}}\left(\mathbf{w}^{(i)}\right)\int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_j,\mathbf{x}_{\pi(j)}}\left(\mathbf{w}^{(j)}\right)\right]\exp\left\{-\frac{1}{2}\int_0^{2\beta}U\left(\mathbf{w}_s^{(i)}-\mathbf{w}_s^{(j)}\right)\,ds\right\}$$

  is the **avoidance probability** for the bridges $\mathbf{w}^{(i)}$ and $\mathbf{w}^{(j)}$.

- There are N permutation jumps and $N(N-1)/2$ distinct jump pairs, so

$$e^{-H_P^{(1)}(\mathbf{X},\pi)}=\left[\prod_{k=1}^{N}\int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)\right]\prod_{i<j}\exp\left\{-\frac{1}{2}\int_0^{2\beta}U\left(\mathbf{w}_s^{(i)}-\mathbf{w}_s^{(j)}\right)\,ds\right\}$$

  (equation 4.7.1) is the probability that all $N(N-1)/2$ jump pairs avoid one another.

4.9 Inclusion/exclusion and collision probabilities

The goal of this section is to reinterpret the avoidance probability of the previous section as an alternating sum of collision probabilities.

Definition 4.9.1. Define

$$\Upsilon\left(\mathbf{w}^{(i)}-\mathbf{w}^{(j)}\right)=1-\exp\left\{-\frac{1}{2}\int_0^{2\beta}U\left(\mathbf{w}_s^{(i)}-\mathbf{w}_s^{(j)}\right)\,ds\right\}.$$

We will frequently abbreviate this as Υ_{ij}. In light of the discussion in the previous section, the expected value of this is the **collision probability** for $\mathbf{w}^{(i)}$ and $\mathbf{w}^{(j)}$.

Then equation 4.7.1 becomes

$$e^{-H_P^{(1)}(\mathbf{X},\pi)}=\left[\prod_{k=1}^{N}\int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)\right]\prod_{i<j}\left(1-\Upsilon\left(\mathbf{w}^{(i)}-\mathbf{w}^{(j)}\right)\right).\tag{4.9.2}$$

Using de Morgan's law, we have

$$P(\text{all avoid})=1-P(\text{any collide}).$$

Let C_ℓ be the event that the ℓth pair $(\mathbf{w}^{(i)},\mathbf{w}^{(j)})$ collides. There are $N(N-1)/2$ such events. The latter term is a union of events, so we may use the inclusion/exclusion principle to write

$$\begin{aligned}1-P(\cup C_\ell)&=1-\sum_i P(C_i)+\sum_{ij}P(C_i\cap C_j)-\sum_{ijk}P(C_i\cap C_j\cap C_k)+\dots\\&+(-1)^m\sum_{m-\text{tuples of jump pairs}}P(m\text{ bridges collide})+\dots\\&+(-1)^{N(N-1)/2}P(\text{all bridges collide}).\end{aligned}$$

Collecting summation symbols, i.e. ranking the terms of $e^{-H_P^{(1)}}$ by increasing m for probabilities of m-tuples of jump pairs colliding, we have

$$e^{-H_P^{(1)}(\mathbf{X},\pi)}=\left[\prod_{k=1}^{N}\int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)\right]\sum_{m=0}^{N(N-1)/2}(-1)^m\sum_{(i_1,j_1),\dots,(i_m,j_m)}\prod_{\ell=1}^{m}\Upsilon\left(\mathbf{w}^{(i_\ell)}-\mathbf{w}^{(j_\ell)}\right)\tag{4.9.3}$$

The first sum is over sizes of subsets of the $N(N-1)/2$ jump pairs; the second sum is over all possible ways of selecting m pairs.

For example, with $N=3$, there are $N(N-1)/2 = 3$ jump pairs: $1,2$; $1,3$; $2,3$. Then

$$\begin{aligned} e^{-H_P^{(1)}(\mathbf{X},\pi)} = 1 & \\ & - P(1,2 \text{ collide}) - P(1,3 \text{ collide}) - P(2,3 \text{ collide}) \\ & + P(1,2 \text{ and } 1,3 \text{ collide}) + P(1,2 \text{ and } 2,3 \text{ collide}) + P(1,3 \text{ and } 2,3 \text{ collide}) \\ & - P(1,2 \text{ and } 1,3 \text{ and } 2,3 \text{ collide}). \end{aligned}$$

Here there is one m value per line; the different P's on that line are indexed by ℓ. In terms of Υ's, we have

$$\begin{aligned} e^{-H_P^{(1)}(\mathbf{X},\pi)} = & \left[\int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_1,\mathbf{x}_{\pi(1)}}\left(\mathbf{w}^{(1)}\right) \int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_2,\mathbf{x}_{\pi(2)}}\left(\mathbf{w}^{(2)}\right) \int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_3,\mathbf{x}_{\pi(3)}}\left(\mathbf{w}^{(3)}\right) \right] \\ & \left(\underbrace{1}_{m=0} - \underbrace{(\Upsilon_{12}+\Upsilon_{13}+\Upsilon_{23})}_{m=1} + \underbrace{(\Upsilon_{12}\Upsilon_{13}+\Upsilon_{12}\Upsilon_{23}+\Upsilon_{13}\Upsilon_{23})}_{m=2} - \underbrace{\Upsilon_{12}\Upsilon_{13}\Upsilon_{23}}_{m=3} \right). \end{aligned}$$

This collection of m-size subsets of the set of jump pairs is the difference between equations 4.9.2 and 4.9.3.

This expression has been obtained using the inclusion/exclusion principle. Notice, however, that one obtains the same expression by distributing the product $(1-\Upsilon_{12})(1-\Upsilon_{13})(1-\Upsilon_{23})$ (for $N=3$) or, in general, $\prod_{i<j}(1-\Upsilon_{ij})$.

4.10 Heuristic for cluster expansion

Moving the integrals through the sums in equation 4.9.3, we obtain

$$e^{-H_P^{(1)}(\mathbf{X},\pi)} = \sum_{m=0}^{N(N-1)/2} (-1)^m \sum_{(i_1,j_1),\ldots,(i_m,j_m)} \left[\prod_{k=1}^{N} \int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right) \right] \prod_{\ell=1}^{m} \Upsilon\left(\mathbf{w}^{(i_\ell)} - \mathbf{w}^{(j_\ell)}\right). \tag{4.10.1}$$

The heuristic (formalized by the cluster expansion as described in section 4.11) is that one may form an approximation by also moving the integrals through the leftmost product.

(For example, let $N=3$. For shorthand, let

$$\int_k = d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right).$$

Then

$$\begin{aligned} e^{-H_P^{(1)}(\mathbf{X},\pi)} &= \left[\int_1\int_2\int_3\right](1-\Upsilon_{12}-\Upsilon_{13}-\Upsilon_{23}+\Upsilon_{12}\Upsilon_{13}+\Upsilon_{12}\Upsilon_{23}+\Upsilon_{13}\Upsilon_{23}-\Upsilon_{12}\Upsilon_{13}\Upsilon_{23}) \\ &= 1 - \int_1\int_2\Upsilon_{12} - \int_1\int_3\Upsilon_{13} - \int_2\int_3\Upsilon_{23} \\ &+ \int_1\int_2\int_3\Upsilon_{12}\Upsilon_{13} + \int_1\int_2\int_3\Upsilon_{12}\Upsilon_{23} + \int_1\int_2\int_3\Upsilon_{13}\Upsilon_{23} - \int_1\int_2\int_3\Upsilon_{12}\Upsilon_{13}\Upsilon_{23}. \end{aligned}$$

The integrals move trivially through the product for $m=0,1$; for $m\geq 2$, the approximations are of the form

$$\left[\int_1\int_2\int_3\Upsilon_{12}\Upsilon_{13}\right] \approx \left[\int_1\int_2\Upsilon_{12}\right]\left[\int_1\int_3\Upsilon_{13}\right] \tag{4.10.2}$$

and so on. Dropping the $m \geq 2$ terms depends on the smallness of this modification. This step is formalized by the cluster expansion in section 4.11. Intuitively, recall that Υ_{12} is the probability that bridges 1 and 2 collide, while $\Upsilon_{12}\Upsilon_{13}$ is the probability of a collision between bridges 1 and 2 *and* bridges 1 and 3. The approximation condition in equation 4.10.2 is that, for weak interactions, these events are weakly correlated and hence nearly independent. This is always true when ij's do not overlap. E.g. for $N = 4$, $\left[\int_1 \int_2 \int_3 \int_4 \Upsilon_{12}\Upsilon_{34}\right] = \left[\int_1 \int_2 \Upsilon_{12}\right] \left[\int_3 \int_4 \Upsilon_{34}\right]$. The approximation applies to overlapping ij's.)

Once the integrals have been moved through the leftmost product of equation 4.10.1, the expectation of $\Upsilon(\mathbf{w}^{(i_\ell)} - \mathbf{w}^{(j_\ell)})$ depends only on the Brownian bridges for $\mathbf{w}^{(i_\ell)}$ and $\mathbf{w}^{(j_\ell)}$.

We define

$$V_{ij} = V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}) = \left[\int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}}\left(\mathbf{w}^{(i)}\right) \int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_j,\mathbf{x}_{\pi(j)}}\left(\mathbf{w}^{(j)}\right)\right] \Upsilon\left(\mathbf{w}^{(i)} - \mathbf{w}^{(j)}\right). \tag{4.10.3}$$

Since we assume small interactions V_{ij},

$$\begin{aligned} e^{-H_P^{(1)}(\mathbf{X},\pi)} &\approx \prod_{i<j}(1 - V_{ij}) \\ &\approx \prod_{i<j}\left(1 - V_{ij} + \frac{V_{ij}^2}{2} - \frac{V_{ij}^3}{6} + \ldots\right) = \prod_{i<j} e^{-V_{ij}} = \exp\left\{-\sum_{i<j} V_{ij}\right\}. \end{aligned} \tag{4.10.4}$$

Here, the first $\approx$ comes from moving the stochastic integrals through the product as discussed at the start of this section, and the second $\approx$ arises from the insertion of negligible higher-order terms in the V_{ij}'s.

For example, with $N = 3$, we have

$$(1 - V_{12})(1 - V_{13})(1 - V_{23}) = 1 - (V_{12} + V_{13} + V_{23}) + (V_{12}V_{13} + V_{12}V_{23} + V_{13}V_{23}) - V_{12}V_{13}V_{23}$$

which we compare to

$$\begin{aligned} &\left(1 - V_{12} + \frac{V_{12}^2}{2} - \ldots\right)\left(1 - V_{13} + \frac{V_{13}^2}{2} - \ldots\right)\left(1 - V_{23} + \frac{V_{23}^2}{2} - \ldots\right) \\ &= 1 - (V_{12} + V_{13} + V_{23}) + (V_{12}V_{13} + V_{12}V_{23} + V_{13}V_{23}) - V_{12}V_{13}V_{23} \\ &+ \left(\frac{V_{12}^2}{2} + \frac{V_{13}^2}{2} + \frac{V_{23}^2}{2}\right) - \left(\frac{V_{12}^2V_{13}}{2} + \frac{V_{12}V_{13}^2}{2} + \frac{V_{12}^2V_{23}}{2} + \frac{V_{12}V_{23}^2}{2} + \frac{V_{13}^2V_{23}}{2} + \frac{V_{13}V_{23}^2}{2}\right) \\ &+ \left(\frac{V_{12}^2V_{13}^2}{4} + \frac{V_{12}^2V_{23}^2}{4} + \frac{V_{13}^2V_{23}^2}{4}\right) \\ &+ \left(\frac{V_{12}^2V_{13}V_{23}}{2} + \frac{V_{12}V_{13}^2V_{23}}{2} + \frac{V_{12}V_{13}V_{23}^2}{2}\right) - \left(\frac{V_{12}V_{13}^2V_{23}^2}{4} + \frac{V_{12}^2V_{13}^2V_{23}}{4} + \frac{V_{12}^2V_{13}V_{23}^2}{4}\right) + \frac{V_{12}^2V_{13}^2V_{23}^2}{8} + \ldots. \end{aligned}$$

We have now achieved one of the goals outlined in section 4.1, namely, to find the logarithm of $e^{H_P^{(1)}}$. Equation 4.10.4 becomes

$$H_P^{(1)}(\mathbf{X}, \pi) = \sum_{1 \leq i < j \leq N} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)})$$

where the jump-pair interaction is as in equation 4.10.3.

4.11 Cluster expansion and jump-pair interactions

This section formalizes the heuristic in section 4.10. This topic is addressed in section 4 of [U07]. Given time constraints leading up to my comprehensive examination, I will first finish other sections of this paper, then complete this section if time permits.

4.12 Simplified jump-pair interactions

When one computes the jump-pair interaction, it is possible to replace the double Brownian bridge by a single Brownian bridge. (See also figure 6.)

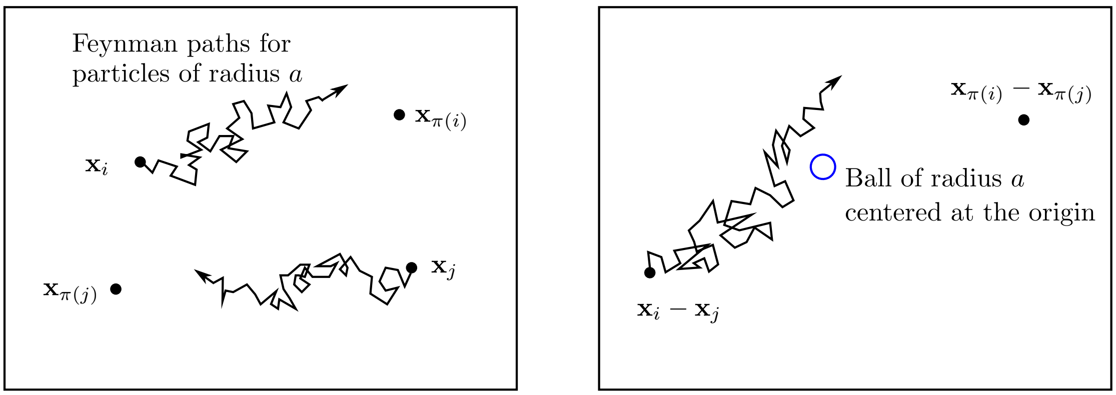

Figure 6: Replacement of double Brownian bridge by single Brownian bridge for jump-pair interactions.

Proposition 4.12.1. *The jump-pair interaction* $V_{ij} = V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)})$ *(equation 4.10.3) satisfies*

$$\int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}}(\mathbf{w}^{(i)}) \int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_j,\mathbf{x}_{\pi(j)}}(\mathbf{w}^{(j)}) \left[1 - \exp\left\{-\frac{1}{2}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right)\, ds\right\}\right]$$
$$= \int d\hat{\mathbf{W}}_{0,4\beta}^{\mathbf{x}_i-\mathbf{x}_j,\mathbf{x}_{\pi(i)},\mathbf{x}_{\pi(j)}}(\mathbf{w}^{(ij)}) \left[1 - \exp\left\{-\frac{1}{4}\int_0^{4\beta} U\left(\mathbf{w}_s^{(ij)}\right)\, ds\right\}\right].$$

Proof. From the definition of $\int d\mathbf{W}$ and $\int d\hat{\mathbf{W}}$ (definitions D.4.5 and D.6.1, respectively), we have

$$\int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}}(\mathbf{w}^{(i)}) \int d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_j,\mathbf{x}_{\pi(j)}}(\mathbf{w}^{(j)}) = \frac{\int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}}(\mathbf{w}^{(i)})}{g_{2\beta}(\mathbf{x}_i - \mathbf{x}_{\pi(i)})} \frac{\int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_j,\mathbf{x}_{\pi(j)}}(\mathbf{w}^{(j)})}{g_{2\beta}(\mathbf{x}_j - \mathbf{x}_{\pi(j)})} \tag{4.12.2}$$

and

$$\begin{aligned}
&\int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_i,\mathbf{x}_{\pi(i)}}(\mathbf{w}^{(i)}) \int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_j,\mathbf{x}_{\pi(j)}}(\mathbf{w}^{(j)}) \left[1-\exp\left\{-\frac{1}{2}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)}-\mathbf{w}_s^{(j)}\right)\, ds\right\}\right] \\
&= \lim_{n\to\infty} \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1 \text{ times}} \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1 \text{ times}} d\mathbf{z}_1^{(i)}\cdots d\mathbf{z}_{n-1}^{(i)}\; d\mathbf{z}_1^{(j)}\cdots d\mathbf{z}_{n-1}^{(j)} \\
&g_{2\beta/n}\left(\mathbf{x}_i-\mathbf{z}_1^{(i)}\right) g_{2\beta/n}\left(\mathbf{z}_1^{(i)}-\mathbf{z}_2^{(i)}\right)\cdots g_{2\beta/n}\left(\mathbf{z}_{n-2}^{(i)}-\mathbf{z}_{n-1}^{(i)}\right) g_{2\beta/n}\left(\mathbf{z}_{n-1}^{(i)}-\mathbf{x}_{\pi(i)}\right) \\
&g_{2\beta/n}\left(\mathbf{x}_j-\mathbf{z}_1^{(j)}\right) g_{2\beta/n}\left(\mathbf{z}_1^{(j)}-\mathbf{z}_2^{(i)}\right)\cdots g_{2\beta/n}\left(\mathbf{z}_{n-2}^{(j)}-\mathbf{z}_{n-1}^{(j)}\right) g_{2\beta/n}\left(\mathbf{z}_{n-1}^{(j)}-\mathbf{x}_{\pi(j)}\right) \\
&\left[1-\exp\left\{\frac{2\beta}{n}\left(-\frac{1}{2}\right)\left(U(\mathbf{x}_i-\mathbf{x}_j)+\sum_{k=1}^{n-1} U\left(\mathbf{z}_k^{(i)}-\mathbf{z}_k^{(j)}\right)\right)\right\}\right].
\end{aligned} \tag{4.12.3}$$

For brevity, let

$$\begin{aligned}
\mathbf{z}_0^{(i)} &= \mathbf{x}_i, & \mathbf{z}_n^{(i)} &= \mathbf{x}_{\pi(i)} \\
\mathbf{z}_0^{(j)} &= \mathbf{x}_j, & \mathbf{z}_n^{(j)} &= \mathbf{x}_{\pi(j)}.
\end{aligned}$$

Then the right-hand side of equation 4.12.3 becomes

$$\begin{aligned}
&\lim_{n\to\infty} \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1 \text{ times}} \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1 \text{ times}} d\mathbf{z}_1^{(i)}\cdots d\mathbf{z}_{n-1}^{(i)}\; d\mathbf{z}_1^{(j)}\cdots d\mathbf{z}_{n-1}^{(j)} \\
&\prod_{k=0}^{n-1} g_{2\beta/n}\left(\mathbf{z}_k^{(i)}-\mathbf{z}_{k+1}^{(i)}\right) \prod_{k=0}^{n-1} g_{2\beta/n}\left(\mathbf{z}_k^{(j)}-\mathbf{z}_{k+1}^{(j)}\right) \left[1-\exp\left\{\frac{2\beta}{n}\left(-\frac{1}{2}\right)\sum_{k=0}^{n-1} U\left(\mathbf{z}_k^{(i)}-\mathbf{z}_k^{(j)}\right)\right\}\right].
\end{aligned}$$

We now make a change of variable. For $k = 0, \ldots, n$, let

$$\mathbf{y}_k^{(ij)} = \mathbf{z}_k^{(i)} - \mathbf{z}_k^{(j)}.$$

The linear map sending $\left(\mathbf{z}_k^{(i)}, \mathbf{z}_k^{(j)}\right)$ to $\left(\mathbf{z}_k^{(i)}, \mathbf{y}_k^{(ij)}\right)$ is

$$\begin{pmatrix} \mathbf{z}_k^{(i)} \\ \mathbf{y}_k^{(ij)} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \mathbf{z}_k^{(i)} \\ \mathbf{z}_k^{(j)} \end{pmatrix}$$

which has Jacobian determinant of absolute value 1, so we may replace

$$d\mathbf{z}_1^{(i)}\cdots d\mathbf{z}_{n-1}^{(i)} d\mathbf{z}_1^{(j)}\cdots d\mathbf{z}_{n-1}^{(j)}$$

with

$$d\mathbf{z}_1^{(i)}\cdots d\mathbf{z}_{n-1}^{(i)} d\mathbf{y}_1^{(ij)}\cdots d\mathbf{y}_{n-1}^{(ij)}.$$

Lemma C.1.4 tells us

$$\begin{aligned}
&g_{2\beta/n}\left(\mathbf{z}_k^{(i)}-\mathbf{z}_{k+1}^{(i)}\right) g_{2\beta/n}\left(\mathbf{z}_k^{(j)}-\mathbf{z}_{k+1}^{(j)}\right) \\
&= g_{4\beta/n}\left((\mathbf{z}_k^{(i)}-\mathbf{z}_k^{(j)})-(\mathbf{z}_{k+1}^{(i)}-\mathbf{z}_{k+1}^{(j)})\right)\; g_{\beta/n}\left(\mathbf{z}_k^{(i)}-\mathbf{z}_{k+1}^{(i)}-\frac{1}{2}\left(\mathbf{z}_k^{(i)}-\mathbf{z}_k^{(j)}\right)+\frac{1}{2}\left(\mathbf{z}_{k+1}^{(i)}-\mathbf{z}_{k+1}^{(j)}\right)\right) \\
&= g_{4\beta/n}\left(\mathbf{y}_k^{(ij)}-\mathbf{y}_{k+1}^{(ij)}\right)\; g_{\beta/n}\left(\mathbf{z}_k^{(i)}-\mathbf{z}_{k+1}^{(i)}-\frac{1}{2}\mathbf{y}_k^{(ij)}+\frac{1}{2}\mathbf{y}_{k+1}^{(ij)}\right) \\
&= g_{4\beta/n}\left(\mathbf{y}_k^{(ij)}-\mathbf{y}_{k+1}^{(ij)}\right)\; g_{\beta/n}\left(\left(\mathbf{z}_k^{(i)}-\mathbf{z}_{k+1}^{(i)}\right)-\frac{1}{2}\left(\mathbf{y}_k^{(ij)}-\mathbf{y}_{k+1}^{(ij)}\right)\right).
\end{aligned}$$

Then we have

$$\lim_{n\to\infty} \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1\text{ times}} \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1\text{ times}} d\mathbf{z}_1^{(i)}\cdots d\mathbf{z}_{n-1}^{(i)}\; d\mathbf{y}_1^{(ij)}\cdots d\mathbf{y}_{n-1}^{(ij)}$$

$$\prod_{k=0}^{n-1} g_{4\beta/n}\left(\mathbf{y}_k^{(ij)}-\mathbf{y}_{k+1}^{(ij)}\right)\prod_{k=0}^{n-1} g_{\beta/n}\left(\left(\mathbf{z}_k^{(i)}-\mathbf{z}_{k+1}^{(i)}\right)-\frac{1}{2}\left(\mathbf{y}_k^{(ij)}-\mathbf{y}_{k+1}^{(ij)}\right)\right)\left[1-\exp\left\{-\frac{\beta}{n}\sum_{k=0}^{n-1}U\left(\mathbf{y}_k^{(ij)}\right)\right\}\right].$$

Re-arranging terms (permissible by Tonelli's theorem due to the non-negativity of the integrand) yields

$$\lim_{n\to\infty} \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1\text{ times}} d\mathbf{y}_1^{(ij)}\cdots d\mathbf{y}_{n-1}^{(ij)}\prod_{k=0}^{n-1} g_{4\beta/n}\left(\mathbf{y}_k^{(ij)}-\mathbf{y}_{k+1}^{(ij)}\right)\left[1-\exp\left\{\frac{4\beta}{n}\left(-\frac{1}{4}\right)\sum_{k=0}^{n-1}U\left(\mathbf{y}_k^{(ij)}\right)\right\}\right]$$

$$\underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1\text{ times}} d\mathbf{z}_1^{(i)}\cdots d\mathbf{z}_{n-1}^{(i)}\prod_{k=0}^{n-1} g_{\beta/n}\left(\left(\mathbf{z}_k^{(i)}-\mathbf{z}_{k+1}^{(i)}\right)-\frac{1}{2}\left(\mathbf{y}_k^{(ij)}-\mathbf{y}_{k+1}^{(ij)}\right)\right).$$

(4.12.4)

The second line of equation 4.12.4 collapses by the iterated Chapman-Kolmogorov proposition (proposition C.1.3):

$$\underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1\text{ times}} d\mathbf{z}_1^{(i)}\cdots d\mathbf{z}_{n-1}^{(i)}\prod_{k=0}^{n-1} g_{\beta/n}\left(\left(\mathbf{z}_k^{(i)}-\mathbf{z}_{k+1}^{(i)}\right)-\frac{1}{2}\left(\mathbf{y}_k^{(ij)}-\mathbf{y}_{k+1}^{(ij)}\right)\right)$$

$$\underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1\text{ times}} d\mathbf{z}_1^{(i)}\cdots d\mathbf{z}_{n-1}^{(i)}\prod_{k=0}^{n-1} g_{\beta/n}\left(\left(\mathbf{z}_k^{(i)}-\frac{\mathbf{y}_k^{(ij)}}{2}\right)-\left(\mathbf{z}_{k+1}^{(i)}-\frac{\mathbf{y}_{k+1}^{(ij)}}{2}\right)\right)$$

$$= g_\beta\left(\left(\mathbf{z}_0^{(i)}-\frac{\mathbf{y}_0^{(ij)}}{2}\right)-\left(\mathbf{z}_n^{(i)}-\frac{\mathbf{y}_n^{(ij)}}{2}\right)\right) = g_\beta\left(\left(\mathbf{x}_i-\frac{\mathbf{x}_i-\mathbf{x}_j}{2}\right)-\left(\mathbf{x}_{\pi(i)}-\frac{\mathbf{x}_{\pi(i)}-\mathbf{x}_{\pi(j)}}{2}\right)\right)$$

$$= g_\beta\left(\frac{\mathbf{x}_i+\mathbf{x}_j}{2}-\frac{\mathbf{x}_{\pi(i)}+\mathbf{x}_{\pi(j)}}{2}\right).$$

With this scale factor pulled out of equation 4.12.4, and recognizing the first line of equation 4.12.4 from definition D.4.5, we now have

$$g_\beta\left(\frac{\mathbf{x}_i+\mathbf{x}_j}{2}-\frac{\mathbf{x}_{\pi(i)}+\mathbf{x}_{\pi(j)}}{2}\right)\int d\mathbf{W}_{0,4\beta}^{\mathbf{x}_i-\mathbf{x}_j,\mathbf{x}_{\pi(i)}-\mathbf{x}_{\pi(j)}}(\mathbf{w}^{(ij)})\left[1-\exp\left\{-\frac{1}{4}\int_0^{4\beta}U\left(\mathbf{w}_s^{(ij)}\,ds\right)\right\}\right].$$

(4.12.5)

It remains to restore the normalizations from equation 4.12.2. From corollary C.1.5 we have

$$g_{2\beta}(\mathbf{x}_i-\mathbf{x}_{\pi(i)})\,g_{2\beta}(\mathbf{x}_j-\mathbf{x}_{\pi(j)}) = g_{4\beta}\left((\mathbf{x}_i-\mathbf{x}_j)-(\mathbf{x}_{\pi(i)}-\mathbf{x}_{\pi(j)})\right)\;g_\beta\left(\frac{(\mathbf{x}_i+\mathbf{x}_j)-(\mathbf{x}_{\pi(i)}+\mathbf{x}_{\pi(j)})}{2}\right).$$

The g_β factor is cancelled by the g_β factor in equation 4.12.5; the $g_{4\beta}$ factor is precisely the normalization factor to convert equation 4.12.5's $d\mathbf{W}$ to $d\hat{\mathbf{W}}$. (See definition D.6.1.) Then equation 4.12.5 becomes

$$\int d\hat{\mathbf{W}}_{0,4\beta}^{\mathbf{x}_i-\mathbf{x}_j,\mathbf{x}_{\pi(i)}-\mathbf{x}_{\pi(j)}}(\mathbf{w}^{(ij)})\left[1-\exp\left\{-\frac{1}{4}\int_0^{4\beta}U\left(\mathbf{w}_s^{(ij)}\,ds\right)\right\}\right]$$

which is what was to be shown. □

4.13 Relation to spatial permutations

Sections 4.6 through 4.12 connect the permutation Hamiltonian, obtained via the bosonic Feynman-Kac formula, with the random-cycle model as defined in section 3. Specifically, we have, in correspondence with equation 3.1.1,

$$H(\mathbf{X}, \pi) = \sum_{i=1}^{N} \frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{1 \le i < j \le N} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}) \tag{4.13.1}$$

where

$$V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}) = \int d\hat{\mathbf{W}}_{0,4\beta}^{\mathbf{x}_i - \mathbf{x}_j, \mathbf{x}_{\pi(i)}, \mathbf{x}_{\pi(j)}}(\mathbf{w}^{(ij)}) \left[1 - \exp\left\{-\frac{1}{4}\int_0^{4\beta} U\left(\mathbf{w}_s^{(ij)}\right) ds\right\}\right]. \tag{4.13.2}$$

5 Model with full jump-pair interactions

Equation 4.13.2 for the jump-pair interactions was

$$V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}) = \int d\hat{\mathbf{W}}_{0,4\beta}^{\mathbf{x}_i - \mathbf{x}_j, \mathbf{x}_{\pi(i)}, \mathbf{x}_{\pi(j)}}(\mathbf{w}^{(ij)}) \left[1 - \exp\left\{ -\frac{1}{4} \int_0^{4\beta} U\left(\mathbf{w}_s^{(ij)}\right) \, ds \right\} \right].$$

This may be interpreted as the probability that a Brownian bridge (figure 6 on page 25) running from $\mathbf{x}_i - \mathbf{x}_j$ to $\mathbf{x}_{\pi(i)} - \mathbf{x}_{\pi(j)}$ in time 4β intersects a ball of radius a centered at the origin. (Proposition 4.12.1 showed that this is exactly equal to the collision probability for two bridges, one running from $\mathbf{x}_i$ to $\mathbf{x}_{\pi(i)}$ and another running from $\mathbf{x}_j$ to $\mathbf{x}_{\pi(j)}$, in time 4β.)

Ueltschi's 2007 paper [U07] has little more to say about this full jump-pair interaction. There are (at least) three things which can be done with it:

- Computing it directly using simulation methods is an interesting statistical problem which will be discussed further in my dissertation. (To date, I have found that simulation of this equation is of prohibitive computational expense. Nonetheless, my dissertation will quantify this expense.)
- One may also hope that this equation could be written in terms of special functions. Our research on this matter, and our contacts with experts in Brownian bridges, has not produced a special-function expression.
- Although one may not simplify all interaction pairs, one may extract the strongest interaction pairs (namely, two-cycles) and simplify those. This is discussed in section 6.

See also section 7 where future research is sketched.

6 Simple model with two-cycle jump-pair interactions

For the simplified two-cycle-interaction model, unlike the fully interacting model of section 5, one obtains expressions for the pressure, critical density, and critical temperature for the weakly interacting Bose gas. These appear as perturbations to the known expressions for the ideal gas.

6.1 Motivation

Equation 4.13.2 is an expression for the jump-pair interaction. In section 5, we reviewed the difficulties in either estimating or simplifying this expression in general.

The pair-jump potential is the collision probability for two bridges, one running from $\mathbf{x}_i$ to $\mathbf{x}_{\pi(i)}$ and another running from $\mathbf{x}_j$ to $\mathbf{x}_{\pi(j)}$, in time 4β; one expects this probability to be highest for two-cycles. (In figure 6, one expects increased collision probability if $\mathbf{x}_{\pi(i)} = \mathbf{x}_j$.) Thus, one may choose to neglect all V_{ij} terms except those involving two-cycles.

Notation 6.1.1. The shorthand notation

$$i \circ\!\!-\pi-\!\!\circ j$$

means that i and j participate in a two-cycle under π, i.e. $\pi(i) = j$, $\pi(j) = i$, and $i < j$.

Then equation 4.13.1 becomes

$$\begin{aligned} H(\mathbf{X}, \pi) &= \sum_{i=1}^{N} \frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{1 \le i < j \le N} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}) \\ \approx \tilde{H}_P(\mathbf{X}, \pi) &= \sum_{i=1}^{N} \frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{i \circ\!-\pi-\!\circ j} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}). \end{aligned} \tag{6.1.2}$$

An unpublished computation of Ueltschi and Betz shows that, for two-cycles, the jump-pair interaction (equation 4.13.2) simplifies significantly to

$$V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_{\pi(i)}, \mathbf{x}_i) = \frac{2a}{\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|} + O(a^2), \tag{6.1.3}$$

where a is the radius of the interparticle hard-core potential U.

The key point is that the Brownian bridges of equation 4.13.2 have been simplified out completely for this two-cycle-interaction model. To estimate expectations of the random variable $\varrho_{m,n}$ (section 3.1), one may simply use Markov-Chain Monte Carlo techniques to sample random permutations with weights derived from equation 6.2.1. (The details of such MCMC simulations will be explained in my dissertation.)

6.2 Hamiltonian with $r_2(\pi)$

Equation 6.1.3 is quite adequate for use in Monte Carlo simulations. A further modification is made, though, which facilitates the computation of thermodynamic properties of the two-cycle-interaction model in the following section.

Letting $r_2(\pi)$ denote the number of two-cycles in the permutation π, one would like to have a simple Hamiltonian of the form

$$H_P^{(\alpha)}(\mathbf{X},\pi) = \sum_{i=1}^{N} \frac{1}{4\beta}\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \alpha r_2(\pi). \tag{6.2.1}$$

It remains to connect the old parameter a with the new parameter α. Note that the distance dependence in equation 6.1.3 needs to be averaged out: in equation 6.2.1, all two-cycles acquire the same weight α regardless of $\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|$.

Proposition 6.2.2. *The first-order approximation*

$$\alpha = \left(\frac{8}{\pi\beta}\right)^{1/2} a + O(a^2) \tag{6.2.3}$$

is valid for computing expectations.

Proof. It may seem odd that the distances $\|\mathbf{x}_i - \mathbf{x}_j\|$ are replaced by a common α. Remember, however, that (see section 3.1) we are averaging over particle positions $\mathbf{x}_i, \mathbf{x}_j \in \Lambda$. Equating the two Hamiltonians in 6.1.2, we have

$$\int_{\Lambda^N} d\mathbf{X} \exp\left\{-\frac{1}{4\beta}\sum_{i=1}^{N}\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2\right\} \exp\left\{-\sum_{i \multimapboth j} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)})\right\}$$
$$= \int_{\Lambda^N} d\mathbf{X} \exp\left\{-\frac{1}{4\beta}\sum_{i=1}^{N}\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2\right\} \exp\left\{-\sum_{i \multimapboth j} \alpha\right\}$$

$$\int_{\Lambda^N} d\mathbf{X} \prod_{i=1}^{N} \exp\left\{-\frac{1}{4\beta}\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2\right\} \prod_{i \multimapboth j} \exp\left\{-V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)})\right\}$$
$$= \int_{\Lambda^N} d\mathbf{X} \prod_{i=1}^{N} \exp\left\{-\frac{1}{4\beta}\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2\right\} \prod_{i \multimapboth j} \exp\left\{\alpha\right\}.$$

By Tonelli's theorem (given the positivity of the integrand) we may iterate the integrals as we wish. All i's which do not participate in two-cycles factor out, canceling on both sides. Since $\pi(i) = j$ and $\pi(j) = i$, and substituting expression 6.1.3 for V, we are left with

$$\prod_{i \multimapboth j} \int_\Lambda \int_\Lambda d\mathbf{x}_i\, d\mathbf{x}_j \, \exp\left\{-\frac{1}{2\beta}\|\mathbf{x}_i - \mathbf{x}_j\|^2\right\} \exp\left\{-\frac{2a}{\|\mathbf{x}_i - \mathbf{x}_j\|}\right\}$$
$$= \prod_{i \multimapboth j} \int_\Lambda \int_\Lambda d\mathbf{x}_i\, d\mathbf{x}_j \, \exp\left\{-\frac{1}{2\beta}\|\mathbf{x}_i - \mathbf{x}_j\|^2\right\} \exp\left\{-\alpha\right\}.$$

It suffices to apply the same technique to each $i \multimapboth j$ pair. Let

$$\mathbf{r}_{ij} = \mathbf{x}_i - \mathbf{x}_j.$$

As in section 4.12, the change-of-variables Jacobian has determinant with absolute value 1, so without need for correction factors we write

$$\int_\Lambda \int_\Lambda d\mathbf{x}_i\, d\mathbf{r}_{ij} \, \exp\left\{-\frac{1}{2\beta}\|\mathbf{r}_{ij}\|^2\right\} \exp\left\{-\frac{2a}{\|\mathbf{r}_{ij}\|}\right\} = \int_\Lambda \int_\Lambda d\mathbf{x}_i\, d\mathbf{r}_{ij} \, \exp\left\{-\frac{1}{2\beta}\|\mathbf{r}_{ij}\|^2\right\} \exp\left\{-\alpha\right\}.$$

Taylor-expanding $\exp(-2a/\|\mathbf{r}_{ij}\|)$ and $\exp(-\alpha)$ to first order, since we are interested in weak interactions, gives us

$$\int_\Lambda \int_\Lambda d\mathbf{x}_i \, d\mathbf{r}_{ij} \, \exp\left\{-\frac{1}{2\beta}\|\mathbf{r}_{ij}\|^2\right\} \left(1 - \frac{2a}{\|\mathbf{r}_{ij}\|}\right) = \int_\Lambda \int_\Lambda d\mathbf{x}_i \, d\mathbf{r}_{ij} \, \exp\left\{-\frac{1}{2\beta}\|\mathbf{r}_{ij}\|^2\right\} (1-\alpha)\,.$$

After distributing the exponentials over the differences, the first products are Gaussians which cancel out on both sides. What is left is

$$2a \int_\Lambda \int_\Lambda d\mathbf{x}_i \, d\mathbf{r}_{ij} \, \frac{\exp\left\{-\frac{1}{2\beta}\|\mathbf{r}_{ij}\|^2\right\}}{\|\mathbf{r}_{ij}\|} = \alpha \int_\Lambda \int_\Lambda d\mathbf{x}_i \, d\mathbf{r}_{ij} \, \exp\left\{-\frac{1}{2\beta}\|\mathbf{r}_{ij}\|^2\right\}.$$

The integral over $d\mathbf{x}_i$ gives the volume of Λ on both sides, which cancels; for $d\mathbf{r}_{ij}$, we pass from Λ to $\mathbb{R}^3$, ignoring boundary corrections which will disappear in the infinite-volume limit. The right-hand integral over $d\mathbf{r}_{ij}$ is $(2\pi\beta)^{3/2}$ (section C.1). Then

$$\begin{aligned}
\alpha &= \frac{2a}{(2\pi\beta)^{3/2}} \int_{\mathbb{R}^3} d\mathbf{r} \, \frac{\exp\left\{-\frac{1}{2\beta}\|\mathbf{r}\|^2\right\}}{\|\mathbf{r}\|} \\
&= \frac{2a}{(2\pi\beta)^{3/2}} \int_{\theta=0}^{\theta=2\pi} d\theta \int_{\phi=0}^{\phi=\pi} d\phi \sin\phi \int_{r=0}^{r=\infty} dr \; re^{-r^2/2\beta} \\
&= \frac{8\pi a}{(2\pi\beta)^{3/2}} \int_{r=0}^{r=\infty} dr \, r \, e^{-r^2/2\beta} \\
&= \frac{8\pi\beta a}{(2\pi\beta)^{3/2}} = \left(\frac{8}{\pi\beta}\right)^{1/2} a.
\end{aligned}$$

(The r integral really should start at $r = 2a$ rather than $r = 0$, since we have a hard-core potential which prohibits $\mathbf{x}_i$ from being within $2a$ of $\mathbf{x}_j$. This would introduce a factor of $e^{-2a^2/\beta}$ into the above. In the small-a regime, though, we set this to 1 without remorse.) □

6.3 Pressure

Here we find the pressure of the two-cycle-interaction model and compare it to the pressure of the ideal gas. The latter is [BU07]:

$$p^{(0)}(\beta,\mu) = -\frac{1}{\beta}\int_{\mathbb{R}^d} \log\left(1 - e^{-\beta\left(4\pi^2\|\mathbf{k}\|^2 - \mu\right)}\right) d\mathbf{k}. \tag{6.3.1}$$

(The **chemical potential** μ is defined in section B.1.

Proposition 6.3.2. *The pressure of the two-cycle-interaction model is*

$$p^{(\alpha)}(\beta,\mu) = p^{(0)}(\beta,\mu) - \frac{e^{2\beta\mu}}{2^{11/2}\pi^{3/2}\beta^{5/2}}(1 - e^{-\alpha}). \tag{6.3.3}$$

Proof. See section 7.1 of [BU07], or section 5 of [U07]. The proof involves a lengthy decomposition into Fourier modes; I will exposit it as time permits. □

6.4 Conjecture for the critical density

Recall from section B.5 (see also equation 3.2.1) that the critical density for the ideal Bose gas is

$$\rho_c^{(0)} = \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{e^{4\beta\pi^2|\mathbf{k}|^2} - 1}. \tag{6.4.1}$$

As I continue to work on this random-cycle project, I certainly have more to learn about thermodynamics. In particular, one might inquire why the partial derivative in the following proposition defines the critical density. ([Huang] approaches the subject from a different perspective than Ueltschi does.) The best I can say at present is:

- The chemical potential is defined to be change in energy per additional particle, with fixed volume and entropy, i.e. $\mu = (\partial E/\partial N)_{S,V}$.
- Particles in the ground state (condensed particles) contribute nothing to the pressure.

Proposition 6.4.2. *The critical density for the two-cycle-interaction model is*

$$\rho_c^{(\alpha)} = \left.\frac{\partial p^{(\alpha)}}{\partial \mu}\right|_{\mu=0-} = \rho_c^{(0)} - \frac{(1-e^{-\alpha})}{2^{9/2}\pi^{3/2}\beta^{3/2}}. \tag{6.4.3}$$

Proof. Differentiating equation 6.4.3 through the integral sign, we obtain

$$\begin{aligned}
\frac{\partial p}{\partial \mu} &= -\frac{1}{\beta}\frac{\partial}{\partial \mu}\left[\int_{\mathbb{R}^d} \log\left(1 - e^{-4\pi^2\beta\|\mathbf{k}\|^2} e^{\beta\mu}\right) d\mathbf{k}\right] - \frac{\partial}{\partial\mu}\left[\frac{e^{2\beta\mu}}{2^{11/2}\pi^{3/2}\beta^{5/2}}(1-e^{-\alpha})\right] \\
&= -\frac{1}{\beta}\int_{\mathbb{R}^d} \frac{-\beta e^{-4\pi^2\beta\|\mathbf{k}\|^2} e^{\beta\mu}}{1 - e^{-4\pi^2\beta\|\mathbf{k}\|^2} e^{\beta\mu}} d\mathbf{k} - \frac{2\beta e^{2\beta\mu}}{2^{11/2}\pi^{3/2}\beta^{5/2}}(1-e^{-\alpha}) \\
\left.\frac{\partial p}{\partial \mu}\right|_{\mu=0-} &= \int_{\mathbb{R}^d} \frac{e^{-4\pi^2\beta\|\mathbf{k}\|^2}}{1 - e^{-4\pi^2\beta\|\mathbf{k}\|^2}} d\mathbf{k} - \frac{(1-e^{-\alpha})}{2^{9/2}\pi^{3/2}\beta^{3/2}} \\
&= \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{e^{4\pi^2\beta\|\mathbf{k}\|^2} - 1} - \frac{(1-e^{-\alpha})}{2^{9/2}\pi^{3/2}\beta^{3/2}}.
\end{aligned}$$

As is familiar from real analysis, differentiation through the integral sign is justified since (i) the integrand is $\mathbf{k}$-integrable for all $\mu < 0$, and (ii) the integrand has continuous partial derivative with respect to μ. □

Conjecture 6.4.4. Infinite cycles occur for densities above ρ_c.

Note that the critical density can be computed; what is not proved is that it corresponds to infinite cycles. The following, weaker result has been proved in [BU07].

Theorem 6.4.5. *For all $b < 1$,*

$$\lim_{V\to\infty} \mathbb{E}_{\Lambda,N}\left(\varrho_{N^b,N}\right) \geq \rho - \frac{4}{(1+e^{-\alpha})^2}\,\rho_c^{(0)}$$

where the limit is taken with fixed ratio $\rho = N/V$.

Compare this to equation 3.2.4 of section 3.2: the ρ_c in $\rho - \rho_c$ acquires the scale factor $4/(1+e^{-\alpha})^2$, and we have only a lower bound.

Late note: A theorem of this type has been proved in the recent paper [BU08].

6.5 Shift in critical temperature

Proposition 6.5.1. *For the weakly interacting two-cycle model,*

$$\frac{T_c^{(a)} - T_c^{(0)}}{T_c^{(0)}} \approx 0.37\rho^{1/3}a.$$

Proof. Recall from section 2.3, and in particular figure 1, that the critical region may be seen as a manifold in (ρ, β, a) space. We will use the result

$$\frac{\partial a}{\partial \rho}\frac{\partial \rho}{\partial \beta}\frac{\partial \beta}{\partial a} = -1$$

from proposition C.4.1. (Since we are working on the critical manifold, we take ρ and β to mean $\rho_c^{(a)}$ and $\beta_c^{(a)}$, respectively.) From equation 3.2.3, the critical line, with $a = 0$, has equation

$$\rho_c^{(0)}\beta_c^{(0)^{3/2}} = \frac{\zeta(3/2)}{(4\pi)^{3/2}} \tag{6.5.2}$$

where $\zeta(z)$ is the Riemann zeta function.

First, we use proposition 6.4.2 for the critical density, then Taylor-expand in the small parameter α and use equation 6.2.3 to relate α and a:

$$\rho_c^{(a)} = \rho_c^{(0)} - \frac{1 - e^{-\alpha}}{(8\pi\beta)^{3/2}}$$

$$\frac{\rho_c^{(a)} - \rho_c^{(0)}}{\rho_c^{(0)}} \approx \frac{-\alpha}{(8\pi\beta)^{3/2}}\frac{(4\pi\beta)^{3/2}}{\zeta(3/2)} = \frac{-8^{1/2}a}{\pi^{1/2}\beta^{1/2}(8\pi\beta)^{3/2}}\frac{(4\pi\beta)^{3/2}}{\zeta(3/2)} = \frac{-a}{\pi^{1/2}\beta^{1/2}\zeta(3/2)}.$$

Letting

$$b = \frac{1}{\zeta(3/2)\pi^{1/2}} \tag{6.5.3}$$

for brevity, we have

$$\frac{\rho_c^{(a)} - \rho_c^{(0)}}{\rho_c^{(0)}} = -\frac{ba}{\beta^{1/2}}.$$

Then

$$a = \frac{-\rho_c^{(a)}\beta^{1/2}}{\rho_c^{(0)}b} + \frac{\beta^{1/2}}{b}$$

and

$$\frac{\partial a}{\partial \rho} = \frac{-\beta^{1/2}}{\rho_c^{(0)}b}.$$

Second, using equation 6.5.2,

$$\rho_c^{(0)} = \frac{\zeta(3/2)}{(4\pi\beta)^{3/2}}$$

and so

$$\frac{\partial \rho_c^{(0)}}{\partial \beta} = \frac{-\zeta(3/2)}{(4\pi\beta)^{3/2}}.$$

For small a (see figure 1 for intuition) we use the approximation

$$\frac{\partial \rho_c^{(a)}}{\partial \beta} \approx \frac{\partial \rho_c^{(0)}}{\partial \beta}.$$

Third, from section 2.3 we expect

$$\frac{T_c^{(a)} - T_c^{(0)}}{T_c^{(0)}} = c\rho^{1/3}a.$$

Putting $\beta = 1/T$ gives

$$\frac{\beta_c^{(a)} - \beta_c^{(0)}}{\beta_c^{(a)}} = -c\rho^{1/3}a$$

which we approximate by

$$\frac{\beta_c^{(a)} - \beta_c^{(0)}}{\beta_c^{(0)}} = -c\rho^{1/3}a.$$

Solving for $\beta_c^{(a)}$ gives

$$\beta_c^{(a)} = \beta_c^{(0)} - \beta_c^{(0)}c\rho^{1/3}a$$

and thus

$$\frac{\partial \beta}{\partial a} = -\beta_c^{(0)}c\rho^{1/3}.$$

Combining the product of all three partial derivatives and using proposition C.4.1, we have

$$\left(\frac{\beta^{1/2}}{\rho_c^{(0)}b}\right)\left(\frac{\zeta(3/2)}{(4\pi\beta)^{3/2}}\right)\left(\beta_c^{(0)}c\rho^{1/3}\right) = 1.$$

Solving for c gives

$$c = \frac{\rho_c^{(0)}\rho^{-1/3}\beta^{5/2}}{\beta_c^{(0)}\beta^{1/2}}\frac{2b\,(4\pi)^{3/2}}{3\,\zeta(3/2)}.$$

Approximating $\beta_c^{(0)}$ and $\rho_c^{(0)}$ by $\beta_c^{(a)}$ and $\rho_c^{(a)}$, we have

$$c = \left(\rho^{2/3}\beta\right)\frac{2b\,(4\pi)^{3/2}}{3\,\zeta(3/2)} = \left(\rho\beta^{3/2}\right)^{2/3}\frac{2b\,(4\pi)^{3/2}}{3\,\zeta(3/2)}.$$

From equation 6.5.2 we know that

$$\rho_c^{(0)}\beta^{3/2} = \frac{\zeta(3/2)}{(4\pi)^{3/2}}$$

which we apply to $\rho_c^{(a)}$ as well. Then

$$c = \left(\frac{\zeta(3/2)}{(4\pi)^{3/2}} \right)^{2/3} \frac{2b\,(4\pi)^{3/2}}{3\,\zeta(3/2)} = \left(\frac{\zeta(3/2)^{2/3}}{(4\pi)} \right) \frac{2b\,(4\pi)^{3/2}}{3\,\zeta(3/2)} = \frac{4b\,\pi^{1/2}}{3\,\zeta(3/2)^{1/3}}.$$

Since

$$b = \frac{1}{\zeta(3/2)\pi^{1/2}},$$

$$c = \frac{4}{3}\zeta(3/2)^{-4/3} \approx 0.37.$$

$\square$

Remark. This result applies for the two-cycle model, where the only permutation jumps that interact are those which participate in two-cycles. When longer cycles are included, the shift in critical temperature is expected to be more pronounced. Thus, this result provides a rough lower bound on the true constant c, which from other methods discussed in section 2.3 is believed to be approximately 1.3. Further work is needed (see the following section) before the random-cycle model can be used to improve on the latter estimate.

7 Future work

7.1 Theoretical directions

My research to date has shown that the full jump-pair interaction (see equation 4.13.2 and section 5) is too computationally intensive for practical use. Ueltschi and Betz have simplified the Brownian bridges out of the jump-pair interaction for the particular case of two-cycles (equation 6.1.3); they also have some unpublished work on approximating the full interaction (to first order in the scattering length a) as a Riemann integral. I have found that this, too, while better than the Brownian bridges, is still computationally expensive. If this integral could be represented as a special function, then the full jump-pair-interacting case could be examined experimentally.

Alternatively, notice that, for the two-cycle-interaction model, the distance dependence in equation 6.1.3 was averaged out in equation 6.2.1. Since we are interested only in expected values of $\rho_{m,n}$, the details of a particular interaction are of minor importance; only the averaged behavior is of final interest. Perhaps equation 4.13.2 may be handled in a manner similar to proposition 6.2.2.

A very recent paper of Betz and Ueltschi [BU08] extends the two-cycle Hamiltonian of section 6 (equation 6.2.1) to the form

$$H_P(\mathbf{X}, \pi) = \sum_{i=1}^{N} \frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{\ell=1}^{N} \alpha_\ell r_\ell(\pi) \tag{7.1.1}$$

where $r_\ell(\pi)$ counts the number of ℓ-cycles in the permutation π. I have yet to evaluate how this recent development affects my own work.

7.2 Numerical directions

Simulations currently underway use the two-cycle-interaction model, with points on a cubic unit lattice. One would like to vary the positions of the points as well, in order to simulate the point-process-configuration model. (See the last paragraph of section 3.1 for a description of the probability measures for these two models.)

Note that the choice between the lattice-configuration and the point-process-configuration models is independent of the choice between the two-cycle-interaction and full jump-pair-interaction models.

If the theoretical work outlined in section 7.1 produces an efficient expression for the full jump-pair interaction, then it will certainly be examined experimentially.

7.3 Statistical directions

Markov-chain Monte Carlo simulations compute sample means of $\varrho_{m,n}$ (see section 3.1) for the lattice and point-process probability measures — producing one mean for a given choice of lattice size N, particle density ρ, inverse temperature β, and interaction parameter a.

We will analyze the error of the resulting sample means. For a large number of trials, one expects a central-limit distribution for the estimated values of $\varrho_{m,n}$; we also desire to have a practical estimator for the variance of the sample mean.

To approach the infinite-volume limit in N, one needs to simulate larger and larger lattice sizes, and then do finite-size scaling on the results. This analysis, involving a regression of a carefully chosen form with due sensitivity to sampling errors, will be a central part of my dissertation work.

8 Acknowledgements

Bill Faris' notes on the Feynman-Kac formula have proved invaluable, as has Janek Wehr's spring 2008 course in stochastic differential equations. Tom Kennedy made it possible for me to participate in this research project, and has been a patient and learned sounding board throughout. Daniel Ueltschi has shared with me his extensive knowledge and his enthusiasm, and has created an environment of great mutual benefit. Each of these gentlemen deserves my gratitude; this work would not have been possible without any of them.

Additionally, much of the work here was done during the Summer School for Current Topics in Mathematical Physics at the Erwin Schrödinger Institute in July 2008. The Institute provided a productive and fruitful atmosphere; the University of Arizona Department of Mathematics helped make the visit possible.

A Quantum mechanics

For information on quantum mechanics, see [Griffiths], [NC], and [Sakurai]; see [Huang], [Widom], and [Pathria] for statistical mechanics. The topics presented here are a digestion of these sources, with unified vocabulary and notation, serving a single purpose: so that I may explain to myself why $\mathrm{Tr}\left(e^{-\beta H}\right)$ is of such central importance.

A.1 Postulates of quantum mechanics

I take elementary quantum mechanics as given; in particular, I will use bra-ket notation without explanation. (I should point out that I take the complex inner product to be linear on the right, in accordance with mathematical-physics convention.) However, I will recall the basic postulates of quantum mechanics in order to smoothly elucidate the usefulness of the otherwise mysterious density matrix. In turn, density matrices are needed to formulate quantum statistical mechanics in section A.8.

(1) To any isolated physical system is associated a separable complex Hilbert space $\mathcal{H}$, called a *state space*, with inner product $\langle \phi \mid \psi \rangle$. States (pure states; see section A.2) of the physical system are described by unit vectors (often called *state vectors* or *wave functions*) in $\mathcal{H}$, i.e. vectors ψ such that $\langle \psi \mid \psi \rangle = 1$. Vectors that are scalar multiples of one another are considered to be equivalent. (If $\psi_1 = c\psi_2$, then, since ψ_1 and ψ_2 have norm 1, $|c| = 1$. That is, $c = e^{i\theta}$ for some real θ. Thus arises the saying that state vectors are distinct up to a *phase factor*.) The state space of a composite system is the tensor product of the state spaces of the component systems.

(2) State vectors evolve in time via *unitary transformations*. Specifically, the unitary operator is described by the *Schrödinger equation*:

$$i\hbar \frac{\partial \psi(t, \mathbf{x})}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi(t, \mathbf{x}) + V(t, \mathbf{x}) \psi(t, \mathbf{x}) = H\psi(t, \mathbf{x})$$

i.e.

$$\frac{\partial \psi}{\partial t} = \frac{-iH}{\hbar} \psi$$

where H is the Hermitian operator

$$H = \frac{-\hbar^2}{2m} \nabla^2 + V.$$

The wave function varies in position and time; the *potential function*, conventionally written with the letter V, may also vary in position and time. The potential represents external interactions with the particle.

We can write down a solution

$$\frac{d\psi}{dt} = \frac{-i}{\hbar} H\psi \tag{A.1.1}$$

$$\psi(t) = e^{-iHt/\hbar} \psi(0). \tag{A.1.2}$$

One checks this solution by differentiating:

$$\frac{d\psi}{dt} = \frac{-iH}{\hbar} e^{-iHt/\hbar} \psi(0) = \frac{-iH}{\hbar} \psi(t) = \frac{-i}{\hbar} H\psi(t).$$

As is well known, the imaginary exponential of a hermitian matrix is unitary. The importance of this is that unitary matrices U are norm-preserving. That is, if $\|\psi\| = 1$ then $\|U\psi\|$ is still 1; probability-density functions remain probability-density functions as they evolve in time. This fact is called the *conservation of probability.*

(3) An observable $\mathcal{O}$ corresponds to a densely defined Hermitian operator $A : \mathcal{H} \to \mathcal{H}$. Since A is Hermitian, $\mathcal{H}$ has an orthonormal basis $\{\phi_j\}$ of eigenvectors of A. Since $\mathcal{H}$ is separable, the basis is a countable set. In the case that A has discrete spectrum, the eigenstates of A have respective (necessarily real) eigenvalues a_j and A has a *spectral decomposition*

$$A = \sum a_j \mid \phi_j \rangle\langle \phi_j \mid$$

(The operators $P_j = \mid \phi_j \rangle\langle \phi_j \mid$ are known as *projection operators.*) A (necessarily square-summable) wave function ψ is a linear combination of the eigenbasis:

$$\psi = \sum_j c_j \phi_j \qquad \text{with} \qquad c_j = \langle \phi_j \mid \psi \rangle \qquad \text{and} \qquad \sum_j |c_j|^2 = 1.$$

A measurement of $\mathcal{O}$ has as its possible outcomes the numbers a_j with probabilities

$$\mathbb{P}(\mathcal{O} = a_j) = |\langle \phi_j \mid \psi \rangle|^2.$$

The expected value of A is

$$\begin{aligned} \langle A \rangle &= \sum_j a_j \mathbb{P}(\mathcal{O} = a_j) = \sum_j a_j |\langle \phi_j \mid \psi \rangle|^2 = \sum_j a_j \langle \psi \mid \phi_j \rangle\langle \phi_j \mid \psi \rangle \\ &= \sum_j a_j \langle \psi \mid \Big(\mid \phi_j \rangle\langle \phi_j \mid \Big) \mid \psi \rangle = \sum_j \langle \psi \mid \Big(a_j \mid \phi_j \rangle\langle \phi_j \mid \Big) \mid \psi \rangle \\ &= \langle \psi \mid A \mid \psi \rangle. \end{aligned}$$

This is the average value or mean of all the observations, averaged over repeated measurements on identical systems.

(4) Immediately after measurement of an observable $\mathcal{O}$, the state of the system is described *only* by an eigenstate ϕ_j of A. This is called the *collapse of the wave function.* The evolution of the single-particle system thereafter is described by the Schrödinger equation, with new initial conditions.

A.2 Pure and mixed states

The terms *pure state* and *mixed state* are horribly misleading. Nonetheless, they are entrenched in the literature and cannot be dispensed with. A pure state is simply a state of a quantum-mechanical system: the adjective *pure* is superfluous. A mixed state not a single state at all: it is a statistical description of a *set* of many states.

Definition A.2.1. An **ensemble** is a list of n distict state vectors $\{\psi_1, \ldots, \psi_n\}$ along with respective probabilities $\{p_1, \ldots, p_n\}$ with $0 \leq p_j \leq 1$ and $\sum_{j=1}^n p_j = 1$. (One may think of an ensemble as a probability mass function.)

Definition A.2.2. A **mixed state** is an ensemble. A **pure state** is (with abuse of notation) either a single state, or an ensemble with $n = 1$, or an ensemble with $n \geq 1$ but only one $p_k = 1$ and the remaining $p_j = 0$ for $j \neq k$.

Remark. Pure and mixed states are not to be confused with the following:

- A quantum-mechanical state is a linear combination of eigenstates. Such states are pure, not mixed.
- Entangled and separable states arise in the theory of multi-particle systems, e.g. the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ of Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. An entangled state is an indecomposable tensor in $\mathcal{H}_1 \otimes \mathcal{H}_2$; a separable state is a decomposable tensor.

A.3 Density matrices

Density matrices are a notational convenience for working with ensembles (mixed states) of quantum systems. I will develop[3] density matrices in three steps: (1) In this section, I will show how to construct a density matrix from an ensemble. (2) In section A.4, I will show how density matrices serve to notationally encapsulate the postulates of quantum mechanics as described in section A.1. (3) In section A.5 I will show how this notation permits one to extend those postulates to the mixed-state case.

Definition A.3.1. A **density matrix** is a positive-definite matrix with trace 1.

Proposition A.3.2. *A density matrix may be obtained from an ensemble by*

$$\rho = \sum_{j=1}^{n} p_j \mid \psi_j \rangle\langle \psi_j \mid .$$

Proof. Let ρ be such a matrix. Fix an orthonormal basis $\{\phi_i\}$ for $\mathcal{H}$. I will use the characterization that a matrix A is positive-definite iff it is Hermitian and $\langle \xi \mid A \mid \xi \rangle > 0$ for all non-zero ξ. To see that ρ is Hermitian, write

$$\rho^* = \left(\sum_{j=1}^{n} p_j \mid \psi_j \rangle\langle \psi_j \mid \right)^* = \sum_{j=1}^{n} p_j \left(\mid \psi_j \rangle\langle \psi_j \mid \right)^* = \sum_{j=1}^{n} p_j \langle \psi_j \mid^* \mid \psi_j \rangle^* = \sum_{j=1}^{n} p_j \mid \psi_j \rangle\langle \psi_j \mid = \rho.$$

Now let $0 \neq \xi \in \mathcal{H}$. Then

$$\langle \xi \mid \rho \mid \xi \rangle = \left\langle \xi \middle| \sum_{j=1}^{n} p_j \mid \psi_j \rangle\langle \psi_j \mid \middle| \xi \right\rangle = \sum_{j=1}^{n} p_j \langle \xi \mid \psi_j \rangle\langle \psi_j \mid \xi \rangle = \sum_{j=1}^{n} p_j \langle \xi \mid \psi_j \rangle\langle \xi \mid \psi_j \rangle^* = \sum_{j=1}^{n} p_j |\langle \xi \mid \psi_j \rangle|^2.$$

Since this is a sum of non-negative real numbers, it is non-negative. But by positive-definiteness of the inner product, it is zero iff either ξ is zero, which it is not by hypothesis, or all of the ψ_j's are zero, which they are not since they all have norm 1.

To see that ρ has trace 1, write

$$\mathrm{Tr}(\rho) = \mathrm{Tr}\left(\sum_{k=1}^{n} p_k \mid \psi_k \rangle\langle \psi_k \mid \right) \tag{A.3.3}$$

$$= \sum_{k=1}^{n} p_k \mathrm{Tr}\left(\mid \psi_k \rangle\langle \psi_k \mid \right). \tag{A.3.4}$$

Write each ψ_k in terms of the orthonormal basis as

$$\psi_k = \sum_{\ell} c_{k\ell} \phi_\ell.$$

Note that $\mid \psi_k \rangle\langle \psi_k \mid$ has ijth matrix element

$$\left(\mid \psi_k \rangle\langle \psi_k \mid \right)_{ij} = c_{ki}\, c_{kj}^*.$$

Then

$$\mathrm{Tr}\left(\mid \psi_k \rangle\langle \psi_k \mid \right) = \sum_i c_{ki}\, c_{ki}^* = \sum_i |c_{ki}|^2 = 1,$$

[3]This development follows, in part, that in `http://electron6.phys.utk.edu/QM1`, retrieved on June 12, 2008.

from which

$$\mathrm{Tr}(\rho) = \sum_{k=1}^{n} p_k = 1.$$

$\square$

Furthermore, we have a criterion for whether a density matrix corresponds to a pure or mixed state.

Proposition A.3.5. *If ρ is a density matrix for an ensemble $\{\psi_1, \ldots, \psi_n\}$, then $\mathrm{Tr}(\rho^2) \leq 1$, with equality if and only if the ensemble is a pure state.*

Proof. First note that for a matrix A, we have

$$\mathrm{Tr}(A^2) = \sum_i \sum_j A_{ij} A_{ji}.$$

Then

$$\begin{aligned}
\mathrm{Tr}(\rho^2) &= \sum_i \sum_j \rho_{ij} \rho_{ji} \\
&= \sum_i \sum_j \left(\sum_{k=1}^{n} p_k c_{ki} c_{kj}^* \right) \left(\sum_{\ell=1}^{n} p_\ell c_{\ell j} c_{\ell i}^* \right) \\
&= \sum_{k=1}^{n} p_k \sum_{\ell=1}^{n} p_\ell \ \sum_i (c_{\ell i}^* c_{ki}) \sum_j (c_{kj}^* c_{\ell j}) \\
&= \sum_{k=1}^{n} p_k \sum_{\ell=1}^{n} p_\ell \ \langle \psi_\ell \mid \psi_k \rangle \langle \psi_k \mid \psi_\ell \rangle \\
&= \sum_{k=1}^{n} p_k \sum_{\ell=1}^{n} p_\ell \ \langle \psi_k \mid \psi_\ell \rangle^* \langle \psi_k \mid \psi_\ell \rangle \\
&= \sum_{k=1}^{n} p_k \sum_{\ell=1}^{n} p_\ell \ |\langle \psi_k \mid \psi_\ell \rangle|^2.
\end{aligned}$$

First suppose that one p_{k_0} is 1 and the rest are zero. (This is the pure case.) Then

$$\mathrm{Tr}(\rho^2) = |\langle \psi_{k_0} \mid \psi_{k_0} \rangle|^2 = 1.$$

Now suppose that at least two p_k's are non-zero. Decompose the sum as

$$\begin{aligned}
\mathrm{Tr}(\rho^2) &= \sum_{k=1}^{n} p_k^2 |\langle \psi_k \mid \psi_k \rangle|^2 + \sum_{k=1}^{n} p_k \sum_{\ell \neq k} p_\ell \ |\langle \psi_k \mid \psi_\ell \rangle|^2 \\
&= \sum_{k=1}^{n} p_k^2 + \sum_{k=1}^{n} \sum_{\ell \neq k} p_k p_\ell \ |\langle \psi_k \mid \psi_\ell \rangle|^2.
\end{aligned}$$

To finish the proof, note that $\sum_{k=1}^{n} p_k^2$ is the diagonal part of $(\sum_{k=1}^{n} p_k)^2$. We have

$$\begin{aligned}
1 = (1)^2 = \left(\sum_{k=1}^{n} p_k \right)^2 &= \sum_{k=1}^{n} \sum_{\ell=1}^{n} p_k p_\ell = \sum_{k=1}^{n} \sum_{\ell \neq k} p_k p_\ell + \sum_{k=1}^{n} p_k^2 \\
\sum_{k=1}^{n} p_k^2 &= 1 - \sum_{k=1}^{n} \sum_{\ell \neq k} p_k p_\ell.
\end{aligned}$$

Then

$$\mathrm{Tr}(\rho^2) = 1 - \sum_{k=1}^{n} \sum_{\ell \neq k} p_k p_\ell (1 - \cos^2 \theta_{k\ell})$$

where

$$\langle \psi_k \mid \psi_\ell \rangle = \|\psi_k\| \, \|\psi_\ell\| \, \cos \theta_{k\ell}.$$

Note that all the terms in the sum are non-negative. If two p_k's are non-zero — without loss of generality, say p_1 and p_2 — then the product $p_1 p_2$ is non-zero. Furthermore, $\cos^2 \theta_{1,2}$ is strictly less than 1. Otherwise, ϕ_1 and ϕ_2 (which are unit vectors) would be identical up to global phase, contradicting the distinctness of the members of the ensemble. Thus, $\mathrm{Tr}(\rho^2) < 1$. □

Remark A.3.6. Two different ensembles can give the same density matrix. In [NC] is a theorem characterizing the conditions under which this can happen.

Lastly, we have two lemmas which will be used in section A.4.

Lemma A.3.7. *The operator ρ is Hermitian. If $\rho = \mid \psi \rangle$, then ρ satisfies $\rho^2 = \rho$.*

Proof. For the first claim,

$$\rho^* = \left(\sum_k p_k \mid \psi_k \rangle \langle \psi_k \mid \right)^* = \sum_k p_k \langle \psi_k \mid^* \mid \psi_k \rangle^* = \sum_k p_k \mid \psi_k \rangle \langle \psi_k \mid = \rho.$$

For the second claim,

$$\rho^2 = \mid \psi \rangle \langle \psi \mid \psi \rangle \mid \psi \rangle = \mid \psi \rangle \langle \psi \mid = \rho$$

since $\langle \psi \mid \psi \rangle = 1$. □

Lemma A.3.8. *For a Hermitian operator A,*

$$\langle \psi \mid A \mid \psi \rangle = \mathrm{Tr}(A \mid \psi \rangle \langle \psi \mid).$$

Proof. The operator $\rho = \mid \psi \rangle \langle \psi \mid$ is Hermitian by lemma A.3.7, so it makes sense to write $\langle \psi \mid A \mid \psi \rangle$. Expand ψ in terms of an orthonormal basis $\{\phi_j\}$ for $\mathcal{H}$ as

$$\psi = \sum_j c_j \phi_j.$$

Recall that

$$\langle \psi \mid A \mid \psi \rangle = \sum_{ik} c_i^* A_{ik} c_k.$$

On the other hand, for matrices C and D,

$$(CD)_{ij} = \sum_k C_{ik} D_{kj} \qquad \text{and} \qquad \mathrm{Tr}(CD) = \sum_{ik} C_{ik} D_{ki},$$

so

$$\mathrm{Tr}(A \mid \psi \rangle \langle \psi \mid) = \sum_{ik} A_{ik} c_k c_i^* = \langle \psi \mid A \mid \psi \rangle.$$

□

A.4 Pure-state density matrices

For this section, fix a state ψ and let

$$\rho = \mid \psi \rangle\langle \psi \mid .$$

Here, four key properties of the density matrix ρ are described, paralleling the four postulates of quantum mechanics listed in section A.1.

(1) The state vector ψ has norm 1. The density matrix ρ has trace 1, as proved in proposition A.3.2.

(2) The state vector ψ evolves in time according to the Schrödinger equation

$$\frac{d\psi}{dt} = \frac{-i}{\hbar} H\psi;$$

the density matrix ρ evolves in time according to

$$\frac{d\rho}{dt} = \frac{-i}{\hbar} [H, \rho]. \tag{A.4.1}$$

Proof. Using the product rule,

$$\frac{d\rho}{dt} = \frac{d \mid \psi \rangle}{dt} \langle \psi \mid + \mid \psi \rangle \frac{d\langle \psi \mid}{dt}.$$

To find $d\langle \psi \mid /dt$, take the adjoint of the Schrödinger equation and recall that the Hamiltonian is Hermitian (so $H^* = H$):

$$\left(\frac{d \mid \psi \rangle}{dt}\right)^* = \left(\frac{-i}{\hbar} H \mid \psi \rangle\right)^*$$

$$\frac{d\langle \psi \mid}{dt} = \frac{i}{\hbar}\langle \psi \mid H^* = \frac{i}{\hbar}\langle \psi \mid H.$$

Then

$$\frac{d\rho}{dt} = \left(\frac{-i}{\hbar} H \mid \psi \rangle\right) \langle \psi \mid + \mid \psi \rangle \left(\frac{i}{\hbar} \langle \psi \mid H\right) = \frac{-i}{\hbar} H\rho + \frac{i}{\hbar}\rho H = \frac{-i}{\hbar} [H, \rho].$$

□

In section A.5 we will find a solution for this equation.

(3) Given an observable $\mathcal{O}$ with operator A, eigenstates ϕ_j, and corresponding eigenvalues a_j, we have

$$\mathbb{P}(\mathcal{O} = a_j) = |\langle \phi_j \mid \psi \rangle|^2 \qquad \text{and} \qquad \langle A \rangle = \langle \psi \mid A \mid \psi \rangle;$$

in terms of ρ, we have

$$\mathbb{P}(\mathcal{O} = a_j) = \mathrm{Tr}(\rho P_j) \qquad \text{and} \qquad \langle A \rangle = \mathrm{Tr}(\rho A)$$

where

$$P_j = \mid \phi_j \rangle\langle \phi_j \mid .$$

Proof. For the first claim,

$$\mathbb{P}(\mathcal{O} = a_j) = |\langle \phi_j \mid \psi \rangle|^2 = \langle \psi \mid \phi_j \rangle\langle \phi_j \mid \psi \rangle = \langle \psi \mid P_j \mid \psi \rangle = \mathrm{Tr}(\rho P_j),$$

where the last step follows from the centrality of trace, along with lemma A.3.8. The second claim also follows from the lemma. □

(4) After measurement of the observable $\mathcal{O}$ with operator A, the state vector ψ is replaced by an eigenstate ϕ_j. The density matrix $\mid \psi \rangle\langle \psi \mid$ is replaced by $\mid \phi_j \rangle\langle \phi_j \mid$.

A.5 Mixed-state density matrices

Now we suppose

$$\rho = \sum_k p_k \mid \psi_k \rangle\langle \psi_k \mid,$$

and we enumerate the postulates of quantum mechanics in terms of the density matrix ρ.

(1) The density matrix ρ has trace 1, as proved in proposition A.3.2.

(2) The density matrix ρ evolves in time according to

$$\frac{d\rho}{dt} = \frac{-i}{\hbar}\,[H, \rho]. \tag{A.5.1}$$

Proof. Using the product rule,

$$\frac{d\rho}{dt} = \sum_k p_k \frac{d \mid \psi_k \rangle}{dt} \langle \psi_k \mid + \sum_k p_k \mid \psi_k \rangle \frac{d\langle \psi_k \mid}{dt}.$$

As in section A.4,

$$\left(\frac{d \mid \psi_k \rangle}{dt}\right)^* = \frac{i}{\hbar}\langle \psi_k \mid H,$$

so

$$\begin{aligned}\frac{d\rho}{dt} &= \sum_k p_k \left(\frac{-i}{\hbar}\, H \mid \psi_k \rangle\right) \langle \psi_k \mid + \sum_k p_k \mid \psi_k \rangle \left(\frac{i}{\hbar}\, \langle \psi_k \mid H\right) \\ &= \frac{-i}{\hbar} \sum_k H p_k \mid \psi_k \rangle\langle \psi_k \mid + \frac{i}{\hbar} \sum_k p_k \mid \psi_k \rangle\langle \psi_k \mid H \\ &= \frac{-i}{\hbar}\, H\rho + \frac{i}{\hbar}\rho H = \frac{-i}{\hbar}\,[H, \rho].\end{aligned}$$

□

Furthermore, if wave functions evolve by a unitary operator U_t via

$$\psi_t = U_t \psi_0,$$

then the density matrix evolves via

$$\rho_t = U_t \rho_0 U_t^*.$$

In particular, if the Hamiltonian is time-independent, we have

$$\rho_t = e^{-iHt/\hbar} \rho_0 e^{iHt/\hbar}. \tag{A.5.2}$$

One verifies by differentiation that A.5.2 solves A.5.1.

(3) Given an observable $\mathcal{O}$ with operator A, eigenstates ϕ_j, and corresponding eigenvalues a_j,

$$\mathbb{P}(\mathcal{O} = a_j) = \mathrm{Tr}(\rho P_j) \qquad \text{and} \qquad \langle\, A \,\rangle = \mathrm{Tr}(\rho A)$$

where

$$P_j = \mid \phi_j \rangle\langle \phi_j \mid .$$

Proof. For the first claim, let $\mathcal{O}_k$ be the observation of ψ_k. Using conditional probability, recalling result 3 from section A.4, and using linearity of trace, we have

$$\begin{aligned}
\mathbb{P}(\mathcal{O} = a_j) &= \sum_k p_k \, \mathbb{P}(\mathcal{O}_k = a_j) \\
&= \sum_k p_k \operatorname{Tr}\left(\mid \psi_k \rangle\langle \psi_k \mid P_j\right) \\
&= \operatorname{Tr}\left(\sum_k p_k \mid \psi_k \rangle\langle \psi_k \mid P_j\right) \\
&= \operatorname{Tr}\left(\left(\sum_k p_k \mid \psi_k \rangle\langle \psi_k \mid\right) P_j\right) \\
&= \operatorname{Tr}(\rho P_j).
\end{aligned}$$

Similarly, for the second claim we have

$$\begin{aligned}
\langle A \rangle &= \sum_k p_k \langle A_k \rangle \\
&= \sum_k p_k \operatorname{Tr}\left(\mid \psi_k \rangle\langle \psi_k \mid A\right) \\
&= \operatorname{Tr}\left(\sum_k p_k \mid \psi_k \rangle\langle \psi_k \mid A\right) \\
&= \operatorname{Tr}(\rho A).
\end{aligned}$$

□

(4) After measurement of the observable $\mathcal{O}$ with operator A, the density matrix ρ is replaced by

$$\sum_j P_j \rho P_j.$$

Proof. First,

$$\begin{aligned}
\sum_j P_j \rho P_j &= \sum_j \left(\mid \phi_j \rangle\langle \phi_j \mid\right) \left(\sum_k p_k \mid \psi_k \rangle\langle \psi_k \mid\right) \left(\mid \phi_j \rangle\langle \phi_j \mid\right) \\
&= \sum_{jk} p_k \mid \phi_j \rangle\langle \phi_j \mid \psi_k \rangle\langle \psi \mid \phi_j \rangle\langle \phi_j \mid \\
&= \sum_{jk} p_k \mid \phi_j \rangle |\langle \phi_j \mid \psi \rangle|^2 \langle \phi_j \mid \\
&= \sum_{jk} p_k |c_{kj}|^2 \mid \phi_j \rangle\langle \phi_j \mid .
\end{aligned}$$

On the other hand, from result 4 in section A.4 we know that each state ψ_k collapses to eigenstate ϕ_j with probability

$$|c_{kj}|^2 = |\langle \phi_j \mid \phi_k \rangle|^2.$$

Thus, again using conditional probability, the post-measurement ensemble should be described by pure-state density matrices $\mid \phi_j \rangle\langle \phi_j \mid$ with probabilities $p_k |c_{kj}|^2$, i.e.

$$\sum_{jk} p_k |c_{kj}|^2 \mid \phi_j \rangle\langle \phi_j \mid = \sum_j P_j \rho P_j.$$

□

A.6 Additional properties of density matrices

Lemma A.6.1. *If $\{\phi_j\}$ is an orthornomal basis for $\mathcal{H}$, then*

$$\sum_j \mid \phi_j \rangle\langle \phi_j \mid = I.$$

Proof. Take an arbitrary vector $\psi \in \mathcal{H}$. Expanded in terms of the basis, this is

$$\psi = \sum_j c_j \phi_j$$

where

$$c_j = \langle \phi_j \mid \psi \rangle.$$

Then

$$\left(\sum_j \mid \phi_j \rangle\langle \phi_j \mid \right) \mid \psi \rangle = \sum_j \mid \phi_j \rangle\langle \phi_j \mid \psi \rangle = \sum_j \mid \phi_j \rangle c_j = \psi = I\psi.$$

□

Lemma A.6.2. *Eigenvectors of a self-adjoint operator H are eigenvectors of $e^{-\beta H}$. That is, if $H\phi_j = E_j \phi_j$ then*

$$e^{-\beta H}\phi_j = e^{-\beta E_j}\phi_j.$$

Proof. This may be justified formally by using the Taylor expansion for the operator exponential:

$$e^{-\beta H}\phi_j = \sum_{k=0}^{\infty} \frac{(-\beta)^k H^k \phi_j}{k!} = \sum_{k=0}^{\infty} \frac{(-\beta)^k E_j^k \phi_j}{k!} = e^{-\beta E_j}\phi_j.$$

□

A.7 Trace in coordinates

With respect to a basis $\{\phi_i\}$, A has matrix element A_{ij}

$$A_{ij} = \langle \phi_i \mid A \mid \phi_j \rangle.$$

Then

$$\mathrm{Tr}(A) = \sum_i A_{ii} = \sum_i \langle \phi_i \mid A \mid \phi_i \rangle. \tag{A.7.1}$$

If $\{\phi_i\}$ is an orthonormal eigenbasis for A, with respective eigenvalues $\{\lambda_i\}$, then

$$\mathrm{Tr}(A) = \sum_i \langle \phi_i \mid \lambda_i \mid \phi_i \rangle = \sum_i \lambda_i \langle \phi_i \mid \phi_i \rangle = \sum_i \lambda_i.$$

Likewise, using lemma A.6.2,

$$\mathrm{Tr}\left(e^{-\beta H}\right) = \sum_i \langle \phi_i \mid e^{-\beta H} \mid \phi_i \rangle = \sum_i \langle \phi_i \mid e^{-\beta E_i} \mid \phi_i \rangle = \sum_i e^{-\beta E_i} \langle \phi_i \mid \phi_i \rangle = \sum_i e^{-\beta E_i}.$$

A.8 Density matrix for the canonical ensemble

Here we work out the density matrix for the canonical ensemble. The p_j's of proposition A.3.2 are

$$p_j = \frac{e^{-\beta E_j}}{Z}.$$

with Z being a to-be-determined normalization factor that makes $\sum_j p_j = 1$. The ϕ_j's are eigenstates of the Hamiltonian with respective eigenvalues E_j. Then

$$\rho = \frac{1}{Z} \sum_j e^{-\beta E_j} \mid \phi_j \rangle\langle \phi_j \mid = \frac{1}{Z} \sum_j e^{-\beta H} \mid \phi_j \rangle\langle \phi_j \mid = \frac{1}{Z} e^{-\beta H} \sum_j \mid \phi_j \rangle\langle \phi_j \mid = \frac{1}{Z} e^{-\beta H}.$$

by lemmas A.6.1 and A.6.2.

It is now clear what the partition function Z is: since trace is linear, for a trace-class operator A we have

$$\mathrm{Tr}\left(\frac{A}{\mathrm{Tr}(A)}\right) = \frac{\mathrm{Tr}(A)}{\mathrm{Tr}(A)} = 1.$$

Thus, to normalize ρ (see property 1 in section A.5),

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right)$$

so

$$\rho = \frac{e^{-\beta H}}{\mathrm{Tr}\left(e^{-\beta H}\right)}.$$

Then property (3) of section A.5 becomes

$$\langle A \rangle = \frac{\mathrm{Tr}\left(A e^{-\beta H}\right))}{\mathrm{Tr}\left(e^{-\beta H}\right)}.$$

B Thermodynamics

Here I collect certain facts about thermodynamics, gleaned from [BU07, U07, LSSY, Huang]. In particular, I note here questions which I would like to resolve to my own satisfaction during my dissertation work.

B.1 Chemical potential

The **chemical potential** μ of a collection of particles is the change in energy that results when a particle is added to the system:

$$dE = \mu\, dN.$$

B.2 Grand-canonical partition function; Fourier space

The partition function N in section 3.1 is what is known as a **canonical partition function**: it involves a fixed particle number N. In statistical mechanics, one also considers a **grand-canonical partition function**, defined as

$$\Xi(\beta, \Lambda, \mu) = \sum_{N \geq 0} e^{\beta \mu N} Z(N).$$

For the two-cycle-interaction model of section 6, we have

$$\begin{aligned}
\Xi(\beta, \Lambda, \mu) &= \sum_{N \geq 0} \frac{e^{\beta\mu N}}{N!} \sum_{\pi \in \mathcal{S}_N} \int_{\Lambda^N} d\mathbf{X}\, e^{-H^{(\alpha)}(\mathbf{X},\pi)} \\
&= \sum_{N \geq 0} \frac{e^{\beta\mu N}}{N!} \sum_{\pi \in \mathcal{S}_N} \int_{\Lambda^N} d\mathbf{X} \exp\left\{-\frac{1}{4\beta} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\}^2\right\} \exp\left\{-\alpha r_2(\pi)\right\} \\
&= \sum_{N \geq 0} \frac{e^{\beta\mu N}}{N!} \sum_{\pi \in \mathcal{S}_N} \exp\left\{-\alpha r_2(\pi)\right\} \int_{\Lambda^N} d\mathbf{X} \prod_{i=1}^{N} \exp\left\{-\frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2\right\}.
\end{aligned}$$

One may write down a grand-canonical partition function in momentum space rather than in position space: one transforms the $\mathbf{x}$ coordinates into $\mathbf{k}$ coordinates. For the two-cycle-interaction model of section 6, we have

$$\hat{X}i(\beta, \Lambda, \mu) = \sum_{N \geq 0} \frac{e^{\beta\mu N}}{N!} \sum_{\pi \in \mathcal{S}_N} \exp\left\{-\alpha r_2(\pi)\right\} \sum_{\mathbf{k}_1, \ldots, \mathbf{k}_N \in \Lambda^*} \prod_{i=1}^{N} \exp\left\{-4\pi^2 \beta \|\mathbf{k}_i\|^2\right\} \delta_{\mathbf{k}_i, \mathbf{k}_{\pi(i)}}.$$

An item to be merged into this discussion is the **occupation number**. Huang, p. 112 [Huang], derives the occupation number for the $\mathbf{k}$th state to be

$$n_{\mathbf{k}} = \frac{e^{\beta\mu}}{e^{\beta E_{\mathbf{k}}} - e^{\beta\mu}} = \frac{1}{e^{\beta(E_{\mathbf{k}} - \mu)} - 1}.$$

B.3 Free energy

The **free energy** is defined in several ways.

In [LSSY], we have

$$F = -\frac{1}{\beta} \log Z.$$

In [U07], the free energy is taken to be the Legendre transform of the pressure:

$$f^{(\alpha)}(\beta, \rho) = \sup_{\mu} \left[\rho\mu - p^{(\alpha)}(\beta, \mu) \right].$$

B.4 Pressure

[Huang] (p. 111) obtains the pressure of the Bose gas from first principles. He sums the momentum distribution for the Bose gas, with pressure in terms of particle flux on the wall of a container.

$$p = \frac{2}{3} \int_{\mathbb{R}^3} \frac{d^3 k}{8\pi^3} \frac{E_{\mathbf{k}}}{e^{\beta(E_{\mathbf{k}} - \mu)} - 1}.$$

[LSSY] define the pressure in terms of a partial derivative involving the free energy:

$$p = -\frac{\partial F}{\partial V} = \rho k_B T.$$

[U07] uses

$$p = \lim_{V \to \infty} \frac{1}{\beta V} \log Z(\beta, \Lambda, \mu).$$

B.5 Density for the Bose gas

[LSSY] (p. 3) declare

$$\rho = \frac{1}{h^3} \int \frac{d\mathbf{k}}{e^{\beta(H_{\mathbf{k}} - \mu)} - 1}.$$

[Huang] (p. 111) has

$$\rho = \frac{1}{2\pi^2} \int_0^\infty dk \frac{k^2}{e^{\beta(H_k - \mu)} - 1}.$$

[U07] uses

$$\rho_c^{(\alpha)} = \left. \frac{\partial p^{(\alpha)}}{\partial \mu} \right|_{\mu = 0-}$$

which yields (equations 6.4.1 and 6.4.3)

$$\begin{aligned} \rho_c^{(\alpha)} &= \left. \frac{\partial p^{(\alpha)}}{\partial \mu} \right|_{\mu = 0-} = \rho_c^{(0)} - \frac{(1 - e^{-\alpha})}{2^{9/2} \pi^{3/2} \beta^{3/2}} \\ \rho_c^{(0)} &= \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{e^{4\beta\pi^2 |\mathbf{k}|^2} - 1}. \end{aligned}$$

It appears that

$$\rho = \frac{\partial p}{\partial \mu} \qquad \text{and} \qquad \rho_c = \left. \frac{\partial p}{\partial \mu} \right|_{\mu = 0-}.$$

C Analysis results

The results here are standard — see, for example, [HN]. They are collected here for ready reference, using notation which is consistent with the rest of the paper. Most of the items here are elaborations on the sketches provided in [Faris], or justifications of it-can-be-shown statements in [U07].

Importantly, here I identify some otherwise-surprising factors of 2 which appear in this paper as well as in [U07] and [BU07]: the generator of Brownian motion is $\nabla^2/2$, but throughout the present work, $H = -\nabla^2$.

C.1 Gaussians

Definition C.1.1. For $\mathbf{x} \in \mathbb{R}^d$, let

$$g_t(\mathbf{x}) = \frac{1}{(2\pi t)^{d/2}} \, e^{-|\mathbf{x}|^2/2t}.$$

Then $g_t(\mathbf{x}-\mathbf{a})$ is a standard Gaussian, with integral 1, having mean $\mathbf{a}$ and variance t in each component.

Proposition C.1.2. *The family of g_t's satisfies a Chapman-Kolmogorov equation:*

$$\int_{\mathbb{R}^d} g_s(\mathbf{x}-\mathbf{z}) g_t(\mathbf{z}-\mathbf{y}) \, d\mathbf{z} = g_{s+t}(\mathbf{x}-\mathbf{y}).$$

Proof. This follows (albeit messily) by completing the square. □

The following proposition is used for the definition of normalized Brownian bridges in section D.6, as well as for the simplified jump-pair interaction in section 4.12.

Proposition C.1.3.

$$\begin{aligned} &\underbrace{\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d}}_{n-1 \textit{ times}} g_{t_1}(\mathbf{x}-\mathbf{z}_1) g_{t_2}(\mathbf{z}_1-\mathbf{z}_2) \cdots g_{t_{n-1}}(\mathbf{z}_{n-2}-\mathbf{z}_{n-1}) g_{t_n}(\mathbf{z}_{n-1}-\mathbf{y}) \\ &\qquad d\mathbf{z}_1 \, d\mathbf{z}_2 \cdots d\mathbf{z}_{n-2} \, d\mathbf{z}_{n-1} \\ &\qquad = g_{t_1+\cdots+t_n}(\mathbf{x}-\mathbf{y}). \end{aligned}$$

Proof. Use induction, iterating the integrals and applying proposition C.1.2. □

The following lemma is used in the proof of proposition 4.12.1 in section 4.12.

Lemma C.1.4.

$$\begin{aligned} g_{2t}(\mathbf{a}_1-\mathbf{a}_2) \, g_{2t}(\mathbf{b}_1-\mathbf{b}_2) &= g_{4t}\left((\mathbf{a}_1-\mathbf{b}_1)-(\mathbf{a}_2-\mathbf{b}_2)\right) \; g_t\left(\mathbf{a}_1-\mathbf{a}_2-\frac{1}{2}(\mathbf{a}_1-\mathbf{b}_1)+\frac{1}{2}(\mathbf{a}_2-\mathbf{b}_2)\right) \\ &= g_{4t}\left((\mathbf{a}_1-\mathbf{b}_1)-(\mathbf{a}_2-\mathbf{b}_2)\right) \; g_t\left(\frac{(\mathbf{a}_1-\mathbf{a}_2)+(\mathbf{b}_1-\mathbf{b}_2)}{2}\right). \end{aligned}$$

Proof. From definition C.1.1, the left-hand side is

$$\frac{1}{(4\pi t)^d} \exp\left\{-\frac{1}{4t}\left(\|\mathbf{a}_1-\mathbf{a}_2\|^2+\|\mathbf{b}_1-\mathbf{b}_2\|^2\right)\right\}.$$

The right-hand side is

$$\frac{1}{(8\pi t)^{d/2}}\,\frac{1}{(2\pi t)^{d/2}}\,\exp\left\{-\frac{1}{8t}\|(\mathbf{a}_1-\mathbf{b}_1)-(\mathbf{a}_2-\mathbf{b}_2)\|^2\right\}\exp\left\{-\frac{1}{2t}\left\|\mathbf{a}_1-\mathbf{a}_2-\frac{(\mathbf{a}_1-\mathbf{b}_1)}{2}+\frac{(\mathbf{a}_2-\mathbf{b}_2)}{2}\right\|^2\right\}$$
$$=\frac{1}{(4\pi t)^d}\,\exp\left\{-\frac{1}{8t}\|(\mathbf{a}_1-\mathbf{b}_1)-(\mathbf{a}_2-\mathbf{b}_2)\|^2\right\}\exp\left\{-\frac{1}{2t}\left\|\frac{\mathbf{a}_1}{2}-\frac{\mathbf{a}_2}{2}+\frac{\mathbf{b}_1}{2}-\frac{\mathbf{b}_2}{2}\right\|^2\right\}$$
$$=\frac{1}{(4\pi t)^d}\,\exp\left\{-\frac{1}{8t}\|(\mathbf{a}_1-\mathbf{a}_2)-(\mathbf{b}_1-\mathbf{b}_2)\|^2\right\}\exp\left\{-\frac{1}{8t}\|(\mathbf{a}_1-\mathbf{a}_2)+(\mathbf{b}_1-\mathbf{b}_2)\|^2\right\}.$$

Since the scale factors are the same, it remains to show that

$$2\|\mathbf{a}_1-\mathbf{a}_2\|^2+2\|\mathbf{b}_1-\mathbf{b}_2\|^2=\|(\mathbf{a}_1-\mathbf{a}_2)-(\mathbf{b}_1-\mathbf{b}_2)\|^2+\|(\mathbf{a}_1-\mathbf{a}_2)+(\mathbf{b}_1-\mathbf{b}_2)\|^2.$$

To see this, let

$$\mathbf{u}=\mathbf{a}_1-\mathbf{a}_2\qquad\text{and}\qquad\mathbf{v}=\mathbf{b}_1-\mathbf{b}_2.$$

Then we only need to show

$$2\|\mathbf{u}\|^2+2\|\mathbf{v}\|^2=\|\mathbf{u}-\mathbf{v}\|^2+\|\mathbf{u}+\mathbf{v}\|^2.$$

But this follows immediately since

$$\|\mathbf{u}\pm\mathbf{v}\|^2=\|\mathbf{u}\|^2\pm 2\mathbf{u}\cdot\mathbf{v}+\|\mathbf{v}\|^2.$$

□

The following corollary is also used in the proof of proposition 4.12.1 in section 4.12. It is nothing more than a relabeling of lemma C.1.4, with

$$\mathbf{a}_1\mapsto\mathbf{x}_1,\quad\mathbf{a}_2\mapsto\mathbf{y}_1,\quad\mathbf{b}_1\mapsto\mathbf{x}_2,\quad\text{and}\quad\mathbf{b}_2\mapsto\mathbf{y}_2.$$

Corollary C.1.5.

$$\begin{aligned}g_{2t}(\mathbf{x}_1-\mathbf{y}_1)\,g_{2t}(\mathbf{x}_2-\mathbf{y}_2)&=g_{4t}\left((\mathbf{x}_1-\mathbf{x}_2)-(\mathbf{y}_1-\mathbf{y}_2)\right)\;g_t\left(\frac{(\mathbf{x}_1-\mathbf{y}_1)+(\mathbf{x}_2-\mathbf{y}_2)}{2}\right)\\&=g_{4t}\left((\mathbf{x}_1-\mathbf{x}_2)-(\mathbf{y}_1-\mathbf{y}_2)\right)\;g_t\left(\frac{(\mathbf{x}_1+\mathbf{x}_2)-(\mathbf{y}_1+\mathbf{y}_2)}{2}\right).\end{aligned}$$

C.2 $e^{-\beta H_0}$ as a convolution operator

We seek to write $e^{-\beta H_0}$ as a convolution operator, where H_0 is a scaled Laplacian. Faris includes the arbitrary scale factor σ^2 in $H_0=-\frac{\sigma^2}{2}\nabla^2$; we simply need to choose $\sigma^2=2$ to fit the present application, then adapt the resulting scale factors to the standard Gaussian notation found in definition C.1.1.

Additionally, we will use $\sigma^2/2=\beta/n$ in sections E.1 and 4.2.

In the following table, $\mathcal{F}$ denotes the Fourier transform; F_β and $\hat{F}_\beta$ denote a Gaussian and its Fourier transform as defined by Faris; g and $\hat{g}$ are as in definition C.1.1.

Arbitrary σ^2			$\sigma^2 = 1$			$\sigma^2 = 2$		
$F_\beta(\mathbf{x})$	$=$	$\dfrac{e^{-\lvert\mathbf{x}\rvert^2/2\sigma^2\beta}}{(2\pi\sigma^2\beta)^{d/2}}$	$F_\beta(\mathbf{x})$	$=$	$\dfrac{e^{-\lvert\mathbf{x}\rvert^2/2\beta}}{(2\pi\beta)^{d/2}}$	$F_\beta(\mathbf{x})$	$=$	$\dfrac{e^{-\lvert\mathbf{x}\rvert^2/4\beta}}{(4\pi\beta)^{d/2}}$
	$=$	$g_{\sigma^2\beta}(\mathbf{x})$		$=$	$g_\beta(\mathbf{x})$		$=$	$g_{2\beta}(\mathbf{x})$
$\hat{F}_\beta(\mathbf{k})$	$=$	$e^{-\sigma^2\beta\lvert\mathbf{k}\rvert^2/2}$	$\hat{F}_\beta(\mathbf{k})$	$=$	$e^{-\beta\lvert\mathbf{k}\rvert^2/2}$	$\hat{F}_\beta(\mathbf{k})$	$=$	$e^{-\beta\lvert\mathbf{k}\rvert^2}$
H_0	$=$	$-\frac{\sigma^2}{2}\nabla^2$	H_0	$=$	$-\frac{1}{2}\nabla^2$	H_0	$=$	$-\nabla^2$
$\mathcal{F}\left(-\frac{\sigma^2}{2}\nabla^2\right)$	$=$	$\frac{\sigma^2}{2}\lvert\mathbf{k}\rvert^2$	$\mathcal{F}\left(-\frac{1}{2}\nabla^2\right)$	$=$	$\frac{1}{2}\lvert\mathbf{k}\rvert^2$	$\mathcal{F}\left(-\nabla^2\right)$	$=$	$\lvert\mathbf{k}\rvert^2$
$\mathcal{F}\left(e^{-\beta H_0}\right)$	$=$	$F_\beta(\mathbf{k})$	$\mathcal{F}\left(e^{-\beta H_0}\right)$	$=$	$F_\beta(\mathbf{k})$	$\mathcal{F}\left(e^{-\beta H_0}\right)$	$=$	$F_\beta(\mathbf{k})$
$(e^{-\beta H_0}f)(\mathbf{x})$	$=$	$(e^{\frac{\sigma^2\beta}{2}\nabla^2}f)(\mathbf{x})$	$(e^{-\beta H_0}f)(\mathbf{x})$	$=$	$(e^{\frac{\beta}{2}\nabla^2}f)(\mathbf{x})$	$(e^{-\beta H_0}f)(\mathbf{x})$	$=$	$(e^{\beta\nabla^2}f)(\mathbf{x})$
	$=$	$F_\beta(\mathbf{x}) * f(\mathbf{x})$		$=$	$F_\beta(\mathbf{x}) * f(\mathbf{x})$		$=$	$F_\beta(\mathbf{x}) * f(\mathbf{x})$
	$=$	$g_{\sigma^2\beta}(\mathbf{x}) * f(\mathbf{x})$		$=$	$g_\beta(\mathbf{x}) * f(\mathbf{x})$		$=$	$g_{2\beta}(\mathbf{x}) * f(\mathbf{x})$

We have used the $*$ notation for the **convolution**:

$$g(\mathbf{x}) * f(\mathbf{x}) = (g * f)(\mathbf{x}) = \int_{\mathbb{R}^d} g(\mathbf{x}-\mathbf{y})f(\mathbf{y})\,d\mathbf{y}.$$

We now prove the claims tabulated above. The proof is split up into a sequence of lemmas.

Definition C.2.1. Following Faris, we define the **Fourier transform** and **inverse Fourier transform** using the non-unitary angular-frequency conventions for sign and scale. Namely, for $f, g : \mathbb{R}^d \to \mathbb{R}$ which are in $L^1 \cap L^2$,

$$(\mathcal{F}f)(\mathbf{k}) = \hat{f}(\mathbf{k}) = \int_{\mathbb{R}^d} f(\mathbf{x})e^{-i\mathbf{k}\cdot\mathbf{x}}\,d\mathbf{x}. \tag{C.2.2}$$

$$(\mathcal{F}^{-1}g)(\mathbf{x}) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} g(\mathbf{k})e^{+i\mathbf{k}\cdot\mathbf{x}}\,d\mathbf{k}. \tag{C.2.3}$$

Lemma C.2.4. *The Fourier transform of the one-dimensional t-variance Gaussian (definition C.1.1) is*

$$\hat{g}_t(k) = e^{-tk^2/2}.$$

Proof. Complete the square, use translation invariance of the integral, and recognize $1/(2\pi)^{1/2}$ as the integral of $e^{-x^2/2t}$:

$$\begin{aligned}(\mathcal{F}g_t) &= \frac{1}{(2\pi t)^{1/2}} \int_{\mathbb{R}} e^{-x^2/2t} e^{-ikx}\, dx \\ &= \frac{1}{(2\pi t)^{1/2}} \int_{\mathbb{R}} \exp\left\{-\frac{1}{2t}(x^2 + 2itkx)\right\} dx \\ &= \frac{1}{(2\pi t)^{1/2}} \int_{\mathbb{R}} \exp\left\{-\frac{1}{2t}(x + itk)^2 - \frac{tk^2}{2}\right\} dx \\ &= \frac{e^{-tk^2/2}}{(2\pi t)^{1/2}} \int_{\mathbb{R}} \exp\left\{-\frac{1}{2t}(x + itk)^2\right\} dx \\ &= \frac{e^{-tk^2/2}}{(2\pi t)^{1/2}} \int_{\mathbb{R}} \exp\left\{-\frac{1}{2t}x^2\right\} dx \\ &= e^{-tk^2/2}.\end{aligned}$$

□

Proposition C.2.5. *The Fourier transform of the d-dimensional t-variance Gaussian (definition C.1.1) is*

$$\hat{g}_t(\mathbf{k}) = e^{-t\|\mathbf{k}\|^2/2}.$$

Proof. First write

$$\begin{aligned}(\mathcal{F}g_t) &= \frac{1}{(2\pi t)^{d/2}} \int_{\mathbb{R}^d} e^{-\|\mathbf{x}\|^2/2t} e^{-i\mathbf{k}\cdot\mathbf{x}}\, d\mathbf{x} \\ &= \left(\frac{1}{2\pi t}\right)^{d/2} \int_{\mathbb{R}^d} \left(\prod_{\ell=1}^{d} e^{-x_j^2/2t} e^{-ik_j x_j}\right) d\mathbf{x}.\end{aligned}$$

Since the integrand is non-negative, by Tonelli's theorem we may iterate the integrals and apply lemma C.2.4 to each. □

Lemma C.2.6. *Let $f : \mathbb{R} \to \mathbb{R}$ be such that $f(x), f'(x)$ and $f''(x)$ are in $L^1 \cap L^2$ and vanish at $\pm\infty$. Then*

$$\mathcal{F}\left(\frac{d^2 f}{dx^2}\right) = -k^2 \hat{f}(k).$$

Proof. Integrate by parts twice, applying the zero boundary conditions:

$$\mathcal{F}\left(\frac{d^2 f}{dx^2}\right) = \int_{\mathbb{R}} \frac{d^2 f}{dx^2} e^{-ikx}\, dx = ik \int_{\mathbb{R}} \frac{df}{dx} e^{-ikx}\, dx = (ik)^2 \int_{\mathbb{R}} f(x) e^{-ikx}\, dx = -k^2 \hat{f}(k).$$

□

Lemma C.2.7. *Let $f : \mathbb{R}^d \to \mathbb{R}$ be such that f and all its first and second partial derivatives are in $L^1 \cap L^2$ and vanish at $\pm\infty$. Then*

$$\mathcal{F}\left(\nabla^2 f\right) = -\|\mathbf{k}\|^2 \hat{f}(\mathbf{k}).$$

Proof. Integrate by parts twice, applying the zero boundary conditions:

$$
\begin{aligned}
\mathcal{F}\left(\nabla^2 f\right) &= \int_{\mathbb{R}^d} \nabla^2 f e^{-i\mathbf{k}\cdot\mathbf{x}}\, d\mathbf{x} \\
&= \int_{\mathbb{R}^d} \left(\sum_{j=1}^{d} \frac{d^2 f}{dx_j^2} \right) \left(\prod_{\ell=1}^{d} e^{-ik_\ell x_\ell} \right) \, d\mathbf{x} \\
&= \sum_{j=1}^{d} \int_{\mathbb{R}^d} \frac{d^2 f}{dx_j^2} \left(\prod_{\ell=1}^{d} e^{-ik_\ell x_\ell} \right) \, d\mathbf{x} \\
&= \sum_{j=1}^{d} (ik_j) \int_{\mathbb{R}^d} \frac{df}{dx_j} \left(\prod_{\ell=1}^{d} e^{-ik_\ell x_\ell} \right) \, d\mathbf{x} \\
&= \sum_{j=1}^{d} (ik_j)^2 \int_{\mathbb{R}^d} f(\mathbf{x}) \left(\prod_{\ell=1}^{d} e^{-ik_\ell x_\ell} \right) \, d\mathbf{x} \\
&= -\|\mathbf{k}\|^2 \hat{f}(\mathbf{k}).
\end{aligned}
$$

□

Definition C.2.8. The **Fourier transform** or **operator transform** of an operator A is

$$\hat{A} = \mathcal{F} A \mathcal{F}^{-1}.$$

Note this this is equivalent to

$$\hat{A}\mathcal{F} = \mathcal{F}A.$$

That is, this is the frequency-domain operator which takes a $\mathbf{k}$ function, back-transforms to an $\mathbf{x}$ function, applies A, and forward-transforms:

$$
\begin{tikzcd}
\text{Spatial domain} & {} \arrow[d, "A"'] & {} \arrow[l, "\mathcal{F}^{-1}"'] \arrow[d, "\hat{A}"] & \text{Frequency domain} \\
& {} \arrow[r, "\mathcal{F}"] & {} &
\end{tikzcd}
$$

Remark C.2.9. As a consequence,

$$
\begin{aligned}
\hat{A} &= \mathcal{F} A \mathcal{F}^{-1} \\
\hat{A}\mathcal{F} &= \mathcal{F} A \\
\hat{A}\mathcal{F} f &= (\mathcal{F} A) f \\
\mathcal{F}(Af) &= \hat{A}\hat{f}.
\end{aligned}
$$

Remark C.2.10. We just saw in lemma C.2.7, with $A = \nabla^2$, that

$$\mathcal{F}(\nabla^2 f) = -\|\mathbf{k}\|^2 \hat{f}.$$

Therefore we conclude that the Fourier transform of the scaled Laplacian is the multiplication operator

$$\mathcal{F}(c\nabla^2) = -c\|\mathbf{k}\|^2.$$

Proposition C.2.11.

$$\mathcal{F}\left(e^{c\,d^2/dx^2}\right) = e^{-ck^2}.$$

Proof. Moving the transform through the infinite sum without justification, we have

$$\begin{aligned}
\mathcal{F}\left(e^{c\,d^2 f/dx^2}\right) &= \mathcal{F}\left(\sum_{j=0}^{\infty} \frac{c^j}{j!}\frac{d^{2j} f}{dx^{2j}}\right) \\
&= \sum_{j=0}^{\infty} \frac{c^j}{j!}\mathcal{F}\left(\frac{d^{2j} f}{dx^{2j}}\right) \\
&= \sum_{j=0}^{\infty} \frac{c^j}{j!}(-k^{2j})\hat{f}(k) \\
&= \left(\sum_{j=0}^{\infty} \frac{-(ck^2)^j}{j!}\right)\hat{f}(k) \\
&= e^{-ck^2}\hat{f}(k).
\end{aligned}$$

□

Proposition C.2.12.

$$\mathcal{F}\left(e^{c\nabla^2}\right) = e^{-c\|\mathbf{k}\|^2}.$$

Proof. TBD. The procedure is similar to C.2.11; there are some combinatorial factors involving mixed partials which I need to work out on paper. □

Proposition C.2.13. *The Fourier transform of a convolution is the product of Fourier transforms:*

$$\mathcal{F}(f * g) = \hat{f}\hat{g}.$$

Proof. Start with

$$\begin{aligned}
\mathcal{F}\,(f * g) &= \mathcal{F}\left(\int_{\mathbb{R}^d} f(\mathbf{y})g(\mathbf{x}-\mathbf{y})\,d\mathbf{y}\right) \\
&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(\mathbf{y})g(\mathbf{x}-\mathbf{y})e^{-i\mathbf{k}\cdot\mathbf{x}} d\mathbf{y}\,d\mathbf{x}.
\end{aligned}$$

Now let $\mathbf{z} = \mathbf{x} - \mathbf{y}$. Then, using Fubini's theorem since imaginary exponentials have modulus one and we assume f, g are L^2 so their product is L^1 (their inner product exists),

$$\begin{aligned}
\mathcal{F}\,(f * g) &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(\mathbf{y})g(\mathbf{z})e^{-i\mathbf{k}\cdot(\mathbf{y}+\mathbf{z})} d\mathbf{y}\,d\mathbf{z} \\
&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(\mathbf{y})e^{-i\mathbf{k}\cdot\mathbf{y}} g(\mathbf{z})e^{-i\mathbf{k}\cdot\mathbf{z}}\,d\mathbf{y}\,d\mathbf{z} \\
&= \int_{\mathbb{R}^d}\left[\int_{\mathbb{R}^d} f(\mathbf{y})e^{-i\mathbf{k}\cdot\mathbf{y}} d\mathbf{y}\right] g(\mathbf{z})e^{-i\mathbf{k}\cdot\mathbf{z}} d\mathbf{z} \\
&= \hat{f}\hat{g}.
\end{aligned}$$

□

Proposition C.2.14. *The exponentiated scaled Laplacian may be written as an integral operator:*

$$\left(e^{c\nabla^2} f\right)(\mathbf{x}) = \int_{\mathbb{R}^d} g_c(\mathbf{x}-\mathbf{y}) f(\mathbf{y})\, d\mathbf{y}.$$

Proof. Let $A = e^{-c\nabla^2}$. Then we need to show

$$\begin{aligned} Af &= g_c * f \\ \mathcal{F}(Af) &= \mathcal{F}(g_c * f) \\ \hat{A}\hat{f} &= \hat{g}_c \hat{f} \\ \hat{A} &= \hat{g}_c. \end{aligned}$$

But this follows from proposition C.2.12. □

C.3 Operator trace

As described in section A.8, we will want to compute $\mathrm{Tr}\left(e^{-\beta H}\right)$. Here is a partial result, assuming that $e^{-\beta H}$ can be written as an integral operator. The construction of that integral operator will need to wait until section E.2.

Proposition C.3.1. *If a trace-class operator A on a separable Hilbert space has a $G(\mathbf{x},\mathbf{y})$ such that*

$$A\, f(\mathbf{x}) = \int G(\mathbf{x},\mathbf{y}) f(\mathbf{y})\, d\mathbf{y},$$

then

$$\mathrm{Tr}(A) = \int G(\mathbf{x},\mathbf{x})\, d\mathbf{x}.$$

Proof. As shown in equation A.7.1, with $\{\phi_j\}$ being a (countable) basis for the (separable) Hilbert space $\mathcal{H}$,

$$\mathrm{Tr}(A) = \sum_j \langle \phi_j \mid A \mid \phi_j \rangle.$$

Then

$$\begin{aligned} \mathrm{Tr}(A) &= \sum_j \langle \phi_j \mid A \mid \phi_j \rangle \\ &= \sum_j \int \int \phi_j^*(\mathbf{x})\, G(\mathbf{x},\mathbf{y})\, \phi_j(\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} \\ &= \int \int G(\mathbf{x},\mathbf{y}) \left(\sum_j \phi_j^*(\mathbf{x})\, \phi_j(\mathbf{y}) \right) d\mathbf{y}\, d\mathbf{x} \\ &= \int \int G(\mathbf{x},\mathbf{y}) \delta(\mathbf{x}-\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} \\ &= \int G(\mathbf{x},\mathbf{x})\, d\mathbf{x}. \end{aligned}$$

The appearance of the delta function is due to the following completeness relation.

Lemma C.3.2. *For all* $\mathbf{x}, \mathbf{y}$,

$$\left(\sum_j \phi_j^*(\mathbf{x})\, \phi_j(\mathbf{y}) \right) = \delta(\mathbf{x} - \mathbf{y}).$$

Proof. Let ψ be an arbitrary wave function. Then it is a linear combination of the basis functions: $\psi(\mathbf{y}) = \sum_j c_j \phi_j(\mathbf{y})$ where $c_j = \int \phi_j^*(\mathbf{x})\psi(\mathbf{x})\, d\mathbf{x}$. Combining these two statements, we have

$$\begin{aligned}
\psi(\mathbf{y}) &= \sum_j \left(\int \phi_j^*(\mathbf{x})\psi(\mathbf{x})\, d\mathbf{x} \right) \phi_j(\mathbf{y}) \\
&= \int \left(\sum_j \phi_j^*(\mathbf{x})\phi_j(\mathbf{y}) \right) \psi(\mathbf{x})\, d\mathbf{x} \\
&= \int \delta(\mathbf{x} - \mathbf{y})\psi(\mathbf{x}) d\mathbf{x}.
\end{aligned}$$

□

□

Remark C.3.3. Note that $G(\mathbf{x}, \mathbf{y})$ only appears in an integral, and thus may be a distribution rather than a function. This will in fact be the case in section E, where the $G(\mathbf{x}, \mathbf{y})$ we construct will contain a delta-function term.

C.4 Triple product of partial derivatives

This is used for the proof of proposition 6.5.1 in section 6.5.

Proposition C.4.1. *Let* $f : \mathbb{R}^3 \to \mathbb{R}$ *be continuously differentiable. Let* (x_0, y_0, z_0) *be a point on the surface*

$$f(x, y, z) = 0$$

where $\partial f/\partial x$, $\partial f/\partial y$, *and* $\partial f/\partial z$ *are non-zero. Then there is a neighborhood of* (x_0, y_0, z_0) *such that*

$$\frac{\partial x}{\partial y}\frac{\partial y}{\partial z}\frac{\partial z}{\partial x} = -1.$$

Proof. Since $\partial f/\partial x \neq 0$, by the implicit function theorem we can solve for x and write

$$f(x(y, z), y, z) = 0.$$

Differentiating with respect to y, we have

$$\begin{aligned}
\frac{\partial f}{\partial x}\frac{\partial x}{\partial y} + \frac{\partial f}{\partial y} &= 0 \\
\frac{\partial x}{\partial y} &= -\frac{\partial f/\partial y}{\partial f/\partial x}.
\end{aligned}$$

Likewise,

$$\frac{\partial y}{\partial z} = -\frac{\partial f/\partial z}{\partial f/\partial y} \qquad \text{and} \qquad \frac{\partial z}{\partial x} = -\frac{\partial f/\partial x}{\partial f/\partial z}.$$

Multiplying the three partials together, we obtain

$$\frac{\partial x}{\partial y}\frac{\partial y}{\partial z}\frac{\partial z}{\partial x} = -\left(\frac{\partial f/\partial y}{\partial f/\partial x}\right)\left(\frac{\partial f/\partial z}{\partial f/\partial y}\right)\left(\frac{\partial f/\partial x}{\partial f/\partial z}\right) = -1.$$

$\square$

D Brownian motion and Brownian bridges

Here I recall some basic results, all in preparation for discussion of the Feynman-Kac formulas in appendix E and section 4. The presentation here is almost entirely an elaboration on [Faris]. For full information, see [GS], [Lawler], or [Øksendal].

D.1 Expectations and covariance

Notation D.1.1. The covariance of $\mathbb{R}^d$-valued random variables

$$\mathbf{X} = \begin{pmatrix} X_1 \\ \vdots \\ X_d \end{pmatrix} \quad \text{and} \quad \mathbf{Y} = \begin{pmatrix} Y_1 \\ \vdots \\ Y_d \end{pmatrix},$$

having respective means $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$, is written

$$\mathrm{Cov}(\mathbf{X}, \mathbf{Y}) = \mathbb{E}[(\mathbf{X} - \boldsymbol{\mu})(\mathbf{Y} - \boldsymbol{\nu})'] = \mathbb{E}[\mathbf{X}\mathbf{Y}'] - \boldsymbol{\mu}\boldsymbol{\nu}'.$$

We write $\mathbf{X}'$ for the transpose of $\mathbf{X}$ from column to row vector. Then $\mathbf{X}\mathbf{Y}'$ and $\boldsymbol{\mu}\boldsymbol{\nu}'$ denote the $d \times d$ outer product of $\mathbf{X}$ and $\mathbf{Y}$ and $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$, respectively, and the expectations are taken componentwise:

$$\mathbb{E}[\mathbf{X}\mathbf{Y}'] = \mathbb{E}\left[\begin{pmatrix} X_1 \\ \vdots \\ X_d \end{pmatrix} \begin{pmatrix} Y_1 & \vdots & Y_d \end{pmatrix}\right] = \begin{pmatrix} \mathbb{E}[X_1Y_1] & \cdots & \mathbb{E}[X_1Y_d] \\ \vdots & & \vdots \\ \mathbb{E}[X_dY_1] & \cdots & \mathbb{E}[X_dY_d] \end{pmatrix}.$$

In case the covariance matrix has constant c along the diagonal and zeroes elsewhere, we write $\mathbb{E}[\mathbf{X}\mathbf{Y}] = cI$.

Notation D.1.2. For a stochastic process $\mathbf{X}_t$, defined on, say, $t \in [0, \infty)$ or $t \in [0, T]$ for some positive real T, and for some Borel set $D \subset \mathbb{R}^d$, we write the conditional probabilities

$$\mathbb{P}_0^{\mathbf{a}}(\mathbf{X}_t \in D) := \mathbb{P}(\mathbf{X}_t \in D \mid \mathbf{X}_0 = \mathbf{a})$$

and

$$\mathbb{P}_{0,T}^{\mathbf{a},\mathbf{b}}(\mathbf{X}_t \in D) := \mathbb{P}(\mathbf{X}_t \in D \mid \mathbf{X}_0 = \mathbf{a}, \mathbf{X}_T = \mathbf{b}).$$

Likewise, we write the conditional expectations

$$\mathbb{E}_0^{\mathbf{a}}[F(\mathbf{X}_t)] := \mathbb{E}[F(\mathbf{X}_t) \mid \mathbf{X}_0 = \mathbf{a}]$$

and

$$\mathbb{E}_{0,T}^{\mathbf{a},\mathbf{b}}[F(\mathbf{X}_t)] := \mathbb{E}[F(\mathbf{X}_t) \mid \mathbf{X}_0 = \mathbf{a}, \mathbf{X}_T = \mathbf{b}].$$

Similarly, conditional covariances are

$$\mathrm{Cov}_0^{\mathbf{a}}(\mathbf{X}_t, \mathbf{Y}_t) := \mathbb{E}[(\mathbf{X}_t - \boldsymbol{\mu}_t)(\mathbf{Y}_t - \boldsymbol{\nu}_t) \mid \mathbf{X}_0 = \mathbf{a}, \mathbf{Y}_0 = \mathbf{a}]$$

and

$$\mathrm{Cov}_{0,T}^{\mathbf{a},\mathbf{b}}(\mathbf{X}_t, \mathbf{Y}_t) := \mathbb{E}[(\mathbf{X}_t - \boldsymbol{\mu}_t)(\mathbf{Y}_t - \boldsymbol{\nu}_t) \mid \mathbf{X}_0 = \mathbf{a}, \mathbf{Y}_0 = \mathbf{a}, \mathbf{X}_T = \mathbf{b}, \mathbf{Y}_T = \mathbf{b}].$$

Notation D.1.3. For N stochastic processes $\mathbf{X}^{(1)}, \ldots, \mathbf{X}^{(N)}$, we write the conditional expectations

$$\mathbb{E}_0^{\mathbf{a}^{(1)},\ldots,\mathbf{a}^{(N)}}[F(\mathbf{X}_t^{(1)}, \ldots, \mathbf{X}_t^{(N)})] := \mathbb{E}\left[F(\mathbf{X}_t^{(1)}, \ldots, \mathbf{X}^{(N)}) \mid \mathbf{X}_0^{(1)} = \mathbf{a}^{(1)}, \ldots, \mathbf{X}_0^{(N)} = \mathbf{a}^{(N)}\right]$$

and

$$\begin{aligned}\mathbb{E}_{0,T}^{\mathbf{a}^{(1)},\mathbf{b}^{(1)};\ldots;\mathbf{a}^{(N)},\mathbf{b}^{(N)}}&[F(\mathbf{X}_t^{(1)}, \ldots, \mathbf{X}_t^{(N)})] \\ &:= \mathbb{E}\left[F(\mathbf{X}_t^{(1)}, \ldots, \mathbf{X}_t^{(N)}) \mid \mathbf{X}_0^{(1)} = \mathbf{a}^{(1)}, \mathbf{X}_T^{(1)} = \mathbf{b}^{(1)}, \ldots, \mathbf{X}_0^{(N)} = \mathbf{a}^{(N)}, \mathbf{X}_T^{(N)} = \mathbf{b}^{(N)}\right].\end{aligned}$$

D.2 Brownian motion

In this section we review fundamental properties of Brownian motion, highlighting its connections with the Gaussian function and laying notational groundwork for the Feynman-Kac formulas in sections E and 4.

Brownian motion (see [Øksendal, Lawler, GS] for more careful treatments) is defined for $t \in [0, \infty) \mapsto \mathbf{b}_t \in \mathbb{R}^d$. It has the following properties:

- $\mathbf{b}_t$ is a stochastic process, or random function of t, which is almost surely continuous (with respect to the probability measure defined below).
- $\mathbf{b}_0 = 0$.
- $\mathbf{b}_t$ has Gaussian distribution with mean 0 and variance t in each of its d components for all $t > 0$, and it has covariance
$$\mathrm{Cov}(\mathbf{b}_s, \mathbf{b}_t) = \mathbb{E}[\mathbf{b}_s \mathbf{b}_t] = (s \wedge t) I$$
where $s \wedge t$ denotes $\min\{s, t\}$. Specifically, the probability density function (PDF) of $\mathbf{b}_t$ at time t is Gaussian with mean 0 and component variances t. For a box
$$D = [\ell^{(1)}, u^{(1)}] \times \cdots \times [\ell^{(d)}, u^{(d)}],$$
we have
$$\mathbb{P}(\mathbf{b}_t \in D) = \int_D g_t(\mathbf{y})\, d\mathbf{y}. \tag{D.2.1}$$
where g_t is definition C.1.1 for the Gaussian with variance t.
- $\mathbf{b}_t$ has *independent increments*: For all $s < t < u < v$, $\mathbf{b}_t - \mathbf{b}_s$ is independent of $\mathbf{b}_v - \mathbf{b}_u$.

It turns out (see also [Faris]) that Brownian motion is uniquely characterized by an extension of equation D.2.1.

Proposition D.2.2. *Brownian motion is uniquely characterized by the following: for all $n \geq 1$, all times $0 < t_1 < \ldots < t_n$, and all boxes*
$$D_k = [\ell_k^{(1)}, u_k^{(1)}] \times \cdots \times [\ell_k^{(d)}, u_k^{(d)}],$$
$$\mathbb{P}\left(\bigcap_{k=1}^{n} \mathbf{b}_{t_k} \in D_k \right) = \int_{D_1} \int_{D_2} \cdots \int_{D_n} g_{t_1}(\mathbf{z}_1) g_{t_2 - t_1}(\mathbf{z}_1 - \mathbf{z}_2) \cdots g_{t_n - t_{n-1}}(\mathbf{z}_{n-1} - \mathbf{z}_n)\, d\mathbf{z}_1\, d\mathbf{z}_2 \cdots d\mathbf{z}_n. \tag{D.2.3}$$

Remark D.2.4. That is, we set up some hoops and calculate the probability that a given realization of the Brownian motion will jump through all of them (figure 7). The only family of functions which jump through such sets of hoops with these normally distributed rates of success is the family of realizations of Brownian motion. This defines a probability measure on continuous functions $f : [0, +\infty) \to \mathbb{R}^d$ with $f(0) = 0$.

Remark. This is equivalent to saying that the joint PDF of the random variables $\mathbf{b}_{t_1}, \ldots, \mathbf{b}_{t_n}$ is
$$g_{t_1}(\mathbf{z}_1) g_{t_2 - t_1}(\mathbf{z}_1 - \mathbf{z}_2) \cdots g_{t_n - t_{n-1}}(\mathbf{z}_{n-1} - \mathbf{z}_n).$$

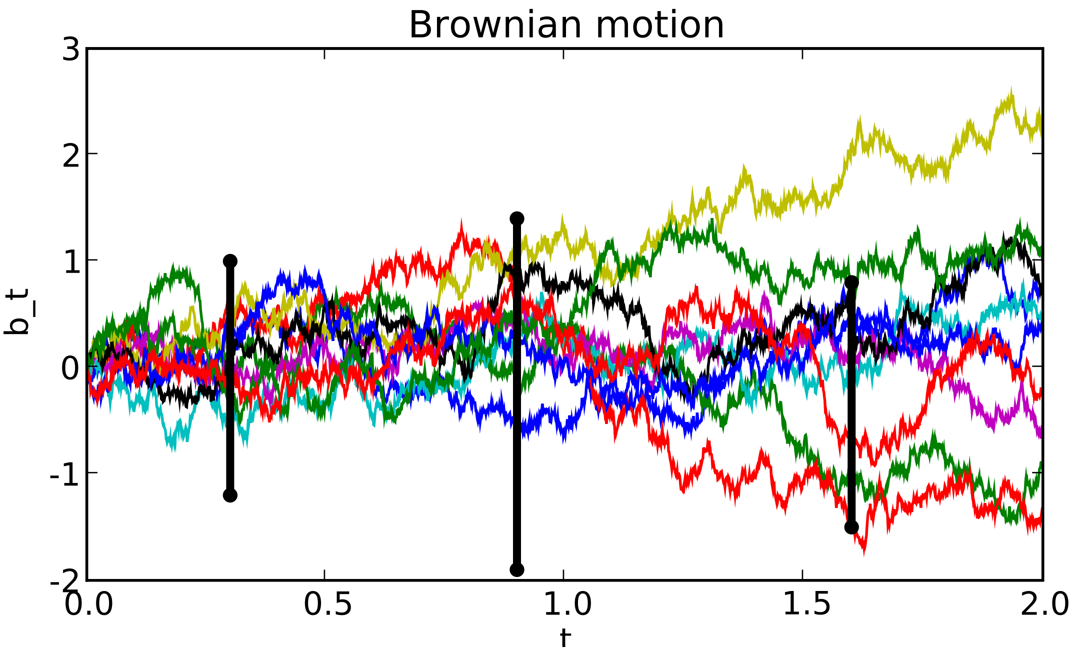

Figure 7: Ten realizations of Brownian motion, moving past three boxes.

Remark D.2.5. Faris points out that one may generalize equation D.2.3. Rephrase it by writing

$$f(\mathbf{b}_{t_1}, \ldots, \mathbf{b}_{t_n}) = \chi_{\cap_{k=1}^n \mathbf{b}_{t_k} \in D_k}(\mathbf{b}_{t_1}, \ldots, \mathbf{b}_{t_n}).$$

Then equation D.2.3 becomes

$$\mathbb{E}[f(\mathbf{b}_{t_1}, \ldots, \mathbf{b}_{t_n})] = \underbrace{\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d}}_{n \text{ times}} g_{t_1}(\mathbf{z}_1) g_{t_2 - t_1}(\mathbf{z}_1 - \mathbf{z}_2) \cdots g_{t_n - t_{n-1}}(\mathbf{z}_{n-1} - \mathbf{z}_n) \\ f(\mathbf{z}_1, \ldots, \mathbf{z}_n)\, d\mathbf{z}_1\, d\mathbf{z}_2 \cdots d\mathbf{z}_n. \tag{D.2.6}$$

This holds not only for the characteristic function χ which appears in equation D.2.3, but for any Borel-measurable f.

Definition D.2.7. We extend this to exponentiated integrals by defining

$$\mathbb{E}\left[\exp\left\{\int_0^T f(\mathbf{b}_t)\, dt\right\}\right] := \lim_{n \to \infty} \underbrace{\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d}}_{n \text{ times}} g_{T/n}(\mathbf{z}_1) g_{T/n}(\mathbf{z}_1 - \mathbf{z}_2) \cdots g_{T/n}(\mathbf{z}_{n-1} - \mathbf{z}_n) \\ \exp\left\{\frac{T}{n} \sum_{j=1}^n f(\mathbf{z}_j)\right\}\, d\mathbf{z}_1 \cdots d\mathbf{z}_n. \tag{D.2.8}$$

Now consider a realization of Brownian motion moving forward in time, having already passed time s with $\mathbf{b}_s = \mathbf{y}$ (figure 8). We want to find the conditional density of $\mathbf{b}_t$.

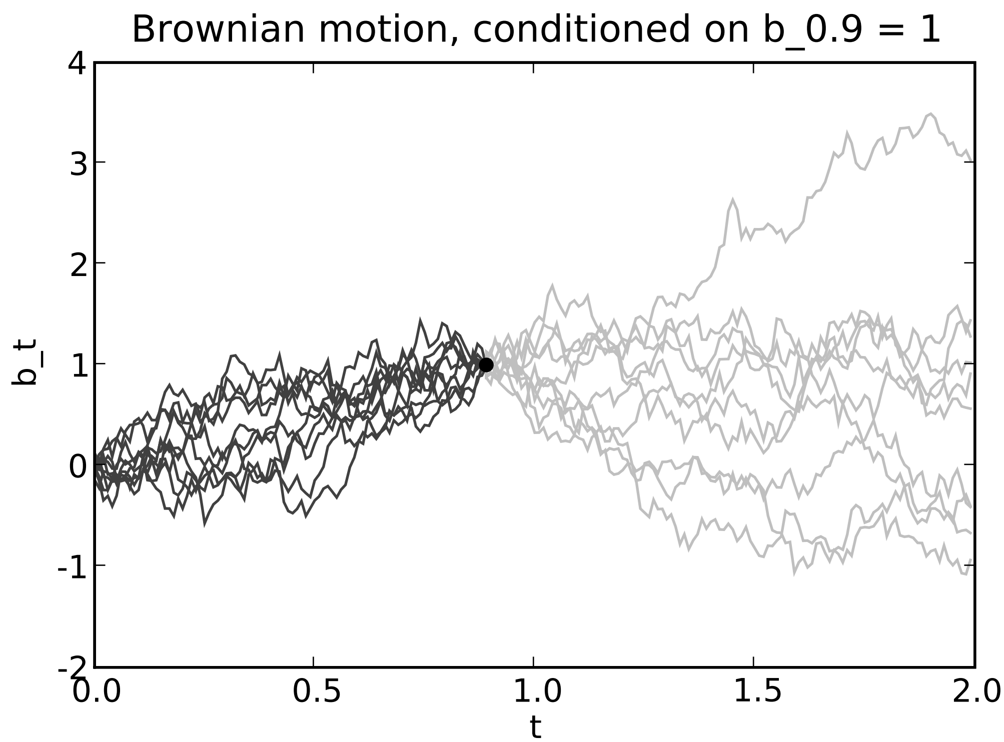

Figure 8: Ten realizations of Brownian motion, conditioned on $\mathbf{b}_s = \mathbf{y}$.

Lemma D.2.9. *The conditional density of* $\mathbf{b}_t$ *given* $\mathbf{b}_s = \mathbf{y}$*, for* $t > s$*, is*

$$g_{t-s}(\mathbf{z} - \mathbf{y}).$$

Proof. This is nothing more than $f_{\mathbf{Z}|\mathbf{Y}}(\mathbf{z} \mid \mathbf{y})$ from elementary probability (see e.g. [GS]), where $\mathbf{Z} = \mathbf{b}_t$ and $\mathbf{Y} = \mathbf{b}_s$. From equation D.2.3, with $n = 2$, the joint density of $\mathbf{Y}$ and $\mathbf{Z}$ is

$$g_{t-s}(\mathbf{z} - \mathbf{y}) g_s(\mathbf{y} - \mathbf{x}).$$

We compute

$$f_{\mathbf{Z}|\mathbf{Y}}(\mathbf{z} \mid \mathbf{y}) = \frac{f_{\mathbf{Z},\mathbf{Y}}(\mathbf{z}, \mathbf{y})}{f_{\mathbf{Y}}(\mathbf{y})} = \frac{g_{t-s}(\mathbf{z} - \mathbf{y}) g_s(\mathbf{y} - \mathbf{x})}{g_s(\mathbf{y} - \mathbf{x})} = g_{t-s}(\mathbf{z} - \mathbf{y}).$$

□

D.3 Shifted Brownian motion

Here we generalize Brownian motion (what [Lawler] calls *standard Brownian motion*) by removing the requirement that the motion start at 0.

Notation D.3.1. For fixed $\mathbf{x}$, we write

$$\mathbf{w}_t^{\mathbf{x}} := \mathbf{x} + \mathbf{b}_t. \tag{D.3.2}$$

If $\mathbf{x}$ is allowed to vary, we simply write $\mathbf{w}_t$. However, this is not well defined as a stochastic process unless we either set a probability distribution for $\mathbf{x}$, or write $\mathbf{w}_t$ inside a conditional expectation. We will take the latter approach in this paper. Also, we take $\mathbb{E}^{\mathbf{x}}[\mathbf{w}_t]$ and $\mathbb{E}[\mathbf{w}_t^{\mathbf{x}}]$ to be equivalent.

Proposition D.3.3. *Shifted Brownian motion has conditional mean and conditional covariance*

$$\mathbb{E}_0^{\mathbf{x}}[\mathbf{w}_t] = \mathbf{x} \qquad \textit{and} \qquad \mathrm{Cov}_0^{\mathbf{x}}[\mathbf{w}_s \mathbf{w}_t] = (s \wedge t)I.$$

Proof. These follow immediately from equation D.3.2, along with the mean and covariance for Brownian motion given in section D.2. $\square$

Proposition D.2.2 becomes the following.

Proposition D.3.4. *For all $n \geq 1$, all times $0 < t_1 < \ldots < t_n$, and all boxes*

$$D_k = [\ell_k^{(1)}, u_k^{(1)}] \times \cdots \times [\ell_k^{(d)}, u_k^{(d)}],$$

we have

$$\mathbb{P}_0^{\mathbf{x}}\left(\bigcap_{k=1}^{n} \mathbf{w}_{t_k} \in D_k\right) = \int_{D_1}\int_{D_2}\cdots\int_{D_n} g_{t_1}(\mathbf{x}-\mathbf{z}_1) g_{t_2-t_1}(\mathbf{z}_1-\mathbf{z}_2)\cdots g_{t_n-t_{n-1}}(\mathbf{z}_{n-1}-\mathbf{z}_n)\, d\mathbf{z}_1\, d\mathbf{z}_2 \cdots d\mathbf{z}_n. \tag{D.3.5}$$

Remark D.3.6. This is equivalent to saying that the joint PDF of the random variables $\mathbf{w}_{t_1}, \ldots, \mathbf{w}_{t_n}$, conditioned on $\mathbf{w}_0 = \mathbf{x}$, is

$$g_{t_1}(\mathbf{z}_1 - \mathbf{x}) g_{t_2-t_1}(\mathbf{z}_1 - \mathbf{z}_2) \cdots g_{t_n-t_{n-1}}(\mathbf{z}_{n-1} - \mathbf{z}_n).$$

Remark D.3.7. Equation D.2.6 becomes

$$\mathbb{E}_0^{\mathbf{x}}[f(\mathbf{w}_{t_1}, \ldots, \mathbf{w}_{t_n})] = \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n \text{ times}} g_{t_1}(\mathbf{x}-\mathbf{z}_1) g_{t_2-t_1)}(\mathbf{z}_1-\mathbf{z}_2)\cdots g_{t_n-t_{n-1}}(\mathbf{z}_{n-1}-\mathbf{z}_n)\, f(\mathbf{z}_1, \ldots, \mathbf{z}_n)\, d\mathbf{z}_1\, d\mathbf{z}_2 \cdots d\mathbf{z}_n. \tag{D.3.8}$$

Definition D.3.9. Definition D.2.7 becomes

$$\mathbb{E}_0^{\mathbf{x}}\left[\exp\left\{\int_0^T f(\mathbf{w}_t)\, dt\right\}\right] := \lim_{n\to\infty} \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n \text{ times}} g_{T/n}(\mathbf{z}_1-\mathbf{x}) g_{T/n}(\mathbf{z}_1-\mathbf{z}_2)\cdots g_{T/n}(\mathbf{z}_{n-1}-\mathbf{z}_n)\, \exp\left\{\frac{T}{n}\sum_{j=1}^{n} f(\mathbf{z}_j)\right\}\, d\mathbf{z}_1 \cdots d\mathbf{z}_n. \tag{D.3.10}$$

D.4 Brownian bridges

[Faris] treats only bridges from $\mathbf{x}$ to $\mathbf{x}$; here, we treat the more general case of bridges from $\mathbf{x}$ to $\mathbf{y}$. This is needed for [BU07], [U07], and in particular for section 4 of this paper.

Definition D.4.1. The **Brownian bridge** running from $\mathbf{x}$ at time 0 to $\mathbf{y}$ at time T is

$$\mathbf{w}^{\mathbf{x},\mathbf{y}}_{0,t,T} = \mathbf{x} + \mathbf{b}_t + \frac{t}{T}\left(\mathbf{y} - \mathbf{x} - \mathbf{b}_T\right). \tag{D.4.2}$$

We may also write this as

$$\mathbf{w}^{\mathbf{x},\mathbf{y}}_{0,t,T} = \frac{(T-t)\mathbf{x} + t\mathbf{y}}{T} + \frac{T\mathbf{b}_t - t\mathbf{b}_T}{T}. \tag{D.4.3}$$

This looks ungainly, but it has the advantage that the mean is precisely the first term.

Notation D.4.4. As in section D.3, if $\mathbf{x}$ and $\mathbf{y}$ are allowed to vary, then we again have simply $\mathbf{w}_t$. We will write $\mathbf{w}_t$ inside a conditional expectation in order to make this notation well defined as a stochastic process. As well, we take $\mathbb{E}^{\mathbf{x},\mathbf{y}}_{0,T}[\mathbf{w}_t]$ and $\mathbb{E}[\mathbf{w}^{\mathbf{x},\mathbf{y}}_{0,t,T}]$ to be equivalent.

Definition D.4.5. As in definition D.3.9, we extend this to exponentiated integrals by defining

$$\begin{aligned}
\mathbb{E}^{\mathbf{x},\mathbf{y}}_{0,T}\left[\exp\left\{\int_0^T f(\mathbf{w}_t)\,dt\right\}\right] &:= \lim_{n\to\infty} \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1 \text{ times}} \\
&\quad g_{T/n}(\mathbf{x}-\mathbf{z}_1)g_{T/n}(\mathbf{z}_1-\mathbf{z}_2)\cdots g_{T/n}(\mathbf{z}_{n-2}-\mathbf{z}_{n-1})g_{T/n}(\mathbf{z}_{n-1}-\mathbf{y}) \\
&\quad \exp\left\{\frac{T}{n}\left(f(\mathbf{x}) + \sum_{j=1}^{n-1} f(\mathbf{z}_j)\right)\right\}\,d\mathbf{z}_1\cdots d\mathbf{z}_{n-1} \\
&:= \int \exp\left\{\int_0^T f(\mathbf{w}_t)\,dt\right\}\,d\mathbf{W}^{\mathbf{x},\mathbf{y}}_{0,T}(\mathbf{w}).
\end{aligned} \tag{D.4.6}$$

Notation D.4.7. In the last line we have defined the notation for the bridge measure as used in [BU07] and [U07].

Proposition D.4.8. *The bridge process $\mathbf{w}^{\mathbf{x},\mathbf{y}}_{T,t}$ has mean*

$$\mathbf{x} + \frac{t}{T}\left(\mathbf{y} - \mathbf{x}\right)$$

and covariance

$$I\left(s \wedge t - \frac{st}{T}\right).$$

Proof. The mean follows immediately from taking the expectation of equation D.4.2. For the covariance, we may take advantage of equation D.4.3 where the mean is readily subtractible, and recall notation D.1.1. Then, since $\mathbb{E}[\mathbf{b}_s\mathbf{b}_t'] = (s \wedge t)I$, we have

$$\begin{aligned}
\mathrm{Cov}^{\mathbf{x},\mathbf{y}}_{0,T}[\mathbf{w}_s, \mathbf{w}_t] &= \frac{1}{T^2}\,\mathbb{E}\left[\left(T\mathbf{b}_s - s\mathbf{b}_T\right)\left(T\mathbf{b}_t - t\mathbf{b}_T\right)'\right] \\
&= \frac{1}{T^2}\,\left(T^2\mathbb{E}[\mathbf{b}_s\mathbf{b}_t'] - sT\mathbb{E}[\mathbf{b}_T\mathbf{b}_t'] - tT\mathbb{E}[\mathbf{b}_s\mathbf{b}_T'] + st\mathbb{E}[\mathbf{b}_S\mathbf{b}_T']\right) \\
&= I\left(s \wedge t - \frac{st}{T}\right).
\end{aligned}$$

□

Remark D.4.9. If $s < t$ we may write this (perhaps more memorably) as

$$I\,\frac{s(T-t)}{T}.$$

Proposition D.4.10. *The difference of two Brownian bridges is twice another Brownian bridge.*

Proof. Let

$$\mathbf{x}_1 + \mathbf{b}_t^{(1)} + \frac{t}{T}\left(\mathbf{y}_1 - \mathbf{x}_1 - \mathbf{b}_T^{(1)}\right) \quad \text{and} \quad \mathbf{x}_2 + \mathbf{b}_t^{(2)} + \frac{t}{T}\left(\mathbf{y}_2 - \mathbf{x}_2 - \mathbf{b}_T^{(2)}\right)$$

be two Brownian bridges, where $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$ are independent Brownian motions. The difference of these bridges is

$$(\mathbf{x}_1 - \mathbf{x}_2) + (\mathbf{b}_t^{(1)} - \mathbf{b}_t^{(2)}) + \frac{t}{T}\left((\mathbf{y}_1 - \mathbf{y}_2) - (\mathbf{x}_1 - \mathbf{x}_2) - (\mathbf{b}_T^{(1)} - \mathbf{b}_T^{(2)})\right).$$

This is a process running from $\mathbf{x}_1 - \mathbf{x}_2$ to $\mathbf{y}_1 - \mathbf{y}_2$ in time T; the statistical properties of the difference of the two Brownian motions remain to be found.

The mean of $\mathbf{b}_t^{(1)} - \mathbf{b}_t^{(2)}$ is zero by linearity of expecation. The covariance is

$$\begin{aligned}\mathbb{E}[(\mathbf{b}_s^{(1)} - \mathbf{b}_s^{(2)})(\mathbf{b}_t^{(1)} - \mathbf{b}_t^{(2)})] &= \mathbb{E}[\mathbf{b}_s^{(1)}\mathbf{b}_t^{(1)}] - \mathbb{E}[\mathbf{b}_s^{(1)}\mathbf{b}_t^{(2)}] - \mathbb{E}[\mathbf{b}_s^{(2)}\mathbf{b}_t^{(1)}] + \mathbb{E}[\mathbf{b}_s^{(2)}\mathbf{b}_t^{(2)}] \\ &= (s \wedge t) - 0 - 0 + (s \wedge t) = 2(s \wedge t),\end{aligned}$$

where the cross terms are zero since $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$ are independent. Reviewing the properties in section D.2 — independence of increments being trivial — shows that the difference of the Brownian motions is twice a Brownian motion. Hence, the difference of the Brownian bridges is twice a Brownian bridge. ☐

D.5 Expectations over delta functions

We continue to follow [Faris] by computing expectations over delta functions. This may seem bizarre, but it is needed in the proof of proposition E.3.1.

Lemma D.5.1. *For the shifted Brownian motion starting at* $\mathbf{x}$*, we have*

$$\mathbb{E}_0^{\mathbf{x}}[\delta(\mathbf{w}_T - \mathbf{y})] = g_T(\mathbf{x} - \mathbf{y})$$

where g_t *is definition C.1.1 for the Gaussian with variance* t*.*

Proof. Using remark D.3.7 for the expectation, we have

$$\mathbb{E}_0^{\mathbf{x}}[\delta(\mathbf{w}_T - \mathbf{y})] = \int_{\mathbb{R}^d} g_T(\mathbf{x} - \mathbf{z})\delta(\mathbf{z} - \mathbf{y})\, d\mathbf{z} = g_T(\mathbf{x} - \mathbf{y}).$$

☐

Lemma D.5.2. *The Wiener-measure covariance of the bridge process* $\mathbf{w}_{T,t}^{\mathbf{x};\mathbf{y}}$ *and the shifted Brownian motion* $\mathbf{w}_T$ *is zero.*

Proof.

$$\begin{aligned}
\mathrm{Cov}\left(\mathbf{w}^{\mathbf{x},\mathbf{y}}_{T,t}, \mathbf{w}_T\right) &= \mathbb{E}\left[\left(\mathbf{w}^{\mathbf{x},\mathbf{y}}_{T,t} - \mathbf{x}\right)\mathbf{w}'_T\right] \\
&= \mathbb{E}\left[\left(\frac{t}{T}(\mathbf{y}-\mathbf{x}) + \mathbf{b}_t - \frac{t}{T}\mathbf{b}_T\right)\mathbf{b}'_T\right] \\
&= \frac{t}{T}(\mathbf{y}-\mathbf{x})\,\mathbb{E}[\mathbf{b}_T]' + \mathbb{E}[\mathbf{b}_t\mathbf{b}'_T] - \frac{t}{T}\,\mathbb{E}[\mathbf{b}_T\mathbf{b}'_T] \\
&= \left(t - \frac{t}{T}T\right) = 0.
\end{aligned}$$

□

The following proposition is needed for our treatment of the Feynman-Kac formula in sections E and 4.4. There, $F(\mathbf{w})$ will be an exponentiated integral in the form of definition D.4.5.

Proposition D.5.3. *Expectations over Brownian bridges and expectations over shifted Brownian motion are related by*

$$\mathbb{E}^{\mathbf{x},\mathbf{y}}_{0,T}[F(\mathbf{w})] = \frac{\mathbb{E}^{\mathbf{x}}_0[F(\mathbf{w})\delta(\mathbf{w}_T - \mathbf{y})]}{g_T(\mathbf{x}-\mathbf{y})}.$$

Proof. We start with the right-hand side. By construction, at time T the Brownian bridge coincides with the Brownian motion conditioned on taking value $\mathbf{y}$ at time T: $\mathbf{w}_T = \mathbf{y} = \mathbf{w}^{\mathbf{x},\mathbf{y}}_T$. Thus

$$\frac{\mathbb{E}^{\mathbf{x}}_0[F(\mathbf{w})\delta(\mathbf{w}_T - \mathbf{y})]}{g_T(\mathbf{x}-\mathbf{y})} = \frac{\mathbb{E}^{\mathbf{x}}_0[F(\mathbf{w}^{\mathbf{x},\mathbf{y}}_T)\delta(\mathbf{w}_T - \mathbf{y})]}{g_T(\mathbf{x}-\mathbf{y})}.$$

By lemma D.5.2, the Wiener-measure covariance of $\mathbf{w}^{\mathbf{x},\mathbf{y}}_{T,t}$ and $\mathbf{w}_T$ is zero. Therefore the expectation factors and the right-hand side becomes

$$\frac{\mathbb{E}^{\mathbf{x}}_0[F(\mathbf{w}^{\mathbf{x},\mathbf{y}}_{T,\cdot})]\,\mathbb{E}^{\mathbf{x}}_0[\delta(\mathbf{w}_T - \mathbf{y})]}{g_T(\mathbf{x}-\mathbf{y})}.$$

By lemma D.5.1, the denominator is equal to the second term in the numerator. Thus the right-hand side equals the left-hand side. □

D.6 Normalized bridges

We modify definition D.4.5 to obtain a normalized measure: we set a scale factor, then prove that it is chosen correctly.

Definition D.6.1. Let

$$d\hat{\mathbf{W}}^{\mathbf{x},\mathbf{y}}_{0,T}(\mathbf{w}) = \frac{1}{g_T(\mathbf{x}-\mathbf{y})}\,d\mathbf{W}^{\mathbf{x},\mathbf{y}}_{0,T}(\mathbf{w}). \tag{D.6.2}$$

Proposition D.6.3. *We have*

$$\int d\hat{\mathbf{W}}^{\mathbf{x},\mathbf{y}}_{0,T}(\mathbf{w}) = 1.$$

Proof. Starting with definition D.4.5 for the non-normalized measure, we have

$$\begin{aligned}\int d\mathbf{W}_{0,T}^{\mathbf{x},\mathbf{y}}(\mathbf{w}) &= \int \exp\left\{\int_0^T 0\,dt\right\} d\mathbf{W}_{0,T}^{\mathbf{x},\mathbf{y}}(\mathbf{w}) \\ &:= \lim_{n\to\infty} \underbrace{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\cdots\int_{\mathbb{R}^d}}_{n-1 \text{ times}} g_{T/n}(\mathbf{x}-\mathbf{z}_1)\cdots g_{T/n}(\mathbf{z}_{n-1}-\mathbf{y})\; d\mathbf{z}_1\cdots d\mathbf{z}_{n-1} \\ &= g_T(\mathbf{x}-\mathbf{y})\end{aligned}$$

where the last step follows from proposition C.1.3. $\square$

E Single-particle Feynman-Kac formulas

The material here is familiar from many references. Here I review it for my own understanding, as well as to fix notation and proof techniques which are used for the derivation of the bosonic Feynman-Kac formula in section 4.

E.1 $e^{-\beta H}$ as expectation

In section C.2, for $H_0 = -\nabla^2$, we saw how to interpret the exponentiated operator

$$e^{-\beta H_0} = e^{\beta \nabla^2}$$

as an integral operator with a Gaussian kernel. We now ask, for $H = -\nabla^2 + U(\mathbf{x})$ where U is a multiplication operator corresponding to a potential energy, how to interpret

$$e^{-\beta H} = e^{-\beta(-\nabla^2 + U(\mathbf{x}))} = e^{\beta(\nabla^2 - U(\mathbf{x}))}.$$

Proposition E.1.1. *For*

$$H = -\nabla^2 + U(\mathbf{x}),$$

we have

$$(e^{-\beta H} f)(\mathbf{x}) = \left(e^{\beta(\nabla^2 - U(\mathbf{x}))} f\right)(\mathbf{x}) = \mathbb{E}_0^{\mathbf{x}} \left[\exp\left\{-\frac{1}{2}\int_0^{2\beta} U(\mathbf{w}_s)\, ds\right\} f(\mathbf{w}_{2\beta})\right].$$

Proof. The Trotter product formula (see [Simon] for a proof) says that for self-adjoint operators A and B,

$$e^{\beta(A+B)} = \lim_{n\to\infty} \left(e^{\beta A/n} e^{\beta B/n}\right)^n. \tag{E.1.2}$$

With $A = \nabla^2$ and $B = -U(\mathbf{x})$, we have

$$\begin{aligned} e^{\beta(\nabla^2 - U(\mathbf{x}))} f(\mathbf{x}) &= \lim_{n\to\infty} \left(e^{\beta\nabla^2/n} e^{-\beta U(\mathbf{x})/n}\right)^n f(\mathbf{x}) \\ &= \lim_{n\to\infty} e^{\beta\nabla^2/n} e^{-\beta U(\mathbf{x})/n} \left(e^{\beta\nabla^2/n} e^{-\beta U(\mathbf{x})/n}\right)^{n-1} f(\mathbf{x}). \end{aligned}$$

Recall that $e^{-\beta U(\mathbf{x})/n}$ is simply a scalar. Using the result of section C.2 to write $e^{\beta\nabla^2/n}$ as an integral operator, we have

$$(e^{-\beta H} f)(\mathbf{x}) = \lim_{n\to\infty} \int_{\mathbb{R}^d} g_{2\beta/n}(\mathbf{x} - \mathbf{z}_1) e^{-\beta U(\mathbf{z}_1)/n} \left(e^{\beta\nabla^2/n} e^{-\beta U(\mathbf{z}_1)/n}\right)^{n-1} f(\mathbf{z}_1)\, d\mathbf{z}_1.$$

Repeating yields

$$(e^{-\beta H} f)(\mathbf{x}) = \lim_{n\to\infty} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} g_{2\beta/n}(\mathbf{x} - \mathbf{z}_1) g_{2\beta/n}(\mathbf{z}_1 - \mathbf{z}_2) e^{-\beta U(\mathbf{z}_1)/n} e^{-\beta U(\mathbf{z}_2)/n} \left(e^{\beta\nabla^2/n} e^{-\beta U(\mathbf{z}_2)/n}\right)^{n-2} f(\mathbf{z}_2)\, d\mathbf{z}_1\, d\mathbf{z}_2,$$

and finally

$$
\begin{aligned}
(e^{-\beta H} f)(\mathbf{x}) &= \lim_{n\to\infty} \underbrace{\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d}}_{n \text{ times}} g_{2\beta/n}(\mathbf{x}-\mathbf{z}_1) g_{2\beta/n}(\mathbf{z}_1-\mathbf{z}_2) \cdots g_{2\beta/n}(\mathbf{z}_{n-1}-\mathbf{z}_n) \\
&\qquad e^{-\beta U(\mathbf{z}_1)/n} e^{-\beta U(\mathbf{z}_2)/n} \cdots e^{-\beta U(\mathbf{z}_n)/n} f(\mathbf{z}_n)\, d\mathbf{z}_1\, d\mathbf{z}_2 \ldots\, d\mathbf{z}_n \\
&= \lim_{n\to\infty} \underbrace{\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d}}_{n \text{ times}} g_{2\beta/n}(\mathbf{x}-\mathbf{z}_1) g_{2\beta/n}(\mathbf{z}_1-\mathbf{z}_2) \cdots g_{2\beta/n}(\mathbf{z}_{n-1}-\mathbf{z}_n) \\
&\qquad \exp\left\{ -\frac{\beta}{n} \sum_{k=1}^n U(\mathbf{z}_k) \right\} f(\mathbf{z}_n)\, d\mathbf{z}_1\, d\mathbf{z}_2 \ldots\, d\mathbf{z}_n.
\end{aligned}
$$

Now we recognize an integrand in the form of definition D.3.9, and we can write

$$
(e^{-\beta H} f)(\mathbf{x}) = \lim_{n\to\infty} \mathbb{E}_0^{\mathbf{x}} \left[\exp\left\{ \frac{2\beta}{n} \left(-\frac{1}{2} \right) \sum_{k=1}^n U(\mathbf{w}_{2k\beta/n}) \right\} f(\mathbf{w}_{2\beta}) \right].
$$

Interchanging limit and expectation by dominated convergence (since the exponential is bounded above by 1) and recognizing the limit of the sum as a Riemann integral, we obtain the desired result:

$$
(e^{-\beta H} f)(\mathbf{x}) = \mathbb{E}_0^{\mathbf{x}} \left[\exp\left\{ -\frac{1}{2} \int_0^{2\beta} U(\mathbf{w}_s)\, ds \right\} f(\mathbf{w}_{2\beta}) \right].
$$

□

Remark E.1.3. Note that in the $U = 0$ case, we have

$$
(e^{-\beta H} f)(\mathbf{x})) = e^{\beta \nabla^2} f(\mathbf{x}) = \mathbb{E}_0^{\mathbf{x}} \left[f(\mathbf{w}_{2\beta}) \right].
$$

Yet in section C.2 we also saw that

$$
e^{\beta \nabla^2} f(\mathbf{x}) = \int_{\mathbb{R}^d} g_{2\beta}(\mathbf{x}-\mathbf{y}) f(\mathbf{y})\, d\mathbf{y}.
$$

These two points of view are reconciled by using the Law of the Unconscious Statistician from elementary probability. Namely, for a measurable function h of a random variable Y,

$$
\mathbb{E}[h(\mathbf{Y})] = \int h(\mathbf{y}) f_{\mathbf{Y}}(\mathbf{y})\, d\mathbf{y}
$$

where $f_{\mathbf{Y}}(\mathbf{y})$ is the PDF for $\mathbf{Y}$. Here, for each fixed β and $\mathbf{x}$, $\mathbf{Y}$ is $\mathbf{w}_{2\beta}$, $h(\mathbf{Y})$ is $f(\mathbf{w}_{2\beta})$, and the PDF of $\mathbf{w}_{2\beta}$ is $g_{2\beta}(\mathbf{y}-\mathbf{x})$ as a function of $\mathbf{y}$ as noted in remark D.3.6.

E.2 $e^{-\beta H}$ as an integral operator

Section C.3 showed how to compute $\mathrm{Tr}\left(e^{-\beta H}\right)$ if $e^{-\beta H}$ can be represented as an integral operator. Proposition E.1.1 constructed the operator's kernel for the $U = 0$ case. Here we construct the kernel for the general case, then apply it to find an expression for the trace.

Proposition E.2.1. *If*

$$H = -\nabla^2 + U(\mathbf{x}),$$

then

$$e^{-\beta H} f(\mathbf{x}) = \int G_{2\beta,U}(\mathbf{x},\mathbf{y}) f(\mathbf{y})\, d\mathbf{y} \tag{E.2.2}$$

where

$$G_{2\beta,U}(\mathbf{x},\mathbf{y}) = \mathbb{E}_0^{\mathbf{x}}\left[\exp\left\{-\frac{1}{2}\int_0^{2\beta} U(\mathbf{w}_s)\, ds\right\} \delta(\mathbf{w}_{2\beta} - \mathbf{y})\right]. \tag{E.2.3}$$

Proof. Inserting equation E.2.3 into the right-hand side of E.2.2 gives

$$\int G_{2\beta,U}(\mathbf{x},\mathbf{y}) f(\mathbf{y})\, d\mathbf{y} = \int \mathbb{E}_0^{\mathbf{x}}\left[\exp\left\{-\frac{1}{2}\int_0^{2\beta} U(\mathbf{w}_s)\, ds\right\} \delta(\mathbf{w}_{2\beta} - \mathbf{y})\right] f(\mathbf{y})\, d\mathbf{y}.$$

Now interchange expectation and integral (by Tonelli's theorem, since the integrand is non-negative) and integrate out the delta function:

$$\begin{aligned}
\int G_{2\beta,U}(\mathbf{x},\mathbf{y}) f(\mathbf{y})\, d\mathbf{y} &= \mathbb{E}_0^{\mathbf{x}}\left[\int \exp\left\{-\frac{1}{2}\int_0^{2\beta} U(\mathbf{w}_s)\, ds\right\} \delta(\mathbf{w}_{2\beta} - \mathbf{y})\, f(\mathbf{y})\, d\mathbf{y}\right] \\
&= \mathbb{E}_0^{\mathbf{x}}\left[\exp\left\{-\frac{1}{2}\int_0^{2\beta} U(\mathbf{w}_s)\, ds\right\} f(\mathbf{w}_{2\beta})\right] \\
&= e^{-\beta H} f(\mathbf{x}).
\end{aligned}$$

where the last step follows from proposition E.1.1. ∎

E.3 $\mathrm{Tr}(e^{-\beta H})$ using Brownian bridges

Proposition E.3.1. *The trace may be computed using Brownian bridges as follows:*

$$\mathrm{Tr}\left(e^{-\beta H}\right) = g_{2\beta}(0) \int \mathbb{E}_{0,2\beta}^{\mathbf{x},\mathbf{x}}\left[\exp\left\{-\frac{1}{2}\int_0^{2\beta} U(\mathbf{w}_s)\, ds\right\}\right] d\mathbf{x}.$$

Proof. Using proposition C.3.1, we have

$$\mathrm{Tr}\left(e^{-\beta H}\right) = \int G_{2\beta,U}(\mathbf{x},\mathbf{x})\, d\mathbf{x};$$

proposition E.2.1 gives us an expression for $G(\mathbf{x},\mathbf{y})$. Setting $\mathbf{y} = \mathbf{x}$ in equation E.2.3, we have

$$\mathrm{Tr}\left(e^{-\beta H}\right) = \int \mathbb{E}_0^{\mathbf{x}}\left[\exp\left\{-\frac{1}{2}\int_0^{2\beta} U(\mathbf{w}_s)\, ds\right\} \delta(\mathbf{w}_{2\beta} - \mathbf{x})\right] d\mathbf{x}.$$

Using proposition D.5.3, we may convert this expectation over Brownian motion into an expectation over Brownian bridges:

$$\mathrm{Tr}\left(e^{-\beta H}\right) = g_{2\beta}(0) \int \mathbb{E}_{0,2\beta}^{\mathbf{x},\mathbf{x}}\left[\exp\left\{-\frac{1}{2}\int_0^{2\beta} U(\mathbf{w}_s)\, ds\right\}\right] d\mathbf{x}.$$

∎

Remark E.3.2. Using definition D.4.5, we may match the notation of [BU07] and [U07]:

$$\operatorname{Tr}\left(e^{-\beta H}\right) = \int d\mathbf{x} \int d\mathbf{W}^{2\beta}_{\mathbf{x}\mathbf{x}}(\mathbf{w}) \, \exp\left\{-\frac{1}{2}\int_0^{2\beta} U(\mathbf{w}_s)\, ds\right\}.$$

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