Remarks on interacting spatial permutations and the Bose gas

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Overview

I exposit Daniel Ueltschi's 2007 paper [U07] *The model of interacting spatial permutations and its relation to the Bose gas* (Qmath 10 proceedings, Romania, Sep. 2007). Also of interest: [GRU], [BU07], [BU08].

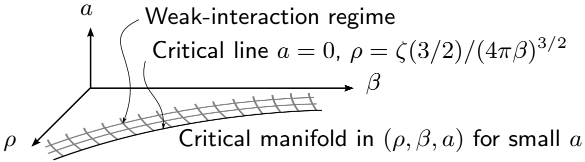
- Problem: determine the effects of interparticle interactions on the critical temperature of Bose-Einstein condensation.
- We begin with a Hamiltonian H for particles with two-body interactions.
- Using a multi-body Feynman-Kac approach involving permutation symmetry of bosonic wave functions, one obtains a Hamiltonian H_P 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.
- Properties of random-cycle models are discussed.
- A simplified two-cycle-interaction model permits analytical determination of the shift in critical temperature.

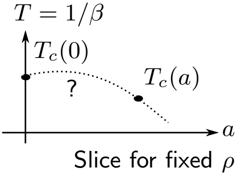
Historical context

Historical context

- Theory: Bose and Einstein (1924): quantum statistics of photons; condensation of non-interacting particles (macroscopic occupation of the ground state of the external potential); critical temperature. Feynman (1953): long permutation cycles should correspond to BEC. Sütő (1993, 2002): BEC implies long cycles in the non-ideal gas; converse for the ideal gas only.
- Experiment: Onnes (1908) liquefied helium. London (1938): drew a connection with BEC but the interactions are strong. Cornell and Wieman (1995): BEC of weakly interacting rubidium gas.
- Shift in critical temperature: The $a = 0$ critical line of the (ρ, β, a) manifold is well understood; off $a = 0$ less is known. Interactions ultimately decrease $T_c^{(a)}$, but for small a, physicists expect

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

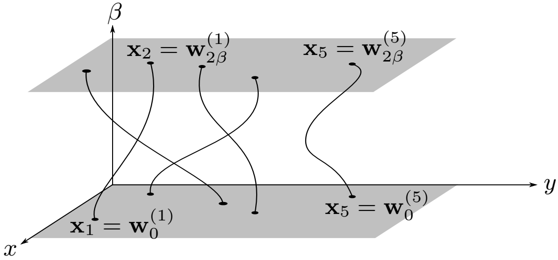




Historical context

- 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*: $c = 1.32$

Bosonic Feynman-Kac formulas



Bosonic Feynman-Kac formulas

We use the canonical partition function as the vehicle for the following transformation:

$$\text{Particle Hamiltonian} \longrightarrow \text{partition function} \longrightarrow \text{permuation Hamiltonian.}$$

A bosonic Feynman-Kac formula effects the transformation in the middle step. 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. U is a hard-core potential of radius a. The pair-interaction Hamiltonian is

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

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

Bosonic Feynman-Kac formulas

Symmetrizing the partition function ($e^{-\beta H}$ is bounded and compact, but this fact is not needed) yields

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

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,

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

Steps to develop a bosonic Feynman-Kac formula:

- Interpret $e^{-\beta H} M_\pi$ as an expectation over Brownian motions, as in the single-particle case.
- Write $e^{-\beta H} M_\pi$ as an integral operator, and find the kernel.
- Compute $\mathrm{Tr}\,(e^{-\beta H} M_\pi)$ in terms of Brownian bridges.
- Sum over $\pi \in \mathcal{S}_N$ to obtain $Z = \mathrm{Tr}_{L^2_{\mathrm{sym}}}(e^{-\beta H})$; define e^{-H_P}.
- Decouple the non-interacting from the interacting terms in the permutation Hamiltonian H_P, so that we may write $e^{-H_P^{(0)}(\mathbf{X},\pi) - H_P^{(1)}(\mathbf{X},\pi)}$.
- Drop all but 2-jump interactions; find the logarithm of $e^{-H_P^{(1)}(\mathbf{X},\pi)}$.

Bosonic Feynman-Kac formulas: $e^{-\beta H} M_\pi$ as expectation

Proposition: With H as above, $e^{-\beta H} f(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)})$ is

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

Proof: Using the Trotter product formula, namely $e^{\beta(A+B)} = \lim_{n\to\infty} \left(e^{\beta A/n} e^{\beta B/n}\right)^n$ with $A = \sum_{i=1}^N \nabla_i^2 \quad \text{and} \quad B = -\sum_{i<j} U(\mathbf{x}_i - \mathbf{x}_j)$, $e^{-\beta H} f(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)})$ is

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

Write $e^{\frac{\beta}{n} \sum_i \nabla_i^2}$ as an integral operator ($\sum_i \nabla_i^2$ is an (Nd)-dimensional Laplacian and $e^{\alpha \nabla^2} f = g_{2\alpha} * f$), and put $\mathbf{Z}^{(k)} = (\mathbf{z}_1^{(k)}, \ldots, \mathbf{z}_N^{(k)})$. Then $e^{-\beta H} f(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)})$ is

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

Bosonic Feynman-Kac formulas: $e^{-\beta H} M_\pi$ as expectation

We recognize an integrand as in the Brownian-motion appendix of my paper, with $\beta_k = 2k\beta/n$, so we can write

$$\lim_{n\to\infty} \int_{\mathbb{R}^{Ndn}} g_{2\beta/n}\left(\mathbf{X} - \mathbf{Z}^{(1)}\right) \cdots g_{2\beta/n}\left(\mathbf{Z}^{(n-1)} - \mathbf{Z}^{(n)}\right)$$
$$e^{\frac{2\beta}{n}\left(-\frac{1}{2}\right)\sum_{i<j}\sum_{k=1}^{n} U\left(\mathbf{z}_i^{(k)} - \mathbf{z}_j^{(k)}\right)} f(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)})\, d\mathbf{Z}^{(1)} \cdots d\mathbf{Z}^{(n)}$$
$$= \mathbb{E}_0^{\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(N)}}\left[e^{-\frac{1}{2}\sum_{i<j}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds} f\left(\mathbf{w}_{2\beta}^{(1)}, \ldots, \mathbf{w}_{2\beta}^{(N)}\right)\right].$$

□

Bosonic Feynman-Kac formulas: $e^{-\beta H} M_\pi$ as an integral operator

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

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

where

$$G_{2\beta,U}(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)}, \mathbf{y}_1, \ldots, \mathbf{y}_N) = \mathbb{E}_0^{\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)}} \left[\exp\left\{ -\frac{1}{2} \sum_{i<j} \int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds \right\} \prod_{i=1}^N \delta\left(\mathbf{w}_\beta^{(i)} - \mathbf{y}^{(i)}\right) \right]. \tag{3}$$

Proof: Insert equation 3 into the right-hand side of 2, interchange expectation and integral, and integrate out the delta function. □

Bosonic Feynman-Kac formulas: Lemma for operator trace

Lemma: 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: Let $\{\phi_j\}$ be a (countable) basis for the Hilbert space. Then

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

□

Bosonic Feynman-Kac formulas: $\mathrm{Tr}\,(e^{-\beta H} M_\pi)$ using Brownian bridges

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

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

Proof: Using the proposition above, 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 3 gives us an expression for G. Then

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

As justified in my paper, we may convert this expectation over Brownian motion into an expectation over Brownian bridges to obtain

$$\mathrm{Tr}\,(e^{-\beta H} M_\pi) =$$

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

The definition of the $d\mathbf{W}$ notation finishes the proof. □

Bosonic Feynman-Kac formulas: Sum over $\pi \in \mathcal{S}_N$

Applying the proposition, we now continue our plan by summing over all permutations:

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

Notationally, we may split this up as

$$\begin{aligned}\mathrm{Tr}_{\,L^2_{\mathrm{sym}}}(e^{-\beta H}) &= \frac{1}{N!} \int d\mathbf{X} \sum_{\pi\in\mathcal{S}_N} e^{-H_P(\mathbf{X},\pi)} \\ e^{-H_P(\mathbf{X},\pi)} &= \left[\prod_{k=1}^{N} \int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}} \left(\mathbf{w}^{(k)}\right)\right] e^{-\frac{1}{2}\sum_{i<j}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)}-\mathbf{w}_s^{(j)}\right)\,ds}.\end{aligned} \tag{4}$$

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.

Bosonic Feynman-Kac formulas: Interacting and non-interacting terms

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

Since $\int d\mathbf{W}_{0,2\beta}^{\mathbf{x}_k,\mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)(1) = g_{2\beta}(\mathbf{x}_k - \mathbf{x}_{\pi(k)}) = \frac{e^{-\frac{1}{4\beta}\|\mathbf{x}_k - \mathbf{x}_{\pi(k)}\|^2}}{(4\pi\beta)^{d/2}}$, we have

$$e^{-H_P(\mathbf{X},\pi)} = \frac{e^{-H_P^{(0)}(\mathbf{X},\pi)}}{(4\pi\beta)^{dN/2}} \quad \text{where} \quad H_P^{(0)}(\mathbf{X},\pi) = \frac{1}{4\beta}\sum_{k=1}^N \|\mathbf{x}_k - \mathbf{x}_{\pi(k)}\|^2. \tag{5}$$

(We ignore the prefactor in equation 5 since it cancels out in the computation of expectations of random variables.) A key point: the β in a permutation Hamiltonian is indeed reciprocated — in contrast to our experience with particle Hamiltonians.

Removing the $U \equiv 0$ assumption, equation 4 is

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

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

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

Bosonic Feynman-Kac formulas: Organize $e^{-H_P^{(1)}}$ by m-jump interactions

- Recall $U(\mathbf{r}) = \infty$ for $\mathbf{r} \le a$, else 0. If $\mathbf{w}_i$ and $\mathbf{w}_j$ do (resp. do not) come within radius a of one another at any Feynman time between 0 and 2β, $\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds = +\infty$ (resp. 0) and $e^{-\frac{1}{2}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds}$ is 0 (resp. 1).
- Shorthand: $\int_k := d\hat{\mathbf{W}}_{0,2\beta}^{\mathbf{x}_k, \mathbf{x}_{\pi(k)}}\left(\mathbf{w}^{(k)}\right)$. Also: $\Upsilon_{ij} := 1 - e^{-\frac{1}{2}\int_0^{2\beta} U\left(\mathbf{w}_s^{(i)} - \mathbf{w}_s^{(j)}\right) ds}$.
- Recall that $\int e^{\int_0^{2\beta} f(\mathbf{w}_s)\, ds}\, d\mathbf{W}_{0,2\beta}^{\mathbf{x},\mathbf{y}}(\mathbf{w}) := \mathbb{E}_{0,2\beta}^{\mathbf{x},\mathbf{y}}\left[e^{\int_0^{2\beta} f(\mathbf{w}_s)\, ds}\right]$. With N permutation jumps and $N(N-1)/2$ distinct jump pairs, $e^{-H_P^{(1)}(\mathbf{X},\pi)} = \left[\prod_{k=1}^N \int_k\right] \prod_{i<j} (1 - \Upsilon_{ij})$ is the probability that all pairs avoid one another.
- $N = 3$ example: $e^{-H_P^{(1)}(\mathbf{X},\pi)}$ is
$$\left[\int_1 \int_2 \int_3\right] (\underbrace{1}_{m=0} - \underbrace{(\Upsilon_{12} + \Upsilon_{13} + \Upsilon_{23})}_{m=1} + \underbrace{(\Upsilon_{12}\Upsilon_{13} + \Upsilon_{12}\Upsilon_{23} + \Upsilon_{13}\Upsilon_{23})}_{m=2} - \underbrace{\Upsilon_{12}\Upsilon_{13}\Upsilon_{23}}_{m=3}).$$
In general,
$$e^{-H_P^{(1)}(\mathbf{X},\pi)} = \left[\prod_{k=1}^N \int_k\right] \sum_{m=0}^{N(N-1)/2} (-1)^m \sum_{(i_1,j_1),\ldots,(i_m,j_m)} \prod_{\ell=1}^m \Upsilon_{i_\ell, j_\ell}.$$
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.

Bosonic Feynman-Kac formulas: Heuristic for cluster expansion

Move the integrals through the sums:

$$e^{-H_P^{(1)}(\mathbf{X},\pi)} = \sum_{m=0}^{N(N-1)/2} (-1)^m \sum_{(i_1,j_1),\ldots,(i_m,j_m)} \left[\prod_{k=1}^{N} \int_k\right] \prod_{\ell=1}^{m} \Upsilon_{i_\ell,j_\ell}.$$

For non-overlapping pairs, certainly $\left[\int_1 \int_2 \int_3 \int_4 \Upsilon_{12}\Upsilon_{34}\right] = \left[\int_1 \int_2 \Upsilon_{12}\right]\left[\int_3 \int_4 \Upsilon_{34}\right]$.

For overlapping pairs, $\left[\int_1 \int_2 \int_3 \Upsilon_{12}\Upsilon_{13}\right] \approx \left[\int_1 \int_2 \Upsilon_{12}\right]\left[\int_1 \int_3 \Upsilon_{13}\right]$ as long as the collisions between bridge pairs $1,2$ and $1,3$ are weakly correlated. (The cluster expansion simply formalizes this.)

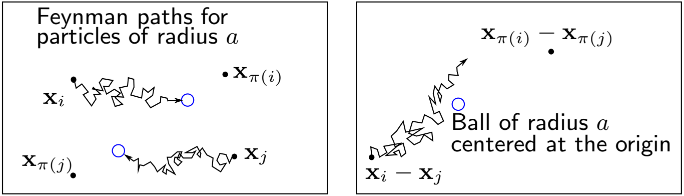
Define $V_{ij} = V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}) = \left[\int_i \int_j\right] \Upsilon_{ij}$. We assume small interactions V_{ij}, so

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

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

Bosonic Feynman-Kac formulas: 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.



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

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

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

Models of spatial permutations

Models of spatial permutations

Here we define and describe two configuration models of spatial permutations from a mathematical point of view. One may relate these models to the physics of the Bose gas, using the derivation just supplied.

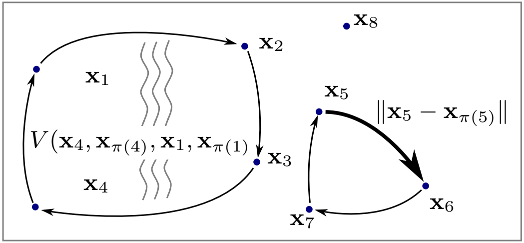


Figure: A configuration of $\mathbf{X}$ and π with $N = 8$.

Models of spatial permutations: Definitions

State space: $\Omega_{\Lambda,N} = \Lambda^N \times \mathcal{S}_N$ where $\mathcal{S}_N$ is the group of permutations of N points.

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

Contributions to the energy of a configuration $(\mathbf{X}, \pi)$:

- The sum of squares of permutation jump lengths. This discourages permutations with long jumps; permutations with many short jumps will be less strongly discouraged.
- The double sum over interactions between permutation jumps. This discourages interacting permutations.

Jump-interaction potentials: We require that V be translation-invariant i.e. for all $\mathbf{a} \in \Lambda$, and for all $\mathbf{x}, \mathbf{y} \in \Lambda$,

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

For BEC, above:

$$V(\mathbf{x}, \mathbf{y}, \mathbf{x}', \mathbf{y}') = \int d\hat{\mathbf{W}}_{0,4\beta}^{\mathbf{x}-\mathbf{x}', \mathbf{y}-\mathbf{y}'}(\mathbf{w}) \left[1 - e^{-\frac{1}{4}\int_0^{4\beta} U(\mathbf{w}_s)\, ds}\right]. \tag{6}$$

Models of spatial permutations: Definitions

Partition functions for a fixed point configuration $\mathbf{X}$ (cubic unit lattice [GRU]) and for an average over point configurations [BU07, U07], 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 on the finite set $\mathcal{S}_N$, for a fixed point configuration $\mathbf{X}$ and for an average over point configurations, respectively:

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

Heuristic for the non-interacting $V = 0$ case:

- 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 $\mathcal{S}_N$.

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

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

Models of spatial permutations: Definitions

Random variables: BEC occurs [Feynman, Sütő] iff there are infinite cycles. These depend on π, not on the geometry of $\mathbf{x}_1, \ldots, \mathbf{x}_N$. Our random variables will depend on π only.

- Define $\ell_i(\pi)$ to be the length of the permutation cycle containing the point $\mathbf{x}_i$. E.g. $\ell_1(\pi) = 4$ in figure 1.
- Let $\rho = \frac{N}{V}$, i.e. ρ is the particle density.
- For $1 \le m \le n \le N$, define

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

  This is the density of sites in cycles of specified length; it takes values between 0 and ρ.
- Related random variable:

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

  This is the fraction of sites in cycles of specified length; it takes values between 0 and 1. For figure 1, we have $f_{2,3}(\pi) = 3/8$.

Models of spatial permutations: Existence of infinite cycles

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 of [BU07], for pure interest: We 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 are in $\mathbb{R}$.

Critical density: We define ρ_c by the following formula. (This is chosen to match the critical density for BEC.)

$$\rho_c^{(0)} = \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{e^{4\beta\pi^2|\mathbf{k}|^2} - 1} = \frac{\zeta(3/2)}{(\beta_c^{(0)} 4\pi)^{3/2}}. \tag{7}$$

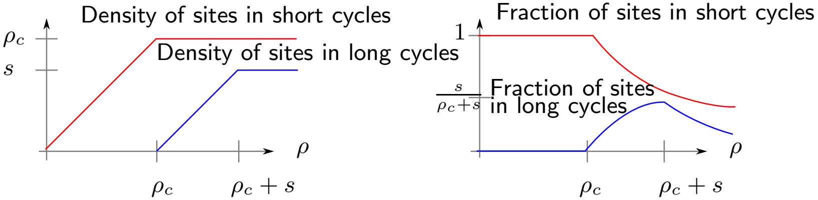
Late note: The recent paper [BU08] produces an expression for $\rho_c^{(a)}$, as well as an analogue of the following theorem for the weakly interacting ($a > 0$) case.

Models of spatial permutations: Existence of infinite cycles

Theorem ([U07], proved in section 1 of [BU07]): In the $U \equiv 0$ case, for any $0 < A < B < 1$ (nominally, A is just above 0 and B is just below 1) and any $s \geq 0$,

$$\lim_{V\to\infty} \mathbb{E}_{\Lambda,N}(f_{1,N^A}) = \begin{cases} 1, & \rho \leq \rho_c^{(0)} \\ \rho_c^{(0)}/\rho, & \rho_c^{(0)} \leq \rho \end{cases} \qquad \lim_{V\to\infty} \mathbb{E}_{\Lambda,N}(f_{N^A,N^B}) = 0$$

$$\lim_{V\to\infty} \mathbb{E}_{\Lambda,N}(f_{N^B,sN}) = \begin{cases} 0, & \rho \leq \rho_c^{(0)} \\ 1 - \rho_c^{(0)}/\rho, & \rho_c^{(0)} \leq \rho \leq s + \rho_c^{(0)} \\ s/\rho, & s + \rho_c^{(0)} \leq \rho. \end{cases} \tag{8}$$



Below $\rho_c^{(0)}$, all sites are in short cycles; as density increases past $\rho_c^{(0)}$ and $\rho_c^{(0)} + s$, a strictly positive fraction are in long cycles; asymptotically, all sites are in long cycles.

Simple model with two-cycle interactions

Simple model with two-cycle interactions: Motivation

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

- Compute it directly using simulation methods: far too expensive.
- Write this equation 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 pairs with highest collision probability (namely, two-cycles) and simplify those. This is the two-cycle-interaction model. (Notation: $i \circ\!\!-\!\pi\!-\!\!\circ j$ for a two-cycle between $\mathbf{x}_i$ and $\mathbf{x}_j$.)

For the simplified two-cycle-interaction model, unlike the fully interacting model, 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.

Simple model with two-cycle interactions: Motivation

The permutation Hamiltonian becomes

$$\begin{aligned} H_P(\mathbf{X},\pi) &= \sum_{i=1}^{N} \frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{1 \le i < j \le N} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}) \\ \approx \tilde{H}_P(\mathbf{X},\pi) &= \sum_{i=1}^{N} \frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \sum_{i \circ\!\text{-}\pi\text{-}\!\circ\, j} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}). \end{aligned} \tag{9}$$

An unpublished computation of Ueltschi and Betz shows that, for two-cycles, the jump-pair interaction (equation 6) simplifies significantly to

$$V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_{\pi(i)}, \mathbf{x}_i) = \frac{2a}{\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|} + O(a^2), \tag{10}$$

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

Key point: the Brownian bridges of equation 6 have been simplified out completely for this two-cycle-interaction model.

Simple model with two-cycle interactions: Hamiltonian with $r_2(\pi)$

Seek a Hamiltonian of the form $H_P^{(\alpha)}(\mathbf{X}, \pi) = \sum_{i=1}^N \frac{1}{4\beta} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|^2 + \alpha r_2(\pi)$. Average out the distance dependence in equation 10 (reasonable since expectations average over $\mathbf{x}$ anyway): here, all two-cycles acquire the same weight α regardless of $\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|$. It remains to connect the old parameter a with the new parameter α.

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

The chemical potential μ 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. An expression for the pressure $p^{(\alpha)}$ is obtained in [U07] using the grand-canonical partition function and occupation numbers for Fourier modes.

Proposition: The critical density for the two-cycle-interaction model is

$$\rho_c^{(\alpha)} = \left.\frac{\partial p^{(\alpha)}}{\partial \mu}\right|_{\mu=0-} = \rho_c^{(0)} - \frac{(1-e^{-\alpha})}{2^{9/2}\pi^{3/2}\beta^{3/2}}. \tag{11}$$

Proof: Differentiate equation 11 through the integral sign. □

Simple model with two-cycle interactions: Lemma for partial derivatives

Lemma: 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

$$\frac{\partial f}{\partial x}\frac{\partial x}{\partial y} + \frac{\partial f}{\partial y} = 0 \qquad\qquad \frac{\partial x}{\partial y} = -\frac{\partial f/\partial y}{\partial f/\partial x}.$$

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

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

□

Simple model with two-cycle interactions: Shift in critical temperature

Proposition: For the two-cycle model with small a,

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

Proof: We will use the lemma for $\frac{\partial a}{\partial \rho}\frac{\partial \rho}{\partial \beta}\frac{\partial \beta}{\partial a} = -1$. (Since we are working on the critical manifold, we take ρ and β to mean $\rho_c^{(a)}$ and $\beta_c^{(a)}$, respectively.)

Taylor-expand $\rho_c^{(a)}$ and use $b = 1/\zeta(3/2)\pi^{1/2}$ for brevity:

$$\frac{\rho_c^{(a)} - \rho_c^{(0)}}{\rho_c^{(0)}} = -\frac{ba}{\beta^{1/2}}; \quad a = \frac{-\rho_c^{(a)}\beta^{1/2}}{\rho_c^{(0)}b} + \frac{\beta^{1/2}}{b} \quad \text{and} \quad \frac{\partial a}{\partial \rho} = \frac{-\beta^{1/2}}{\rho_c^{(0)}b}.$$

Using equation 7 for $\rho_c^{(0)}$ and $\partial\rho_c^{(a)}/\partial\beta \approx \partial\rho_c^{(0)}/\partial\beta$,

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

From $(T_c^{(a)} - T_c^{(0)})/T_c^{(0)} = c\rho^{1/3}a$ with $\beta = 1/T$, we obtain

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

Simple model with two-cycle interactions: Shift in critical temperature

Combining the product of all three partial derivatives and using the lemma on the triple product of partial derivatives, 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, along with some algebra, gives

$$c = \frac{\rho_c^{(0)}\rho^{-1/3}\beta^{5/2}}{\beta_c^{(0)}\beta^{1/2}}\,\frac{2b\,(4\pi)^{3/2}}{3\,\zeta(3/2)} = \frac{4b\,\pi^{1/2}}{3\,\zeta(3/2)^{1/3}} \approx 0.37.$$

□

Remark: This result applies for the two-cycle model. 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 above is believed to be approximately 1.3. Further work is needed before the random-cycle model can be used to improve on the latter estimate.

Future work

Future work

Theory: Seek a computationally tractable expression for the full jump-pair interaction, perhaps involving averaging over positions as was done for the two-cycle model.

Experiments: 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.

Statistical analysis: Markov-chain Monte Carlo simulations map (N, β, ρ, a) to sample mean of $\varrho_{m,n}$. 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 do finite-size scaling.

Thank you for attending!