Spatial random permutations & infinite cycles

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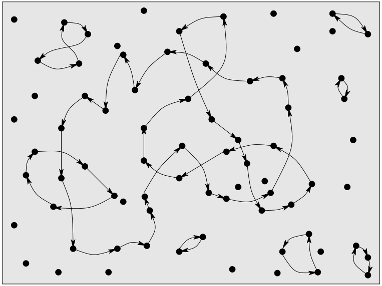
Outline

1. Spatial random permutations
2. Lattice permutations
3. Existence of infinite cycles
4. Spatial permutations and quantum bosonic systems
5. A simple model of interacting permutations

Spatial random permutations



Fix the positions $\mathbf{x} = (x_1, \dots, x_N)$

A permutation π has probability

$$\mathrm{Prob}(\pi) = \frac{1}{Y(\mathbf{x})} \exp\Big\{ -\sum_{i=1}^{N} \xi(x_i - x_{\pi(i)}) - \sum_{i<j} V\big(x_i, x_{\pi(i)}, x_j, x_{\pi(j)}\big) \Big\}$$

$$\equiv \frac{1}{Y(\mathbf{x})} \exp\big\{ -H(\mathbf{x}, \pi) \big\}$$

The main question: length of cycles
$\ell_i(\pi)$: length of cycle containing i

$$\rho_{mn}(\pi) = \frac{1}{V} \#\{i = 1, \dots, N : m \leqslant \ell_i(\pi) \leqslant n\}$$

Thermodynamic limit $N, V \to \infty$ with fixed density $\rho = N/V$

Are there infinite cycles?

Infinite volume measure

$B_{ij} = \{\pi : \pi(i) = j\}$: "cylinder set"
$\mathbf{x}$: realization of point process on $\mathbb{R}^d$. For fixed $\mathbf{x}$,

$$\nu(B_{ij}) = \lim_{\Lambda \to \mathbb{R}^d} \frac{1}{Y(\mathbf{x})} \sum_{\pi \in B_{ij} \cap \mathcal{S}_N} \mathrm{e}^{-H(\mathbf{x},\pi)}$$

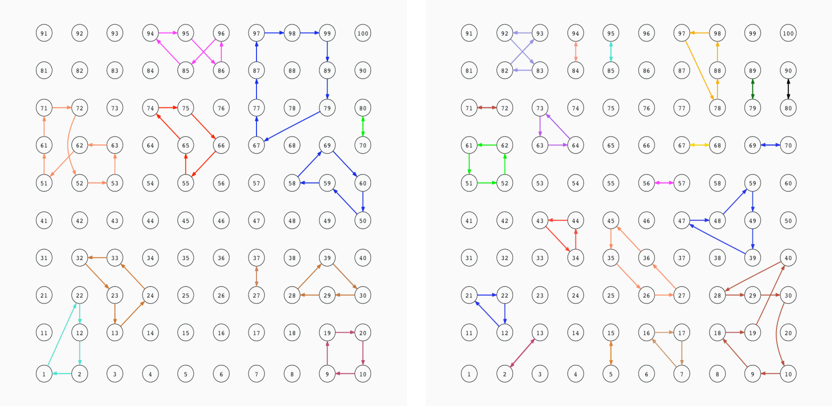
(Limit exists at least on a subseq. by compactness argument)
We need ν to be a measure on σ-algebra Σ generated by $\{B_{ij}\}$

Extension Theorem (Betz, U)
If $\sum_j \nu(B_{ij}) = 1$ ∀ fixed i , then ν extends as a probability measure on Σ

This allows to define the probability for infinite cycles to be present
Condition of the theorem clearly fulfilled if $\mathrm{e}^{-\xi(x)} = 0$ for x large
Condition not yet established for $\xi(x) = \frac{1}{4\beta}|x|^2$ and β large

Monte Carlo simulations (dimension $d = 2$)

Step ∞



(Courtesy of Daniel Gandolfo and Jean Ruiz, CNRS, Marseille)

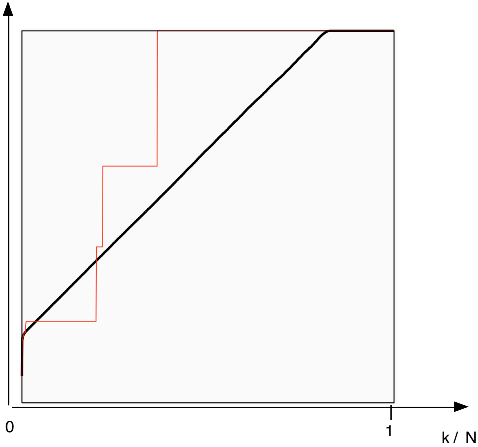
Monte Carlo simulations: cycle distribution

Simulation of a large $3d$ system in equilibrium.

Cubic lattice with $L = 30$, $\beta = 0.5$.

The graph shows the number of sites in cycles of length $\leqslant k$, as a function of k/N .
red = current
black = average

Conclusion: "infinite" cycles appear!



Gandolfo, Ruiz, U (J. Stat. Phys. 129, 2007)

Main result

State space: $\Omega_{\Lambda,N} = \Lambda^N \times \mathcal{S}_N$
Expectation of random variable includes averaging over positions:

$$E_{\Lambda,N}(\varrho_{mn}) = \frac{1}{Z} \int_{\Lambda^N} \mathrm{d}\mathbf{x} \sum_{\pi \in \mathcal{S}_N} \varrho_{mn}(\pi)\, \mathrm{e}^{-H(\mathbf{x},\pi)}\,, \qquad H(\mathbf{x},\pi) = \sum_{i=1}^{N} \xi(x_i - x_{\pi(i)})$$

Theorem (Betz, U)
There exists ρ_{c} such that, for any $0 < a < b < 1$ and any $s \geqslant 0$,

$$\text{(a)} \qquad \lim_{V\to\infty} E_{\Lambda,\rho V}(\varrho_{1,V^a}) = \begin{cases} \rho & \text{if } \rho \leqslant \rho_{\mathrm{c}} \\ \rho_{\mathrm{c}} & \text{if } \rho \geqslant \rho_{\mathrm{c}} \end{cases}$$

$$\text{(b)} \qquad \lim_{V\to\infty} E_{\Lambda,\rho V}(\varrho_{V^a,V^b}) = 0$$

$$\text{(c)} \qquad \lim_{V\to\infty} E_{\Lambda,\rho V}(\varrho_{V^b,sV}) = \begin{cases} 0 & \text{if } \rho \leqslant \rho_{\mathrm{c}} \\ s & \text{if } 0 \leqslant s \leqslant \rho - \rho_{\mathrm{c}} \\ \rho - \rho_{\mathrm{c}} & \text{if } 0 \leqslant \rho - \rho_{\mathrm{c}} \leqslant s \end{cases}$$

Critical density

The critical density is exactly known!
Let $\int \mathrm{e}^{-\xi(x)} \, \mathrm{d}x = C < \infty$, and define $\varepsilon(k)$ through

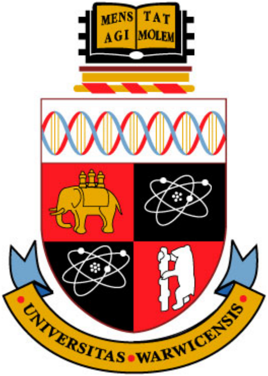
$$C \, \mathrm{e}^{-\varepsilon(k)} = \int_{\mathbb{R}^d} \mathrm{e}^{-2\pi \mathrm{i} k x} \, \mathrm{e}^{-\xi(x)} \, \mathrm{d}x$$

This assumes that $\widehat{\mathrm{e}^{-\xi}} \geqslant 0$.
Notice that $\varepsilon(0) = 0$ and $\varepsilon(k) > a|k|^2$ near $k = 0$. Then

$$\rho_{\mathrm{c}} = \int_{\mathbb{R}^d} \frac{\mathrm{d}k}{\mathrm{e}^{\varepsilon(k)} - 1}$$

Our theorem extends an earlier result of Sütő (2002) for the quantum Bose gas

Quantum Bose gas



Notice the quantum symbolism!

Bose-Einstein condensation for ideal gas

Hamiltonian for N bosons in box $\Lambda \subset \mathbb{R}^d$:

$$\mathbf{H} = -\sum_{i=1}^{N} \Delta_i \qquad \text{in } L^2_{\mathrm{sym}}(\Lambda^N)$$

In Fourier space: $\operatorname{Tr} \mathrm{e}^{-\beta \mathbf{H}} = \sum_{(n_k) : \sum_k n_k = N} \prod_{k \in \Lambda^*} \mathrm{e}^{-\beta k^2 n_k}$

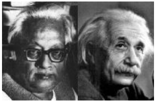
Expectation of zero mode:

$$\frac{\langle n_0 \rangle}{V} = \frac{\sum_{(n_k)} n_0 \prod_{k \in \Lambda^*} \mathrm{e}^{-\beta k^2 n_k}}{\operatorname{Tr} \mathrm{e}^{-\beta \mathbf{H}}} \longrightarrow \begin{cases} 0 & \text{if } \rho \leqslant \rho_{\mathrm{c}} \\ \rho - \rho_{\mathrm{c}} & \text{if } \rho \geqslant \rho_{\mathrm{c}} \end{cases}$$

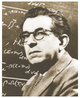
with critical density

$$\rho_{\mathrm{c}} = \frac{1}{(4\pi\beta)^{d/2}} \sum_{n \geqslant 1} n^{-\frac{d}{2}}$$

Brief history



1924-25: Bose & Einstein understand that the ideal Bose gas displays "macroscopic occupation of zero mode"

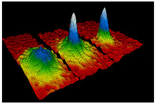


1938: F. London suggests that superfluidity is related to BEC

What does BEC mean in interacting systems?

1947: Боголюбов's microscopic theory of superfluidity
1951-53: Matsubara & Feynman consider the length of permutation cycles

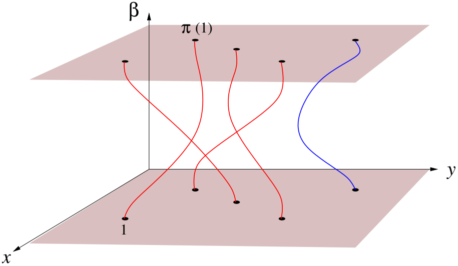
1956: Penrose & Onsager introduce correct order parameter, the "off-diagonal long-range order"



1995: BEC finally observed (Cornell, Wieman, Ketterle)

Feynman-Kac representation for the Bose gas

$$\mathbf{H} = -\sum_{i=1}^{N} \Delta_i + \sum_{i<j} U(x_i - x_j) \qquad \text{in } L^2_{\mathrm{sym}}(\Lambda^N)$$



$$\operatorname{Tr} \mathrm{e}^{-\beta \mathbf{H}} = \sum_{\pi} \frac{1}{N!} \int \mathrm{d}x_1 \dots \mathrm{d}x_N \int \mathrm{d}W^{2\beta}_{x_1 x_{\pi(1)}}(w_1) \dots \mathrm{d}W^{2\beta}_{x_N x_{\pi(N)}}(w_N)$$

$$\exp\Big\{ -\tfrac{1}{2} \sum_{i<j} \int_0^{2\beta} U\big(w_i(s) - w_j(s)\big) \mathrm{d}s \Big\}$$

Calculation of interactions between jumps

From the Feynman-Kac representation:

$$\mathrm{Tr}\ \mathrm{e}^{-\beta \mathbf{H}} = \frac{1}{N!}\int_{\Lambda^N} \mathrm{d}\mathbf{x} \sum_{\pi} \mathrm{e}^{-H(\mathbf{x},\pi)}$$

with

$$\mathrm{e}^{-H(\mathbf{x},\pi)} = \Big[\prod_{i=1}^{N} \int \mathrm{d}W^{2\beta}_{x_i x_{\pi(i)}}(\omega_i)\Big] \exp\Big\{-\tfrac{1}{2}\sum_{i<j}\int_0^{2\beta} U\big(w_i(s)-w_j(s)\big)\mathrm{d}s\Big\}$$

We introduce the normalised measure $\mathrm{d}\widehat{W}^{\beta}_{xy}$ so as to extract the Gaussian weights. Then we expand using a cluster expansion

$$\begin{aligned}
\mathrm{e}^{-H(\mathbf{x},\pi)} &= \prod_{i=1}^{N} \mathrm{e}^{-\frac{1}{4\beta}|x_i - x_{\pi(i)}|^2} \Big[\prod_{i=1}^{N} \int \mathrm{d}\widehat{W}^{2\beta}_{x_i x_{\pi(i)}}(\omega_i)\Big]\, \mathrm{e}^{-\frac12 \sum \int_0^{2\beta} U(\omega_i(s)-\omega_j(s))\mathrm{d}s} \\
&= \mathrm{e}^{-H^{(0)}(\mathbf{x},\pi)} \Big[\prod_{i=1}^{N} \int \mathrm{d}\widehat{W}^{2\beta}_{x_i x_{\pi(i)}}(\omega_i)\Big] \prod_{b=\{i,j\}} \big(1 - \Upsilon(\omega_b)\big) \\
&= \mathrm{e}^{-H^{(0)}(\mathbf{x},\pi)} \Big[\prod_{i=1}^{N} \int \mathrm{d}\widehat{W}^{2\beta}_{x_i x_{\pi(i)}}(\omega_i)\Big] \sum_{k \geqslant 0} (-1)^k \sum_{\{b_1,\dots,b_k\}} \prod_{m=1}^{k} \Upsilon(\omega_{b_m})
\end{aligned}$$

For small interactions: Υ is small, the typical k is a small fraction of the volume, and the bonds are sparse and do not overlap. In which case

$$\Big[\prod_{i=1}^{N} \int \mathrm{d}\widehat{W}^{2\beta}_{x_i x_{\pi(i)}}(\omega_i)\Big] \prod_{m=1}^{k} \Upsilon(\omega_{b_m}) = \prod_{m=1}^{k} V(x_{i_m}, x_{\pi(i_m)}, x_{j_m}, x_{\pi(j_m)})$$

with $V(x,y,x',y') = \int \mathrm{d}\widehat{W}^{2\beta}_{xy}(\omega) \int \mathrm{d}\widehat{W}^{2\beta}_{x'y'}(\omega')\Upsilon(\omega - \omega')$

This is the two-body jump interaction between jumps $x \mapsto y$ and $x' \mapsto y'$!

Model of spatial permutations with interactions

The interaction above can be simplified further:

$$V(x,y,x',y') = \int \Big[1 - \mathrm{e}^{-\frac{1}{4}\int_0^{4\beta} U(\omega(s))\mathrm{d}s}\Big] \mathrm{d}\widehat{W}^{4\beta}_{x-x',y-y'}(\omega)$$

If U is hard core potential with radius a , $V(\cdot)$ is probability that Brownian bridge from $x - x'$ to $y - y'$ hits ball of radius a centered at origin

Is there a simple expression involving special functions???

The Hamiltonian, exact to lowest order in a :

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

In need of Monte-Carlo simulations

Bose-Einstein condensation

Conjecture: Critical temperature for infinite cycles $\equiv$ critical temperature for Bose-Einstein condensation (*in* $d = 3$ *, if interactions are weak*)

A major question: Do interactions enhance or discourage Bose-Einstein condensation?

Here: repulsive interactions only; characterized by their scattering length a

Many studies, mostly by path integral Monte-Carlo techniques

Effects of interactions on critical temperature

$\mathbf{H} = -\sum_{i=1}^{N} \Delta_i + \sum_{i<j} U(x_i - x_j)$, $U(x) \geqslant 0$ with scattering length a

1964 Huang: $\frac{\Delta T_{\rm c}}{T_{\rm c}} \sim (a\rho^{1/3})^{3/2}$, increases

1971 Fetter & Walecka: $\frac{\Delta T_{\rm c}}{T_{\rm c}}$ decreases

1982 Toyoda: $\frac{\Delta T_{\rm c}}{T_{\rm c}}$ decreases

1992 Stoof: $\frac{\Delta T_{\rm c}}{T_{\rm c}} = c\, a\rho^{1/3} + o(a\rho^{1/3}), \quad c > 0$

1996 Bijlsma & Stoof: $c = 4.66$

1997 Grüter, Ceperley, Laloë: $c = 0.34$

1999 Holzmann, Grüter, Laloë: $c = 0.7$; Holzmann, Krauth: $c = 2.3$; Baym et. al.: $c = 2.9$

2000 Reppy et. al.: $c = 5.1$

2001 Kashurnikov, Prokof'ev, Svistunov: $c = 1.29$; Arnold, Moore: $c = 1.32$

2004 Kastening: $c = 1.27$; Nho, Landau: $c = 1.32$

Simplified model ($d = 3$)

$$H(\mathbf{x},\pi) = \frac{1}{4\beta}\sum_{i=1}^{N} \left|x_i - x_{\pi(i)}\right|^2 + \sum_{i<j} V\big(x_i, x_{\pi(i)}, x_j, x_{\pi(j)}\big)$$

$$\tilde{H}(\mathbf{x},\pi) = \qquad + \sum_{\substack{i<j \\ \pi(i)=j,\pi(j)=i}} V\big(x_i, x_{\pi(i)}, x_j, x_{\pi(j)}\big)$$

$$H^{(\alpha)}(\mathbf{x},\pi) = \qquad + \alpha N_2(\pi)$$

Recall that $E_{\Lambda,N}(\varrho_{mn}) = \frac{1}{Z} \sum_{\pi} \varrho_{mn}(\pi) \int_{\Lambda^N} \mathrm{d}\mathbf{x}\ \mathrm{e}^{-\tilde{H}(\mathbf{x},\pi)}$

The substitution $\tilde{H} \mapsto H^{(\alpha)}$ is exact, provided that for any π

$$\int_{\Lambda^N} \mathrm{d}\mathbf{x}\ \mathrm{e}^{-\tilde{H}(\mathbf{x},\pi)} = \int_{\Lambda^N} \mathrm{d}\mathbf{x}\ \mathrm{e}^{-H^{(\alpha)}(\mathbf{x},\pi)}$$

Everything factorizes according to cycles. The equation reduces to

$$\int_{\Lambda^2} \mathrm{d}x_1 \mathrm{d}x_2\, \mathrm{e}^{-\frac{1}{2\beta}|x_1-x_2|^2 - V(x_1,x_2,x_2,x_1)} = \int_{\Lambda^2} \mathrm{d}x_1 \mathrm{d}x_2\, \mathrm{e}^{-\frac{1}{2\beta}|x_1-x_2|^2 - \alpha}$$

We find $\alpha = (\frac{8}{\pi\beta})^{1/2} a + O(a^2)$

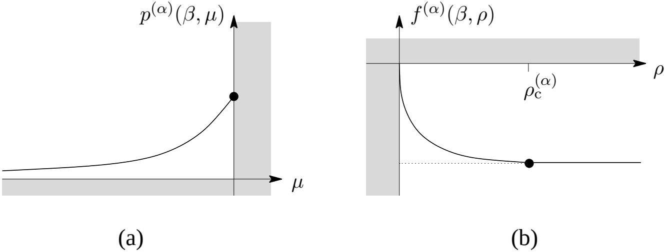
Pressure of simple model

The pressure $p^{(\alpha)}(\beta,\mu)$ can be exactly computed. One gets

$$p^{(\alpha)}(\beta,\mu) = -\frac{1}{\beta}\int_{\mathbb{R}^3} \log\bigl(1 - \mathrm{e}^{-\beta(|2\pi k|^2-\mu)}\bigr)\mathrm{d}k - \frac{\mathrm{e}^{2\beta\mu}}{2^{11/2}\pi^{3/2}\beta^{5/2}}\bigl(1 - \mathrm{e}^{-\alpha}\bigr)$$

Free energy obtained by Legendre transform:

$$f^{(\alpha)}(\beta,\rho) = \sup_{\mu}\bigl[\rho\mu - p^{(\alpha)}(\beta,\mu)\bigr]$$



Critical temperature

The critical density:

$$\rho_{\mathrm{c}}^{(\alpha)} = \frac{\partial p^{(\alpha)}}{\partial \mu}\Big|_{\mu=0-} = \rho_{\mathrm{c}}^{(0)} - \frac{1}{2^{9/2}\pi^{3/2}\beta^{3/2}}(1 - \mathrm{e}^{-\alpha})$$

Using $\alpha = (\frac{8}{\pi\beta})^{1/2} a$, we find

$$\frac{T_{\mathrm{c}}^{(a)} - T_{\mathrm{c}}^{(0)}}{T_{\mathrm{c}}^{(0)}} = 0.37\,\rho^{1/3} a + o(a)$$

To be compared with expected constant 1.3

Theorem (Betz, U)

For any $0 < b < 1$,

$$\lim_{V\to\infty} E_{\Lambda,\rho V}(\varrho_{V^b,\rho V}) \geqslant \rho - \frac{4}{(1+\mathrm{e}^{-\alpha})^2}\rho_{\mathrm{c}}^{(0)}$$

Conclusion

- An interesting probabilistic model: random permutations with spatial structure
- Occurrence of infinite, macroscopic cycles; proved in “one-body” model
- Relation with Bose-Einstein condensation, through Feynman-Kac representation
- Much work to do: existence of infinite domain measure, typical behavior of cycle random variables
- Effects of interactions on occurrence of infinite cycles