

The critical temperature of the dilute Bose gas: A tentative exact approach using spatial permutations

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Joint work with **VOLKER BETZ** (University of Warwick)

Bose-Einstein condensation for ideal gas

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

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

In Fourier space: $\text{Tr } e^{-\beta \mathbf{H}} = \sum_{(n_k): \sum_k n_k = N} \prod_{k \in \Lambda^*} e^{-\beta k^2 n_k}$, $\Lambda^* = \frac{2\pi}{L} \mathbb{Z}^d$

Expectation of zero mode:

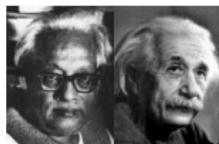
$$\frac{\langle n_0 \rangle}{V} = \frac{\sum_{(n_k)} n_0 \prod_{k \in \Lambda^*} e^{-\beta k^2 n_k}}{\text{Tr } e^{-\beta \mathbf{H}}} \longrightarrow \begin{cases} 0 & \text{if } \rho \leq \rho_c \\ \rho - \rho_c & \text{if } \rho \geq \rho_c \end{cases}$$

with critical density

$$\rho_c = \frac{\zeta\left(\frac{d}{2}\right)}{(4\pi\beta)^{d/2}}$$

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

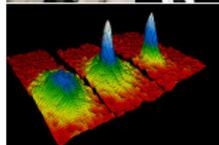


1951-53: **Matsubara & Feynman** consider the length of permutation cycles

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



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



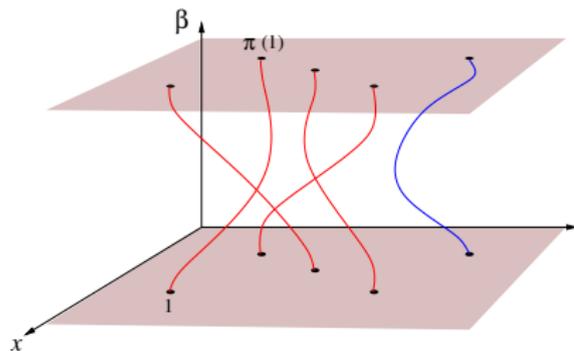
Interacting Bose gas: Feynman-Kac representation

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

U : repulsive pair potential, $N = \rho|\Lambda|$

Feynman-Kac representation of the partition function:

$$\begin{aligned} \text{Tr } e^{-\beta H} &= \frac{1}{N!} \sum_{\pi \in \mathcal{S}_N} \int dx_1 \dots dx_N \\ &\int dW_{x_1 x_{\pi(1)}}^{2\beta}(\omega_1) \dots dW_{x_N x_{\pi(N)}}^{2\beta}(\omega_N) \\ &\exp \left\{ -\frac{1}{2} \sum_{i < j} \int_0^{2\beta} U(\omega_i(s) - \omega_j(s)) ds \right\} \end{aligned}$$



Conjecture 1

CONJECTURE 1. The critical temperature for Bose-Einstein condensation is identical to the critical temperature for the occurrence of infinite cycles.

This was proved by Sütő ('93, '02) for the ideal gas ($U = 0$).

Model of “spatial random permutations”

We write $\text{Tr} e^{-\beta H} = \frac{1}{Z} \sum_{\pi \in \mathcal{S}_N} \int dx_1 \dots dx_N e^{-H_1(\mathbf{x}, \pi)}$, with

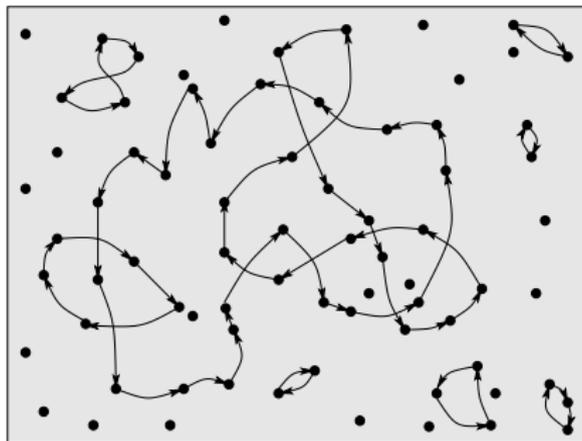
$$e^{-H_1(\mathbf{x}, \pi)} = \int dW_{x_1 x_{\pi(1)}}^{2\beta}(\omega_1) \dots dW_{x_N x_{\pi(N)}}^{2\beta}(\omega_N) \exp\left\{-\frac{1}{2} \sum_{i < j} \int_0^{2\beta} U(\omega_i(s) - \omega_j(s)) ds\right\}$$

U has scattering length a . A cluster expansion leads to $H_1 = H_2 + \mathcal{O}(a^2)$ with

$$H_2(\mathbf{x}, \pi) = \frac{1}{4\beta} \sum_{i=1}^N |x_i - x_{\pi(i)}|^2 + \sum_{i < j} V(x_i, x_{\pi(i)}, x_j, x_{\pi(j)})$$

The 2-jump interaction $V(\cdot)$ is given by the integral kernel of $e^{2\beta\Delta} - e^{2\beta(\Delta-U)}$

Spatial random permutations



$$\mathbb{E}_N(\theta) = \frac{1}{Z_N} \sum_{\pi \in \mathcal{S}_N} \int_{\Lambda^n} dx_1 \dots dx_N \theta(x, \pi) e^{-H_2(x, \pi)}$$

with

$$H_2(x, \pi) = \frac{1}{4\beta} \sum_{i=1}^N |x_i - x_{\pi(i)}|^2 + \sum_{i < j} V(x_i, x_{\pi(i)}, x_j, x_{\pi(j)}).$$

Conjecture 2

CONJECTURE 2. The critical temperature of the model H_2 is identical to that of the model H_1 , up to a correction $o(a)$.

From 2-jump interactions to cycle weights

Goal: replace the 2-jump interactions $\sum_{i<j} V_{ij}(\mathbf{x}, \pi)$ by cycle weights $\sum_{\ell \geq 1} \alpha_{\ell} r_{\ell}(\pi)$ in such a way that critical density remains identical (to lowest order)

Let θ be a random variable that depends only on the permutation, not on the positions. Its expectation can be written as

$$E(\theta) = \frac{1}{Z_2} \sum_{\pi} \theta(\pi) Z^{(\pi)} \int d\mu^{(\pi)}(\mathbf{x}) e^{-\sum_{i<j} V_{ij}(\mathbf{x}, \pi)}$$

where $\mu^{(\pi)}$ is a probability measure that depends on π , given by

$$d\mu^{(\pi)}(\mathbf{x}) = \frac{1}{Z^{(\pi)}} e^{-H_0(\mathbf{x}, \pi)} d\mathbf{x}, \quad Z^{(\pi)} = \int e^{-H_0(\mathbf{x}, \pi)} d\mathbf{x}$$

From 2-jump interactions to cycle weights

Introduce a “permutation free energy” by

$$e^{-F(\pi)} = \int d\mu^{(\pi)}(\mathbf{x}) e^{-\sum_{i<j} V_{ij}(\mathbf{x},\pi)}$$

Main idea: take the integral inside the exponential

$$e^{-F(\pi)} \approx \exp\left\{-\int d\mu^{(\pi)}(\mathbf{x}) \sum_{i<j} V_{ij}(\mathbf{x},\pi)\right\}$$

Justification: think in terms of typical positions. For given permutation, let \mathbf{y} be typical realization of measure $\mu^{(\pi)}$, and let \mathbf{z} be typical realization of measure

$$\frac{1}{\text{normalization}} e^{-H_0(\mathbf{x},\pi)} e^{-\sum_{i<j} V_{ij}(\mathbf{x},\pi)} .$$

From 2-jump interactions to cycle weights

For all macroscopic observables A we expect that

$$A(\mathbf{y}) = A(\mathbf{z}) (1 + O(a))$$

This holds in particular when macroscopic observable is $\sum_{i<j} V_{ij}(\mathbf{x}, \pi)$

We have $e^{-F(\pi)} \approx e^{-\sum_{i<j} V_{ij}(\mathbf{z}, \pi)}$.

We replace it by $e^{-F(\pi)} \approx e^{-\sum_{i<j} V_{ij}(\mathbf{y}, \pi)}$, the difference of free energies should be of order $O(a^2)$.

We get the new Hamiltonian

$$H_3(\mathbf{x}, \pi) = H_0(\mathbf{x}, \pi) + \sum_{i<j} \int V_{ij}(\mathbf{y}, \pi) d\mu^{(\pi)}(\mathbf{y}).$$

CONJECTURE 3. The critical temperature of the model H_3 is identical to that of the model H_2 , up to a correction $o(a)$.

From 2-jump interactions to cycle weights

Define the weights

$$\alpha_\ell = \sum_{i,j \in \gamma, i < j} \int V_{ij}(\mathbf{x}, \gamma) d\mu^{(\gamma)}(\mathbf{x}), \quad \gamma = (2, \dots, \ell, 1)$$

$$\alpha_{\ell, \ell'} = \frac{1}{2} \sum_{i \in \gamma, j \in \gamma'} \int V_{ij}(\mathbf{x}, \gamma \cup \gamma') d\mu^{(\gamma \cup \gamma')}(\mathbf{x}), \quad \gamma \cup \gamma' = (2, \dots, \ell, 1)(\ell + 2, \dots, \ell + \ell', \ell + 1)$$

Then

$$H_3(\mathbf{x}, \pi) = \frac{1}{4\beta} \sum_i |x_i - x_{\pi(i)}|^2 + \sum_{\ell \geq 1} (\alpha_\ell - \alpha_{\ell, \ell}) r_\ell(\pi) + \sum_{\ell, \ell' \geq 1} \alpha_{\ell, \ell'} r_\ell(\pi) r_{\ell'}(\pi)$$

where $r_\ell(\pi)$ is the number of ℓ -cycles in the permutation π

Intermission: effects of interactions on crit. temperature

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

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

Effects of interactions on critical temperature

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A partial but rigorous result:

Theorem (with Robert Seiringer, 2009)

There is no BEC when $\frac{\Delta T_c}{T_c} > 5.09 \sqrt{a\rho^{1/3}}$

Back to the cycle model for the Bose gas

$$H_3(\mathbf{x}, \pi) = \frac{1}{4\beta} \sum_i |x_i - x_{\pi(i)}|^2 + \sum_{\ell \geq 1} (\alpha_\ell - \alpha_{\ell,\ell}) r_\ell(\pi) + \sum_{\ell, \ell' \geq 1} \alpha_{\ell, \ell'} r_\ell(\pi) r_{\ell'}(\pi)$$

A computation gives

$$\alpha_{\ell, \ell'} = \frac{4\pi\beta\ell\ell'a}{|\Lambda|}$$

(to first order). Then

$$\sum_{\ell, \ell' \geq 1} \alpha_{\ell, \ell'} r_\ell(\pi) r_{\ell'}(\pi) = \frac{4\pi\beta a N^2}{|\Lambda|}$$

is constant in the canonical ensemble. This term can be dismissed!

We also get

$$\alpha_\ell = \frac{\ell a}{(4\pi\beta)^{1/2}} \sum_{j=1}^{\ell-1} \left(\frac{\ell}{j(\ell-j)} \right)^{3/2}$$

(to first order)

We have $\lim_{\ell \rightarrow \infty} \frac{\alpha_\ell}{\ell} = \frac{2\zeta(\frac{3}{2})a}{(4\pi\beta)^{1/2}}$. Define $\alpha'_\ell = \alpha_\ell - \frac{2\zeta(\frac{3}{2})a\ell}{(4\pi\beta)^{1/2}}$. Then

$$\sum_{\ell \geq 1} \alpha'_\ell r_\ell(\pi) = \sum_{\ell \geq 1} \alpha_\ell r_\ell(\pi) - \frac{2\zeta(\frac{3}{2})aN}{(4\pi\beta)^{1/2}}$$

so that both weights yield the same Gibbs distribution.

$$H_4 = \frac{1}{4\beta} \sum_i |x_i - x_{\pi(i)}|^2 + \sum_{\ell \geq 1} \alpha'_\ell r_\ell(\pi)$$

CONJECTURE 4. The critical temperature of the model H_4 is identical to that of the model H_3 , up to a correction $o(a)$.

Critical density

Since $\frac{\alpha'_\ell}{\ell} \rightarrow 0$, we have the formula for the critical density:

$$\rho_c^{(a)} = \sum_{\ell \geq 1} \frac{e^{-\alpha'_\ell}}{(4\pi\beta\ell)^{3/2}}$$

This is computed by analogy to the ideal Bose gas. Is it relevant for the occurrence of infinite cycles?

- **Sütő** proved it for $\alpha'_\ell \equiv 0$ ('93, '02)
- With **Betz**, we proved it when $\alpha'_\ell \rightarrow 0$ faster than $1/\log \ell$ ('10)

Here, one can check that $\alpha'_\ell = -\frac{6-3\gamma_{1/2}}{(4\pi\beta)^{1/2}} a (1 + O(\ell^{-1/5}))$

The weights are **negative**, and $\alpha'_\ell \not\rightarrow 0$, but we conjecture that the formula for the critical density applies nonetheless

CONJECTURE 5. The critical density of the model H_5 is given by the formula above.

Change in critical density

We get

$$\begin{aligned}\frac{\rho_c^{(a)} - \rho_c^{(0)}}{\rho_c^{(0)}} &= -\frac{2a}{(4\pi\beta)^2} \sum_{\ell \geq 1} \frac{1}{\ell^{1/2}} \left[\frac{1}{2} \sum_{j=1}^{\ell-1} \left(\frac{\ell}{j(\ell-j)} \right)^{3/2} - \zeta(3/2) \right] \\ &= +\frac{2\sqrt{\pi}}{\zeta(3/2)} a\beta^{-1/2}\end{aligned}$$

This implies that

$$\frac{T_c^{(a)} - T_c^{(0)}}{T_c^{(0)}} = -\frac{8\pi}{3\zeta(\frac{3}{2})^{4/3}} a\rho^{1/3} = -2.33 a\rho^{1/3}$$

This contradicts the consensus of the physics literature!!!
(Constant is +1.3)

A verification: the free energy

In Oberwolfach, an excellent suggestion of **ROBERT SEIRINGER**: calculate the **free energy** of the simplified model, and compare it with the one of the dilute Bose gas, which is known explicitly (**Seiringer '08**, **Yin '09**)

We have that

$$f(\beta, \rho) = 4\pi a\rho(\rho + 2\rho_c) + \hat{f}(\beta, \rho),$$

with \hat{f} the free energy of the model with weights $\{\alpha'_\ell\}$. We find

$$\hat{f}(\beta, \rho) = f^{(0)}(\beta, \rho) + \begin{cases} 4\pi a\rho(\rho - 2\rho_c) & \text{if } \rho \leq \rho_c \\ -4\pi a\rho_c^2 & \text{if } \rho \geq \rho_c \end{cases}$$

Then one recovers the free energy of the dilute Bose gas:

$$f(\beta, \rho) = f^{(0)}(\beta, \rho) + 4\pi a[2\rho^2 - (\rho - \rho_c)_+^2]$$

(All identities are valid to first order in $a\rho^{1/3}$ only)

Conclusion

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- We neglect the fluctuations of a certain macroscopic observable
- The formula for the critical density has not been rigorously established for our weights
- Despite these caveats, our method should give the right critical temperature. The discrepancy with the physics literature is puzzling.

THANK YOU!