The Critical Temperature of Dilute Bose Gases

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Joint work with R. Seiringer (Princeton University)
Program

1. Bose-Einstein condensation
2. Effects of interactions on critical temperature
3. The density bound
4. Feynman-Kac representation
5. Estimates of integral kernels
Quantum many-body system

$N$ particles in box $\Lambda \subset \mathbb{R}^d$
State space is Hilbert space $\bigotimes_{i=1}^N L^2(\Lambda) \cong L^2(\Lambda^N)$

Hamiltonian given by Schrödinger operator

$$H = - \sum_{i=1}^N \Delta_i + \sum_{i<j} U(x_i - x_j)$$

with $\Delta_i = \sum_{\nu=1}^d \frac{\partial^2}{\partial x_{i,\nu}^2}$ the Laplacian and $U \geq 0$ a function with compact support. (Periodic boundary conditions)

System of identical bosons: state space is $L^2_{\text{sym}}(\Lambda^N)$, the space of $L^2$ functions that are symmetric with respect to $N$ arguments
Bose-Einstein condensation

Understood by Einstein in 1924 for the ideal gas (no interactions)

Fourier space: $\Lambda_* = \frac{1}{L} \mathbb{Z}^d$

$$\ell^2_{\text{sym}}(\Lambda^N_*) \cong \text{span} \left\{ \mathbf{n} \in \mathbb{N}^{\Lambda_*} : \sum_{k \in \Lambda_*} n_k = N \right\}$$

The space spanned by occupation numbers.

Hamiltonian is now a multiplication operator:

$$H|\mathbf{n}\rangle = \sum_{k \in \Lambda_*} 4\pi^2 k^2 n_k |\mathbf{n}\rangle$$
Bose-Einstein condensation

Statistical mechanics: Expectation of observables (i.e. self-adjoint operators on state space) is defined by

$$\langle A \rangle = \frac{\text{Tr } A e^{-\beta H}}{\text{Tr } e^{-\beta H}}$$

where $\beta = 1/T$ is inverse temperature

Let $\rho = N/|\Lambda|$ the particle density, and consider the observable $A = \frac{n_0}{L^3}$

with $n_0 = n_{k=0}$
Bose-Einstein condensation \((d = 3)\): There is a critical density,
\[
\rho_c = \frac{\zeta(3/2)}{(4\pi\beta)^{3/2}} \quad \text{(with } \zeta(3/2) = \sum n^{-3/2} = 2.612... \text{)}
\]
such that
\[
\lim_{L,N \to \infty} \frac{\text{Tr} \frac{n_0}{L^3} e^{-\beta H}}{\text{Tr} e^{-\beta H}} = \begin{cases} 
0 & \text{if } \rho \leq \rho_c \\
\rho - \rho_c & \text{if } \rho \geq \rho_c 
\end{cases}
\]

Alternatively, there is a critical temperature \(T_c = 4\pi(\rho/\zeta(3/2))^{2/3}\)

Physical manifestations of BEC: superfluidity, superconductivity. Also present in optics and in turbulence.
The **scattering length** $a$ is a number that characterizes the potential function for dilute quantum systems. Hard core potentials: $a$ is the radius of the hard core. For integrable potentials, $a_0 = \frac{1}{8\pi} \int U(x)dx$ is the first Born approximation to the scattering length. Otherwise, let $R$ be larger than the radius $R_0$ of $U$, and consider the energy functional

$$
\mathcal{E}_R(\psi) = \int_{B_R} \left( |\nabla \psi(x)|^2 + U(x)|\psi(x)|^2 \right) dx
$$

with $B_R$ the ball of radius $R$ in $\mathbb{R}^3$. Let $\psi_0$ be the minimizer of $\mathcal{E}_R$ over $H^1$ functions that satisfy the boundary condition $\psi_0(x) = 1$ when $|x| = R$. $\psi_0$ is spherically symmetric and it satisfies the equation

$$
-\Delta \psi_0(x) + U(x)\psi_0(x) = 0
$$

For $R_0 \leq |x| \leq R$, we have

$$
\psi_0(x) = \frac{1 - a/|x|}{1 - a/R}
$$

for a number $a$, the **scattering length**. Cf Lieb, Seiringer, Solovej, Yngvason, *The Mathematics of the Bose Gas and its Condensation*
Effects of particle interactions on critical temperature

\[ H = - \sum_{i=1}^{N} \Delta_i + \sum_{i<j} U(x_i - x_j) , \quad U(x) \geq 0 \text{ with scattering length } a \]
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2000 Reppy et. al.: \( c = 5.1 \)
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A partial but rigorous result:

**Theorem** (with R. Seiringer, 2009)

*There is no BEC when* \( \frac{\Delta T_c}{T_c} > 5.09 \sqrt{a \rho^{1/3}} \)
Grand-canonical ensemble

(Laplace transform with respect to $N$)

$$\langle A \rangle = \frac{1}{Z} \sum_{N \geq 0} z^N \text{Tr}_{L^2_{\text{sym}}(\Lambda^N)} A e^{-\beta H}$$

Parameters are $\beta, \Lambda, z$ ($z$ : fugacity)

The density is given by $\rho(z) = \langle N \rangle / |A|$ ; $\rho(z)$ is increasing in $z$

FACT: There is no Bose-Einstein condensation when $z < 1$. This holds for any repulsive interaction (see Bratteli-Robinson)

We need information on $\rho(z)$

Known: $\rho^{(0)}(z) = (4\pi\beta)^{-3/2} \sum_{n \geq 1} z^n / n^{3/2}$

**Theorem** (with R. Seiringer, 2009)

$$\rho(z) \geq \rho^{(0)}(z) - C \frac{a}{\beta^2 \sqrt{-\log z}}$$
The density bound

Illustration

\[
\rho \sim a \beta^{-2}
\]

\[
\rho \sim a^{1/2} \beta^{-7/4}
\]

\[
\rho^{(0)} < \rho < \rho_c
\]

\[
\rho_c^{(0)} < \rho_c < \rho_0
\]

\[
0 < z_0 < 1 < z_c
\]
Feynman-Kac representation for the Bose gas

◊ Allows to get suitable bounds, by dropping certain terms

Let $W_{xy}^t$ be the Wiener measure for the Brownian bridge between $x$ and $y$ in time $t$. Let $\omega = (x, k, \omega)$ stand for a “winding path” from $x$ to $x$ in time $2\beta k$, and

$$V(\omega) = \frac{1}{2} \sum_{0 \leq \ell < m \leq k-1} \int_0^{2\beta} U(\omega(2\ell \beta + s) - \omega(2m \beta + s)) \, ds$$

Define the measure $\mu$ by

$$\int d\mu(\omega) \cdots \equiv \sum_{k \geq 1} \frac{z^k}{k} \int_{\Lambda} dx \int dW_{xx}^{2\beta k}(\omega) \, e^{-V(\omega)} \cdots$$
Feynman-Kac representation for the Bose gas

The partition function $Z = \sum_{N \geq 0} z^N \text{Tr} \ e^{-\beta H}$ is then given by

$$Z = \sum_{n \geq 0} \frac{1}{n!} \int d\mu(\omega_1) \ldots d\mu(\omega_n) e^{-\sum_{1 \leq i < j \leq n} V(\omega_i, \omega_j)}$$

where the two-path interaction is

$$V(\omega, \omega') = \frac{1}{2} \sum_{\ell=0}^{k-1} \sum_{\ell'=0}^{k'-1} \int_0^{2\beta} U(\omega(2\beta \ell + s) - \omega'(2\beta \ell' + s)) ds$$
Feynman-Kac representation

Space-time picture
Feynman-Kac representation for the Bose gas

Similarly, the density \( \rho(z) \) is given by

\[
\rho(z) = \frac{1}{|\Lambda|Z} \sum_{n \geq 1} \frac{1}{(n-1)!} \int d\mu(\omega_1) k_1 \int d\mu(\omega_2) \ldots \int d\mu(\omega_n) e^{-\sum_{1 \leq i < j \leq n} V(\omega_i, \omega_j)}
\]

Since \( V \geq 0 \), one immediately gets the upper bound

\[
\rho(z) \leq \frac{1}{|\Lambda|} \int d\mu(\omega_1) k_1 \leq \rho(0)(z)
\]

For the lower bound, one uses \( e^{-\sum_i V_i} \geq 1 - \sum_i (1 - e^{-V_i}) \) in various ways, to obtain

\[
\rho(z) \geq \rho(0)(z) - \frac{C}{\beta^3 \sqrt{-\log z}} \int K(x,y) dx dy
\]

where \( K(x,y) \equiv \int \left[ 1 - e^{-\frac{1}{4} \int_0^4 \beta U(\omega(s)) ds} \right] dW_{xy}^{4\beta}(\omega) \) is the integral kernel of \( e^{2\beta \Delta} - e^{\beta(2\Delta - U)} \) (Feynman-Kac formula)
Scattering estimates

It remains to study the quantity

\[ a(\beta) \equiv \frac{1}{8\pi\beta} \int K(x, y)dxdy \]

Using \(1 - e^{-u} \leq u\), we have

\[
\int K(x, y)dxdy \leq \frac{1}{4} \int_0^{4\beta} ds \int dy \int dW_{y, 0}^{4\beta}(\omega) \int dx U(\omega(s) + x)
= \beta \int U(z)dz
\]

In scattering theory, \(a_0 = \frac{1}{8\pi} \int U(z)dz\) is called the first Born approximation of the scattering length

Then \(a(\beta) \leq a_0\). OK if potential \(U\) is integrable and small in a suitable sense. One needs another method for more general potentials.
Variational principle

\[
a(\beta) = \frac{1}{8\pi} \inf_{\psi \in H^1(\mathbb{R}^d)} \left[ \int_{\mathbb{R}^d} \left( 2|\nabla \psi(x)|^2 + U(x)|1 - \psi(x)|^2 \right) dx + \frac{1}{\beta} \langle \psi | f(\beta(-2\Delta + U)) | \psi \rangle \right]
\]

where \( f \) is the decreasing function

\[
f(t) = t \frac{1 - e^{-t}}{t - 1 + e^{-t}}
\]

Notice that \( 1 \leq f \leq 2 \). The variational principle shows that \( a(\beta) \) is decreasing in \( \beta \) and that

\[
\lim_{\beta \to 0} a(\beta) = a_0, \quad \lim_{\beta \to \infty} a(\beta) = a
\]

Then \( a \leq a(\beta) \leq a_0 \). One can also show that

\[
a(\beta) = a(1 + O(\sqrt{a\beta^{-1/2}}))
\]
Two more scattering estimates

We also need to estimate the following expressions:

\[ a'(\beta) = (8\pi\beta)^{1/2} \int K(x, x)dx \]

\[ a''(\beta) = (8\pi\beta)^{1/2} \int K(x, -x)dx \]

Lemma

\[ \max\{a'(\beta), a''(\beta)\} \leq 2^{d/2} a(\beta/2) \]

For \( d = 3 \), we can also show that

\[ \lim_{\beta \to \infty} a'(\beta) = a, \quad \lim_{\beta \to \infty} a''(\beta) = a \]

We do not control \( a' \) and \( a'' \) as well as we control \( a \), but this is not important for our purpose.
Conclusion

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THANK YOU!