BOSE-EINSTEIN CONDENSATION
IN THE PRESENCE OF ONE IMPURITY

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0. INTRODUCTION

1. α-VORTEX AND CONTACT INTERACTION

2. 2D BOSE-EINSTEIN CONDENSATION

$$\alpha \neq 0 \qquad \alpha = 0 \qquad \alpha = -\frac{1}{2}$$

3. CONCLUSION

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0. INTRODUCTION

- Original Bose-Einstein Condensation (**BEC**) is a **I-order phase transition in momentum space** **it occurs for an ideal gas of free particles in 3D** (three space dimensions)

BUT NOT IN 1-2D

⋆ Standard 3D case ⋆

- Consider a system of N non-interacting Bose particles of mass m in a cubic volume $V = L^3$ with Hamiltonian

$$H_N = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m}$$

$$\mathbf{p} = \frac{2\pi\hbar}{L}\mathbf{n} \; ; \qquad \mathbf{n} = (n_x, n_y, n_z)$$

• The **single-particle energies** , the **total energy** and the **total number of particles** are given by

$$\varepsilon_{\mathbf{p}} = \frac{\mathbf{p}^2}{2m} \quad , \quad E = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} n_{\mathbf{p}}$$

$$N = \sum_{\mathbf{p}} n_{\mathbf{p}} \quad , \quad n_{\mathbf{p}} \in \mathbf{N}$$

• From Grand Canonical Partition Function $Z(z, V, T)$ of ideal Bose-system we obtain the

equation of state

• $$\beta P \equiv \frac{1}{V} \ln Z(z, V, T) = -\frac{1}{V} \sum_{\mathbf{p}} \ln \left(1 - z e^{-\beta \varepsilon_{\mathbf{p}}}\right)$$

• $$\langle n \rangle_{3D} \equiv \frac{\langle N \rangle}{V} = \frac{1}{V} z \frac{\partial}{\partial z} \ln Z(z, V, T) = \frac{1}{V} \sum_{\mathbf{p}} \frac{z e^{-\beta \varepsilon_{\mathbf{p}}}}{1 - z e^{-\beta \varepsilon_{\mathbf{p}}}}$$

$$z = e^{\beta \mu} \in [0, 1] \ , \quad \beta = \frac{1}{KT}$$

• Now the **main point** :

$*$ **thermodynamic limit** $*$

$$\langle N \rangle \ , \ V \to \infty \ , \quad \langle n \rangle = \text{const}$$

$*$ **continuum limit** $*$

$$\sum_{\mathbf{p}} \longrightarrow \frac{V}{h^3} \int \ d^3p$$

whenever possible! **BUT** the sums in state equation **diverge** as $z \to 1$, because of the term in $\mathbf{p} = 0$.

$*$ `The single term` $\mathbf{p} = 0$ `may be` $*$

$*$ `as important as the entire sum` $*$

• We split off the terms corresponding to $\mathbf{p} = 0$ and replace the rest of the sums by integrals $\lambda \equiv h/\sqrt{2\pi m K T}$

$$\bullet \quad \beta P = \frac{1}{\lambda^3} g_{5/2}(z) - \frac{1}{V} \ln(1-z)$$

$$\bullet \quad \langle n \rangle_{3D} = \frac{1}{\lambda^3} g_{3/2}(z) + \frac{z}{V(1-z)} \equiv \frac{1}{\lambda^3} g_{3/2}(z) + \langle n_0 \rangle_{3D} \qquad (\heartsuit)$$

$$g_s(z) = \frac{z}{\Gamma(s)} \int_0^\infty dx \frac{x^{s-1} e^{-x}}{1 - z e^{-x}} = \sum_{l=0}^{\infty} \frac{z^l}{l^s}$$

$\star$ **Some comments** $\star$

- **1.** Above state equations are strictly true

$*$ **only in the absence of external fields** $*$

- **2.** $g_{3/2}(z)$ is a **bounded** , positive, monotonically increasing function of z

- **3.** $\langle n_0 \rangle_{3D}$ is a **finite number** in **the limits**

$$V \to \infty \ , \quad z \to 1$$

a finite fraction of all particles

occupy the single level with $\mathbf{p} = 0$

$$\textbf{iff} \quad \frac{\lambda^3}{v} \geq g_{3/2}(1) = \zeta(3/2)$$

a finite fraction of the particles

occupies the fundamental level

BEC PHENOMENON

⋆ Standard 2D case ⋆

∘ State equation in 2D space dimensions for **free** Bose gas

- $\beta P = \frac{1}{\lambda^2} g_2(z) - \frac{1}{A} \ln(1-z)$

- $\langle n \rangle_{2D} = \frac{1}{\lambda^2} g_1(z) + \frac{z}{A(1-z)}$

  $A \equiv L^2$

BUT now $g_1(z)$ is an **unbounded** , positive, monotonically increasing function of z *i.e.*

- $\lim_{z \to 1} g_1(z) = \infty$

no finite fraction of Bose-particles will

ever fill the fundamental level $\mathbf{p} = 0$

NO BEC IN 2D FREE CASE

$\star$ **Important remark** $\star$

• In the presence of **EXTERNAL FIELDS the previous**

$*$ **naive continuum limit does not work** $*$

• The density of the 1-particle quantum states can be obtained as the inverse **Laplace transform** of the 1-particle partition function per unit volume.

• **IN GENERAL** the **state equation** for an ideal Bose gas

$$\bullet \quad \beta P = \int_0^\infty dE \, \frac{\beta \tau(E, V; a)}{1 - e^{\beta(E-\mu)}}$$

$$\bullet \quad \langle n \rangle = - \int_0^\infty dE \, \frac{\rho(E, V; a)}{1 - e^{\beta(E-\mu)}}$$

$\rho(E, V; a)$ is *the density of 1-particle states,*

$\tau(E, V; a)$ is *the no. of 1-particle states up to energy* E

$$\rho(E, V; a) \equiv \frac{\partial}{\partial E} \tau(E, V; a)$$

$$Z(T, V, a) = \int_0^\infty dE \, \rho(E, V; a) e^{-\beta E}$$

$a \equiv$ external field parameters

1. α-VORTEX AND CONTACT INTERACTION

- Starting point is the classical 1-particle Hamiltonian in 2D

- $H(\phi) = \frac{1}{2m}\left[\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{r})\right]^2 \quad , \qquad \mathbf{p}, \mathbf{r} \in \mathbf{R}^2$
- $A_j(x_1, x_2) = \frac{\phi}{2\pi}\epsilon_{jk}\frac{x_k}{r^2} \quad , \qquad r \equiv \sqrt{x_1^2 + x_2^2}$
- $\alpha = \frac{\phi}{\phi_0} = \frac{e\phi}{hc}$
- $\phi_0 \equiv \frac{hc}{e} \sim 10^{-4}\text{G} \times \text{cm}^2$

- When $\alpha \in \mathbf{Z}$ the hamiltonian operator is equivalent to the one with $\alpha = 0$ up to gauge transformations on **single valued wave functions** $\Longrightarrow \quad -1 < \alpha \leq 0$

- The **AB vector potential** is a good classical description of one **point-like impurity** .

• Now the **main point**

$*$ quantization of classical Hamiltonian $*$

$*$ leads to **SYMMETRIC** operator $*$

$\Downarrow$

FIND A SELF-ADJOINT OPERATOR

$\Updownarrow$

• Self-adjoint extension of Hamiltonian leads to genuine **QM** concept of **CONTACT INTERACTION** (CI).

(*Fermi 1936*)

$\odot$ (1+1)D **CI** is **equivalent** to δ-potential

$\odot$ (2+1)D **CI** is **NOT equivalent** to δ-potential .

Correct mathematical framework is to find Self-Adjoint Extensions (SAEs) of the symmetric hamiltonian operator.

(*Albeverio 1988*)

- **Most general rotational invariant solution** of the radial eigenvalue problem is

$$\odot \qquad \psi(kr)_l = A_l J_{|l+\alpha|} + B_l N_{|l+\alpha|}$$

◦ where $J_{|l+\alpha|}$ and $N_{|l+\alpha|}$ are Bessel and Neumann functions of order $|l+\alpha|$ respectively.

- To select a definite solution, we have to choose **the boundary conditions** for the radial wave functions **at the origin** (impurity position) in such a way to ensure the **self-adjointness of the Hamiltonian quantum operator** .

- We have to impose square integrability of wave functions around impurity position.

$\odot$ In so doing the coefficients A and $B = 0$ are uniquely fixed **BUT** for S-**wave function**.

- The **improper eigenfunctions** belonging to the **continuous** part of the **spectrum** are given by

- $$\psi_l(k,r) = \sqrt{k} J_{|l+\alpha|}(kr)\ , \qquad l \in \mathbf{Z} - \{0\}$$

- $$\psi_0(k,r;E_0) = A(k;\alpha,E_0) J_{|\alpha|}(kr) + B(k;\alpha,E_0) N_{|\alpha|}(kr)$$

- $$N_{|\alpha|}(kr) \sim -\frac{\csc \pi|\alpha|}{\Gamma(1-|\alpha|)} \left(\frac{kr}{2}\right)^{-|\alpha|} \qquad (r \sim 0)$$

○ $J_{|\alpha|}$ and $N_{|\alpha|}$ being Bessel and Neuman functions of order $|\alpha|$ respectively.

- The coefficients $A(k;\alpha,E_0)$ and $B(k;\alpha,E_0)$

$*$ **are NOT uniquely fixed** $*$

- $$\frac{B(k;\alpha,E_0)}{A(k;\alpha,E_0)} = \frac{\sin(\pi\alpha)}{\cos(\pi\alpha) + \mathrm{sgn}(E_0)\left(\hbar^2 k^2/2m|E_0|\right)^{\alpha}}$$

$-\infty \leq E_0 < +\infty$ is some suitable **energy scale**

∘ The **normalizable bound state** is provided by

- $$\langle r|\psi_B\rangle = \psi_B(\kappa, r) = \frac{\kappa}{\pi}\sqrt{\frac{\sin(\pi\alpha)}{\alpha}}K_\alpha(\kappa r)$$

$$\hbar\kappa \equiv \sqrt{2m|E_0|}$$

K_α being Bessel function of imaginary argument

of order $|\alpha|$.

$*$ **SAEs of the differential hamiltonian operator** $*$

$$\Updownarrow$$

Supply the hamiltonian differential operator with the

BOUNDARY CONDITIONS ON THE WAVEFUNCTION

at the impurity position

$$\Updownarrow$$

$\circ$ The self-adjoint $O(2)$ **rotational invariant** Hamiltonian is thus defined by the **spectral decompositions**

$$\bullet \quad H(\alpha, E_0) = \sum_{l=-\infty}^{+\infty} \int_0^\infty dk \frac{\hbar^2 k^2}{2m} |l, k\rangle \langle k, l| + \vartheta(-E_0) |\psi_B\rangle \langle \psi_B| \qquad (\clubsuit)$$

where ϑ is the usual Heaviside's step distribution and

$$\bullet \quad \langle r, \theta | l, k \rangle = \frac{\exp\{il\theta\}}{\sqrt{2\pi}} \psi_l(k, r; \alpha, E_0) \ , \qquad k \geq 0$$

⋆ Remarks ⋆

1. $H(\alpha, E_0)$ **spectral decompositions**

provide the **correct mathematical framework**

CI in QM

2. **Bound state exists** $\Leftrightarrow$ $-\infty < E_0 < 0$

whose energy is just E_0

3. More **generally** , the physical meaning of the characteristic energy scale E_0 is given by the **resonance energy** , according to the following pattern

- $$E_{\rm res} = \begin{cases} |E_0|(\sec\pi\alpha)^{1/|\alpha|} \ , & \text{if} \ \ 0 < |\alpha| < 1/2 \ , \quad E_0 < 0 \ ; \\ |E_0| \ , & \text{if} \ (1/2) < |\alpha| < 1 \ , \quad E_0 < 0 \ ; \end{cases}$$

- $$E_{\rm res} = E_0|\sec\pi\alpha|^{1/|\alpha|} \ , \qquad \text{if} \ (1/2 <)|\alpha| < 1 \ , \quad E_0 \geq 0$$

4. Existence of the Contact Interaction

corresponds to the

presence of a locally square integrable singularity

of the wave function at the impurity position

5. In the limit

$$E_0 \to -\infty$$

Contact Interaction is removed

`* The domain of the Hamiltonian is that of *`

`* the regular wave functions on the whole plane *`

Impurity is a pure AB α non-integer vortex

6. In the limits

$$\alpha \to 0 \ , \quad E_0 \to -\infty$$

`* The two dimensional free particle Hamiltonian *`

`* is truly recovered *`

Friedrichs' limit

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JUST IN FRIEDRICHS' LIMIT

BOSE-EINSTEIN CONDENSATION

DISAPPEARS IN 2D CASE

IN THE PRESENCE OF

CONTACT INTERACTION

NO MATTER HOW WEAK IT IS

NON-VANISHING CRITICAL TEMPERATURE

FOR BOSE-EINSTEIN TRANSITION

ALWAYS EXISTS

2. 2D BOSE-EINSTEIN CONDENSATION

- In order **to discuss BEC** it is necessary to compute the **average number of particles at thermal equilibrium** ; to do this we evaluate:

∘ **I)** `the diagonal Heat-Kernel`

$$G(\alpha, \beta, E_0; r)$$

∘ **II)** `the one-particle partition function`

$$Z_{\mathrm{2D}}(\alpha, \beta, E_0)$$

∘ **III)** `the density of 1-particle states`

$$\rho(E; \alpha, |E_0|)$$

∘ **IV) the average particles density at thermal equilibrium**

$$\langle n(\alpha, |E_0|) \rangle_{2D}$$

○ **I)** `The diagonal Heat-Kernel`

• According to the spectral decomposition (♣), after **separation** of the **free particle Hamiltonian**

$$H_0 \equiv H(0, -\infty)$$

contribution, the **diagonal Heat-Kernel** becomes

$$G(\alpha, \beta, E_0; r) \equiv \ G_{\rm int}(\alpha, \beta, E_0; r) + G_0(\beta)$$

$$= \langle \mathbf{r} \, | [\exp\{-\beta H(\alpha, E_0)\} - \exp\{-\beta H_0\}] | \, \mathbf{r} \rangle + \ \lambda^{-2}$$

$$= I(\alpha; r) + I(-\alpha; r) - 2I(0; r) - I_0(\alpha; r) - I_0(-\alpha; r)$$

$$+ I_0(0; r) + \ \vartheta(-E_0) e^{-\beta E_0} \, |\psi_B(\kappa r)|^2 + \mathcal{I}_0(\alpha, E_0; r) + \lambda^{-2}$$

(♠)

• The translation invariant **free particle diagonal Heat-Kernel** is nothing but the **inverse square thermal wavelength** λ.

In equation (♠) we have set

$$I(\alpha;r) = \int_0^\infty \frac{dk}{2\pi}\ ke^{-\beta\hbar^2 k^2/2m} \sum_{l=0}^{\infty}\ [J_{l+\alpha}(kr)]^2$$

$$I_0(\alpha;r) = \int_0^\infty \frac{dk}{2\pi}\ ke^{-\beta\hbar^2 k^2/2m}\ \ [J_\alpha(kr)]^2$$

$$\mathcal{I}_0(\alpha, E_0; r) =$$

$$\int_0^\infty \frac{dk}{2\pi}\ \frac{k\exp\{-\beta\hbar^2 k^2/2m\}}{1+\tan^2[\pi\mu(k)]+2\tan[\pi\mu(k)]\cos(\alpha\pi)}$$

$$\times \left\{\tan^2[\pi\mu(k)]\, J_{-\alpha}^2(kr) + J_\alpha^2(kr) + \right.$$

$$\left. +\ 2\ \tan[\pi\mu(k)]\, J_{-\alpha}(kr)\, J_\alpha(kr)\right\}$$

$$\tan[\pi\mu(k)] \equiv \mathrm{sgn}(E_0)\left[\frac{2m|E_0|}{\hbar^2 k^2}\right]^{|\alpha|}$$

◦ **II)** `The one-particle partition function`

• It is very **important to realize** that

$$G_{\mathrm{int}}(\alpha, \beta, E_0; r)$$

is integrable on the whole plane !

• We have to evaluate integrals of the type

$$I_\alpha = \int d^2\mathbf{r} \int_0^\infty dk\, k e^{-\beta k^2} \sum_{j=0}^{\infty} \left[J_{2j+\alpha}(kr)\right]^2$$

which is **manifestly divergent** as it stands !

(Arovas, Comtet et al.)

◦ Here we adopt the following definition

• $$I_\alpha = \sum_{j=0}^{\infty} \int_0^\infty dk\, k e^{-\beta k^2} \int d^2\mathbf{r}\ \left[J_{2j+\alpha}(kr)\right]^2$$
$$\equiv \lim_{\omega\to 1} \sum_{j=0}^{\infty} \int_0^\infty dk\ k e^{-\beta k^2} \int d^{2\omega}\mathbf{r} \left[J_{2j+\alpha}(kr)\right]^2$$

i.e. we employ **dimensional regularization**

.

• This leads to the following **UNIQUE** result for the

1-particle partion function

• $$Z_{\rm 2D}(\alpha,\beta,E_0) = \frac{\rm A}{\lambda^2} + \frac{\alpha(\alpha+1)}{2} + \vartheta(-E_0)e^{\beta|E_0|}$$

$$+\frac{\alpha\sin(\pi\alpha)}{\pi}\int_0^\infty \frac{dx}{x^{1+\alpha}}\frac{{\rm sgn}(E_0)\ e^{-\beta|E_0|x}}{1+2{\rm sgn}(E_0)x^{|\alpha|}\cos(\pi\alpha)+x^{2|\alpha|}}$$

(Υ)

∘ From the above expression we obtain the specific notable cases $\alpha\to 0$ and $\alpha=-1/2$

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(i) The one-particle partition function in 2D in the presence of **pure contact interaction** *i.e.* $\alpha \to 0$

$$Z_{\rm 2D}(0,\beta,E_B) = \frac{\rm A}{\lambda^2} + e^{\beta|E_B|} - \int_0^\infty \frac{dE}{E} \frac{e^{-\beta E}}{\ln^2(-E/E_B) + \pi^2}$$
$$= \frac{\rm A}{\lambda^2} + \nu(\beta|E_B|) \ , \qquad E_B < 0$$

$$\nu(x) \equiv \int_0^\infty \frac{x^t}{\Gamma(t+1)} dt$$

- In 2D **bound state is always present** for any

$$-\infty < E_B < 0$$

.

(ii) The one-particle partition function in 3D in the presence of **pure contact interaction** *i.e.* $\alpha = -1/2$

$\odot$ *Thanks to dimensional transmutation, the latter case just corresponds to the value* $\alpha = -1/2$*, up to a suitable redefinition of the free part*

$$Z_{3\mathrm{D}}(\beta, E_0) = \frac{\mathrm{V}}{\lambda^3} + \vartheta(-E_0)e^{\beta|E_0|}$$

$$+\frac{1}{2}\mathrm{sgn}(E_0)e^{\beta|E_0|}\mathrm{erfc}(\sqrt{\beta|E_0|})$$

◦ **III)** `The density of 1-particle states`

- From the Laplace inverse transform of (Υ)

$$\varrho(E;\alpha,|E_0|) = \frac{\alpha\sin(\pi\alpha)E^{|\alpha|-1}}{\pi|E_0|^{\alpha}\left[E^{2|\alpha|}+|E_0|^{2|\alpha|}+2\mathrm{sgn}(E_0)(E|E_0|)^{|\alpha|}\cos(\pi\alpha)\right]}\ .$$

◦ **IV) The mean density at thermal equilibrium**

- $$\begin{aligned}\langle n\rangle_{2\mathrm{D}} &= \lambda^{-2}g_1(z)+\frac{z\alpha(\alpha+1)}{2\mathrm{A}(1-z)}\\ &+\vartheta(-E_0)\frac{z}{\mathrm{A}(z_0-z)}+\vartheta(E_0)\frac{z}{\mathrm{A}(1-z)}\\ &+\mathrm{sgn}(E_0)\frac{z}{\mathrm{A}}\int_0^\infty dE\ \frac{\varrho(E;\alpha,|E_0|)e^{-\beta E}}{1-z\exp\{-\beta E\}}\end{aligned} \qquad (\heartsuit)$$

$$z_0\equiv\exp\{\beta E_0\}\ ,\qquad g_1(z)=-\ln(1-z)$$

$\star$ **Comments** $\star$

- Thanks to analytic continuation the very last term in ($\heartsuit$) admits a finite limit when $z \to 1$ and $E_0 \geq 0$

- The range of fugacity is

  $\odot$ $0 \leq z \leq z_0 < 1$ if $E_0 < 0$

  $\odot$ $0 \leq z < 1$ if $E_0 \geq 0$

- **BEC occurs only in the presence of the bound state**

Only for the sub-family of the self-adjoint extensions of the symmetric Hamiltonian

$$-\infty < E_0 < 0$$

Critical temperature (**specific area**) **does'nt depend upon** α , is the **unique** solutions of

$$\ln\left(1 - e^{\beta E_0}\right) = -\frac{h^2 \beta}{2\pi m} \langle n \rangle_{2\mathrm{D}} \qquad (\diamondsuit)$$

- **2D contact interaction** can be obtained from the **basic formula** (♡) in the limit $\alpha \to 0$

Treating separately the cases

$$E_0 \geq 0 \quad \text{and} \quad -\infty < E_0 < 0$$

$$\langle n \rangle_{2\mathrm{D}}\big|_{\alpha=0} =$$

$$\frac{g_1(z)}{\lambda^2} + \vartheta(E_0)\frac{z}{\mathrm{A}(1-z)} + \vartheta(-E_0)\frac{z}{\mathrm{A}(z_0 - z)}$$

$$-\,\vartheta(-E_0)\frac{z}{\mathrm{A}}\int_0^\infty \frac{dE}{E}\;\frac{e^{-\beta E}}{1 - z\exp\{-\beta E\}}\,\frac{1}{\ln^2(-E/E_0) + \pi^2}$$

- **BEC does not occur if** $E_0 \geq 0$
- **BEC occurs iff** $-\infty < E_0 < 0$

and the critical temperature is **always** fixed by (◇)

- The very same formula can be also obtained directly from (**i**) as it does.

- **3D contact interaction** can be obtained, up to irrelevant terms in the thermodynamic limit, from the **basic formula** (♡) for $\alpha = -1/2$

$$\langle n \rangle_{\rm 3D} = \lambda^{-3} g_{\frac{3}{2}}(z) + \vartheta(-E_0)\frac{z}{\mathrm{V}(z_0 - z)} + \vartheta(E_0)\frac{z}{\mathrm{V}(1-z)}$$
$$+ \,\mathrm{sgn}(E_0)\frac{z}{\mathrm{V}}\int_0^\infty dE\ \frac{\varrho(E;\alpha = -\frac{1}{2}, |E_0|)e^{-\beta E}}{1 - z\exp\{-\beta E\}}$$

- **Bose-Einstein condensation always exists in 3D**

- **Critical temperature** and/or **density do depend upon the sign of the parameter characterizing the self-adjoint extension of the Hamiltonian**

⊙ $E_0 \geq 0$ (**absence of the bound state**)

$$\lambda^3 \langle n \rangle_{\rm 3D} = \zeta(3/2)$$

⊙ $-\infty < E_0 < 0$ (**presence of the bound state**)

$$g_{\frac{3}{2}}(z_0) = \lambda^3 \langle n \rangle_{\rm 3D}$$

3. CONCLUSION

- **CI -presence of bound state- makes possible the occurrence of BEC in 2D**

- In the presence of AB-potential the half-family **without bound state** ($E_0 \geq 0$) of the self-adjoint extensions **does not allow BEC**, whilst the remaining half-family **with bound state** ($-\infty < E_0 < 0$) **leads to BEC and the critical temperature is independent of** α

- **CI in 3D shifts the critical temperature from its conventional value**