Calculations on Bose-Einstein Condensation Using Zeta Functions

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Development in technology allowed mankind to obtain ultracold Bose-Einstein gas

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New experimental discoveries

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Theoretical explanation

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Calculation on Bose-Einstein condensation (BEC)

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“Spectral Functions in Mathematics and Physics” by K. Kirsten

Three dimensional ideal Bose-Einstein gas

$$\left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{x})\right)\phi_k(\mathbf{x}) = E_k\phi_k(\mathbf{x})$$

Magnetic traps are modelled by harmonic oscillator potentials

$$V(\mathbf{x}) = \frac{\hbar m}{2}\left(\omega_1 x_1^2 + \omega_2 x_2^2 + \omega_3 x_3^2\right)$$

Grand canonical description of Bose-Einstein gas

Partition function

$$\Xi(\mu,\beta)=\prod_{k=0}^{\infty}\frac{1}{1-e^{-\beta(E_k-\mu)}}$$

Partition sum

$$q=\ln\Xi=-\sum_{k=0}^{\infty}\ln\left(1-e^{-\beta(E_k-\mu)}\right)=q_0-\sum_{k=1}^{\infty}\ln\left(1-e^{-\beta(E_k-\mu)}\right)$$

Number of particles

$$N=\frac{1}{\beta}\frac{\partial}{\partial\mu}q=\sum_{k=0}^{\infty}\frac{1}{e^{\beta(E_k-\mu)}-1}=N_0+\sum_{k=1}^{\infty}\frac{1}{e^{\beta(E_k-\mu)}-1}$$

We define the condensation temperature T_C by $\mu=E_0$, $N_0=0$.

Deformation of q

$$q = q_0 - \sum_{k=1}^{\infty} \ln\left(1 - e^{-\beta(E_k - \mu)}\right)$$

$$= q_0 + \sum_{k=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{n} e^{-\beta n(E_k - \mu)}$$

$$= q_0 + \sum_{k=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{n} e^{-\beta n(E_k - E_0 + \mu_C - \mu)}$$

$$= q_0 + \sum_{k=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{n} e^{-\beta n(\mu_C - \mu)} e^{-\beta n(E_k - E_0)}$$

Mellin transformation

$$\mathcal{M}\{f(x)\} = F(\alpha) = \int_0^\infty f(x)x^{\alpha-1}dx$$

$$\mathcal{M}^{-1}\{F(\alpha)\} = f(x) = \frac{1}{2\pi i}\int_{b-i\infty}^{b+i\infty} F(\alpha)x^{-\alpha}d\alpha$$

Integral representation of the exponential

$$\Gamma(\alpha) = \int_0^\infty e^{-x}x^{\alpha-1}dx$$

$$e^{-x} = \frac{1}{2\pi i}\int_{b-i\infty}^{b+i\infty} \Gamma(\alpha)x^{-\alpha}d\alpha$$

Integral description of q

$$q = q_0 + \sum_{k=1}^{\infty}\sum_{n=1}^{\infty}\frac{1}{2\pi i}\int_{b-i\infty}^{b+i\infty} d\alpha \Gamma(\alpha) n^{-\alpha-1}\left\{\beta\left(E_k - E_0\right)\right\}^{-\alpha} e^{-\beta n(\mu_C - \mu)}$$

$$= q_0 + \frac{1}{2\pi i}\int_{b-i\infty}^{b+i\infty} d\alpha \Gamma(\alpha)\beta^{-\alpha} Li_{1+\alpha}\left(e^{-\beta(\mu_C-\mu)}\right)\zeta_{Spectral}(\alpha)$$

Polylogarithm $$Li_p(x) = \sum_{n=1}^{\infty}\frac{x^n}{n^p}$$

Spectral zeta function $$\zeta_{Spectral}(\alpha) = \sum_{k=1}^{\infty}\left(E_k - E_0\right)^{-\alpha}$$

Consider a Hermitian $N \times N$ matrix P with eigenvalues λ_n .

(In our case of BEC, $P = -\frac{\hbar^2}{2m}\Delta + \frac{\hbar m}{2}\left(\omega_1 x_1^2 + \omega_2 x_2^2 + \omega_3 x_3^2\right).$)

$$\ln \det P = \sum_{n=1}^{N} \ln \lambda_n = -\frac{d}{ds}\sum_{n=1}^{N} \lambda_n^{-s}\Big|_{s=0} = -\frac{d}{ds}\zeta_P(s)\Big|_{s=0}$$

Spectral zeta function derived from P

$$\zeta_P(s) = \sum_{n=1}^{N} \lambda_n^{-s}$$

$$N \to \infty \qquad \zeta_P(s) = \sum_{n=1}^{\infty} \lambda_n^{-s}$$

Heat kernel $K(t)$

$$\begin{cases} \left(\frac{\partial}{\partial t} + P\right) K(t, x, x') = 0 \\ \mathcal{B} K(t, x, x')\big|_{x \in \partial \mathcal{M}} = 0 \\ \lim_{t \to 0} K(t, x, x') = \delta(x, x') \end{cases}$$

$$K(t) = \int_{\mathcal{M}} dx Tr_V K(t, x, x')$$

$$t \to 0 \qquad K(t) \sim \sum_{k=0}^{\infty} a_k t^{-j_k} \quad (j_i > j_{i+1})$$

The relation between the spectral zeta function $\zeta_P(s)$ and the heat kernel $K(t)$

$$\operatorname{Res}\zeta_P(\alpha = j_k) = \frac{a_k}{\Gamma(j_k)}$$

$$K(t) \sim \sum_{k=0}^{\infty} a_k t^{-j_k}$$

We can now use the residue theorem to calculate the integral of q .

Calculation of the integral by taking only the two rightmost poles of $\zeta_{Spectral}(\alpha)$

$$q = q_0 + \beta^{-j_0} Li_{1+j_0}\left(e^{-\beta(\mu_C - \mu)}\right)a_0 + \beta^{-j_1} Li_{1+j_1}\left(e^{-\beta(\mu_C - \mu)}\right)a_1$$

Number of particles

$$N = \frac{1}{\beta}\frac{\partial}{\partial \mu} q$$

$$N = N_0 + \beta^{-j_0} Li_{j_0}\left(e^{-\beta(\mu_C - \mu)}\right)a_0 + \beta^{-j_1} Li_{j_1}\left(e^{-\beta(\mu_C - \mu)}\right)a_1$$

$$\because \frac{\partial}{\partial x} Li_p(x) = \frac{1}{x} Li_{p-1}(x)$$

$$N = \beta_C^{\ -j_0}\zeta(j_0)a_0 + \beta_C^{\ -j_1}\zeta(j_1)a_1$$

$$\because Li_p\left(e^{-x}\right) = \sum_{l=1}^{\infty}\zeta(p-l)\frac{(-x)^l}{l!} \cong \zeta(p) \qquad (x \to 0) \quad (p > 1) \quad (j_0 > j_1 > 1)$$

$\zeta(\alpha)$: Riemann zeta function

Condensation temperature in the bulk limit

$$T_0 = \frac{1}{k_B}\left(\frac{N}{\zeta(j_0)a_0}\right)^{\frac{1}{j_0}}$$

Corrections due to finite-N effect

$$T_C = T_0(1+\delta)$$

$$\downarrow$$

$$N = \left\{\frac{1}{k_B T_0}(1-\delta)\right\}^{-j_0}\zeta(j_0)a_0 + \left\{\frac{1}{k_B T_0}(1-\delta)\right\}^{-j_1}\zeta(j_1)a_1$$

$$\delta = -\frac{\zeta(j_1)a_1}{j_0\zeta(j_0)^{\frac{j_1}{j_0}}a_0^{\frac{j_1}{j_0}}N^{\frac{j_0-j_1}{j_0}} + j_1\zeta(j_1)a_1} \cong -\frac{\zeta(j_1)a_1}{j_0\zeta(j_0)^{\frac{j_1}{j_0}}a_0^{\frac{j_1}{j_0}}N^{\frac{j_0-j_1}{j_0}}}$$

$$\therefore T_C = T_0\left(1-\frac{\zeta(j_1)a_1}{j_0\zeta(j_0)^{\frac{j_1}{j_0}}a_0^{\frac{j_1}{j_0}}}\frac{1}{N^{\frac{j_0-j_1}{j_0}}}\right)$$

Calculations to determine j_k , a_k

Energy eigenvalues $$E_{n_1 n_2 n_3} = \hbar \sum_{i=1}^{3} \omega_i \left(n_i + \frac{1}{2} \right) \quad , \quad n_i \in \mathbf{N}_0$$

$$K(t) = e^{-\frac{1}{2}\hbar(\omega_1+\omega_2+\omega_3)} \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} e^{-t\hbar(n_1\omega_1+n_2\omega_2+n_3\omega_3)}$$

$$\cong \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} e^{-t\hbar(n_1\omega_1+n_2\omega_2+n_3\omega_3)} \qquad \Leftarrow \frac{1}{2}\hbar(\omega_1+\omega_2+\omega_3) = 0$$

$$= \frac{1}{1-e^{-t\hbar\omega_1}} \frac{1}{1-e^{-t\hbar\omega_2}} \frac{1}{1-e^{-t\hbar\omega_3}} \qquad (t \to 0)$$

Maclaurin series of $\dfrac{x}{e^x - 1}$

$$f(x) = \frac{x}{e^x - 1} = \sum_{n=0}^{\infty} \frac{B_n}{n!} x^n$$

B_n : Bernoulli numbers

$$g(x) = f^{-1}(x) = \frac{e^x - 1}{x} = \sum_{r=1}^{\infty} \frac{x^{r-1}}{r!}$$

$$\Rightarrow f(x) g(x) = 1$$

$$\therefore \left(1 + \frac{x}{2!} + \frac{x^2}{3!} + \cdots\right)\left(B_0 + B_1 x + B_2 \frac{x^2}{2!} + \cdots\right) = 1$$

$$B_0 = 1, \qquad B_1 + \frac{1}{2} B_0 = 0 \quad \therefore B_1 = -\frac{1}{2}$$

Recurrence relation of Bernoulli numbers

$$\left(\sum_{r=1}^{\infty}\frac{x^{r-1}}{r!}\right)\left(\sum_{m=0}^{\infty}\frac{B_m}{m!}x^m\right)=1$$

$$\sum_{m=0}^{n}\frac{B_m}{(n+1-m)!\,m!}=\begin{cases}1 & (n=0)\\ 0 & (n\geq 1)\end{cases} \qquad (n=(r-1)+m)$$

$$\sum_{m=0}^{n-1}\frac{B_m}{(n+1-m)!\,m!}+\frac{B_n}{n!}=0 \qquad (n\geq 1)$$

$$B_n=-\frac{1}{n+1}\sum_{m=0}^{n-1}\frac{(n+1)!}{(n+1-m)!\,m!}B_m=-\frac{1}{n+1}\sum_{m=0}^{n-1}\binom{n+1}{m}B_m$$

Using the series representation $\dfrac{x}{e^x - 1} = \sum_{n=0}^{\infty} \dfrac{B_n}{n!} x^n$,

we can obtain the Laurent series of $\dfrac{1}{1 - e^{-t\hbar\omega_i}}$.

$$\frac{1}{1 - e^{-t\hbar\omega_i}} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} B_n (\hbar\omega_i t)^{n-1}$$

$$= \frac{1}{\hbar\omega_i t} + \frac{1}{2} + \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} B_n (\hbar\omega_i t)^{n-1} \qquad (i = 1, 2, 3)$$

$$K(t) = \frac{1}{1-e^{-t\hbar\omega_1}} \frac{1}{1-e^{-t\hbar\omega_2}} \frac{1}{1-e^{-t\hbar\omega_3}}$$

$$= \left(\frac{1}{\hbar\omega_1 t} + \frac{1}{2} + \cdots \right)\left(\frac{1}{\hbar\omega_2 t} + \frac{1}{2} + \cdots \right)\left(\frac{1}{\hbar\omega_3 t} + \frac{1}{2} + \cdots \right)$$

$$= \frac{1}{\hbar^3\omega_1\omega_2\omega_3} t^{-3} + \frac{1}{2\hbar^2}\left(\frac{1}{\omega_1\omega_2} + \frac{1}{\omega_1\omega_3} + \frac{1}{\omega_2\omega_3} \right) t^{-2} + \cdots$$

$$j_0 = 3, \quad j_1 = 2$$

$$a_0 = \frac{1}{\hbar^3\omega_1\omega_2\omega_3}, \quad a_1 = \frac{1}{2\hbar^2}\left(\frac{1}{\omega_1\omega_2} + \frac{1}{\omega_1\omega_3} + \frac{1}{\omega_2\omega_3} \right)$$

$$K(t) \sim \sum_{k=0}^{\infty} a_k t^{-j_k} \quad (j_i > j_{i+1})$$

Number of particles

$$N = \left(k_B T_C\right)^3 \zeta(3) \frac{1}{\hbar^3 \omega_1 \omega_2 \omega_3} + \left(k_B T_C\right)^2 \zeta(2) \frac{1}{2\hbar^2} \left(\frac{1}{\omega_1 \omega_2} + \frac{1}{\omega_1 \omega_3} + \frac{1}{\omega_2 \omega_3} \right)$$

Condensation temperature

$$T_C = T_0 \left(1 - \frac{\zeta(2)}{3\zeta(3)^{\frac{2}{3}}} \gamma N^{-\frac{1}{3}} \right)$$

$$T_0 = \frac{\hbar}{k_B} \left(\omega_1 \omega_2 \omega_3\right)^{\frac{1}{3}} \left(\frac{N}{\zeta(3)} \right)^{\frac{1}{3}}$$

$$\gamma = \frac{1}{2} \left(\omega_1 \omega_2 \omega_3\right)^{\frac{2}{3}} \left(\frac{1}{\omega_1 \omega_2} + \frac{1}{\omega_1 \omega_3} + \frac{1}{\omega_2 \omega_3} \right)$$

Calculation of the condensation temperature using the data from an experiment by J.R. Ensher, D.S. Jin, M.R. Matthews, C.E. Wieman and E.A. Cornell (1996) [3].

$$\omega_1 = \omega_2 = \frac{746\pi}{\sqrt{8}} \left[s^{-1}\right], \quad \omega_3 = 746\pi \left[s^{-1}\right], \quad N = 40000$$

$$T_0 = 2.88 \times 10^{-7} \left[K\right] = 288 \left[nK\right]$$

$$T_C = 0.976 T_0 = 281 \left[nK\right]$$

Condensation temperature reported by Ensher et al.

$$T_C = 0.94 T_0 = 280 \left[nK\right]$$

According to T. Haugset, H. Haugerud and J.O. Anderson (1997) [4], the number of particles can also be calculated using the Euler-Maclaurin summation formula.

$$\sum_{n=a}^{b} f(n) = \int_a^b dx f(x) + \frac{1}{2}\left[f(b) + f(a)\right] - \frac{1}{12}\left[f'(b) - f'(a)\right] + \cdots$$

$$\left(\sum_{n=a}^{b} f(n) = \int_a^b dx f(x) + \frac{1}{2}\left[f(b) + f(a)\right] + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!}\left[f^{(2k-1)}(b) - f^{(2k-1)}(a)\right]\right)$$

Isotropic potential

$$N = \sum_{n=0}^{\infty} \frac{g_n}{e^{\beta(n\hbar\omega - \mu)} - 1}$$

Energy degeneracy

$$g_n = \frac{(n+1)(n+2)}{2}$$

Anisotropic potential

$$N = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} \frac{1}{e^{\beta\{\hbar(n_1\omega_1 + n_2\omega_2 + n_3\omega_3) - \mu\}} - 1}$$

The formula of N

$$N = \frac{1}{b_1 b_2 b_3} Li_3(z) + \frac{1}{2}\left(\frac{1}{b_1 b_2} + \frac{1}{b_1 b_3} + \frac{1}{b_2 b_3}\right) Li_2(z)$$

$$z = e^{\beta\mu} \ , \qquad b_i = \beta\hbar\omega_i \qquad (i = 1, 2, 3)$$

By setting $E_0 = 0$ and $\mu = 0$, N is expressed as below.

$$N = (k_B T_C)^3 \zeta(3) \frac{1}{\hbar^3 \omega_1 \omega_2 \omega_3} + (k_B T_C)^2 \zeta(2) \frac{1}{2\hbar^2}\left(\frac{1}{\omega_1 \omega_2} + \frac{1}{\omega_1 \omega_3} + \frac{1}{\omega_2 \omega_3}\right)$$

The same result can also be obtained by using a density of states approach [6].

References

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