7 Quantenstatistik & Bose-Einstein Kondensation

Statistischer Operator & Dichtematrix

Erwartungswerte $(\langle\psi|\psi\rangle = 1)$

$$\langle \mathcal{O} \rangle = \langle \psi | \mathcal{O} | \psi \rangle \tag{7.1}$$

können mit Hilfe des statistischen Operators W als Spur geschrieben werden,

$$W = |\psi\rangle\langle\psi| \tag{7.2}$$

mit

$$\begin{aligned} \langle \mathcal{O} \rangle &= \mathrm{Sp}\, W \mathcal{O} \\ &= \sum_n \langle \varphi_n | \psi \rangle \langle \psi | \mathcal{O} | \varphi_n \rangle \\ &= \sum_n \langle \psi | \mathcal{O} | \varphi_n \rangle \langle \varphi_n | \psi \rangle = \langle \psi | \mathcal{O} | \psi \rangle \end{aligned} \tag{7.3}$$

Offensichtlich erfüllt W die Eigenschaft, daß

$$\mathrm{Sp}\, W = 1 \quad (= \langle \psi | \psi \rangle = 1) \tag{7.4}$$

sowie

$$\mathrm{Sp}\, W^2 = 1 \tag{7.5}$$

Gl. (7.5) definiert einen reinen Zustand.

Nun können wir einen allgemeinen Quantenzustand mit einem stat. Operator mit Gl. (7.4) definieren mit

$$\langle O \rangle = Sp\, W O$$

und

$$\boxed{Sp\, W = 1} \qquad (\text{Normierung}) \qquad (7.6)$$

Es gilt nicht mehr allgemein Gl. (7.5), sondern $Sp\, W^2 \leq 1$. Für

$$\boxed{Sp\, W^2 < 1} \qquad (7.7)$$

spricht man von einem gemischten Zustand.

Dies lässt sich mit dem Dichteoperator darstellen

$$\rho = \sum_{n,m} \rho_{nm} |\varphi_n\rangle\langle\varphi_m| \qquad (7.8)$$

mit

$$\rho_{nm} = \langle \varphi_n | W | \varphi_m \rangle$$

Es gilt

$$\sum \rho_{nn} = 1 \quad \leftarrow \text{Gl. } (7.4) \qquad (7.9)$$

und

$$\sum \rho_{nm} \underbrace{\rho_{mn}}_{=\rho^*_{nm}} \leq 1 \quad \leftarrow \text{Gl. } (7.7)$$

Beispiel: Wir betrachten einen Zustand mit Drehimpuls (Spin) $j = 1/2$. Dieser hat 2 Einstellungen, magn. Quantenzahl $m = \pm 1/2$, Spin up $\Uparrow$ und Spin down $\Downarrow$. (Zweizustandssyst.)

Ein allgemeiner Zustand ist dann eine lineare Überlagerung

$$|\psi\rangle = \lambda_1 |\uparrow\rangle + \lambda_2 |\downarrow\rangle$$

mit

$$\lambda_1 \lambda_1^* + \lambda_2 \lambda_2^* = 1 \,, \quad \leftarrow \langle\psi|\psi\rangle = 1 \qquad (7.10)$$

$$\langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = 1 \,, \quad \langle\uparrow|\downarrow\rangle = 0$$

Eine allgemeine Dichtematrix ist

$$\rho = \rho_{++} |\uparrow\rangle\langle\uparrow| + \rho_{+-} |\uparrow\rangle\langle\downarrow| + \rho_{-+} |\downarrow\rangle\langle\uparrow| + \rho_{--} |\downarrow\rangle\langle\downarrow|$$

mit

$$\rho_{++} + \rho_{--} = 1 \qquad (7.11)$$

$$\uparrow$$

$$\mathrm{Sp}\, \rho = 1$$

Drehimpulsalgebra für $j = 1/2$:

Wir suchen $s_i = \hat{L}_i$ und $|\uparrow\rangle, |\downarrow\rangle$ mit

$$\vec{S}^2 |\uparrow\rangle = \frac{3}{4}\hbar^2 |\uparrow\rangle$$
$$\vec{S}^2 |\downarrow\rangle = \frac{3}{4}\hbar^2 |\downarrow\rangle \quad (7.12)$$

← (6.77) & (6.82) p. 171b, 171c
↙ (6.86)

und

$$S_z |\uparrow\rangle = \frac{1}{2}\hbar |\uparrow\rangle$$
$$S_z |\downarrow\rangle = -\frac{1}{2}\hbar |\downarrow\rangle \quad (7.13)$$

mit

$$[S_i, S_j] = i\hbar\, \varepsilon_{ijk}\, S_k \quad (7.14)$$

Wir definieren

$$S_i = \hbar\, \sigma_i/2 \quad \text{mit} \quad \vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$$

und

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (7.15)$$

und damit

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (7.16)$$

und $$\vec{S}^2 = \frac{\hbar^2}{4}\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right] = \frac{3}{4}\hbar^2\, \mathbb{1}$$

Die Spur von ρ^2 ist

$$\mathrm{Sp}\,\rho^2 = \rho_{++}^2 + 2\rho_{+-}\underbrace{\rho_{-+}}_{\rho_{+-}^*} + \rho_{--}^2 \leq 1 \qquad (7.17)$$

(Beweis über $\mathrm{Sp}\,\rho = \sum_n \rho_n = 1 \longrightarrow \rho_n \leq 1$

ρ_n: EW von ρ ≥ 0

$$\mathrm{Sp}\,\rho^2 = \sum_n \rho_n^2 < 1$$

Spin-Statistik:

Betrachten wir nun Zustände mit zwei Teilchen und Wellenfkt. $\Psi(\vec{x}_1, \vec{s}_1; \vec{x}_2, \vec{s}_2)$

($\vec{x}_1, \vec{x}_2$: Ort; $\vec{s}_1, \vec{s}_2$: Spin)

dann gilt

$$\Psi(\vec{x}_1, \vec{s}_1; \vec{x}_2, \vec{s}_2) = \pm \Psi(\vec{x}_2, \vec{s}_2; \vec{x}_1, \vec{s}_2)$$

$+$: Bosonen (7.18)

$-$: Fermionen

Für Fermionen folgt das Pauli-Prinzip!

$$\Psi(\vec{x}, \vec{s}; \vec{x}, \vec{s}) = -\Psi(\vec{x}, \vec{s}; \vec{x}, \vec{s}) = 0 \qquad (7.18)$$

Damit können sich Fermionen <u>nicht</u> am selben Ort mit demselben Spin aufhalten, d.h.

$$|\uparrow\uparrow\rangle = 0 \qquad (7.20)$$

↑ zwei Teilchen Zustand

Dies hat sehr weitreichende Konsequenzen:

<u>Thermische Verteilungsfkt.:</u>

$$\rho = \frac{\sum_n |n\rangle\langle n| \, e^{-\beta(E_n - \mu n)}}{\sum_n e^{-\beta(E_n - \mu n)}} \qquad (7.21)$$

$\beta = \frac{1}{k_B T}$; μ: chem. pot.; n: Teilchenzahl; Nenner: Normierung auf 1

Fermi-Dirac (Fermionen): $n = 0, 1$ Pauli-Prinzip

Verteilungsfkt. für 1 Zustand: $(E_0 = 0)$

$$\rho_1 = \frac{1}{e^{\beta(E_1 - \mu)} + 1}$$

Bose-Einstein Condensation

Cold quantum gases

Constants

$$\hbar = 1$$

$1.01 \times 10^{-34}\,\mathrm{J\,s}$

$$k_B = 1$$

$1.38 \times 10^{-23}\,\mathrm{m^2\,kg\,s^{-2}\,K^{-1}}$

$$c = 1$$

$3.00 \times 10^{8}\,\mathrm{m\,s^{-1}}$

$$2m = 1$$

$$\mathbf{100}\mathrm{MeV} = \mathbf{1.16 \times 10^{12} K}$$

Bose-Einstein condensation

Hamiltonian & dispersion of a free boson gas

- **Hamiltonian of a free bose gas (in a box with volume V)**

$$H = \sum_{\vec{q}} \frac{\vec{q}^{\,2}}{2m} \, a^\dagger_{\vec{q}} a_{\vec{q}} \qquad \textbf{with} \qquad [a_{\vec{q}}\,,\, a^\dagger_{\vec{q}\,'}] = \delta(\vec{q} - \vec{q}\,')$$

- **occupation number**

$$\hat{n}_{\vec{q}} = a^\dagger_{\vec{q}} a_{\vec{q}}$$

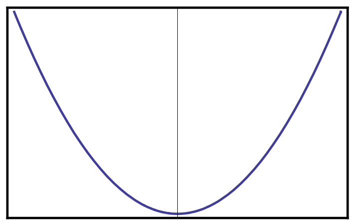
total occupation number

$$\hat{N} = \sum_{\vec{q}} a^\dagger_{\vec{q}} a_{\vec{q}}$$

- **Dispersion relation**

$$E_q = \frac{q^2}{2m}$$

with $q = \sqrt{\vec{q}^{\,2}}$



Bose-Einstein condensation

Partition function & free energy

- **Partition function of a free bose gas**

$$Z = \mathrm{Tr}\, e^{-\beta(H - \mu N)}$$

$\beta = \frac{1}{k_B T}$ **chemical potential**

Free Energy

$$F = k_B T \log Z$$

- **Computation of Free Energy**

$$F = k_B T \log \prod_{\vec{q}} \sum_{n_{\vec{q}}} e^{-\beta\left(\frac{\vec{q}^{\,2}}{2m} - \mu\right) n_{\vec{q}}} \;=\; k_B T \log \prod_{\vec{q}} \frac{1}{1 - e^{-\beta\left(\frac{\vec{q}^{\,2}}{2m} - \mu\right)}}$$

$$\hat{n}_{\vec{q}} |n_{\vec{q}}\rangle = n_{\vec{q}} |n_{\vec{q}}\rangle$$ **occupation number basis**

Bose-Einstein condensation

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$$e^{-\beta\left(\frac{\vec{q}^{\,2}}{2m}-\mu\right)} < 1$$

convergence of sum over $n_{\vec{q}}$

Bose-Einstein condensation

Partition function & free energy

- **Partition function of a free bose gas**

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)}$$

Free Energy

$$F = k_B T \log Z$$

$$\beta = \frac{1}{k_B T}$$

- **Computation of Free Energy**

$$F = -k_B T \sum_{\vec{q}} \log\left(1-e^{-\beta\left(\frac{\vec{q}^{\,2}}{2m}-\mu\right)}\right)$$

$$e^{-\beta\left(\frac{\vec{q}^{\,2}}{2m}-\mu\right)} < 1 \rightarrow \mu < 0$$

Bose-Einstein condensation

Partition function & free energy

- **Partition function of a free bose gas**

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)}$$

Free Energy

$$F = k_B T \log Z$$

$$\beta = \frac{1}{k_B T}$$

- **Computation of Free Energy**

without zero mode with $\vec{q} = 0$

$$F = -k_B T \log(1-z) - k_B T \sum_{\vec{q}}{}' \log\left(1 - z\, e^{-\beta \frac{\vec{q}^2}{2m}}\right)$$

with fugacity $z = e^{\beta\mu} < 1$

Bose-Einstein condensation

Equation of state & continuum limit

- **Computation of Free Energy**

$$z = e^{\beta\mu}$$

$$F = -k_B T \log(1-z) - k_B T \sum_{\vec{q}}{}' \log\left(1 - z\, e^{-\beta \frac{\vec{q}^2}{2m}}\right)$$

- **Equation of state**

$$N = -\frac{\partial F}{\partial \mu} = \frac{z}{1-z} + \sum_{\vec{q}}{}' \frac{z\, e^{-\beta \frac{\vec{q}^2}{2m}}}{1 - z\, e^{-\beta \frac{\vec{q}^2}{2m}}}$$

- **Continuum limit with volume V**

$$N = \frac{z}{1-z} + V \int{}' \frac{d^3 q}{(2\pi)^3} \frac{z\, e^{-\beta \frac{\vec{q}^2}{2m}}}{1 - z\, e^{-\beta \frac{\vec{q}^2}{2m}}}$$

N_0 ⟸ **occupation number of zero mode**

Bose-Einstein condensation

Equation of state & continuum limit

- **Computation of Free Energy**

$$z = e^{\beta\mu}$$

$$F = -k_B T \log(1-z) - k_B T \sum_{\vec{q}}{}' \log\left(1 - z\, e^{-\beta\frac{\vec{q}^{\,2}}{2m}}\right)$$

- **Equation of state**

$$N = -\frac{\partial F}{\partial \mu} = \frac{z}{1-z} + \sum_{\vec{q}}{}' \frac{z\, e^{-\beta\frac{\vec{q}^{\,2}}{2m}}}{1 - z\, e^{-\beta\frac{\vec{q}^{\,2}}{2m}}}$$

- **Continuum limit with volume V**

$$N = \frac{z}{1-z} + V \int' \frac{d^3q}{(2\pi)^3} \frac{z\, e^{-\beta\frac{\vec{q}^{\,2}}{2m}}}{1 - z\, e^{-\beta\frac{\vec{q}^{\,2}}{2m}}}$$

$$\Downarrow$$

$$z = \frac{N_0}{1+N_0}$$

Bose-Einstein condensation

Equation of state & continuum limit

- **Equation of state**

$$z = e^{\beta\mu}$$

$$N = \frac{z}{1-z} + V \int' \frac{d^3q}{(2\pi)^3} \frac{z\, e^{-\beta\frac{\vec{q}^{\,2}}{2m}}}{1 - z\, e^{-\beta\frac{\vec{q}^{\,2}}{2m}}}$$

$$\lambda_{\mathrm{dB}} = \frac{1}{\sqrt{2\pi m k_B T}}$$

deBroglie wavelength

$$g_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty x^{n-1} \frac{ze^{-x}}{1 - ze^{-x}}$$

polygamma function

Bose-Einstein condensation

Bose-Einstein condensation in 3d

- **Equation of state for density** $n = N/V$ $\qquad z = e^{\beta\mu}$

$$n = \frac{1}{V}\frac{z}{1-z} + \frac{1}{\lambda_{\rm dB}^3} g_{\frac{3}{2}}(z)$$

$$\lambda_{\rm dB} = \frac{1}{\sqrt{2\pi m k_B T}} \qquad g_n(z) = \frac{1}{\Gamma(n)}\int_0^\infty x^{n-1}\frac{ze^{-x}}{1-ze^{-x}}$$

deBroglie wavelength $\qquad$ **polygamma function**

- **Limits**
  - $\mathbf{N_0 = O(1)}$: $z < 1$
  - $\mathbf{N_0 = O(V)}$: $z \to 1 - O(1/V)$ ⟸ **macroscopic occupation of zero mode**

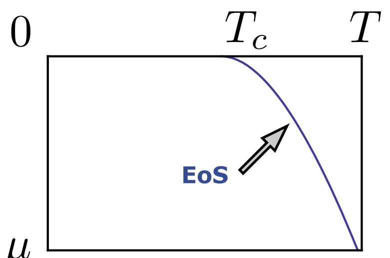
Bose-Einstein condensation

Bose-Einstein condensation in 3d

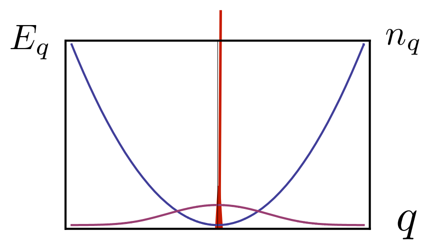
$$n = N/V$$

$$n = \frac{1}{V}\frac{z}{1-z} + \frac{1}{\lambda_{\rm dB}^3} g_{\frac{3}{2}}(z)$$

$\mathbf{N_0 = O(1)}$ $\qquad$ $\mathbf{N_0 = O(V)}$



fixed density



$\mathbf{T_c}$: $n\,\lambda_{\rm dB}^3 = g_{\frac{3}{2}}(1)$

macroscopic occupation of zero mode

Bose-Einstein condensation

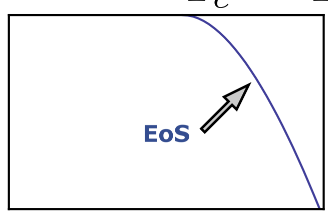
Bose-Einstein condensation in 3d

- **Equation of state for density** $n = N/V$

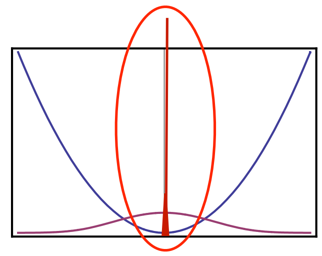
$$n = \frac{1}{V}\frac{z}{1-z} + \frac{1}{\lambda_{\mathrm{dB}}^3} g_{\frac{3}{2}}(z)$$

$\mathbf{N_0 = O(1)}$

$\mathbf{N_0 = O(V)}$



fixed density



macroscopic occupation of zero mode

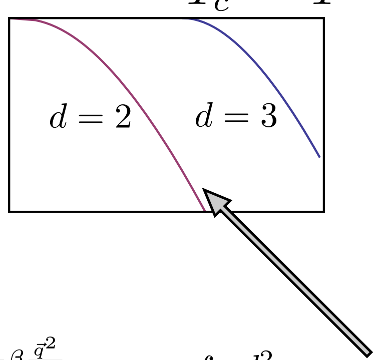
Bose-Einstein condensation

Bose-Einstein condensation in 2d & 3d

- **Equation of state for density** $n = N/V$

$$n = \frac{1}{V}\frac{z}{1-z} + \frac{1}{\lambda_{\mathrm{dB}}^3} g_{\frac{3}{2}}(z)$$

EoS



- **d=2**

$$n \simeq \int \frac{d^2q}{(2\pi)^2} \frac{z e^{-\beta\frac{\vec{q}^2}{2m}}}{1 - z e^{-\beta\frac{\vec{q}^2}{2m}}} \xrightarrow{z\to 1} \int \frac{d^2q}{(2\pi)^2} \frac{z e^{-\beta\frac{\vec{q}^2}{2m}}}{(1-z) + z\beta\frac{q^2}{2m}}$$

infrared singularity
reflects Mermin-Wagner