AQT, June 24, 2011

<u>Recap:</u> 2nd quantization for fermions and bosons

$$(\mathbb{P}_\pm f)(x_1,\dots,x_N) = \frac{1}{N!}\sum_{\pi\in S_N} (\pm 1)^\pi f(x_{\pi(1)},\dots,x_{\pi(N)}).$$

N not fixed: Fock space

$$\mathcal{F}_\pm = \bigoplus_{N\geq 0} \mathcal{H}_\pm^{(N)} \qquad \mathcal{H}_\pm^{(N)} = \mathbb{P}_\pm \otimes^N \mathcal{H}.$$

$(e_\alpha)_\alpha$ an ~~basis~~ ONB of $\mathcal{H}$ $\Rightarrow \mathbb{P}_\pm(e_{\alpha_{i_1}} \otimes e_{\alpha_{i_2}} \cdots \otimes e_{\alpha_{i_N}})$

$i_1 \leq i_2 \leq \dots$ a basis of $\mathcal{H}_\pm^{(N)}$.
orthogonal

$$n_\alpha = |\{k\in\{1,\dots,N\} : i_k = \alpha\}|$$

$\Rightarrow$ can characterize such states by their occupation numbers n_α, $\alpha\in A$.

Creation & annihilation operators satisfy

$$[a_\alpha, a^*_\beta] = \delta_{\alpha\beta}\cdot 1 \qquad \text{bosons}$$

$$\{a_\alpha, a^*_\beta\} = \delta_{\alpha\beta}\cdot 1 \qquad \text{fermions.}$$

etc. $[n_\alpha, n_\beta] = 0$

For $f\in\mathcal{H}$, $f = \sum_\alpha f_\alpha e_\alpha$, $f_\alpha\in\mathbb{C}$, set

$$a^*(f) = \sum_\alpha f_\alpha a^*_\alpha$$

$$\left(\Rightarrow \quad a(f) = \sum_\alpha \overline{f_\alpha}\, a_\alpha \right)$$

Then $[a(f), a^*(g)]_\mp = \sum_\alpha \overline{f_\alpha} g_\alpha \cdot 1 = \langle f|g\rangle 1$

(CCR/CAR in basis-independent form)

and

$$a^*(f)\mathbb{P}_\pm(\varphi_1\otimes\ldots\otimes\varphi_n) = \sqrt{n+1}\,\mathbb{P}_\pm(f\otimes\varphi_1\otimes\ldots\otimes\varphi_n)$$

$$a(f)\mathbb{P}_\pm(\varphi_1\otimes\ldots\otimes\varphi_n) = \mathbb{P}_\pm\sqrt{n}\Big(\langle f|\varphi_1\rangle\varphi_2\otimes\ldots\otimes\varphi_n \pm \langle f|\varphi_2\rangle\varphi_1\otimes\varphi_3\otimes\ldots\otimes\varphi_n + \ldots\Big)$$

The basis independence implies that the algebra of operators generated by the a and a^* is independent of the choice of basis in the 1-particle space $\mathcal{H}$:
if U is unitary on $\mathcal{H}$ and

$$f_\alpha = Ue_\alpha,$$

then the family $b^*_\alpha = a^*(f_\alpha)$ $b_\alpha = a(f_\alpha)$ $\alpha\in A$
generates the same algebra as $(a^*_\alpha, a_\alpha)_{\alpha\in A}$.

Obviously if $Ue_\alpha = \sum_\beta U_{\beta\alpha}e_\beta$

$$b^*_\alpha = a^*\Big(\sum_\beta U_{\beta\alpha}e_\beta\Big) = \sum_\beta U_{\beta\alpha}\,a^*(e_\beta)$$

$$= \sum_\beta U_{\beta\alpha}\,a^*_\beta$$

transforms with the same unitary

$$[b_\alpha, b^*_{\alpha'}]_\pm = \langle Ue_\alpha|Ue_{\alpha'}\rangle\,1 = \langle e_\alpha|e_{\alpha'}\rangle 1 = \delta_{\alpha\alpha'}\cdot 1.$$

Representation of operators on $\mathcal{H}_{\pm}^{(N)}$ and $\mathcal{F}$.

Assume first that H is an operator on $\mathcal{H}$ with $H = H^*$, and that H has an ONB of eigenvectors $(e_\alpha)_\alpha$. Then

$$H = \sum_\alpha E_\alpha |e_\alpha\rangle\langle e_\alpha|$$

with $E_\alpha \in \mathbb{R}$. Then, on the N-particle space,

$$H^{(N)} = H \otimes \mathbb{1} \dots \otimes \mathbb{1} + \mathbb{1} \otimes H \otimes \dots \otimes \mathbb{1} = \sum_{i=1}^{N} H_i$$

with H_i acting on particle i. But if the particles are identical, this just counts occupation numbers:

$$H^{(N)} | n \rangle = \sum_\alpha E_\alpha n_\alpha | n \rangle$$

$$= \sum_\alpha E_\alpha a_\alpha^* a_\alpha | n \rangle$$

so

$$H^{(N)} = \sum_\alpha E_\alpha a_\alpha^* a_\alpha$$

Since the RHS is not explicitly N-dependent, this extends to an operator on $\mathcal{F}$:

$$H = \sum_\alpha E_\alpha \underbrace{a_\alpha^* a_\alpha}_{\underline{n}_\alpha} .$$

(number operator)

For example, for a gas of noninteracting particles in a box, with spin S,

$$H = \sum_{s=-S}^{S} \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^d} E_s(k)\, a^*_{k,s}\, a_{k,s}$$

(Often $E_s(k)$ is spin-independent.)

More generally, a one-particle operator B can be written as

$$B = \sum_{\alpha,\alpha'} |e_\alpha\rangle \underbrace{\langle e_\alpha | B e_{\alpha'}\rangle}_{B_{\alpha\alpha'}} \langle e_{\alpha'}|$$

and on $\mathcal{F}$ it becomes

$$B = \sum_{\alpha,\alpha'} B_{\alpha\alpha'}\, a^*_\alpha\, a_{\alpha'}$$

A two-body interaction U can similarly be written as

$$U = \sum_{\alpha,\alpha',\beta,\beta'} |e_\alpha \otimes e_{\alpha'}\rangle \langle e_\alpha \otimes e_{\alpha'} | U e_\beta \otimes e_{\beta'}\rangle \cdot \langle e_\beta \otimes e_{\beta'}|$$

and the corresponding operator on $\mathcal{F}$ is

$$U = \sum_{\alpha,\alpha',\beta,\beta'} U_{\alpha\alpha';\beta\beta'} \, a_\alpha^* a_{\alpha'}^* a_\beta a_{\beta'}$$

An important example is a two body interaction for the particles in a box. Here, "$e_\alpha = |k\rangle$"

$$\langle x | k \rangle = L^{-d/2} e^{ik\cdot x}$$

so $U(x_1, x_2) = u(x_1 - x_2)$ has matrix elements

$$\langle k_1, k_2 | U | k_2' k_1' \rangle = (L^{-d/2})^4 \cdot \int dx_1 \, dx_2 \, dx_1' \, dx_2' \; e^{-ik_1x_1 - ik_2x_2} e^{ik_2'x_2' + ik_1'x_1'} \underbrace{\langle x_1, x_2 | u | x_2' x_1' \rangle}_{\delta(x_1 - x_2')\,\delta(x_2 - x_1')\, u(x_1 - x_1')}$$

$$= L^{-2d} \int d^dx \, d^dy \; u(x-y) \, e^{-ix(k_1 - k_1')} e^{iy(k_2 - k_2')}$$

$$\underset{x-y=\xi}{=} L^{-2d} \int d^dy \left(\int d^d\xi \; u(\xi) \, e^{-i\xi(k_1 - k_1')} \right) \cdot e^{iy(k_2 - k_2' + k_1 - k_1')}$$

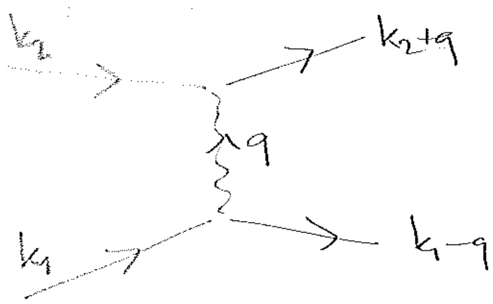
$$= L^{-d} \, \delta_{k_1+k_2,\, k_1'+k_2'} \cdot \hat{u}(k_1 - k_1')$$

(6) Thus, here

$$U = L^{-d} \sum_{k_1,k_2,k_1',k_2'} \hat{u}(k_1-k_1')\, a^*_{k_1} a^*_{k_2} a_{k_2'} a_{k_1'}\, \delta_{k_1+k_2,\, k_2'+k_1'}$$

$$= L^{-d} \sum_{k_1,k_2,q} \hat{u}(q)\, a^*_{k_1} a^*_{k_2} a_{k_2+q}\, a_{k_1-q}$$

$\left(k_1 - k_1' = q \quad k_1' = k_1 - q \right)$



Assume particles without interaction.

$$\rho = \frac{1}{Z} e^{-\beta H}$$

where $Z = \mathrm{Tr}(e^{-\beta H})$. Inserting

$$H = \sum_\alpha E_\alpha \underline{n}_\alpha$$

and using $[\underline{n}_\alpha, \underline{n}_\beta] = 0$ for all α, β,
we get $e^{-\beta H} = \prod_\alpha e^{-\beta E_\alpha \underline{n}_\alpha}$

$$Z = \mathrm{Tr}(e^{-\beta H}) = \sum_n \langle n | e^{-\beta H} n \rangle$$

$$= \sum_{(n_\alpha)_\alpha} \prod_{\alpha \in A} e^{-\beta E_\alpha n_\alpha}$$

$$= \prod_{\alpha \in A} \sum_{n_\alpha} \left(e^{-\beta E_\alpha}\right)^{n_\alpha}$$

<u>Bosons:</u> $n_\alpha \in \mathbb{N}_0$. The sum converges only if $E_\alpha > 0$ for all α, then

$$Z_+ = \prod_{\alpha \in A} \frac{1}{1 - e^{-\beta E_\alpha}}$$

Fermions: $n_\alpha \in \{0, 1\}$.

$$Z_- = \prod_{\alpha \in A} \left(1 + e^{-\beta E_\alpha}\right).$$

The average occupation number is then

$$\langle n_\alpha \rangle = \mathrm{Tr}(\rho \, \underline{n}_\alpha)$$

$$= \begin{cases} \dfrac{1}{e^{\beta E_\alpha} - 1} & \text{bosons} \\[2ex] \dfrac{1}{e^{\beta E_\alpha} + 1} & \text{fermions.} \end{cases}$$

With $E_\alpha = \epsilon_\alpha - \mu$, this becomes the Bose-Einstein and Fermi-Dirac distributions.

In general:

$$\mathrm{Tr}_{\gamma(N)}(\rho \, a^\dagger_\alpha a_\beta) = (\tilde{\rho}_1)_{\alpha\beta} \qquad \tilde{\rho}_1 = N \cdot \mathrm{Tr}_{2..N} \rho$$

$$\mathrm{Tr}_{\gamma(N)}(\rho \, a^\dagger_\alpha a^\dagger_{\alpha'} a_\beta a_{\beta'}) = (\tilde{\rho}_2)_{\alpha\alpha',\beta\beta'} \qquad \tilde{\rho}_2 = N(N-1) \, \mathrm{Tr}_{3..N} \rho.$$

Take diagonal case; $\langle a^\dagger_\alpha a_\alpha \rangle = \langle n_\alpha \rangle = n_\alpha$

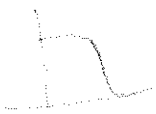
$\sum n_\alpha = N$, not 1.

7.4 Das wechselwirkende Bosegas

Hamiltonoperator

$$H = \sum_k \frac{\hbar^2 k^2}{2m} a_k^* a_k$$

$$+ \frac{1}{2V} \sum_{p,k,q} \tilde{U}(q)\, a_{k+q}^* a_{p-q}^* a_p a_k$$



$\tilde{U}(q) > 0$ (abstoßende WW) $\hat{u}(0) > 0.$

$\tilde{U}$ nicht sehr stark, $\tilde{U}(q) = \hat{U}(-q)$

$U=0$ ground state is: $n_0 = N$, $n_k = 0$ for all $k \neq 0$. low-lying excitations $E(k) \sim \frac{\hbar^2 k^2}{2m}$. quadratic in k.

T klein; niedrigliegende Anregungen.

2 Teilchengruppen:

(a) im Kondensat: $k = 0$

(b) in angeregten Zuständen: $k \neq 0$.

Die Theorie ist sehr schwierig und wir betrachten hier nur eine näherungsweise Behandlung, die aber den Kern der Sache trifft (stammt von NN Bogolubov, 1947).

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1) Wir vernachlässigen die WW der Teilchen außerhalb des Kondensats: ∘ most particles in the ground state at $k=0$ only few excitations.

$$H \to \sum_{k\neq 0} \frac{\hbar^2 k^2}{2m} a_k^* a_k$$

$$+ \frac{1}{2V} \tilde{U}(0)\, a_0^* a_0^* a_0 a_0$$

$$+ \frac{1}{2V} \sum_{k\neq 0} \tilde{U}(k) \left[a_k^* a_{-k}^* a_0 a_0 + a_0^* a_0^* a_k a_{-k} + 2 a_k^* a_0^* a_k a_0 \right]$$

2) $$\frac{1}{V} a_0^* a_0 |\psi\rangle = \frac{N_0}{V} |\psi\rangle$$

$$\frac{1}{V} a_0 a_0^* |\psi\rangle = \frac{N_0+1}{V} |\psi\rangle = \frac{N_0}{V}|\psi\rangle + \frac{1}{V}|\psi\rangle$$

$N_0 \sim V \Rightarrow$ Kommutatorterm vernachlässigbar

$\Rightarrow$ behandle a_0^*, a_0 als vertauschbare Größen, also als komplexe Zahlen; wähle sie sogar reell: $a_0 = \bar{a}_0 = \sqrt{N_0} = \sqrt{V n_0}$

wobei $n_0 = \frac{N_0}{V}$

(*) It is this assumption which leads to particle nonconservation in H_B: in principle is still conserved. By throwing out the commutator, we have essentially made the condensate into a reservoir that is so large: adding or removing particles does no longer change anything.

Damit erhalten wir Bogoliubov's Hamiltonop.

$$H_B = \frac{\tilde{U}(0)}{2} N_0 \cdot n_0$$

$$+ \sum_{k \neq 0} \left[\left(\frac{\hbar^2 k^2}{2m} + n_0 \tilde{U}(k) \right) a_k^* a_k + \frac{1}{2} n_0 \tilde{U}(k) \left(a_k^* a_{-k}^* + a_k a_{-k} \right) \right]$$

(*)

Bogoliubov - Transformation:

$$a_k = u_k A_k + v_k A_{-k}^*$$

ist kanonisch, wenn

$$[A_k, A_{k'}^*] = \delta_{kk'}. \quad [A_k, A_{k'}] = 0.$$

analogy to canonical transf. in classical mechanics.

NB: $a_\alpha \to e^{i\varphi} a_\alpha$ is a symmetry of the Hamiltonian, it's broken here!

Das gilt, wenn $|u_k|^2 - |v_k|^2 = 1$.

Wähle u_k, v_k reell, nur von $|k|$ abhängig.

Exercise: verify this.

$$H_B = E_0 + \sum_{k \neq 0} \varepsilon(k) A_k^* A_k$$

$$+ \sum_{k \neq 0} F(k) \left(A_k^* A_{-k}^* + A_k A_{-k} \right)$$

$$E_0 = \frac{\tilde{U}(0)}{2} N_0 n_0 + \sum_{k \neq 0} \left(n_0 \tilde{U}(k) \left(v_k^2 + u_k v_k \right) + \frac{\hbar^2 k^2}{2m} v_k^2 \right)$$

$$F(k) = n_0 \tilde{U}(k) \left(u_k v_k + \frac{1}{2} (u_k^2 + v_k^2) \right) + \frac{\hbar^2 k^2}{2m} u_k v_k.$$

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m} (u_k^2 + v_k^2) + n_0 \tilde{U}(k) (u_k + v_k)^2$$

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H_B diagonal $\Leftrightarrow F(k) = 0.$

$$\Longrightarrow \quad u_k^2 + v_k^2 = -2 c_k u_k v_k \,, \qquad c_k = \frac{\frac{\hbar^2 k^2}{2m} + n_0 \tilde{U}(k)}{n_0 \tilde{U}(k)} > 0. \;(>1)$$

$$u_k^2 - v_k^2 = 1$$

$$\Longrightarrow \ldots \Longrightarrow u_k = \sqrt{\frac{1}{2}\left(1 + \frac{c_k}{\sqrt{c_k^2 - 1}}\right)}$$

$$v_k = -\sqrt{\frac{1}{2}\left(-1 + \frac{c_k}{\sqrt{c_k^2 - 1}}\right)}$$

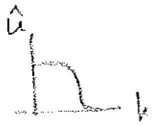
$$u_k v_k = -\frac{1}{2} \frac{1}{\sqrt{c^2 - 1}} \;; \quad u_k^2 + v_k^2 = \frac{c}{\sqrt{c^2 - 1}} .$$

Damit wird

$$H_B = E_0 + \sum_{k \neq 0} \varepsilon(k) A_k^* A_k$$

$$E_0 = \frac{N_0}{2} n_0 \hat{U}(0) + \frac{1}{2} \sum_{k \neq 0} \left[\frac{\hbar |k|}{\sqrt{2m}} \sqrt{\frac{\hbar^2 k^2}{2m} + 2 n_0 \tilde{U}(k)} - \left(\frac{\hbar^2 k^2}{2m} + n_0 \tilde{U}(k) \right) \right]$$

$$\varepsilon(k) = \frac{\hbar |k|}{\sqrt{2m}} \cdot \sqrt{\frac{\hbar^2 k^2}{2m} + 2 n_0 \tilde{U}(k)}$$

assume  i.e. $\hat{u}' \ll 0$ in some region $k \approx k_0 > 0$. Then

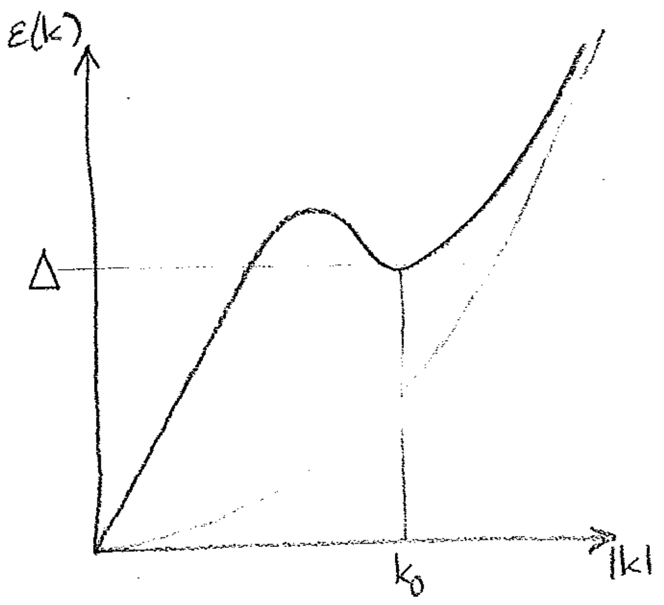
$$\frac{\partial}{\partial k}\left(\varepsilon(k)^2\right) \approx \frac{\partial}{\partial k}\left(k^4 + \alpha k^2 \hat{u}(k) \right)$$

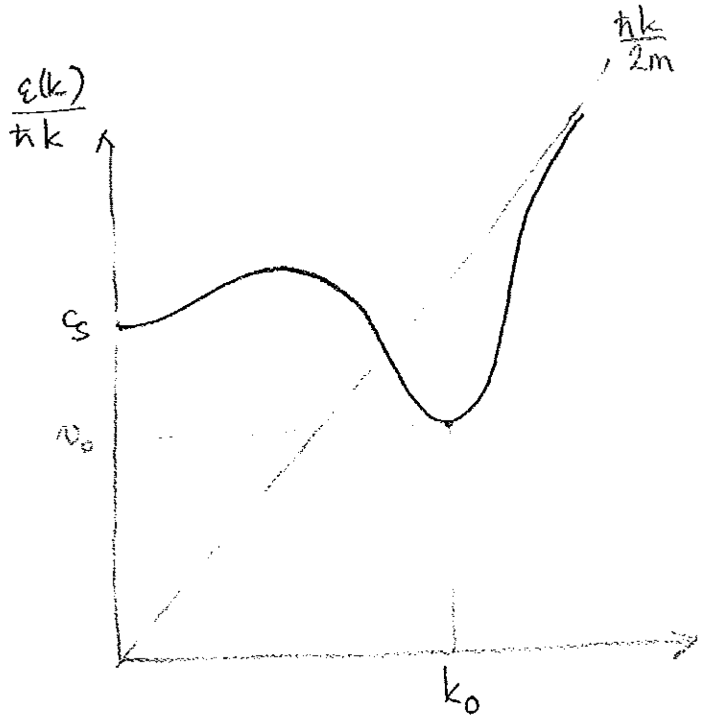
$$= 4k^3 + 2\alpha k \hat{u} + \alpha k^2 \hat{u}'(k) < 0 \quad \text{for } k \approx k_0$$

for a suitable choice of parameters.

Die Bedingung, dass $F(k) = 0$ ist, ist äquivalent dazu, dass E_0 minimal wird!

Die $A_k^{(\alpha)}$ beschreiben Quasiteilchen, nicht mehr tatsächliche Teilchen!
Ihre Dispersionsrelation ist nun (für $U \neq 0$) ganz anders als $\frac{\hbar^2 k^2}{2m}$:





$$c_s = \left.\frac{\partial \varepsilon}{\partial(\hbar k)}\right|_{k=0} = \sqrt{\frac{n_0 \tilde{U}(0)}{m}}$$

Schallgeschwindigkeit, wie bei Phononen (später!)

k klein: $\varepsilon(k) \sim \hbar k c_s$

k groß (asymptotisch) $\varepsilon(k) \sim \frac{\hbar^2 k^2}{2m}$

dazwischen ein Minimum!

Thermodynamische Eigenschaften:

nun die eines idealen Quasiteilchengases

Unterschied zu vorher:

- $\varepsilon(k)$ anders
- keine Teilchenzahlerhaltung ($\mu = 0$). condensate acts as a reservoir!

Mittlere Energie (V groß)

$$U = E_0 + \frac{V}{(2\pi)^3} \int d^3k \, \frac{\varepsilon(k)}{e^{\beta \varepsilon(k)} - 1}$$

Wärmekapazität:

$$C_V = \frac{\partial U}{\partial T}$$

β groß: dominanter Beitrag von $k \approx 0$

Bei etwas höherer Temperatur trägt noch die Umgebung des Minimums bei, allerdings mit einem Faktor $e^{-\beta\Delta}$ unterdrückt, wobei $\Delta = \varepsilon(k_0)$ ist.

Also, näherungsweise

$$E = E_0 + E_{Ph} + E_R$$

$$E_{Ph} = \frac{V}{(2\pi)^3} \int_{|k| \leq \tilde{k}} d^3k \, \frac{\varepsilon_{Ph}(k)}{e^{\beta \varepsilon_{Ph}(k)} - 1} \qquad \varepsilon_{Ph}(k) = c_s \cdot \hbar k$$

$$E_R = \frac{V}{(2\pi)^3} \int_{||k|-k_0| \leq k_1} d^3k \, \frac{\varepsilon_R(k)}{e^{\beta \varepsilon_R(k)} - 1}$$

$$\varepsilon_R(k) = \Delta + \frac{\hbar^2}{2M} (k - k_0)^2$$

Wenn man, statt $\hat{U}(k)$ vorzugeben, die Größen Δ, M, k_0 an das Spektrum anpasst, so erhält man

$$\frac{\Delta}{k_B} = 8.5 \text{ K}, \quad k_0 = 1.9 \cdot 10^8 \text{ cm}^{-1}, \quad M = 0.16 \, m_{He}$$

Ph ... Phononen
R ... Rotonen

} Landau hatte in phän. hydrodyn. Theorie diese beiden Terme identifiziert; hier ist das einfach eine Näherung!

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In E_{Ph} lassen wir wegen der Dominant von $k \approx 0$ die Beschränkung $|k| \le \tilde{k}$ fallen und erhalten

$$E_{Ph} = \frac{V}{(2\pi)^3} c_s \hbar \int \frac{d^3k \cdot k}{e^{\beta \hbar c_s k} - 1}$$

$$= \frac{V}{(2\pi)^3} \frac{(kT)^4}{(\hbar c_s)^3} \cdot \underbrace{\Gamma(4)}_{6} \underbrace{g_4(1)}_{\zeta(4)}$$

$$\frac{E_{Ph}}{N} = \frac{v}{(2\pi)^3} \cdot 6 \zeta(4) \frac{(kT)^4}{(\hbar c_s)^3} .$$

Δ ist groß genug, um $(e^{\beta \varepsilon_R} - 1)^{-1} \approx e^{-\beta \varepsilon_R}$ zu setzen (Boltzmannverteilung).

Außerdem: nahe am Minimum: $k^2 dk \approx k_0^2 dk$

$$\Rightarrow E_R = \frac{V}{2\pi^2} k_0^2 \int_{k_0-k_1}^{k_0+k_1} dk \, \varepsilon_R e^{-\beta \varepsilon_R} = - \frac{V}{2\pi^2} k_0^2 \frac{\partial}{\partial \beta} \int dk \, e^{-\beta \varepsilon_R}$$

$$= - \frac{V}{2\pi^2} k_0^2 \cdot \frac{\partial}{\partial \beta} \left(e^{-\beta \Delta} \cdot \frac{\sqrt{2 M \pi k_B T}}{\hbar} \right)$$

Diskussion der spontanen Symmetrie-brechung $a_k \to e^{i\alpha} a_k$

$V \to \infty$, etc.

exp. Nachweis der Quasiteilchen

$$E_R = \frac{V}{\pi} k_0^2 \frac{\sqrt{2\pi M k_B T}}{h} \left(\Delta + \frac{k_B T}{2} \right) e^{-\Delta / k_B T}$$

Wärmekapazität

$$C_V = C_V^{(Ph)} + C_V^{(R)}$$

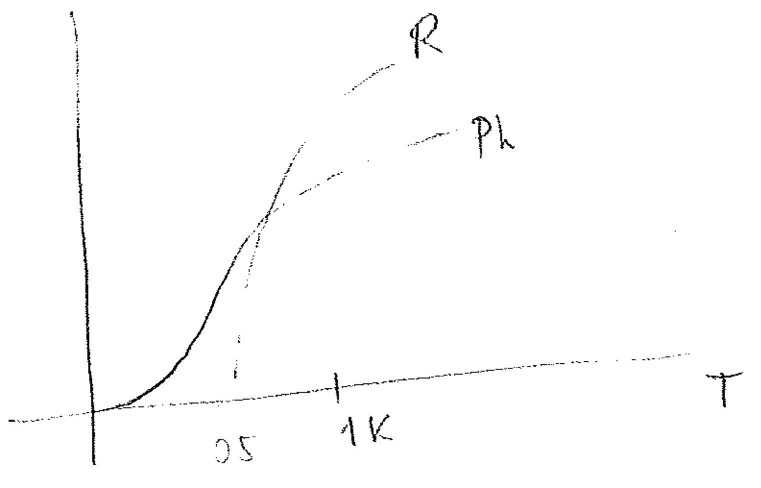
$$C_V^{(Ph)} = k_B V \cdot \frac{2\pi^2}{15} \left(\frac{k_B T}{\hbar c_s} \right)^3$$

$$C_V^{(R)} = k_B V \frac{k_0^2}{\pi h} \cdot (2\pi M k_B T)^{1/2} \cdot \left[\frac{3}{4} + \frac{\Delta}{k_B T} + \left(\frac{\Delta}{k_B T} \right)^2 \right] e^{-\Delta / k_B T}$$

Für $T \to 0$ dominiert $C_V^{(Ph)}$,

$$C_V \sim T^3$$

Für größere T (1–2°K) wird $C_V^{(R)}$ größer



stimmt mit Experiment gut überein.