Pauli Paramagnetism

$$\varepsilon^{\pm}(p) = \varepsilon(p) \mp g\mu_B H$$

$\varepsilon^{+}(p) = \frac{p^2}{2m} - g\mu_B H$ $\quad \uparrow^{H} \uparrow \vec{\mu}$ $\qquad \mu_B = \frac{e\hbar}{2mc}$

$\varepsilon^{-}(p) = \frac{p^2}{2m} + g\mu_B H$ $\quad \uparrow^{H} \downarrow \vec{\mu}$

$N = N^{+} + N^{-}$ $\qquad \varepsilon = \frac{p^2}{2m}$ $\qquad s = 1/2$

$$\boxed{M = N^{+} g\mu_B + gN^{-}(-\mu_B) = g\mu_B (N^{+} - N^{-})}$$

$$\boxed{\begin{aligned}\tilde{g}(\varepsilon) &= \frac{1}{2} g(\varepsilon) \\ &= \frac{2\pi V}{h^3}(2m)^{3/2}\varepsilon^{1/2}\end{aligned}}$$

$$N_{\pm} = \int_0^{\infty} \tilde{g}(\varepsilon) \langle n_{\pm}(\varepsilon, H)\rangle = \int_0^{\infty} \tilde{g}(\varepsilon) \frac{d\varepsilon}{e^{\beta(\varepsilon \mp g\mu_B H - \mu)} + 1}$$

$g\mu_B H \ll \mu$

$$N_{\pm} = \int_0^{\infty} \tilde{g}(\varepsilon) \langle n_{\pm}(\varepsilon, H)\rangle \, d\varepsilon = \int_0^{\infty} \tilde{g}(\varepsilon) \langle n(\varepsilon \mp g\mu_B H)\rangle$$

$$\simeq \int_0^{\infty} \tilde{g}(\varepsilon) \left\{ \langle n(\varepsilon)\rangle \mp \frac{\partial}{\partial \varepsilon} \langle n(\varepsilon)\rangle g\mu_B H \right\} d\varepsilon$$

$$= \int_0^{\infty} \tilde{g}(\varepsilon) \langle n(\varepsilon)\rangle \, d\varepsilon \mp \int_0^{\infty} \tilde{g}(\varepsilon) \frac{\partial \langle n(\varepsilon)\rangle}{\partial \varepsilon} d\varepsilon \cdot g\mu_B H$$

(integr. by parts) $$= \int_0^{\infty} \tilde{g}(\varepsilon) \langle n(\varepsilon)\rangle \, d\varepsilon \pm \int_0^{\infty} \frac{\partial \tilde{g}(\varepsilon)}{\partial \varepsilon} \langle n(\varepsilon)\rangle \, d\varepsilon \, g\mu_B H$$

$$M = g\mu_B(N^{+} - N^{-}) = 2g^2\mu_B^2 H \int_0^{\infty} \frac{\partial \tilde{g}(\varepsilon)}{\partial \varepsilon} \langle n(\varepsilon)\rangle \, d\varepsilon$$

but $2\tilde{g}(\varepsilon) = g(\varepsilon)$

$$= g^2\mu_B^2 H \int_0^{\infty} \frac{\partial g(\varepsilon)}{\partial \varepsilon} \langle n(\varepsilon)\rangle \, d\varepsilon = g^2\mu_B^2 H \left\{ \int_0^{\mu} \frac{\partial g}{\partial \varepsilon} d\varepsilon + \frac{\pi^2}{6}(kT)^2 \left.\frac{\partial^2 g}{\partial \varepsilon^2}\right|_{\mu} \right\}$$

$$= g^2\mu_B^2 H \left\{ g(\mu) + \frac{\pi^2}{6}(kT)^2 g''(\mu) \right\} \quad \ldots$$

$$g(\varepsilon) = \frac{4\pi V}{h^3}(2m)^{3/2}\,\varepsilon^{1/2}$$

and

$$\mu(T) \cong \varepsilon_F\left(1 - \frac{\pi^2}{12}\left(\frac{kT}{\varepsilon_F}\right)^2\right)$$

$$\chi = \left(\frac{\partial M}{\partial H}\right)_{H\to 0} = g^2\mu_B^2\, g(\mu)\left(1 + \frac{\pi^2}{6}(kT)^2\frac{g''(\mu)}{g(\mu)}\right)$$

$\uparrow$ Landé factor

$$= g^2\mu_B^2\,\frac{4\pi V}{h^3}(2m)^{3/2}\mu^{1/2}\left(1 + \frac{\pi^2}{6}(kT)^2\left(-\frac{1}{4}\right)\frac{1}{\mu^2}\right) \simeq$$

$$\simeq g^2\mu_B^2\,\frac{4\pi V}{h^3}(2m)^{3/2}\mu^{1/2}\left(1 - \frac{\pi^2}{24}\left(\frac{kT}{\mu}\right)^2\right)$$

$$N \simeq \frac{2}{3}\,\frac{4\pi V}{h^3}(2m)^{3/2}\mu^{3/2}\left\{1 + \frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2\right\}$$ from earlier

$$\frac{\chi}{N} \simeq \frac{3g^2\mu_B^2}{2\mu}\,\frac{1 - \frac{\pi^2}{24}\left(\frac{kT}{\mu}\right)^2}{1 + \frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2} \simeq \frac{3(\mu_B g)^2}{2\,\varepsilon_F}$$ $g = 2$ Landé factor for electrons

$$\boxed{\chi \simeq \frac{3}{2}\,\frac{N g^2\mu_B^2}{\varepsilon_F}}$$

$$\mu^* = g\mu_B$$

"excitable" fraction of e^-

classical: (Curie law) $$\chi \sim \frac{N\mu_B^2 g^2}{kT} = \frac{N\left(\frac{kT}{\varepsilon_F}\right)\mu_B^2 g^2}{kT} \simeq \frac{N\mu_B^2}{\varepsilon_F}$$

first order correction:

$$\boxed{\frac{\chi}{N} \simeq \frac{3}{2}\,\frac{\mu^{*2}}{\varepsilon_F}\left(1 - \frac{\pi^2}{12}\left(\frac{kT}{\varepsilon_F}\right)^2\right)}$$

from $\left(1 + \frac{1}{12}a\right)\left(1 - \frac{1}{24}a\right)\left(1 - \frac{1}{8}a\right)$

$$\simeq 1 - \frac{-2 + 1 + 3}{24}a = 1 - \frac{1}{12}a$$

Bose-Einstein condensation

discussion of $N = (2s+1)\frac{V}{\lambda^3} f_{3/2}(z)$ $\qquad z = e^{\mu/kT}$

$$\lambda = \left(\frac{h^2}{2\pi m k T}\right)^{1/2}$$

$s=0$ for simplicity

$$\frac{N}{V} = \frac{(2\pi m k T)^{3/2}}{h^3} \bar{f}_{3/2}(z)$$

$$(1) \quad \frac{N}{V} = \frac{(2\pi m k T)^{3/2}}{h^3} \frac{1}{\Gamma(3/2)} \int_0^\infty \frac{x^{1/2}\, dx}{e^x e^{-\mu/kT} - 1}$$

from the B-E distribution: $\langle n(\varepsilon)\rangle = \frac{1}{e^{\frac{\varepsilon-\mu}{kT}} - 1}$

it follows that μ cannot be larger than the minimum single-particle energy level. $\varepsilon = 0$, i.e., $\mu \leq 0$. Otherwise $\langle n(\varepsilon)\rangle$ could be negative for $\varepsilon < \mu$, which is clearly not physically sound

Assume we keep N, V constant, i.e., density $\frac{N}{V}$ = fixed. Then <u>decrease</u> the temperature T. To keep the left hand side of (1) constant, <u>μ must be increased</u> ($\bar{f}_{3/2}(e^{\mu/kT})$ is a monotonic increasing function of μ). But its upper bound from physical considerations is $\mu = 0$, at which the integral is <u>finite</u>.

Thus Eq. (1) yields the obviously flawed conclusion that particles "disappear" below some T_c.

T_c is defined then (1) at which Eq. (1) stops to be valid: (at this point μ reaches its maximum value $\mu = 0$):

$$\frac{N}{V} = \frac{(2\pi m k T_c)^{3/2}}{h^3} \underbrace{\frac{1}{\Gamma(3/2)} \int_0^\infty \frac{x^{1/2}\,dx}{e^x - 1}}_{f_{3/2}(1) \,=\, \zeta(3/2) \,\simeq\, 2.612}$$

[math note: $\displaystyle\int_0^\infty \frac{x^{\nu-1}\,dx}{e^x - 1} = \int e^{-x} \frac{x^{\nu-1}\,dx}{1 - e^{-x}} = \int_0^\infty x^{\nu-1} e^{-x} \sum_{n=0}^\infty e^{-nx}\,dx$

$$= \sum_{n=0}^\infty \int e^{-x(n+1)} x^{\nu-1}\,dx \overset{y \equiv x(n+1)}{=} \sum_{n=0}^\infty \frac{1}{(n+1)^\nu} \int e^{-y} y^{\nu-1}\,dy$$

$$= \Gamma(\nu) \sum_{n=0}^\infty \frac{1}{(n+1)^\nu} = \Gamma(\nu) \sum_{\ell=1}^\infty \frac{1}{\ell^\nu} = \Gamma(\nu)\,\zeta(\nu)$$

Riemann zeta function]

(2) $$\boxed{\frac{N}{V} = \frac{(2\pi m k T_c)^{3/2}}{h^3}\,\zeta(3/2)}$$

for fixed density, N/V, this equation defines T_c

$\zeta(3/2) \simeq 2.612$

To understand the "physics" below T_c, we have to go back to the "basics", i.e., how Eq. (1) was obtained.

$$\bar{p} = \hbar \bar{k} \qquad k_x = \frac{2\pi}{L} n_x \qquad n_x = 0, \pm 1, \pm 2, \ldots$$

$$N = \sum_{\bar{k}} \langle n_{\bar{k}} \rangle = \sum_{\bar{p}} \langle n_{\bar{p}} \rangle \qquad p_x = \hbar \frac{2\pi}{L} n_x = \frac{h}{L} n_x \qquad n_x = 0, \pm 1, \pm 2, \ldots$$

$$\frac{N}{V} = \frac{1}{V} \sum_{\bar{p}} \langle n_{\bar{p}} \rangle = \frac{1}{V} \sum_{\bar{p}} \frac{1}{e^{\frac{\varepsilon(\bar{p}) - \mu}{kT}} - 1} \qquad \varepsilon(\bar{p}) = \frac{p^2}{2m}$$

$$= \frac{1}{V} \frac{1}{e^{-\mu/kT} - 1} + \frac{1}{V} \sum_{|\bar{p}|>0} \frac{1}{e^{\frac{\varepsilon(\bar{p}) - \mu}{kT}} - 1}$$

$T > T_c$, $\mu < 0$: No matter how small $|\mu|$ is, the first term vanishes in the $N \to \infty$, $V \to \infty$, $\frac{N}{V} = \text{const.}$ normal thermodynamic limit

e.g. $|\mu|/kT \ll 1$: $\frac{1}{V} \frac{1}{e^{-\mu/kT} - 1} \simeq \frac{1}{V} \frac{kT}{|\mu|} \xrightarrow[V \to \infty]{} 0$ $\quad \mu \neq 0$

For the remaining sum: $$\frac{N}{V} \cong \frac{1}{V} \sum_{|\bar{p}|>0} \frac{1}{e^{\frac{\varepsilon(\bar{p}) - \mu}{kT}} - 1} = \frac{1}{V} \sum_{|\bar{p}|>0} \frac{V}{h^3} \frac{\Delta p_x \Delta p_y \Delta p_z}{e^{\frac{\varepsilon(\bar{p}) - \mu}{kT}} - 1}$$

$$L = V^{1/3} \qquad \xrightarrow[V \to \infty]{} \int_{h/L}^{\infty} \frac{4\pi p^2 dp}{h^3} \frac{1}{e^{\frac{\varepsilon(\bar{p}) - \mu}{kT}} - 1} \simeq \frac{1}{h^3} \int_0^{\infty} \frac{4\pi p^2 \, dp}{e^{\frac{\varepsilon(\bar{p}) - \mu}{kT}} - 1}$$

from this Eq. (1) follows by $x \equiv \frac{p^2}{2mkT}$ $\quad \left(\varepsilon(\bar{p}) = \frac{p^2}{2m} \right)$

$T < T_c$:

μ can become arbitrarily close to 0 as $V \to \infty$ $(N \to \infty)$, i.e., $|\mu| \sim 1/V$. In this case occupation in the ground state becomes macroscopic

$$\frac{N_0}{V} = \frac{\langle n_0 \rangle}{V} = \frac{1}{V}\frac{1}{e^{-\mu/kT}-1} \simeq \frac{1}{V}\frac{kT}{|\mu|} \sim \mathcal{O}(1)$$

Thus the ground-state contribution for $\frac{N_0}{V}$ tends to a nonzero density of particles in the ground state.

For the first excited state (and above):

$$\frac{N_1}{V} = \frac{\langle n_1 \rangle}{V} = \frac{1}{V}\frac{1}{e^{\frac{\varepsilon_1-\mu}{kT}}-1} \simeq \frac{1}{V}\frac{kT}{\varepsilon_1} \sim \frac{1}{V}\frac{kT}{1/V^{2/3}} \sim \mathcal{O}\left(1/V^{1/3}\right)$$

$$\frac{N_1}{N_0} \sim \mathcal{O}\left(\frac{1}{V^{1/3}}\right) \to 0$$

GS is macroscopically occupied, other states are not.
$\langle n_p \rangle$ is a smooth function of $(\bar{p})$ for $|\bar{p}|>0$.

for $V \to \infty$;

$$\mu \sim \mathcal{O}\left(\frac{1}{N_0}\right) \sim \mathcal{O}(1/V) \to 0$$

$$\frac{N}{V} = \frac{N_0}{V} + \frac{1}{V}\sum_{|\bar{p}|>0} \frac{1}{e^{\frac{\varepsilon(\bar{p})}{kT}}-1} \xrightarrow[V\to\infty]{} \frac{N_0}{V} + \frac{1}{h^3}\int_{h/L}^{\infty} \frac{4\pi p^2\,dp}{e^{\varepsilon(\bar{p})/kT}-1}$$

$$\longrightarrow \frac{N_0}{V} + \frac{1}{h^3}\int_0^{\infty} \frac{4\pi p^2\,dp}{e^{\varepsilon(\bar{p})/kT}-1} =$$

$$= \frac{N_0}{V} + \frac{(2\pi m kT)^{3/2}}{h^3} f^{-}_{3/2}(1)$$

(3)
$$\boxed{= \frac{N_0}{V} + \frac{(2\pi m kT)^{3/2}}{h^3}\,\zeta(3/2)}$$

Thus:

$\boxed{T > T_c:}$ $$\frac{N}{V} = \frac{(2\pi mkT)^{3/2}}{h^3} f_{3/2}(e^{\mu/kT})$$

yields solution for fixed $\frac{N}{V}$

where T_c is given by:
$$\frac{N}{V} = \frac{(2\pi mkT_c)^{3/2}}{h^3} \zeta(3/2)$$

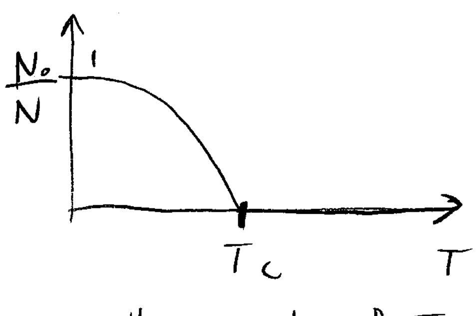
$\boxed{T < T_c:}$ $\mu \equiv 0$ in the thermodynamic limit, and the ground state is macroscopically occupied

$$\frac{N}{V} = \frac{N_0}{V} + \frac{(2\pi mkT)^{3/2}}{h^3} \zeta(3/2)$$

$\hookrightarrow \frac{V}{h^3}(2\pi mkT)^{3/2} \zeta(3/2)$: number of Bose particles above the ground state

Combining: $$\boxed{\frac{N}{V} = \frac{N_0}{V} + \frac{N}{V}\left(\frac{T}{T_c}\right)^{3/2}}$$

$$\Rightarrow \quad N_0 = N\left(1 - \left(\frac{T}{T_c}\right)^{3/2}\right) \qquad (\text{for } T < T_c)$$



$$\boxed{\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^{3/2}} \qquad (\#)$$

near the vicinity of T_c: $T = T_c - \Delta$ $\qquad \frac{\Delta}{T_c} \ll 1$

$$\frac{N_0}{N} = 1 - \left(\frac{T_c - \Delta}{T_c}\right)^{3/2} = 1 - \left(1 - \frac{\Delta}{T_c}\right)^{3/2} \simeq 1 - \left(1 - \tfrac{3}{2}\frac{\Delta}{T_c}\right) = \frac{3}{2}\frac{\Delta}{T_c} = \frac{3}{2}\frac{T_c - T}{T_c}$$

Thus, $\boxed{\frac{N_0}{N} \simeq \frac{3}{2}\frac{T_c - T}{T}}$ for $T \lesssim T_c$

Thermodynamic Behavior below T_c:

$\boxed{T < T_c}$ $E = \sum_{\bar{p}} \varepsilon(\bar{p}) \langle n_p \rangle$ or $\frac{E}{V} = \frac{1}{V} \sum_{\bar{p}} \langle n_{\bar{p}} \rangle \varepsilon(\bar{p})$

Here the $\bar{p} = 0$ contribution will not cause any problems since $\varepsilon(\bar{p} = 0) = 0$. The particles in the ground state do not contribute towards the total energy (and pressure).

Thus,

$$E = \frac{3}{2} kT\, V \frac{(2\pi mkT)^{3/2}}{h^3} f_{5/2}\left(e^{\mu/kT}\right)$$

remains correct for both $T > T_c$ and $T < T_c$

In particular, for $\boxed{T < T_c \quad \mu \equiv 0}$ for $V \to \infty$

$$\boxed{E = \frac{3}{2} kT\, V \frac{(2\pi mkT)^{3/2}}{h^3} \zeta\left(5/2\right)}$$ $\zeta(5/2) \simeq 1.341$

$$\boxed{\begin{array}{l} E = \text{const.}\, V \cdot T^{5/2} \\ C_V = \text{const.}\, V \cdot T^{3/2} \end{array}}$$

and exploiting $PV = \frac{2}{3} E$:

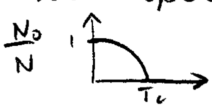
$$\boxed{P = \text{const.}\, T^{5/2}}$$ independent of the density!

increasing the density will simply "force" more particle in the ground state. These particles carry no kinetic energy, thus do not contribute to E and P.

Thermodynamic Behavior in the vicinity of T_c ($T < T_c$ and $T \gtrsim T_c$)

The Bose-Einstein condensation as a phase transition

"order parameter": $$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^{3/2} \simeq \frac{3}{2}\frac{T_c - T}{T_c} \quad \text{for } T \lesssim T_c$$



$$\frac{N_0}{N} \simeq 0 \quad \text{for } T \geqslant T_c$$

I. The chemical potential $\mu(T)$ for $T \gtrsim T_c$

In this case

$$N = V\frac{(2\pi mkT)^{3/2}}{h^3} f_{3/2}^-\left(e^{-\alpha}\right) \quad (T > T_c) \qquad \alpha \equiv -\mu/kT \ll 1$$

and

$$N = V\frac{(2\pi mkT_c)^{3/2}}{h^3} \underbrace{f_{3/2}^-(1)}_{\zeta(3/2)} \qquad (\text{at } T = T_c)$$

$$\Rightarrow \left(\frac{T_c}{T}\right)^{3/2} = \frac{f_{3/2}^-(e^{-\alpha})}{\zeta(3/2)} \qquad \zeta(\nu) = \sum_{\ell=1}^{\infty}\frac{1}{\ell^\nu}$$

need small α ($\ll 1$) expansion of $f_\nu^-(e^{-\alpha})$:

---

for $\nu < 1$ and non-integer $\nu > 1$:

$$\boxed{f_\nu^-(e^{-\alpha}) = \Gamma(1-\nu)\,\alpha^{\nu-1} + \sum_{\ell=0}^{\infty}\frac{(-1)^\ell}{\ell!}\zeta(\nu-\ell)\,\alpha^\ell}$$

e.g. $f_{3/2}^{-}(e^{-\alpha}) \simeq \Gamma(-\tfrac{1}{2})\,\alpha^{1/2} + \zeta(\tfrac{3}{2}) + \sigma(\alpha)$

$$f_{5/2}^{-}(e^{-\alpha}) \simeq \Gamma(-\tfrac{3}{2})\,\alpha^{3/2} + \zeta(\tfrac{5}{2}) - \zeta(\tfrac{3}{2})\alpha + \sigma(\alpha^2)$$

$$\simeq \zeta(\tfrac{5}{2}) - \zeta(\tfrac{3}{2})\alpha \quad + \sigma(\alpha^{3/2})$$

Note: $\Gamma(\nu) = \frac{1}{\nu}\Gamma(\nu+1)$

$\zeta(\tfrac{3}{2}) \simeq 2.612$
$\zeta(\tfrac{5}{2}) \simeq 1.341$

$$\Gamma(-\tfrac{1}{2}) = \frac{1}{(-\tfrac{1}{2})}\Gamma(\tfrac{1}{2}) = -2\sqrt{\pi}$$

$$\Gamma(-\tfrac{3}{2}) = \frac{1}{(-\tfrac{3}{2})}\Gamma(-\tfrac{1}{2}) = -\tfrac{2}{3}(-2\sqrt{\pi}) = \tfrac{4}{3}\sqrt{\pi}$$

$$\left(\frac{T_c}{T}\right)^{3/2} \simeq \frac{\zeta(\tfrac{3}{2}) - 2\sqrt{\pi}\,\alpha^{1/2}}{\zeta(\tfrac{3}{2})} = 1 - \frac{2\sqrt{\pi}}{\zeta(\tfrac{3}{2})}\alpha^{1/2} \qquad (\alpha \equiv -\mu/kT)$$

$T \gtrsim T_c$

$\alpha \ll 1$ let $T = T_c + \Delta$ $\quad \Delta/T_c \ll 1$

$$\left(\frac{T_c}{T_c+\Delta}\right)^{3/2} = \frac{1}{(1+\Delta/T_c)^{3/2}} \simeq \frac{1}{1+\tfrac{3}{2}\frac{\Delta}{T_c}} \simeq 1 - \tfrac{3}{2}\frac{\Delta}{T_c} = 1 - \tfrac{3}{2}\frac{T-T_c}{T_c}$$

$$\Rightarrow \quad 1 - \tfrac{3}{2}\frac{T-T_c}{T_c} \simeq 1 - \frac{2\sqrt{\pi}}{\zeta(\tfrac{3}{2})}\sqrt{-\mu/kT}$$

$$-\mu/kT \cong \left(\frac{3\,\zeta(\tfrac{3}{2})}{4\sqrt{\pi}}\right)^2 \left(\frac{T-T_c}{T_c}\right)^2$$

(5) $$\boxed{\mu \simeq -kT\left(\frac{3\,\zeta(\tfrac{3}{2})}{4\sqrt{\pi}}\right)^2\left(\frac{T-T_c}{T_c}\right)^2}$$ for $T \gtrsim T_c$

II The energy and the specific heat around the transition point T_c

$$E = \frac{3}{2} kT\, V \frac{(2\pi mkT)^{3/2}}{h^3}\, \zeta\left(\tfrac{5}{2}\right) \qquad \text{for } T < T_c$$

$$E = \frac{3}{2} kT\, V \frac{(2\pi mkT)^{3/2}}{h^3}\, \bar{f}_{5/2}(e^{-\alpha}) \qquad \text{for } T > T_c$$

Thus, for $T \gtrsim T_c$:

$$\bar{f}_{5/2}(e^{-\alpha}) \simeq \zeta\left(\tfrac{5}{2}\right) - \zeta\left(\tfrac{3}{2}\right)\alpha$$

i.e.

$$E = \begin{cases} \frac{3}{2} kT\, V \frac{(2\pi mkT)^{3/2}}{h^3}\, \zeta\left(\tfrac{5}{2}\right) & \text{for } T < T_c \\ \frac{3}{2} kT\, V \frac{(2\pi mkT)^{3/2}}{h^3}\left(\zeta\left(\tfrac{5}{2}\right) - \zeta\left(\tfrac{3}{2}\right)\alpha\right) & \text{for } T \gtrsim T_c \end{cases}$$

where $\boxed{\alpha \simeq \left(\frac{3\,\zeta(3/2)}{4\sqrt{\pi}}\right)^2 \left(\frac{T - T_c}{T_c}\right)^2}$ (see (5))