Thermodynamical Properties of a Rotating Ideal Bose Gas

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In Ref. [6] an amount of $3 \times 10^5$ atoms of $^{87}\text{Rb}$ is set into rotation with another laser beam acting as a stirrer. The laser creates an anisotropic potential in the $xy$-plane which rotates with frequency $\Omega$. In the corotating frame, the resulting trapping potential can be written as

$$V_{\text{rot}}(x, \Omega) = \frac{M}{2} \left( \omega^2_0 - \Omega^2 \right) r^2 + \frac{M}{2} \omega^2 z^2 + \frac{k}{4} r^4,$$

where $\omega_0 = \omega_x - 4U_0 M^{-1} w^{-2} = 2\pi \times 64.8 \text{ Hz}$ and $M$ is the atomic mass. The last term in (1) corresponds to the quartic anharmonicity with $k = 8U_0 w^{-4} = 2.6 \times 10^{-11} \text{ J m}^{-4}$.

In the following we treat the Bose gas in the anharmonic trap (1) within the grand-canonical ensemble and determine the critical temperature, the condensate fraction, and the heat capacity of the Bose gas within a semiclassical approximation. In our discussion the rotation frequency $\Omega$ appears as a control parameter. The Paris experiment [6] allows rotation frequencies $\Omega$ up to $1.04 \times \omega_\perp$.

However, in the present theoretical discussion, we consider arbitrarily large rotation frequencies. In Fig. 1 we depict how the trapping potential (1) varies with increasing rotation frequency $\Omega$. For small rotation frequencies $\Omega < \omega_\perp$, the potential (1) is convex, for the critical rotation frequency $\Omega = \omega_\perp$ it is purely quartic in the perpendicular plane, and for a fast rotation frequency $\Omega > \omega_\perp$ the trap has the shape of a Mexican hat. In our discussion, we focus on two particular rotation frequencies, namely the critical rotation frequency $\Omega = \omega_\perp$ and the limit of an infinite fast rotation frequency $\Omega \rightarrow \infty$ as the potential reduces to power laws in both cases. Such potentials were investigated some time ago as they lead to analytic formulas for the respective thermodynamical properties [7, 8]. Note that the case $\Omega \rightarrow \infty$ corresponds to a trap where the bosons are confined to a cylinder of radius $r_{\text{cycl}} = \sqrt{M^2 \omega^2_z (\Omega^2 - \omega^2_\perp)/(\hbar k)}$. Thus, the above mentioned experimental restriction $r_{\text{cycl}} < w/2$ allows to determine a maximum rotation frequency $\Omega_{\text{max}}$ for which the anharmonic potential (1) of the Paris experiment is

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valid. The resulting value $\Omega_{\text{max}} = 1.08 \times \omega_\perp$ shows that considering an infinite rotation frequency $\Omega \to \infty$ is not suitable for this experiment.

II. IDEAL BOSE GAS IN ROTATING TRAP

We consider $N$ particles of an ideal Bose gas which are distributed over various quantum states $\nu$ of the system. These states are characterized by the population $n_n$ of the one-particle state $n$ of the trap (1), such that the energy levels are $E_\nu = \sum_n n_n E_n$, where $E_n$ denotes the one-particle energy. Correspondingly, the number of particles in state $\nu$ are given by $N_\nu = \sum_n n_n$. The resulting grand-canonical ensemble is determined by its partition function

$$Z = \sum_\nu \exp \left[ -\beta (E_\nu - \mu N_\nu) \right],$$

where $\beta = 1/(k_B T)$ denotes an inverse temperature, $k_B$ is Boltzmann’s constant, and $\mu$ is the chemical potential. The corresponding grand-canonical free energy $F = -(1/\beta) \ln Z$ allows to calculate all relevant thermodynamical quantities [9, 10]. Around the minimum, the trap (1) has a small curvature so that the energy levels are close to each other. With increasing rotation frequency, the curvature decreases until the critical rotation frequency $\Omega = \omega_\perp$ is reached. Not until the rotation frequency overcompensates the harmonic part of the trap, the curvature increases again. Thus, for all experimentally realized rotation frequencies $0 \leq \Omega \leq 1.04 \times \omega_\perp$, our system can be described by the discrete ground state $E_0$, which must be retained quantum-mechanically, plus a continuum of states above $E_0$. Within this semiclassical approximation, we can set the ground-state energy $E_0$ to zero so that the grand-canonical free energy of the ideal Bose gas reads

$$F = N_0(\mu_c - \mu)$$

The critical chemical potential $\mu_c$, where the condensation emerges, is determined by the condition $H(x, p) - \mu_c > 0$ and is therefore given by $\mu_c = \min_x V_{\text{rot}}(x, \Omega)$. Due to (1) it reads explicitly

$$\mu_c = \begin{cases} 0 & ; \Omega \leq \omega_\perp, \\
-\frac{M^2}{4k} (\omega_\perp^2 - \Omega^2) & ; \Omega > \omega_\perp. \end{cases}$$

Performing the phase-space integral in (3), we obtain

$$F = N_0(\mu_c - \mu) - \frac{\zeta_4(e^{\beta \mu}, \Omega)}{\beta^4 \hbar^4 \omega_z (\omega_\perp^2 - \Omega^2)},$$

where we have introduced the generalized $\zeta$-function

$$\zeta_4(e^{\beta \mu}, \Omega) = \sum_{j=1}^{\infty} \frac{e^{2j\beta \mu}}{j^4 \sqrt{\Omega \gamma T}} \left( \omega_\perp^2 - \Omega^2 \right)^2 \exp \left[ j \gamma T \left( \omega_\perp^2 - \Omega^2 \right)^2 \right] \text{erfc} \left[ \sqrt{j \gamma T} \left( \omega_\perp^2 - \Omega^2 \right) \right]$$

with the complementary error function

$$\text{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^{\infty} dt \, e^{-t^2}.$$
generalized $\zeta$-function (7) reduces to the polylogarithmic function
\[
\lim_{\nu \to \nu_0} \zeta_\nu(z, \Omega) = \zeta_\nu(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^\nu}, \quad (9)
\]
which is related to the Riemann $\zeta$-function via
\[
\zeta_\nu(1) = \zeta(\nu) = \sum_{j=1}^{\infty} \frac{1}{j^\nu}. \quad (10)
\]

Furthermore, we note that in the limit of the critical rotation frequency $\Omega \to \omega_\perp$, the generalized $\zeta$-function (7) reads
\[
\lim_{\Omega \to \omega_\perp} \frac{\zeta_\nu(z, \Omega)}{\omega^2_{\perp} - \Omega^2} = \sqrt{\pi \gamma_T} \zeta_{\nu-1/2}(z) \quad (11)
\]
and in the limit of an infinite fast rotation it is approximated by
\[
\frac{\zeta_\nu(z, \Omega)}{\omega^2_{\perp} - \Omega^2} \approx 2\sqrt{\pi \gamma_T} \sum_{j=1}^{\infty} \frac{z^j e^{\gamma_T}(\omega^2_{\perp} - \Omega^2)^j}{j^{\nu-1/2}}; \quad \Omega \to \infty, \quad (12)
\]

III. CONDENSATE DENSITY

From the grand-canonical free energy (6) we read off that the number of particles $N = -(\partial F/\partial \mu)_{T,V}$ of an ideal Bose gas is given by a sum of $N = N_0 + N_c$ of particles in the ground state $N_0$ and particles in excited states $N_c$:
\[
N = N_0 + \frac{\zeta_3(\mu, \Omega)}{\beta^3 \hbar \omega_{\perp}(\omega^2_{\perp} - \Omega^2)}. \quad (13)
\]
The critical temperature $T_c$ at which the condensation emerges can be found from Eq. (13) by setting $N_0 = 0$ and $\mu = \mu_c$. For undercritical rotation frequencies $\Omega < \omega_\perp$ and vanishing anharmonicity $k \downarrow 0$, we apply (9) so that the critical temperature reads
\[
T_c = \frac{\hbar \omega_{\perp}}{k_B} \left( \frac{\omega^2_{\perp} - \Omega^2}{\omega^2_{\perp} \zeta(3)} \right)^{1/3}; \quad k = 0. \quad (14)
\]

For a non-vanishing anharmonicity $k$, the critical temperature can not be determined explicitly because it appears in Eq. (13) transcendentally. However, there are two special cases in which we obtain an analytical expression for the critical temperature. At first, for the critical rotation $\Omega = \omega_\perp$, we find with (11) [11]:
\[
T_c = \frac{\hbar \omega_{\perp}}{k_B} \left( \frac{4k h}{\pi M^2 \omega^2_{\perp}} \right)^{1/5} \left( \frac{\zeta(5/2)}{N} \right)^{2/5}. \quad (15)
\]
Secondly, the limit of an infinite fast rotation frequency $\Omega \to \infty$ leads with (12) to the critical temperature
\[
T_c = \frac{\hbar \omega_{\perp}}{k_B} \left( \frac{k h}{\pi M^2 \omega^2_{\perp}} \right)^{1/5} \left( \frac{\zeta(5/2)}{N} \right)^{2/5}, \quad (16)
\]
which is by a factor $(1/4)^{1/5} \approx 0.76$ smaller than the previous one. A numerical evaluation of the critical temperature obtained from (13) is shown in Fig. 2 for the values of the Paris experiment [12]. For the non-rotating trap, we see that the anharmonicity only slightly affects the critical temperature. With increasing rotation frequency $\Omega$, the critical temperature decreases and the difference between the harmonic and the anharmonic trap is clearly seen. At the critical rotation frequency $\Omega = \omega_\perp$, the critical temperature is $T_c = 63.5$ kN which is about three times smaller than the one estimated for the Paris experiment [6].

From the number of particles (13), we also obtain the condensate fraction in the temperature regime $T < T_c$. Here the chemical potential coincides with the critical

FIG. 3: Condensate fraction versus reduced temperature. The solid line corresponds to the condensate fraction (19) of a Bose gas in the trap (1) for the rotation frequency $\Omega = 0$ and the parameters of the Paris experiment [6]. The dashed line corresponds to the condensate fraction at the critical $\Omega = \omega_\perp$ and at the infinite fast $\Omega \to \infty$ rotation frequency given by Eq. (18).

FIG. 4: Condensate fraction versus reduced temperature. The critical temperature is evaluated for various rotation frequencies $\Omega$, the solid line corresponds to $\Omega = 0$ to which the temperature is normalized. The other lines are for $\Omega = \omega_{\perp}/\sqrt{2}$ (short dashes), $\Omega = \omega_\perp$ (longer dashes), and $\Omega = \sqrt{3/2} \times \omega_\perp$ (long dashes).
one given by Eq. (5). For undercritical rotation frequencies $\Omega < \omega_\perp$ and vanishing anharmonicity $k \downarrow 0$, we use (9) so that the condensate fraction is given by

$$\frac{N_0}{N} = 1 - \left( \frac{T}{T_c} \right)^3 ; k = 0.$$  

(17)

Furthermore, applying (11) and (12) in the cases $\Omega = \omega_\perp$ and $\Omega \rightarrow \infty$, respectively, yields with the critical chemical potential (5) the following condensate fraction:

$$\frac{N_0}{N} = 1 - \left( \frac{T}{T_c} \right)^{5/2}.$$  

(18)

Here, $T_c$ is given by (14) and (15), (16), respectively. In general, the condensate fraction is given by

$$\frac{N_0}{N} \approx \begin{cases} 
1 - \frac{k_B \zeta(3)}{Nh^4 \omega (\omega^2 - \Omega^2)} T^3 ; \Omega < \omega_\perp, \\
1 - \frac{M \sqrt{\pi k_B T \zeta(5/2)}}{N \sqrt{2 \pi T \omega^2}} T^{5/2} ; \Omega > \omega_\perp.
\end{cases}$$  

(20)

The temperature dependence of the condensate fraction $N_0/N$ following from (19) is shown in Fig. 3 and Fig. 4. From this we read off that the temperature dependence of the condensate fraction depends crucially on the rotation frequency and is thus not universal.

IV. HEAT CAPACITY

The heat capacity follows from the grand-canonical free energy $F = U - TS - \mu N$, where $U$ is the internal energy and $S$ is the entropy, according to

$$C = \frac{\partial U}{\partial T} \bigg|_{N,V}.$$  

(21)

Within the grand-canonical ensemble, the heat capacity has to be determined separately in the two regimes $T > T_c$ and $T < T_c$.

A. Gase Phase

At first, we treat the gas phase where $N_0 = 0$ and determine the entropy via the thermodynamical relation

$$S = -(\partial F/\partial T)_{V,\mu}.$$  

$$\frac{S_\geq}{k_B N} = \frac{7 \zeta_4(e^{\beta \mu}, \Omega)}{2 \zeta_3(e^{\beta \mu}, \Omega)} + \gamma_T (\omega_\perp^2 - \Omega^2)^2 \frac{\zeta_3(e^{\beta \mu})}{\zeta_5(e^{\beta \mu}, \Omega)}$$

$$- \left[ \beta \mu + \gamma_T (\omega_\perp^2 - \Omega^2)^2 \right]$$  

(22)

The internal energy $U = F + TS + \mu N$ then follows from (6), (13), (22) and reads

$$\frac{U_\geq}{N k_B T} = \frac{5 \zeta_4(e^{\beta \mu}, \Omega)}{2 \zeta_3(e^{\beta \mu}, \Omega)}$$

$$+ \gamma_T (\omega_\perp^2 - \Omega^2)^2 \left[ \frac{\zeta_3(e^{\beta \mu})}{\zeta_5(e^{\beta \mu}, \Omega)} - 1 \right].$$  

(23)

Finally, the heat capacity (21) for temperatures above $T_c$ is given by

$$\frac{C_\geq}{k_B N} = \frac{35 \zeta_4(e^{\beta \mu}, \Omega)}{4 \zeta_3(e^{\beta \mu}, \Omega)} - \frac{25 \zeta_4(e^{\beta \mu}, \Omega)}{4 \zeta_3(e^{\beta \mu}, \Omega)}$$

$$+ \gamma_T (\omega_\perp^2 - \Omega^2)^2 \frac{11 \zeta_3(e^{\beta \mu})}{2 \zeta_3(e^{\beta \mu}, \Omega)} - \frac{5 \zeta_3(e^{\beta \mu})}{2 \zeta_3(e^{\beta \mu}, \Omega)}$$

$$+ \gamma_T^2 (\omega_\perp^2 - \Omega^2)^4 \frac{12 \zeta_3(e^{\beta \mu})}{\zeta_5(e^{\beta \mu}, \Omega)} - \frac{9 \zeta_3(e^{\beta \mu})}{\zeta_5(e^{\beta \mu}, \Omega)}.$$  

(24)

To obtain this result, we have determined the derivative $(\partial \beta \mu/\partial T)_{V,\mu}$ from (13). In the limit $k \downarrow 0$ of a harmonic trap, the heat capacity (24) reduces to the well-known result

$$\frac{C_\geq}{k_B N} = \frac{12 \zeta_4(e^{\beta \mu}, \Omega)}{\zeta_3(e^{\beta \mu}, \Omega)} - \frac{9 \zeta_3(e^{\beta \mu})}{\zeta_5(e^{\beta \mu}, \Omega)} ; k = 0.$$  

(25)

Again, both cases $\Omega = \omega_\perp$ and $\Omega \rightarrow \infty$ yield the same analytic expression:

$$\frac{C_\geq}{k_B N} = \frac{\zeta_4(3/2, e^{\beta \mu + \gamma_T (\omega_\perp^2 - \Omega^2)^2})}{4 \zeta_3(3/2, e^{\beta \mu + \gamma_T (\omega_\perp^2 - \Omega^2)^2})} - \frac{25 \zeta_5/2(3/2, e^{\beta \mu + \gamma_T (\omega_\perp^2 - \Omega^2)^2})}{4 \zeta_3(3/2, e^{\beta \mu + \gamma_T (\omega_\perp^2 - \Omega^2)^2})}.$$  

(26)
Now, we investigate the heat capacity (24) in the high temperature limit $T \to \infty$. To this end we use a large $T$-expansion of the generalized $\zeta$-function (7):

$$\zeta_\nu(z, \Omega) \approx e^{\beta \mu \left(\sqrt{\pi/\nu}T (\omega_+^2 - \Omega^2) - 2\gamma_T (\omega_+^2 - \Omega^2)^2 \right) + \ldots}$$

$$+ \frac{e^{2\beta \mu}}{2^\nu} \left[ \sqrt{2\gamma_T (\omega_+^2 - \Omega^2)} - 4\gamma_T (\omega_+^2 - \Omega^2)^2 \right] + \ldots$$

Inserting the expansion (27) into the number of particles (13), we find for the first order of the fugacity $e^{\beta \mu} \approx 2N \sqrt{\hbar^2 \omega_+^2 k / \pi M^2 k_B^2 T^2}$, so that the heat capacity (24) behaves like

$$\frac{C_\nu}{k_B N} \approx \frac{5}{2} + \frac{\gamma_T}{4 \sqrt{\pi}} (\omega_+^2 - \Omega^2) - \frac{\gamma_T^3 (4 - \pi)}{32 \pi^3/2} (\omega_+^2 - \Omega^2)^3.$$  

(28)

Thus, the heat capacity approaches the Dulong-Petit law in an anharmonic trap limit $T \to \infty$, $C_\nu/(k_B N) = 5/2$ which is 1/2 smaller than the corresponding one in the harmonic trap. Furthermore, the first $\Omega$ dependent term in (28) changes its behavior, from being larger ($\Omega > \omega_+^2$) than the limit to being smaller ($\Omega < \omega_+^2$), see Fig. 5.

At the critical point, the harmonic heat capacity (25) reduces for small rotation frequencies $\Omega < \omega_+$ to

$$\lim_{T \to T_c} \frac{C_\nu}{k_B N} = \frac{12 \zeta(4)}{\zeta(3)} - \frac{9 \zeta(3)}{\zeta(2)} \approx 4.23 ; k = 0.$$  

(29)

In both limits $\Omega = \omega_+$, and $\Omega \to \infty$, the heat capacity (26) at the critical point is given by

$$\lim_{T \to T_c} \frac{C_\nu}{k_B N} = \frac{35 \zeta(7/2)}{4 \zeta(5/2)} - \frac{25 \zeta(5/2)}{4 \zeta(3/2)} \approx 4.14.$$  

(30)

### B. Condensate Phase

Now we turn to the condensate phase $T < T_c$ where the chemical potential is given by (5). For the entropy, we obtain

$$S_\nu \approx \left( \frac{T}{T_c} \right)^3 \left\{ \frac{7 \zeta_3 (e^{\beta \mu}, \Omega)}{2 \zeta_3 (e^{\beta \mu}, \Omega)} - \beta \mu \frac{\zeta_3 (e^{\beta \mu}, \Omega)}{\zeta_3 (e^{\beta \mu}, \Omega)} \right\} + \gamma_T (\omega_+^2 - \Omega^2)^2 \left[ \zeta_3 (e^{\beta \mu}, \Omega) - \zeta_3 (e^{\beta \mu}, \Omega) \right].$$

(31)

The internal energy below the critical temperature reads

$$\frac{U_\nu}{N k_B T} = \left( \frac{T}{T_c} \right)^3 \left\{ \frac{11 \zeta_3 (e^{\beta \mu}, \Omega)}{2 \zeta_3 (e^{\beta \mu}, \Omega)} - 5 \Theta (\omega_+ - \Omega) \frac{\zeta_3 (e^{\beta \mu}, \Omega)}{\zeta_3 (e^{\beta \mu}, \Omega)} \right\} + \mu_c N,$$

(32)

where $\Theta$ denotes the Heaviside function. Thus, we find for the heat capacity below the critical temperature with help of Eq. (5)

$$\frac{C_\nu}{k_B N} = \left( \frac{T}{T_c} \right)^3 \left\{ \frac{35 \zeta_3 (e^{\beta \mu}, \Omega)}{4 \zeta_3 (e^{\beta \mu}, \Omega)} \right\} + \gamma_T (\omega_+^2 - \Omega^2)^2 \left[ \zeta_3 (e^{\beta \mu}, \Omega) - \zeta_3 (e^{\beta \mu}, \Omega) \right].$$

(33)

In the limit $k \downarrow 0$, Eq. (33) simplifies to

$$\frac{C_\nu}{k_B N} = \frac{12 \zeta(4)}{\zeta(3)} \left( \frac{T}{T_c} \right)^3 ; k = 0.$$  

(34)

Thus, at the critical point it has the value

$$\lim_{T \to T_c} \frac{C_\nu}{k_B N} = \frac{12 \zeta(4)}{\zeta(3)} \approx 10.80 ; k = 0.$$  

(35)

In both limits $\Omega = \omega_+$ and $\Omega \to \infty$, the heat capacity is given by

$$\frac{C_\nu}{k_B N} = \frac{35 \zeta(7/2)}{4 \zeta(5/2)} \left( \frac{T}{T_c} \right)^{5/2}$$

(36)

so that the heat capacity (33) at the critical point reduces to

$$\lim_{T \to T_c} \frac{C_\nu}{k_B N} = \frac{35 \zeta(7/2)}{4 \zeta(5/2)} \approx 7.35.$$  

(37)

In the low temperature limit $T \downarrow 0$, the heat capacity (33) tends to zero in accordance with the third law of thermodynamics. We note that the low-temperature limit of the heat capacity (38) has the same power-law behavior as the corresponding one of the condensate fraction (20):

$$\frac{C_\nu}{k_B N} \approx \left\{ \begin{array}{ll}
\frac{35k_B^3 \zeta_3 (4)}{4Nh^2 \omega_+^2 (\omega_+^2 - \Omega^2)^2} T^3 ; & \Omega < \omega_+ \\
\frac{35M \sqrt{\pi/8} k_B^{5/2} \zeta_3 (7/2)}{4N k_B h^2 \omega_+^2} T^{5/2} ; & \Omega > \omega_+.
\end{array} \right.$$  

(38)
the critical temperature $T_c$ of the anharmonic trap (1) for varying rotation frequencies. The lines correspond to $\Omega = 0$ (solid), $\Omega = \omega_{\perp}$ (long dashes), and $\Omega = 2\omega_{\perp}$ (short dashes). The gray solid line corresponds to the Dulong-Petit law, the first term of (28). We note that for $\Omega = 2\omega_{\perp}$ and $T > T_c$ the heat capacity approaches the Dulong-Petit limit from below (see Fig. 5).

Fig. 6 shows the temperature dependence of the heat capacity for the values of the Paris experiment without rotation [6]. We see that the effect of the anharmonicity is rather small. According to Ehrenfest's classification, the discontinuity at the critical temperature characterizes the phase transition to be of second order. In Fig. 7 we show how the heat capacity depends on the rotation frequency $\Omega$. Here, the rotation has a huge influence on the temperature dependence of the heat capacity.

V. CONCLUSIONS

We have determined a semiclassical approximation for the critical temperature $T_c$ at which the condensation of a rotating ideal Bose gas occurs in the anharmonic trap (1). We have found that condensation is possible even in the overcritical rotation regime $\Omega > \omega_{\perp}$ which is in contrast with the harmonic trap where the condensate gets lost, when the rotation frequency $\Omega$ gets close to the trap frequency $\omega_{\perp}$. Our value for the critical temperature $T_c \approx 64 \text{nK}$ at the critical rotation frequency $\Omega = \omega_{\perp}$ yields $k_B T_c / \hbar \omega_{\perp} \approx 120 \gg 1$ which justifies a posteriori our semiclassical treatment. However, the value $T_c \approx 64 \text{nK}$ is about three times smaller than the one estimated in the Paris experiment [6]. This huge discrepancy could not be explained with the circumstance that our semiclassical analysis of the rotating ideal Bose gas neglects three important aspects, namely finite-size corrections, interactions between the particles, and the effect of vortices in the condensate. All three should have the effect of lowering the critical temperature. In a harmonic trap, it was found numerically that the finiteness of the system slightly lowers the critical temperature [13] which was also shown analytically [14, 15]. Furthermore, an additional weak repulsive two-particle contact interaction leads to a negative shift of just a few percent [16, 17]. Therefore, we conclude that our semiclassical findings ask for a revised experimental measurement of the critical temperature for a rotating Bose gas.

For the condensate fraction, we can state that the low-temperature behavior crucially depends on the rotation frequency $\Omega$. It shows a non-uniform temperature dependence which is in between the two power-laws $T^{5/2}$ and $T^3$.

The heat capacity of the rotating ideal Bose gas is discontinuous at the critical temperature. It tends in agreement with the third law of thermodynamics to zero in the low temperature limit $T \downarrow 0$, and approaches the Dulong-Petit law (28) in the high temperature limit $T \rightarrow \infty$ from above ($\Omega \leq \omega_{\perp}$) or from below ($\Omega > \omega_{\perp}$).

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