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Theoretical Statistical Physics

Solution to Exercise Sheet 11

1 Symmetric states (1 point)

The (anti-)symmetrized many-particle states are defined as

$$|\alpha_1, \dots, \alpha_n\rangle_\pm = \mathcal{P}_\pm |\alpha_1\rangle \otimes \cdots \otimes |\alpha_n\rangle = \frac{1}{n!} \sum_{\pi \in S_n} (\pm 1)^\pi |\alpha_{\pi(1)}\rangle \otimes \cdots \otimes |\alpha_{\pi(n)}\rangle \tag{1}$$

Show that

$$|\alpha_1, \alpha_2, \alpha_3\rangle_- = -|\alpha_2, \alpha_1, \alpha_3\rangle_- \tag{2}$$

$$|\alpha_1, \alpha_2, \alpha_3\rangle_+ = +|\alpha_2, \alpha_1, \alpha_3\rangle_+. \tag{3}$$

Written out explicitly, the states (2) and (3) are

$$\begin{aligned} |\alpha_1, \alpha_2, \alpha_3\rangle_\pm = \frac{1}{3!}\Big(&|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes |\alpha_3\rangle \pm |\alpha_1\rangle \otimes |\alpha_3\rangle \otimes |\alpha_2\rangle \pm |\alpha_2\rangle \otimes |\alpha_1\rangle \otimes |\alpha_3\rangle \\ &+ |\alpha_2\rangle \otimes |\alpha_3\rangle \otimes |\alpha_1\rangle + |\alpha_3\rangle \otimes |\alpha_1\rangle \otimes |\alpha_2\rangle \pm |\alpha_3\rangle \otimes |\alpha_2\rangle \otimes |\alpha_1\rangle \Big). \end{aligned} \tag{4}$$

Exchanging $|\alpha_1\rangle$ and $|\alpha_2\rangle$, we get

$$\begin{aligned} |\alpha_2, \alpha_1, \alpha_3\rangle_\pm &= \frac{1}{3!}\Big(|\alpha_2\rangle \otimes |\alpha_1\rangle \otimes |\alpha_3\rangle \pm |\alpha_2\rangle \otimes |\alpha_3\rangle \otimes |\alpha_1\rangle \pm |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes |\alpha_3\rangle \\ &\qquad + |\alpha_1\rangle \otimes |\alpha_3\rangle \otimes |\alpha_2\rangle + |\alpha_3\rangle \otimes |\alpha_2\rangle \otimes |\alpha_1\rangle \pm |\alpha_3\rangle \otimes |\alpha_1\rangle \otimes |\alpha_2\rangle \Big) \\ &= \pm\frac{1}{3!}\Big(|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes |\alpha_3\rangle \pm |\alpha_1\rangle \otimes |\alpha_3\rangle \otimes |\alpha_2\rangle \pm |\alpha_2\rangle \otimes |\alpha_1\rangle \otimes |\alpha_3\rangle \\ &\qquad + |\alpha_2\rangle \otimes |\alpha_3\rangle \otimes |\alpha_1\rangle + |\alpha_3\rangle \otimes |\alpha_1\rangle \otimes |\alpha_2\rangle \pm |\alpha_3\rangle \otimes |\alpha_2\rangle \otimes |\alpha_1\rangle \Big) \\ &= \pm |\alpha_1, \alpha_2, \alpha_3\rangle_\pm. \end{aligned} \tag{5}$$

2 Number fluctuations (2 points)

Consider the occupation probability

$$\langle n_k \rangle_g = -\frac{1}{\beta} \frac{\partial}{\partial \epsilon_k} \ln(Z_g) \tag{6}$$

of a single mode k both in an ideal Bose and Fermi gas in the grand canonical ensemble. Compute the fluctuations of the occupation probability, $\langle n_k^2 \rangle - \langle n_k \rangle^2$, and express it in terms of $\langle n_k \rangle$. Show that the fluctuations of the total particle number $\Delta N = \langle N^2 \rangle - \langle N \rangle^2$ scale linearly with volume.

Ideal quantum gases are systems containing a large number of non-interacting particles. Each individual particle occupies a state that is in no way altered from that of a solitary particle. The total energy is simply the sum of individual particle energies. Quantum gases thus form tensor products of states out of a single-particle Hilbert space $\mathcal{H}$, making them perfectly suited for a description i.t.o. elements of a Fock space $\mathcal{F}_\pm$. In order to compute the statistics of such systems, we first need the grand partition function $Z_g^\pm$.

Computing it requires a basis for $\mathcal{F}_\pm$. The occupation number basis consists of states of the form

$$\begin{aligned} |\{n_i\}_i^\pm\rangle = |n_0, n_1, n_2, \dots\rangle_\pm &= \mathcal{P}_\pm \bigotimes_{i=0}^{\infty} |\psi_i\rangle^{\otimes n_i} \\ &= \mathcal{P}_\pm |\psi_0\rangle^{\otimes n_0} \otimes |\psi_1\rangle^{\otimes n_1} \otimes \dots . \end{aligned} \tag{7}$$

It draws upon a single-particle basis $\{|\psi_n\rangle\}_{n\in\mathbb{N}_0}$ of $\mathcal{H}$ to denote with n_i the number of particles in state $|\psi_i\rangle$ with $i \in \mathbb{N}_0$ where i labels all basis elements of $\mathcal{H}$.[1]

States of the form (7) offer the huge advantage that they are eigenstates of both the number operator $\hat{N}$ and the Hamiltonian $\hat{H}$ on $\mathcal{F}_\pm$:

$$\hat{N}\,|n_0, n_1, \dots, n_k\rangle_\pm = \sum_{i=0}^{\infty} n_i\,|n_0, n_1, \dots, n_k\rangle_\pm, \tag{8}$$

$$\hat{H}\,|n_0, n_1, \dots, n_k\rangle_\pm = \sum_{i=0}^{\infty} n_i\,\epsilon_i\,|n_0, n_1, \dots, n_k\rangle_\pm. \tag{9}$$

ϵ_i here denotes the energy of the single-particle state $|\psi_i\rangle$.

Equipped with a basis, we can calculate the grand partition function on $\mathcal{F}_\pm$ as the trace over the grand canonical weighting factor,

$$Z_g^\pm = \mathrm{tr}_{\mathcal{F}_\pm}\big(e^{-\beta(\hat{H}-\mu\,\hat{N})}\big) = \sum_{N=0}^{\infty} \sum_{\{n_i\}_i^\pm} \langle\{n_i\}_i^\pm|e^{-\beta(\hat{H}-\mu\,\hat{N})}|\{n_i\}_i^\pm\rangle\,\delta_{N,\sum n_i}. \tag{10}$$

This is a rather complicated sum running over all possible combinations of occupation numbers n_i of all single-particle states $|\psi_i\rangle \in \mathcal{H}$. The Kronecker symbol ensures that in each term of the sum over N only configurations with the correct number of total particles appear. If we had instead chosen to work in the canonical ensemble, we would still have this restriction but the sum over N (and the fugacity $z^{\hat{N}} = e^{\beta\mu\hat{N}}$), would be absent from the partition function, making the evaluation of Z_c extremely difficult. The sum over all possible number of particles turns out to be a crucial advantage of the grand canonical ensemble when it comes to quantum gases.

We make full use of it by dropping both the sum over N and the Kronecker symbol. This lets the n_i roam freely, so to speak. We still sum over all possibilities of distributing an arbitrary number of particles (up to infinitely many) onto the single-particle states in $\mathcal{H}$, thus still taking into account every possible value for the total particle number N. By furthermore using (8) and (9), $Z_g^\pm$ factorizes into

$$\begin{aligned} Z_g^\pm &= \sum_{\{n_i\}_i^\pm} e^{-\beta\sum_{j=0}^{\infty} n_j(\epsilon_j-\mu)} \underbrace{\langle\{n_i\}_i^\pm|\{n_i\}_i^\pm\rangle}_{=1} \\ &= \sum_{n_0^\pm=0}^{\infty\text{ or }1} \sum_{n_1^\pm=0}^{\infty\text{ or }1} \sum_{n_2^\pm=0}^{\infty\text{ or }1} \cdots \prod_{j=0}^{\infty} e^{-\beta\,n_j(\epsilon_j-\mu)} = \prod_{j=0}^{\infty} \sum_{n_j^\pm=0}^{\infty\text{ or }1} e^{-\beta\,n_j(\epsilon_j-\mu)}. \end{aligned} \tag{11}$$

For fermions, the sum over n_j^- contains only two terms,

$$Z_g^- = \prod_{j=0}^{\infty}\Big(1 + e^{-\beta\,(\epsilon_j-\mu)}\Big), \tag{12}$$

[1] We are working exclusively with separable Hilbert spaces here. This guarantees that even if the number of basis vectors becomes infinite, they remain countable since any separable Hilbert space $\mathcal{H}$ contains a countable subset with countable basis whose span is dense in $\mathcal{H}$.

while for bosons, we may use the geometric series to get

$$Z_g^+ = \prod_{j=0}^{\infty} \frac{1}{1 - e^{-\beta\,(\epsilon_j - \mu)}}. \tag{13}$$

There is an important point to consider here. The geometric series will only converge if $\epsilon_j - \mu > 0\ \forall\, j$, i.e. if all single-particle energies are larger than the chemical potential. Since we take $\hat{H}$ to be a trace class operator, i.e. a compact operator for which a trace may be defined such that it is finite and basis-independent, it follows that the spectrum $\{\epsilon_j\}_j$ of eigenvalues of $\hat{H}$ can accumulate only at zero. To understand why, remember that in general, we are operating on infinite-dimensional Hilbert spaces $d = \dim(\mathcal{H}) = \infty$. Since $\hat{H}^\dagger = \hat{H}$ is self-adjoint, the set of eigenvectors $B = \{|\epsilon_j\rangle\}_j$ of $\hat{H}$ form an orthogonal basis of $\mathcal{H}$. The cardinality of the basis is $|B| = d$, i.e. there are infinitely many basis vectors. The trace of $\hat{H}$ evaluated in its eigenbasis therefore gives an infinite sum over all eigenvalues times their degeneracy. This will only be finite if the $\{\epsilon_j\}_j$ form a null sequence, i.e. if $\lim_{j\to\infty} \epsilon_j = 0$. To cut a long story short, the bosonic grand partition function can only be computed in this way for systems with $\mu < 0$ to ensure $\epsilon_j - \mu > 0\ \forall\, j$. For fermions, due to their capped occupation number, μ remains unrestricted.

Now that we have an explicit expression for $Z_g^\pm$, we can use it to calculate occupation numbers for all single-particle states by differentiating w.r.t. that state's energy as in (6). To see this, note that

$$\begin{aligned}\langle n_k\rangle_\pm &= \frac{1}{Z_g^\pm}\,\mathrm{tr}_{\mathcal{F}_\pm}\big(n_i\, e^{-\beta(\hat{H} - \mu\,\hat{N})}\big) = \frac{1}{Z_g^\pm} \prod_{j=0}^{\infty} \sum_{n_j} n_k\, e^{-\beta\, n_j (\epsilon_j - \mu)} \\ &= \frac{1}{Z_g^\pm} \prod_{j=0}^{\infty} \sum_{n_j} \Big(-\frac{1}{\beta}\frac{\partial}{\partial \epsilon_k}\Big) e^{-\beta\, n_j(\epsilon_j - \mu)} = -\frac{1}{\beta}\frac{1}{Z_g^\pm}\frac{\partial}{\partial\epsilon_k} Z_g^\pm = -\frac{1}{\beta}\frac{\partial}{\partial \epsilon_k}\ln\big(Z_g^\pm\big).\end{aligned} \tag{14}$$

Inserting (12) and (13) gives

$$\begin{aligned}\langle n_k\rangle_\pm &= \pm\frac{1}{\beta}\frac{\partial}{\partial\epsilon_k}\sum_{j=0}^{\infty} \ln\big(1 \mp e^{-\beta\,(\epsilon_j - \mu)}\big) = \pm\frac{1}{\beta}\,\frac{1}{1 \mp e^{-\beta\,(\epsilon_k - \mu)}}\,\frac{\partial}{\partial \epsilon_k}\big(\mp e^{-\beta\,(\epsilon_k-\mu)}\big) \\ &= \frac{e^{-\beta\,(\epsilon_k - \mu)}}{1 \mp e^{-\beta\,(\epsilon_k-\mu)}} = \frac{1}{e^{\beta\,(\epsilon_k - \mu)} \mp 1}.\end{aligned} \tag{15}$$

These are the familiar Bose-Einstein and Fermi-Dirac distributions, respectively.

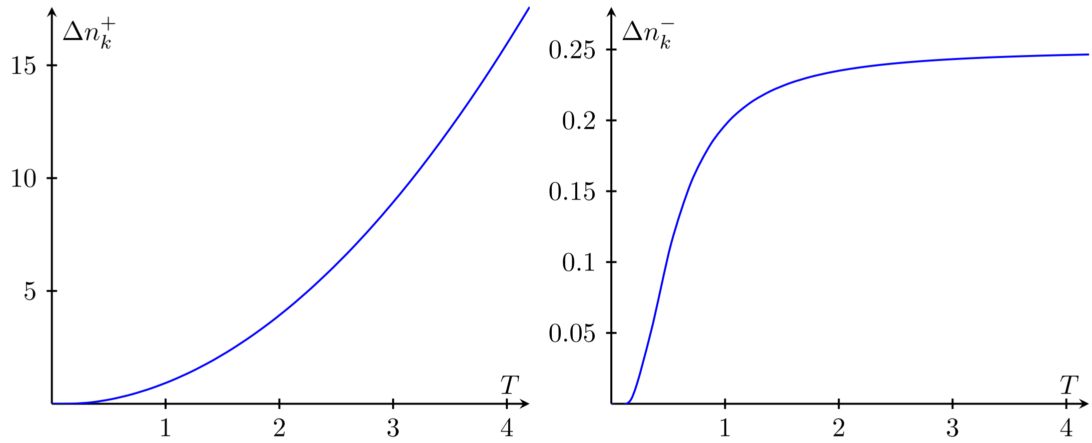
To obtain fluctuations of the occupation number, we need $\langle n_k^2\rangle$. Just like $\langle n_k\rangle$, we can compute it by differentiation,

$$\langle n_k^2\rangle_\pm = \frac{1}{\beta^2}\frac{1}{Z_g^\pm}\frac{\partial^2}{\partial^2\epsilon_k} Z_g^\pm = \frac{e^{-\beta(\epsilon_k-\mu)} + 1}{\big(e^{-\beta(\epsilon_k-\mu)} \mp 1\big)^2} = \big(e^{-\beta(\epsilon_k-\mu)} + 1\big)\,\langle n_k\rangle_\pm^2. \tag{16}$$

This results in the bosonic respectively fermionic fluctuations

$$\begin{aligned}\Delta n_k^\pm = \langle n_k^2\rangle_\pm - \langle n_k\rangle_\pm^2 &= \big(e^{-\beta(\epsilon_k-\mu)} + 1\big)\,\langle n_k\rangle_\pm^2 - \langle n_k\rangle_\pm^2 \\ &= e^{-\beta(\epsilon_k-\mu)}\,\langle n_k\rangle_\pm^2.\end{aligned} \tag{17}$$

The prefactor $e^{-\beta(\epsilon_k-\mu)}$ strongly suppresses fluctuations for states of energy ϵ_k much bigger than the chemical potential. For fermions, where $\langle n_k\rangle_-$ is limited to at most one particle, (17) suggests that even for high temperatures, thermal fluctuations remain small whereas for bosons we expect a strictly monotonic increase/decrease depending on the sign of $\epsilon_k - \mu$. We can plot $\Delta n_k^\pm$ as functions of T for constant $\epsilon_k - \mu > 0$ to confirm this.



Note that Δn_k^- is bounded by $1/4$ as $T \to \infty$. We can understand why if we write it as a function of β, ϵ_k, and μ explicitly,

$$\Delta n_k^- = \frac{1}{2\cosh[\beta(\epsilon_k - \mu)] + 2}, \tag{18}$$

which approaches $1/4$ for $\epsilon_k \neq \mu$ because $\cosh(\pm\infty) = 1$. Wrtiting out Δn_k^+ gives

$$\Delta n_k^+ = \frac{1}{\left[2\sinh\left(\frac{\beta}{2}(\epsilon_k - \mu)\right)\right]^2}. \tag{19}$$

To find the dependence of fluctuations of the total particle number $\Delta N = \sum_k n_k$ on the volume V, we can use that in non-interacting gases, occupation numbers of different modes are uncorrelated, i.e. $\langle n_k n_l \rangle = \langle n_k \rangle \langle n_l \rangle$ for $k \neq l$. We can therefore decompose the expectation values of N and N^2 into sums of expectation values of n_k and n_k^2,

$$\begin{aligned}
\Delta N = \langle N^2 \rangle - \langle N \rangle^2 &= \left\langle \left(\sum_k n_k \right)^2 \right\rangle - \left\langle \sum_k n_k \right\rangle^2 \\
&= \left\langle \sum_k n_k \sum_j n_j \right\rangle - \sum_k \langle n_k \rangle \sum_j \langle n_j \rangle \\
&= \sum_k \langle n_k^2 \rangle + \sum_{k \neq j} \langle n_k n_j \rangle - \sum_{k \neq j} \langle n_k \rangle \langle n_j \rangle - \sum_k \langle n_k \rangle^2 \\
&= \sum_k \langle n_k^2 \rangle - \sum_k \langle n_k \rangle^2 = \sum_k \Delta n_k,
\end{aligned} \tag{20}$$

which is proportional to V because Δn_k is V-independent and the number of modes scales linearly with volume.

3 Relativistic Fermi gas (4 points)

Consider an ideal Fermi gas in three dimensions with ultra-relativistic dispersion relation $\epsilon(\boldsymbol{k}) = \hbar c |\boldsymbol{k}|$ in a very large volume.

a) Compute the grand canonical potential Ω, the average energy and the average number of particles as functions of T, V, and μ.

b) Show that $U = 3pV$.

c) Determine the Fermi energy and the pressure of the gas at $T = 0$ as functions of density.

a) From the fermionic partition function of the ideal quantum gas derived in exercise 2, it is easy to find the grand canonical potential. Let the particles under consideration have spin s and be confined to a box of volume $V = L^3$, then

$$\begin{aligned}\Omega^-(T,V,\mu) &= -\frac{1}{\beta}\ln(Z_g^-) \overset{(12)}{=} -\frac{1}{\beta}\sum_j \ln\left(1+e^{-\beta(\epsilon_j-\mu)}\right)\\ &= -\frac{g_s}{\beta}\sum_{\boldsymbol{k}\in\frac{2\pi}{L}\mathbb{Z}^3}\ln\left(1+z\,e^{-\beta\hbar c|\boldsymbol{k}|}\right),\end{aligned}\tag{21}$$

where $g_s = 2s+1$ is the spin degeneracy and $z = e^{\beta\mu}$ denotes the fugacity. We used that the sum over single-particle states $|\psi_j\rangle \in \mathcal{H}$ becomes a sum over all possible values for the spin σ and three-momentum $\boldsymbol{k}$,

$$\sum_j = \sum_{\sigma=-s}^{s}\sum\nolimits_{\boldsymbol{k}\in\frac{2\pi}{L}\mathbb{Z}^3}.\tag{22}$$

Considering the problem asymptotically for large volumes, the discrete (Riemann) sum (21) translates into the following integral (we get a measure by multiplying and dividing the term $\frac{(2\pi)^3}{L^3}$ which limits to an infinitesimal volume element of momentum space for $L\to\infty$),

$$\begin{aligned}\Omega^-(T,V,\mu) &= -\frac{g_s}{\beta}\frac{V}{(2\pi)^3}\int_{\mathbb{R}^3}\ln\left(1+z\,e^{-\beta\hbar c|\boldsymbol{k}|}\right)\mathrm{d}^3k\\ &= -\frac{g_s}{\beta}\frac{V}{(2\pi)^3}4\pi\int_0^\infty k^2\ln\left(1+z\,e^{-\beta\hbar ck}\right)\mathrm{d}k\\ &= -\frac{g_s}{\beta}\frac{V}{2\pi^2}\left(-\int_0^\infty\frac{k^3}{3}\frac{(-z\beta\hbar c)e^{-\beta\hbar ck}}{1+z\,e^{-\beta\hbar ck}}\right)\mathrm{d}k\\ &= -\frac{g_s}{\beta}\frac{V}{6\pi^2}\frac{1}{(\beta\hbar c)^3}\int_0^\infty\frac{x^3}{z^{-1}\,e^x+1}\mathrm{d}x\\ &\equiv -\frac{g_s}{\pi^2\beta}\frac{V}{(\beta\hbar c)^3}f_4^-(z),\end{aligned}\tag{23}$$

where we transformed to spherical coordinates in the second step, partially integrated with vanishing boundaries in the third, substituted $x = \beta\,\hbar\,c\,k$, $\mathrm{d}x = \beta\,\hbar\,c\,\mathrm{d}k$ in the fourth, and defined the integral function

$$f_\nu^\pm(z) = \frac{1}{\Gamma(\nu)}\int_0^\infty\frac{x^{\nu-1}}{z^{-1}\,e^x\mp 1}\mathrm{d}x,\tag{24}$$

in the last line.

The average energy is given by the Hamiltonian's grand canonical expectation value,

$$\begin{aligned}U(T,V,\mu) &= \langle\hat{H}\rangle_g = \frac{1}{Z_g^-}\mathrm{tr}_{\mathcal{H}}\left(\hat{H}e^{-\beta(\hat{H}-\mu\hat{N})}\right)\\ &= \sum_{\sigma=-s}^{s}\sum_{\boldsymbol{k}}\frac{\hbar c|\boldsymbol{k}|}{z^{-1}e^{\beta\hbar c|\boldsymbol{k}|}+1}\xrightarrow{V\to\infty} g_s\frac{V}{(2\pi)^3}4\pi\int_0^\infty\frac{\hbar\,c\,k}{z^{-1}\,e^{\beta\hbar ck}+1}k^2\,\mathrm{d}k\\ &= \frac{g_s}{2\pi^2\beta}\frac{V}{(\beta\hbar c)^3}\int_0^\infty\frac{x^3}{z^{-1}e^x+1}\mathrm{d}x = \frac{3g_s}{\pi^2\beta}\frac{V}{(\beta\hbar c)^3}f_4^-(z)\end{aligned}\tag{25}$$

Finally, the average particle number derives from the number operator's expectation value,

$$\begin{aligned}N(T,V,\mu) &= \langle\hat{N}\rangle_g = \frac{1}{Z_g^-}\mathrm{tr}_{\mathcal{H}}\left(\hat{N}\,e^{-\beta(\hat{H}-\mu\hat{N}}\right)\\ &= \sum_{\sigma=-s}^{s}\sum_{\boldsymbol{k}}\langle n_{\boldsymbol{k}}\rangle\xrightarrow{V\to\infty} g_s\frac{V}{(2\pi)^3}4\pi\int_0^\infty\frac{k^2\,\mathrm{d}k}{z^{-1}e^{\beta\hbar ck}+1} = \frac{g_s}{\pi^2}\frac{V}{(\beta\hbar c)^3}f_3(z).\end{aligned}\tag{26}$$

where we used $\langle n_k\rangle_g = \frac{\partial\Omega^-}{\partial\epsilon(k)} = \frac{1}{z^{-1}e^{\beta\epsilon(k)}+1}$.

b) The pressure is given by the derivative of the grand potential (23) w.r.t. volume,

$$p = -\frac{\partial \Omega^-}{\partial V} = \frac{g_s}{\pi^2 \beta} \frac{f_4^-(z)}{(\beta \hbar c)^3}. \tag{27}$$

Comparing (25) and (27), we see that

$$U = 3pV. \tag{28}$$

c) To determine the energy and pressure of a relativistic Fermi gas in the $T \to 0$ limit, we employ an asymptotic expansion of $f_\nu^-(z)$ for $\ln(z) = \beta\mu \gg 1$,

$$f_\nu^-(e^{\beta\mu}) = \frac{(\beta\mu)^\nu}{\Gamma(\nu+1)} \left(1 + 2\sum_{j=1}^{n} (2j)! \binom{\nu}{2j} \left(1 + 2^{1-2j}\right) \zeta(2k)\, (\beta\mu)^{-2j} + \mathcal{O}\big[(\beta\mu)^{-2n-1}\big]\right), \tag{29}$$

where $\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}$, $s \in \mathbb{C}$ is the Riemann zeta function. We only need to consider the leading order behaviour,

$$f_4^-(e^{\beta\mu}) = \frac{(\beta\mu)^4}{4!} + \mathcal{O}\big[(\beta\mu)^3\big]. \tag{30}$$

to find that $\beta \to \infty$ with μ fixed results in the Fermi energy and pressure

$$E_\mathrm{F} = U(0, V, \mu) = \frac{g_s}{8\pi^2} \frac{V\mu^4}{(\hbar c)^3}, \tag{31}$$

$$p_\mathrm{F} = P(0, V, \mu) = \frac{g_s}{24\pi^2} \frac{\mu^4}{(\hbar c)^3}. \tag{32}$$

The reason they are non-zero is the Pauli principle. It prevents identical fermions from occupying the same state more than once. Macroscopic condensation into the ground state as in bosonic systems near absolute zero is therefore impossible. Instead, a Fermi system at $T = 0$ fills up all available energy states from the bottom up, a configuration known as full degeneracy. Adding particles or compressing the system forces the particles into higher-energy states. The necessary energy must be introduced into the system by a compression force performing work against the resisting pressure (32).

To express (31) and (32) in terms of the Fermi density, we may again apply the asymptotic expansion of $f_\nu^-(e^{\beta\mu})$, this time to (26) to find

$$\rho_\mathrm{F} = \frac{1}{V} N(0, V, \mu) = \frac{g_s}{6\pi^2} \frac{\mu^3}{(\hbar c)^3}, \tag{33}$$

which gives

$$E_\mathrm{F} = \frac{3}{4} \rho_\mathrm{F} V \mu, \tag{34}$$

$$p_\mathrm{F} = \frac{1}{4} \rho_\mathrm{F} \mu. \tag{35}$$

Note that the Fermi pressure depends exclusively on the density of the fermions, while the Fermi Energy, being an extensive quantity, also scales linearly with volume.

4 Two-dimensional Bose gas (3 points)

Consider a two-dimensional ideal Bose gas in a box of side length L with periodic boundary conditions and dispersion relation $\epsilon(\boldsymbol{k}) = \boldsymbol{k}^2/2m$.

a) Calculate the grand canonical partition function Z_g^+ and obtain the limit

$$\lim_{A\to\infty} \frac{1}{A} \ln[Z_g^+(z,A,T)] \tag{36}$$

where $A = L^2$ is the area available to the system, and $z = e^{\beta\mu}$ denotes the fugacity.

b) Explicitly find the average number of particles per unit area as a function of z and T.

c) Show that no macroscopic occupation of the $\boldsymbol{k} = \boldsymbol{0}$ mode is necessary at any density. What are the consequences for Bose-Einstein condensation?

a) The partition function for the ideal Bose gas of spin-s particles confined to a two-dimensional box of side length L reads

$$Z_g^+ = \prod_{\boldsymbol{k}\in\frac{2\pi}{L}\mathbb{Z}^2} \prod_{\sigma=-s}^{s} \frac{1}{1-e^{-\beta\,[\epsilon(\boldsymbol{k})-\mu]}} = \prod_{\boldsymbol{k}\in\frac{2\pi}{L}\mathbb{Z}^2} \left(1-e^{-\beta\,(\boldsymbol{k}^2/2m-\mu)}\right)^{-g_s}, \tag{37}$$

where we used that the dispersion relation $\epsilon(\boldsymbol{k}) = \boldsymbol{k}^2/2m$ is independent of σ, so the product over spin states just gives the degeneracy $g_s = 2s+1$. To write Z_g^+ as a momentum integral, we take the logarithm and perform the continuum limit in the resulting sum,

$$\begin{aligned}
\ln(Z_g^+) &= -g_s \frac{L^2}{(2\pi)^2} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{(2\pi)^2}{L^2} \ln\left(1 - z\,e^{-\frac{\beta}{2m}\boldsymbol{k}^2}\right) - g_s \ln(1-z) \\
&\xrightarrow{L\to\infty} -g_s \frac{A}{(2\pi)^2}\, 2\pi \int_0^\infty k \ln\left(1 - z\,e^{-\frac{\beta}{2m}k^2}\right) \mathrm{d}k - g_s\ln(1-z) \\
&\overset{\text{part. int.}}{=} g_s \frac{A}{2\pi} \int_0^\infty \frac{k^2}{2} \frac{\frac{\beta}{m} k\, z\, e^{-\frac{\beta}{2m}k^2}}{1 - z\,e^{-\frac{\beta}{2m}k^2}} \mathrm{d}k - g_s \ln(1-z) \\
&= g_s \frac{A}{2\pi}\frac{\beta}{m} \int_0^\infty \frac{k^3}{z^{-1}e^{\frac{\beta}{2m}k^2} - 1} \mathrm{d}k - g_s\ln(1-z) \\
&= g_s \frac{A}{2\pi}\frac{\beta}{m}\frac{2m^2}{\beta^2} \int_0^\infty \frac{x}{z^{-1}e^x - 1}\mathrm{d}x - g_s\ln(1-z) \\
&= g_s \frac{A}{\pi}\frac{m}{\beta} f_2^+(z) - g_s\ln(1-z).
\end{aligned} \tag{38}$$

The limit (36) gives the pressure

$$\beta\, p = -\lim_{A\to\infty} \frac{\beta}{A}\Omega = \lim_{A\to\infty}\frac{1}{A}\ln(Z_g^+) = \frac{g_s}{\pi}\frac{m}{\beta} f_2^+(z). \tag{39}$$

b) The average number of particles per unit area, i.e. the areal density, is given by

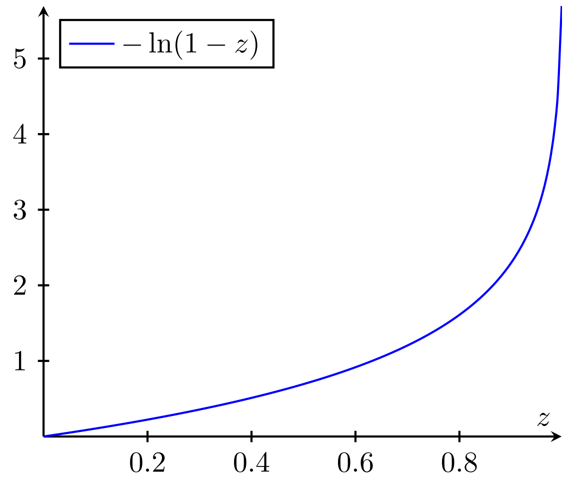
$$\begin{aligned}
\frac{1}{A} N(T,A,\mu) &= \frac{1}{A}\langle \hat{N}\rangle_g = \frac{1}{A}\frac{1}{Z_g^+}\,\mathrm{tr}\left(\hat{N} e^{-\beta(\hat{H}-\mu\hat{N})}\right) \\
&= \frac{1}{A}\sum_{\sigma=-s}^{s}\left(\frac{A}{(2\pi)^2}\sum_{\boldsymbol{k}\neq 0}\frac{(2\pi)^2}{L^2}\langle n_{\boldsymbol{k}}\rangle + \langle n_{\boldsymbol{0}}\rangle\right) \\
&= \frac{g_s}{(2\pi)^2}\, 2\pi \int_0^\infty \frac{k}{z^{-1}e^{\beta\epsilon(k)} - 1}\,\mathrm{d}k + \frac{g_s}{A}\frac{z}{1-z} \\
&= \frac{g_s}{2\pi}\frac{m}{\beta}\int_0^\infty \frac{\mathrm{d}x}{z^{-1}e^x - 1} + \frac{g_s}{A}\frac{z}{1-z} \\
&= \frac{g_s}{2\pi}\frac{m}{\beta} f_1^+(z) + \frac{g_s}{A}\frac{z}{1-z}.
\end{aligned} \tag{40}$$

c) For the three-dimensional ideal Bose gas discussed in the lecture, we had calculated the number of particles per unit volume to be

$$\frac{N}{V} = \frac{g_s}{\lambda^3} f_{3/2}^{+}(z) + \frac{g_s}{V} \frac{z}{1-z}, \tag{41}$$

where $\lambda = h/\sqrt{2\pi m k_\mathrm{B} T}$ denotes the thermal de Broglie wavelength. We had argued that since $\lambda^{-3} \propto T^{\frac{3}{2}}$ and the integral function $f_{3/2}^{+}(z)$ is bounded from above by $f_{3/2}^{+}(1) = \zeta(3/2) \approx 2.61$ for $z \in [0, 1]$[2], the occupation numbers of all states but the zero mode tend to zero as $T \to 0$, which requires $z \to 1$ so that the zero mode occupation diverges. Otherwise, it would not be able to account for the macroscopic density ρ_F at $T = 0$ all on its own. This is Bose-Einstein condensation.

In two dimensions, the situation is different. While $f_1^{+}(z) = -\ln(1-z)$ is still monotonic for $z \in [0, 1]$, it is no longer bounded. Instead, it diverges as $z \to 1$.



Hence, we can no longer argue that as $T \to 0$, the term $\frac{g_s}{2\pi}\frac{m}{\beta} f_1^{+}(z)$ in (40) must vanish because $\beta^{-1} \propto T$ will be countered by $f_1^{+}(z) \to \infty$ if $z = 1$, i.e. if $\mu = 0$. So if the thermal mode occupation doesn't vanish at absolute zero, nothing forces the zero mode occupation to become macroscopic, meaning no Bose-Einstein condensation will take place.

[2] Recall that we had used $\mu < 0$ and thus $z = e^{\beta\mu} < 1$ to apply the geometric series in the calculation of the bosonic partition function. Otherwise the sum over occupation numbers wouldn't even have been convergent.