Physics 7602 Midterm Exam – Spring 2019

- Closed-book exam: no notes, no phone
- Please begin each of the 3 problems on a new page.

Problem 1. (33 points)
A gas of identical bosons is in equilibrium at temperature $T = 1/\beta$ and chemical potential μ. If the bosons have the nonrelativistic energy-momentum relation $\varepsilon = \vec{p}^{\,2}/2m$, the number of bosons in a volume V can be expressed as

$$N = \frac{V}{(2\pi\hbar)^3}\int d^3p \frac{1}{e^{\beta(p^2/2m-\mu)}-1} = \frac{V(2m)^{3/2}}{4\pi^2\hbar^3}\int_0^\infty d\varepsilon \frac{\varepsilon^{1/2}}{e^{\beta(\varepsilon-\mu)}-1} = \frac{V}{\Gamma(\frac{3}{2})}\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2}\int_0^\infty dx \frac{x^{1/2}}{e^{-\beta\mu}e^x-1}.$$

4 A. Suppose the bosons instead have the relativistic energy-momentum relation $\varepsilon = |\vec{p}|c$. Express the number N as an integral over ε.

$$N = \frac{V}{(2\pi\hbar)^3}\int d^3p \frac{1}{e^{\beta(pc-\mu)}-1} = \frac{V}{(2\pi\hbar)^3} 4\pi \int_0^\infty p^2 dp \frac{1}{e^{\beta(pc-\mu)}-1}$$

$\varepsilon = pc$
$d\varepsilon = c\,dp$

$$= \frac{4\pi V}{(2\pi\hbar)^3}\frac{1}{c^3}\int_0^\infty \varepsilon^2 d\varepsilon \frac{1}{e^{\beta(\varepsilon-\mu)}-1}$$

4 B. Suppose the bosons instead are nonrelativistic particles in 2 dimensions. Express the number N of bosons in an area A as an integral over the momentum vector $\vec{p} = (p_x, p_y)$.

$$N = \frac{A}{(2\pi\hbar)^2}\int_{-\infty}^{\infty} dp_x \int_{-\infty}^{\infty} dp_y \frac{1}{\exp(\beta[\frac{1}{2m}(p_x^2+p_y^2)-\mu]) - 1}$$

4 C. Suppose the bosons instead are norelativistic atoms in 3 dimensions in the trapping potential $V(\vec{r}) = \frac{1}{2}m\omega^2\vec{r}^{\,2}$. Express the number N of bosons as an integral over the momentum and position vectors $\vec{p}$ and $\vec{r}$.

$$N = \frac{1}{(2\pi\hbar)^3}\int d^3r \int d^3p \frac{1}{\exp(\beta[\frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 r^2 - \mu]) - 1}$$

4 D. Using the expression for N above with an integral over a dimensionless variable x, deduce the critical temperature T_c for the onset of Bose-Einstein condensation. (You do not need to evaluate the integral over x.)

$$T = T_c \Longrightarrow \mu = 0$$

$$N = \frac{V}{\Gamma(\frac{3}{2})}\left(\frac{mkT_c}{2\pi\hbar^2}\right)^{3/2}\int_0^\infty dx \frac{x^{1/2}}{e^x-1} \Longrightarrow kT_c = \left(\frac{\Gamma(\frac{3}{2})}{\int_0^\infty dx \frac{x^{1/2}}{e^x-1}}\frac{N}{V}\right)^{2/3}\frac{2\pi\hbar^2}{m}$$

If the nonrelativistic bosons are in equilibrium at a temperature T below the critical temperature T_c, the number of bosons in a volume V can be expressed as

$$N = N_0 + \zeta_{3/2} V \left(\frac{mkT}{2\pi\hbar^2} \right)^{3/2} .$$

4 E. Use this expression for N to deduce the critical temperature T_c for the onset of Bose-Einstein condensation.

$$T = T_c \implies N_0 = 0$$

$$N = \zeta_{3/2} V \left(\frac{mkT_c}{2\pi\hbar^2} \right)^{3/2} \implies kT_c = \left(\frac{1}{\zeta_{3/2}} \frac{N}{V} \right)^{2/3} \frac{2\pi\hbar^2}{m}$$

4 F. Use the expression for N above to derive the number N_0 of atoms in the condensate as a function of N and the ratio T/T_c.

$$N = N_0 + \zeta_{3/2} V \left(\frac{mkT_c}{2\pi\hbar^2} \right)^{3/2} \left(\frac{T}{T_c} \right)^{3/2} = N_0 + N \left(\frac{T}{T_c} \right)^{3/2}$$

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

5 At a temperature T below T_c, the ideal gas is a mixture of two coexisting phases.
G. Describe each of the two phases as explicitly and concisely as possible.

Bose-Einstein condensate: $[1-(T/T_c)^{3/2}]N$ bosons all in the lowest energy state

thermal gas: $(T/T_c)^{3/2} N$ bosons at temperature T
chemical potential 0

4 H. The entropy per particle is 0 in one of the coexisting phases and 1.284 in the other phase. What is the total entropy S at a temperature T below T_c as a function of N and T/T_c?

$$S = \left[1 - (T/T_c)^{3/2} \right] N \cdot 0 + (T/T_c)^{3/2} N \cdot 1.284$$

$$= 1.284 \left(T/T_c \right)^{3/2} N$$

Problem 2. (33 points)

The ^{6}Li isotope has atomic number 3 and atomic weight near 6.

3 A. List all the constituents of a neutral ^{6}Li atom. Explain how can you determine from the constituents that the atom is a fermion.

nucleus with 3 protons and 3 neutrons plus 3 electrons

9 fermions: odd $\Longrightarrow$ fermion

In the grand canonical ensemble, each single-particle state is in thermal equilibrium at temperature $T = 1/\beta$ and in chemical equilibrium at chemical potential μ.

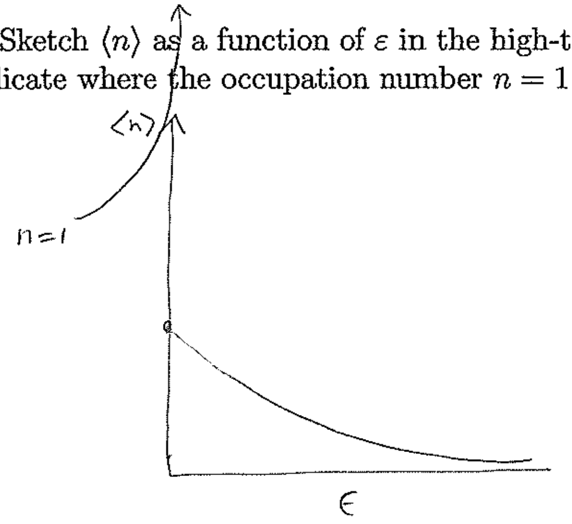
4 B. What are all the possible values of the occupation number n for a single-particle state with energy ε? What are the probabilities for each of those occupation numbers?

fermion $\Longrightarrow$ $n = 0, 1$ $\quad P_0 = \dfrac{1}{1+e^{-\beta(\epsilon-\mu)}} \quad P_1 = \dfrac{e^{-\beta(\epsilon-\mu)}}{1+e^{-\beta(\epsilon-\mu)}}$

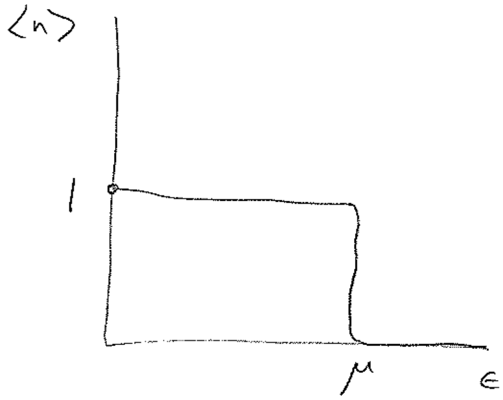
3 C. Write down the average occupation number $\langle n\rangle$ for a single-particle state with energy ε.

$$\langle n\rangle = \frac{1}{e^{\beta(\epsilon-\mu)}+1}$$

3 D. Sketch $\langle n\rangle$ as a function of ε in the high-temperature limit.
Indicate where the occupation number $n = 1$ is on the vertical scale.



3 E. Sketch $\langle n\rangle$ as a function of ε in the low-temperature limit.
Indicate where the occupation number $n = 1$ is on the vertical scale.



The energy of a ^{6}Li atom in the lowest hyperfine state trapped in a 3-dimensional harmonic-oscillator potential is

$$\varepsilon = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + \frac{1}{2}m\omega^2(x^2 + y^2 + z^2).$$

A large number N of ^{6}Li atoms all in the lowest hyperfine state are trapped in the potential and cooled down to the absolute zero of temperature.

3 F. Given the Fermi energy ε_F, deduce the Fermi momentum p_F beyond which all momentum states are unoccupied.

$$\varepsilon < \varepsilon_F \Longrightarrow \frac{1}{2m}p^2 < \varepsilon_F \Longrightarrow p < \sqrt{2m\varepsilon_F} \equiv p_F$$

3 G. Given the Fermi energy ε_F, deduce the Fermi radius R_F beyond which all position states are unoccupied.

$$\varepsilon < \varepsilon_F \Longrightarrow \frac{1}{2}m\omega^2 r^2 < \varepsilon_F \Longrightarrow r < \sqrt{\frac{2\varepsilon_F}{m\omega^2}} \equiv R_F$$

3 H. Express N at a general temperature $T = 1/\beta$ and chemical potential μ as an integral over the position and momentum vectors of a single atom.

$$N = \frac{1}{(2\pi\hbar)^3}\int d^3r\, d^3p \frac{1}{\exp\left(\beta\left[\frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 r^2 - \mu\right]\right) + 1}$$

5 I. Derive the expression for N at $T = 0$ as an integral over the energy ε of a single atom. (The solid angle in D dimensions is $2\pi^{D/2}/\Gamma(D/2)$.
The gamma function satisfies $\Gamma(n+1) = n\,\Gamma(n)$, $\Gamma(1) = 1$, $\Gamma(\frac{1}{2}) = \sqrt{\pi}$.)

$$\Omega_6 = \frac{2\pi^3}{\Gamma(3)} = \pi^3$$

$$N = \frac{1}{(2\pi\hbar)^3}\int d^3r \int d^3p\, \Theta\left(\varepsilon_F - \frac{1}{2m}p^2 - \frac{1}{2}m\omega^2 r^2\right)$$

$$= \frac{1}{(2\pi\hbar)^3}\frac{1}{(m\omega)^3}\int d^6P\, \Theta\left(\varepsilon_F - \frac{1}{2m}P^2\right)$$

$$= \frac{1}{(2\pi m\hbar\omega)^3}\Omega_6 \int_0^\infty P^5 dP\, \Theta\left(\varepsilon_F - \frac{1}{2m}P^2\right)$$

$$= \frac{1}{(2\pi m\hbar\omega)^3}\pi^3 \frac{(2m)^3}{2}\int_0^{\varepsilon_F}\varepsilon^2 d\varepsilon$$

$$= \frac{1}{2(\hbar\omega)^3}\frac{\varepsilon_F^3}{3}$$

3 J. Deduce the Fermi energy ε_F as a function of N.

$$N = \frac{1}{(\hbar\omega)^3}\frac{\varepsilon_F^3}{6} \Longrightarrow \varepsilon_F = (6N)^{1/3}\hbar\omega$$

Problem 3. (34 points)

Two nitrogen atoms can form a diatomic molecule. The nucleus for the ^{14}N isotope is a boson with spin 1. The nucleus for the ^{15}N isotope is a fermion with spin $\frac{1}{2}$.

The possible quantum numbers for the total nuclear spin of the ^{14}N-^{15}N molecule are $i = \frac{1}{2}$, which has 2 spin states, and $i = \frac{3}{2}$, which has 4 spin states.

3 A. What are the possible quantum numbers i for the total nuclear spin of the $(^{14}\mathrm{N})_2$ molecule? How many spin states are there for each one?

$$i = |1-1|, \ldots, 1+1 = 0, 1, 2$$

i	$2i+1$
0	1
1	3
2	5

A rotation of the molecule by an angle π around an axis perpendicular to its symmetry axis changes the rotational wavefunction by a factor of $(-1)^\ell$, where ℓ is the orbital angular momentum quantum number.

For the $(^{14}\mathrm{N})_2$ molecule, the interchange of the nuclei changes the nuclear spin wavefunction by a factor of $(-1)^i$, where i is the total nuclear spin quantum number.

3 B. What are the allowed values of ℓ and i for the $(^{14}\mathrm{N})_2$ molecule?

rotation by π interchanges the nuclei
multiplies state by $(-1)^\ell(-1)^i$

boson : $(-1)^\ell(-1)^i = +1$

$i = 0, 2 : \ \ell = 0, 2, 4, \ldots$

$i = 1 \ : \ \ell = 1, 3, 5, \ldots$

In a gas of diatomic nitrogen molecules, the only degrees of freedom from internal motion that are important at low temperatures are rotations.

For the ^{14}N-^{15}N molecule, the rotational partition function at temperature $T = 1/\beta$ is

$$Z_{\mathrm{rot}} = \sum_{\ell=0}^{\infty}(2\ell+1)\exp(-\beta\ell(\ell+1)\hbar^2/2I),$$

where I is the moment of inertia of the molecule. The nuclear-spin partition function is

$$Z_{\mathrm{nuc}} = 3 \cdot 2.$$

4 C. What is the rotational/nuclear-spin partition function $Z_{\mathrm{rot/nuc}}$ for the $(^{14}\mathrm{N})_2$ molecule?

$$Z_{\mathrm{rot/nuc}} = (1+5)\sum_{\substack{\ell=0 \\ \ell \text{ even}}}^{\infty}(2\ell+1)\exp(-\beta\ell(\ell+1)\hbar^2/2I) + 3\sum_{\substack{\ell=0 \\ \ell \text{ odd}}}^{\infty}(2\ell+1)\exp(-\beta\ell(\ell+1)\hbar^2/2I)$$

3 D. What is the temperature scale below which rotations freeze out due to quantum effects?

freezeout $\Longrightarrow \ell = 1, 2, 3, \ldots$ exponentially suppressed

$$\Longrightarrow \beta\hbar^2/I > 1 \qquad \Longrightarrow kT < \hbar^2/I$$

In the high-temperature limit, the rotational partition function Z_{rot} simplifies.

4 E. Derive a simple expression for Z_{rot} for the ^{14}N-^{15}N molecule as a function of T by approximating the sum over ℓ by an integral over the dimensionless variable $x = \beta\ell(\ell+1)\hbar^2/2I$.

$$dx = (2\ell+1)d\ell \ \beta\hbar^2/2I \qquad Z_{\mathrm{rot}} \simeq \int_0^\infty d\ell\,(2\ell+1)\exp\left(-\beta\ell(\ell+1)\hbar^2/2I\right)$$

$$= \frac{2I}{\beta\hbar^2}\int_0^\infty dx\, e^{-x} = \frac{2I}{\hbar^2}kT \cdot 1$$

At higher temperatures, vibrations in the distance r between the two nuclei become important. The relevant term in the Hamiltonian can be approximated by

$$H_{\text{vib}} = \overset{\frac{1}{2}\mu}{\left(\frac{1}{m}\right)}\dot{r}^2 + \frac{1}{2}V''(r_0)(r-r_0)^2,$$

where r_0 is the equilibrium radius that minimizes the interatomic potential $V(r)$ and m is the mass of a single nitrogen atom.

4 F. Identify the eigenvalues of H_{vib}.

$$H_{\text{vib}} = \frac{1}{2}\mu\dot{r}^2 + \frac{1}{2}\mu\omega^2(r-r_0)^2 \quad \text{where } V''(r_0) = \mu\omega^2 \Longrightarrow \omega = \sqrt{V''(r_0)/\mu}$$

$$= \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2(r-r_0)^2$$

eigenvalues: $\mathcal{E}_n = (n+\frac{1}{2})\hbar\omega \quad n = 0,1,2,\ldots$

4 G. What is the vibrational partition function Z_{vib} at temperature $T = 1/\beta$.

$$Z_{\text{vib}} = \sum_{n=0}^{\infty} \exp\left(-\beta(n+\tfrac{1}{2})\hbar\omega\right)$$

$$= e^{-\beta\hbar\omega/2}\frac{1}{1-e^{-\beta\hbar\omega}} = \frac{1}{2\sinh(\beta\hbar\omega/2)}$$

3 H. What is the temperature scale below which vibrations freeze out due to quantum effects?

freezeout: $n = 1,2,\ldots$ exponentially suppressed

$$\Longrightarrow \beta\hbar\omega > 1 \quad \Longrightarrow \quad kT < \hbar\omega$$

In the high-temperature limit, the vibrational partition function Z_{vib} can be simplified if nonharmonic corrections and couplings to rotations are ignored.

3 I. Derive a simple expression for Z_{vib} as a function of T.

$$Z_{\text{vib}} \simeq \frac{1}{2(\beta\hbar\omega/2)} = \frac{kT}{\hbar\omega}$$

OR

$$Z_{\text{vib}} \simeq \int_0^{\infty} dn\, e^{-\beta n\hbar\omega} = \frac{1}{\beta\hbar\omega}\int_0^1 dx\, e^{-x} = \frac{kT}{\hbar\omega}$$

The partition function for a single ^{14}N-^{15}N molecule in a volume V in thermal equilibrium at temperature T is

$$V\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2} Z_{\text{rot}}\, Z_{\text{vib}}\, Z_{\text{nuc}}.$$

3 J. What is the Helmholtz free energy F for a large number N of ^{14}N-^{15}N molecules in the volume V at temperature T?

$$Z_N = \frac{1}{N!}Z_1^N = \frac{1}{N!}\left[V\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2} Z_{\text{rot}}\, Z_{\text{vib}}\, Z_{\text{nuc}}\right]^N$$

$$= e^{-\beta F}$$

$$F = -kT\log Z_N = -kT\left(N\log\left[V\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2} Z_{\text{rot}}\, Z_{\text{vib}}\, Z_{\text{nuc}}\right] - (N\log N - N)\right)$$

$$= -NkT\left[\log\left(V\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2}\right) + \log Z_{\text{rot}} + \log Z_{\text{vib}} + \log Z_{\text{nuc}} - \log N + 1\right]$$