National University of Singapore

PC4241 Statistical Mechanics

(Semester I: AY2009-10, 26 November)

Time Allowed: Two Hours

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains **FOUR** questions and comprises **FOUR** printed pages.
2. All questions carry equal marks.
3. Answer any **THREE** questions.
4. This is a CLOSED BOOK examination.
5. One A4 double-sided sheet of formulae and equations is allowed.

1. A monatomic crystal of N atoms has N lattice sites and M interstitial sites. The energy of an atom at an interstitial site exceeds that at a lattice site by an amount ε.

   (i) Use the microcanonical ensemble to calculate the entropy of the crystal in the state where n of the N atoms are at interstitial sites. Hence, determine the temperature of the crystal in this state.

   (ii) Show that n at temperature T is given by

   $$\frac{n^2}{(N-n)(M-n)} = e^{-\frac{\varepsilon}{kT}} .$$

   Hence, obtain n for $\varepsilon >> kT$ and $\varepsilon << kT$.

   (iii) Use this model for defects in a crystal with $M = N$. Obtain the defect concentration at very low and very high temperatures. Comment on the results.

2. Consider a one-dimensional harmonic oscillator which is in thermal equilibrium with a heat reservoir at absolute temperature T.

   (i) According to classical mechanics, the Hamiltonian for such an oscillator is given by

   $$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 .$$

   Find the partition function for the oscillator and obtain the relation between its mean energy and the temperature.

   (ii) According to quantum mechanics, the energy levels of the oscillator are given by

   $$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0,1,2,...$$

   Find the partition function and the mean energy of the oscillator.

   (iii) Comment on the limits of validity of the classical description.

   $$\left[\int_{-\infty}^{\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}\right]$$

3. The parametric equations of state for the Bose gas are given by

$$\frac{\lambda^3 P}{kT} = g_{\frac{5}{2}}(z) \ , \qquad \lambda^3 n = g_{\frac{3}{2}}(z) \ ,$$

where λ is the thermal wavelength, z the fugacity and the Bose function $g_k(z) = \sum_{l=1}^{\infty} z^l / l^k$.

(i) Obtain the energy U of the gas as a function of $g_{\frac{5}{2}}(z)$ and hence show that

$$U = \frac{3}{2} PV \ .$$

(ii) Show that the fugacity z is given by

$$z = n\lambda^3 \left[1 - \frac{n\lambda^3}{2^{\frac{3}{2}}} - \dots \right] .$$

(iii) Show that at high temperatures

$$\frac{\lambda^3 P}{kT} \approx n\lambda^3 - \frac{\left(n\lambda^3\right)^2}{2^{\frac{5}{2}}} ,$$

$$U \approx \frac{3}{2} NkT \left(1 - 2^{-\frac{5}{2}} n\lambda^3 \right) .$$

Comment on the result of U .

4. Consider an ideal gas of N free electrons, each of mass m, enclosed in a cube of volume V at low temperatures. Its density of states $f(\varepsilon)$ and chemical potential μ are given respectively by

$$f(\varepsilon)=\frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\varepsilon^{\frac{1}{2}},$$

$$\mu=\varepsilon_F\left[1-\frac{\pi^2}{12}\left(\frac{kT}{\varepsilon_F}\right)^2+\ldots\right].$$

(i) Use the Sommerfeld expansion

$$\int_0^\infty n(\varepsilon)G'(\varepsilon)\,d\varepsilon=G(\mu)+\frac{\pi^2}{6}(kT)^2G''(\mu)+\ldots$$

to show that

$$U=\frac{3}{5}N\varepsilon_F\left[1+\frac{5\pi^2}{12}\left(\frac{kT}{\varepsilon_F}\right)^2+\ldots\right].$$

(ii) Show that the pressure P, the grand potential Ω_G, the entropy S and the Helmholtz free energy F of the free electron gas are given respectively by

$$P=\frac{2}{5}\frac{N}{V}\varepsilon_F\left[1+\frac{5}{12}\pi^2\left(\frac{kT}{\varepsilon_F}\right)^2+\ldots\right],$$

$$\Omega_G=-\frac{2}{5}N\varepsilon_F\left[1+\frac{5}{12}\pi^2\left(\frac{kT}{\varepsilon_F}\right)^2+\ldots\right],$$

$$S=\frac{1}{2}N\pi^2k^2\frac{T}{\varepsilon_F},$$

$$F=\frac{3}{5}N\varepsilon_F\left[1-\frac{5}{12}\pi^2\left(\frac{kT}{\varepsilon_F}\right)^2+\ldots\right].$$

(iii) Comment on the expressions of P and S.

Ng S C

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