School of Physics & Astronomy

# Statistical Physics

## PHYS11024 (SCQF Level 11)

**Tuesday 26th April, 2016 09:30 – 11:30**
**(May Diet)**

**Please read full instructions before commencing writing.**

**Examination Paper Information**

Answer **TWO** questions

**Special Instructions**

- Electronic Calculators must **not** be used during this examination.
- Attach supplied anonymous bar codes to *each* script book.

**Special Items**

- School supplied barcodes

**Chairman of Examiners:** Prof S Playfer
**External Examiner:** Prof S Clark

ANONYMITY OF THE CANDIDATE WILL BE MAINTAINED DURING THE MARKING OF THIS EXAMINATION.

**1.** (a) State the canonical partition function for an assembly of $N$ particles occupying microstates denoted by $\{E_i\}$. **[2]**

(b) If $C_V = \partial\langle E\rangle/\partial T$ is the heat capacity at constant volume show that

$$C_V = -k\beta^2 \frac{\partial\langle E\rangle}{\partial\beta},$$

where $\beta = 1/(kT)$, $k$ being Boltzmann's constant. **[3]**

(c) Hence show that the mean squared energy fluctuations for a canonical distribution is given by

$$\left\langle (E - \langle E\rangle)^2 \right\rangle = kT^2 C_V\,.$$ **[5]**

(d) Show that

$$\frac{\partial^2}{\partial\beta^2}\langle E\rangle = \left\langle (E - \langle E\rangle)^3 \right\rangle,$$

**[5]**

and hence that

$$\left\langle (E - \langle E\rangle)^3 \right\rangle = k^2\left[T^4\frac{\partial C_V}{\partial T} + 2T^3 C_V\right].$$ **[5]**

(e) For an ideal gas of $N$ particles, where $\langle E\rangle = \frac{3}{2}NkT$ show that

$$\frac{\langle (E - \langle E\rangle)^2\rangle}{\langle E\rangle^2} = \frac{2}{3N}\,.$$ **[2]**

(f) Find the equivalent result to part (e) for

$$\frac{\langle (E - \langle E\rangle)^3\rangle}{\langle E\rangle^3}\,.$$ **[3]**

**2.** (a) The Hamiltonian for a classical statistical mechanical system comprised of $N$ identical particles of mass $m$ in volume $V$ is given by

$$H(\{\vec{q}\},\{\vec{p}\}) = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j} U_{ij}\,,$$

(where $U_{ij} = U(|\vec{q}_i - \vec{q}_j|)$ is a two-body interaction and $\beta = 1/(kT)$). Show that the canonical partition function

$$Z = \frac{1}{N!\,h^{3N}} \int \prod_{i=1}^{N} d^3q_i\, d^3p_i\, e^{-\beta H(\{\vec{q}\},\{\vec{p}\})}\,,$$

can be written as

$$Z = Z_{\text{ideal}}\, Q\,,$$

where $Z_{\text{ideal}}$ is the partition function for an ideal gas and $Q$ is a correction factor due to the two-body interactions. **[3]**

(b) Show that the free energy, $F$, for the system described in (a) is given by

$$F = -kTN \ln\left(\frac{Ve}{N}\left(\frac{2\pi mkT}{h^2}\right)^{3/2}\right) - kT\ln Q\,.$$ **[6]**

(c) It can be shown that the first correction to $Q$ due to the interactions is given by

$$Q = \left(1 - \frac{2}{V}B_2\right)^{N(N-1)/2}\,,$$

where $B_2$, the second virial coefficient is given by

$$B_2 = \tfrac{1}{2}\int d^3r\,[1 - e^{-\beta U(r)}]\,.$$

Find the free energy, $F$, of the system. **[4]**

(d) For the potential

$$U(r) = \xi e^{-\alpha r^2}\,, \quad \text{where } \alpha > 0\,,$$

where $\xi$ is a small parameter, compute $B_2$ to lowest order in $\xi$. **[5]**

(e) Hence show that the equation of state is given by

$$P = \frac{NkT}{V} + \frac{1}{2}\xi\left(\frac{\pi}{\alpha}\right)^{3/2}\left(\frac{N}{V}\right)^2\,.$$ **[5]**

and determine the entropy, $S$. **[2]**

[**Hints:** The Gaussian integral $\int_{-\infty}^{\infty} dx\, \exp[-\alpha x^2] = \sqrt{\pi/\alpha}$, $\alpha > 0$ and Stirling's approximation $\ln N! = N\ln N - N$ for large $N$ may be quoted.]

**3.** The spin $s$ Ising model in $d$ dimensions in an external magnetic field $h$ is given by

$$E = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i \,,$$

where $S_i = -s, -s+1, \ldots, 0, \ldots, s-1, s$ (there being $2s+1$ integer values in total). The sum is over nearest neighbours with coupling $J > 0$.

(a) Develop Weiss mean field theory by considering all contributions involving $S_i$ to show that the single–spin Boltzmann distribution is given by

$$p(S_i) \approx \frac{e^{-\beta \epsilon_{\mathrm{mf}}(S_i)}}{\sum_{S_j=-s}^{s} e^{-\beta \epsilon_{\mathrm{mf}}(S_j)}} \,,$$

where

$$\epsilon_{\mathrm{mf}}(S_i) = -(Jzm + h) S_i \,,$$

and $z = 2d$ is the coordination number and $m$ is the average magnetisation. **[6]**

(b) State the Weiss mean field consistency relation. **[2]**

(c) Show for this model that the mean field consistency equation is given by

$$m = (s + \tfrac{1}{2}) \coth[(s + \tfrac{1}{2})\alpha] - \tfrac{1}{2} \coth(\tfrac{1}{2}\alpha) \,,$$

where $\alpha = \beta(Jzm + h)$. **[5]**

(d) Consider now the zero magnetic field case (i.e. $h = 0$). By expanding the right hand side of this equation to $O(m^3)$ show first that the $O(m)$ terms give the critical temperature as

$$T_c = \frac{Jz}{3k}\, s(s+1) \,.$$ **[6]**

(e) Secondly show including the $O(m^3)$ terms gives the magnetisation close to the critical point

$$m^2 \approx \frac{5}{3} \frac{s^2(s+1)^2}{(s+\frac{1}{2})^2 + \frac{1}{4}} (-t) \,.$$

where $t$ is the reduced temperature $t = (T - T_c)/T_c$. **[5]**

(f) What is the corresponding critical exponent? **[1]**

[**Hints:** The following may be quoted

$$\sum_{n=-s}^{s} e^{\alpha n} = \frac{\sinh\left[(s+\frac{1}{2})\alpha\right]}{\sinh(\frac{1}{2}\alpha)} \,,$$

$$\coth(x) = \frac{1}{x} + \frac{1}{3}x - \frac{1}{45}x^3 + O(x^5) \,.$$

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