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Solutions in Advanced Statistical Physics

Solution 1: The Langmuir lattice gas

a.) isothermal compressibility

$$P(N,V) = \binom{V}{N} \rho^N (1-\rho)^{V-N} \to \langle N \rangle = V\rho, \quad \langle (N - \langle N \rangle)^2 \rangle = V\rho(1-\rho) \equiv (\Delta N)^2$$

Hence

$$\kappa_T = \beta V (\Delta N)^2 / N^2 = \beta \left(\frac{V}{N} \right)^2 \rho(1-\rho) \stackrel{\rho \ll 1}{\longrightarrow} \beta \frac{V}{N} = \frac{1}{P}.$$

Ideal gas : $PV = NkT \to \kappa_T = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T = \frac{N}{V} \frac{kT}{P^2} = \frac{1}{P}$

b.) Poisson distribution

$$\frac{P(N+1,V)}{P(N,V)} = \frac{V\rho}{N+1} \frac{1 - \frac{N}{V}}{1-\rho} \to \frac{V\rho}{N+1}.$$

Hence $P(N+1,V) = \frac{V\rho}{N+1} P(N,V) = \cdots = \frac{(V\rho)^{N+1}}{(N+1)!} P(0,V)$. By normalization, $P(0,V) = e^{-V\rho}$.

c.) Using Stirling's formular $N! \approx N^N e^{-N} \sqrt{2\pi N}$,

$$\begin{aligned} P(N,V) &\sim \exp\left[V \ln V - (V-N) \ln(V-N) - N \ln N + N \ln \rho + (V-N) \ln(1-\rho) \right] \\ &= \exp\left[-V \left((1-n) \ln \frac{1-n}{1-\rho} + n \ln \frac{n}{\rho} \right) \right] = \exp[-V s_\rho(n)] \end{aligned}$$

The maximum of $s_\rho(n)$ occurs at $n = \rho$ because

$$\frac{ds_\rho(n)}{dn} = \ln \left(\frac{n(1-\rho)}{\rho(1-n)} \right), \quad \frac{d^2 s_\rho(n)}{dn^2} = \frac{1}{n(1-n)} > 0$$

Hence around $n \simeq \rho$, $s_\rho(n) \simeq \frac{1}{2} \frac{(n-\rho)^2}{\rho(1-\rho)}$ and $P(N,V) \sim \frac{\sqrt{V}}{\sqrt{2\pi\rho(1-\rho)}} \exp(-\frac{V}{2} \frac{(n-\rho)^2}{\rho(1-\rho)})$

Solution 2: Shannon entropy

a.) canonical and grandcanonical distribution

Constraint $\sum_s P^{(s)} = 1, \quad \sum_s E^{(s)}P^{(s)} = \langle E\rangle, \quad \sum_s N^{(s)}P^{(s)} = \langle N\rangle$. Let $\lambda_1,\ \lambda_2$, and λ_3 be the Lagrange multipliers for the corresponding constraint and let

$$\psi[P^{(s)}] = -\,k\sum_s P^{(s)}(\ln P^{(s)} - 1) + \lambda_1\left(1 - \sum_s P^{(s)}\right) \\ +\lambda_2\left(\langle E\rangle - \sum_s E^{(s)}P^{(s)}\right) - \lambda_3\left(\langle N\rangle - \sum_s N^{(s)}P^{(s)}\right).$$

Then to maximize the entropy is equivalent to maximize ψ.

$$\frac{\partial\psi}{\partial P^{(s)}} = 0 \rightarrow P^{(s)} = \exp\left(-\frac{\lambda_1}{k} - \frac{\lambda_2}{k}E^{(s)} + \frac{\lambda_3}{k}N^{(s)}\right)$$

From three constraints, $\lambda_1,\ \lambda_2$, and λ_3 are calculated. Actually, $\lambda_2 = \frac{\partial\psi}{\partial\langle E\rangle} = \frac{1}{T}$, $\lambda_3 = -\frac{\partial\psi}{\partial\langle N\rangle} = \frac{\mu}{T}$, and $\lambda_1 = k\ln y$. Since $\frac{\partial^2 S}{\partial P^{(s)2}} = -1/P^{(s)} < 0$, the extremum is maximum.

b) Three properties

i) is clear from the above derivation.

Alternative)

Let $\varphi(x) = x\ln x$. Since $\varphi(x)$ is a convex function, $\varphi\left(\frac{1}{\Omega}\sum_{k=1}^{\Omega} a_k\right) \leq \frac{1}{\Omega}\sum_{k=1}^{\Omega}\varphi(a_k)$ for positive a_k's. If $a_k = p_k \ \left(\sum_{k=1}^{\Omega} p_k = 1\right)$,

$$\varphi(1/\Omega) = -\ln\Omega/\Omega \leq \frac{1}{\Omega}\sum_{k=1}^{\Omega} p_k\ln p_k. \rightarrow S[P^{(s)}] \leq S[P^{(s)} = 1/\Omega] = \ln\Omega$$

ii) trivial

iii) Let $s_0 = 0,\ s_K = \Omega$.

$$S[P^{(s)}] = -k\sum_{r=1}^{K}\bar{P}_r\sum_{q=s_{r-1}+1}^{s_r}\frac{P^{(q)}}{\bar{P}_r}\ln P^{(q)}, \quad S[\bar{P}^{(r)}] = -k\sum_{r=1}^{K}\bar{P}_r\sum_{q=s_{r-1}+1}^{s_r}\frac{P^{(q)}}{\bar{P}_r}\ln\bar{P}_r$$

$$\Rightarrow S[P^{(s)}] - S[\bar{P}^{(r)}] = -k\sum_{r=1}^{K}\bar{P}_r\sum_{q=s_{r-1}+1}^{s_r}\frac{P^{(q)}}{\bar{P}_r}\ln\frac{P^{(q)}}{\bar{P}_r} = \sum_{r=1}^{K}\bar{P}_r S[P(s|r)].$$

c) uniqueness theorem

Let $f(\Omega) \equiv S_\Omega\left(\frac{1}{\Omega}, \ldots, \frac{1}{\Omega}\right)$. Since

$$S_\Omega\left(\frac{1}{\Omega-1}, \ldots, \frac{1}{\Omega-1}, 0\right) < S_\Omega\left(\frac{1}{\Omega}, \ldots, \frac{1}{\Omega}\right) = f(\Omega) \quad \text{[by property i)]},$$
$$S_\Omega\left(\frac{1}{\Omega-1}, \ldots, \frac{1}{\Omega-1}, 0\right) = S_{\Omega-1}\left(\frac{1}{\Omega-1}, \ldots, \frac{1}{\Omega-1}\right) = f(\Omega-1) \quad \text{[by property ii)]},$$

$f(\Omega)$ is an increasing function ($f(\Omega-1) < f(\Omega)$). Let $\Omega = LM$ with integers L and M. From property iii),

$$S_\Omega(\overbrace{\underbrace{\frac{1}{\Omega}, \ldots, \frac{1}{\Omega}}_{L}, \ldots, \underbrace{\frac{1}{\Omega}, \ldots, \frac{1}{\Omega}}_{L}}^{\Omega}) = S_M\left(\frac{1}{M}, \ldots, \frac{1}{M}\right) + M \cdot \frac{1}{M} S_L\left(\frac{1}{L}, \ldots, \frac{1}{L}\right),$$

that is, $f(LM) = f(L) + f(M)$. Hence $f(\Omega) = c\ln(\Omega)$ with c positive. Now go back to the original problem. Let $P_i = \frac{q_i}{N}$ with (arbitrary) positive integers q_i and N. ¿From normalization, $\sum_{i=1}^{\Omega} q_i = N$. By property iii),

$$f(N) = S_N(\overbrace{\underbrace{\frac{1}{N}, \ldots, \frac{1}{N}}_{q_1}, \underbrace{\frac{1}{N}, \ldots, \frac{1}{N}}_{q_2}, \ldots, \underbrace{\frac{1}{N}, \ldots, \frac{1}{N}}_{q_\Omega}}^{N}) = S(P_1, \ldots, P_\Omega) + \sum_{i=1}^{\Omega} P_i f(q_i).$$

Hence

$$S(P_1, \ldots, P_\Omega) = \sum_i P_i(f(N) - f(q_i)) = \sum_i P_i c \ln(N/q_i) = -c\sum_i P_i \ln P_i.$$

Since S is supposed to be continuous, the above relation should be true for all real numbers.

Solution 3: Irreversibility of diffusion

$$\frac{\partial}{\partial t} S[P] = -k\int d\vec{r}\,(\ln P + 1)\frac{dP}{dt} = -Dk\int d\vec{r}\,(\ln P + 1)\nabla^2 P = Dk\int d\vec{r}\,\frac{(\nabla P)^2}{P} > 0$$

Solution 4: Entropic elasticity

a) entropy

Let m be the number of steps to the right $\to m = \frac{N}{2} + \frac{R}{2\ell}$.

$$\Omega(R) = \binom{N}{m} \to S = k\ln\Omega(R) \simeq -kN\left(\frac{1+x}{2}\ln\frac{1+x}{2} + \frac{1-x}{2}\ln\frac{1-x}{2}\right)$$
$$\simeq -kN\left(\frac{x^2}{2} - \ln 2\right),$$

where $x = \dfrac{R}{\ell N}$.

b) tension

$$f = -T\frac{\partial S}{\partial R} = -\frac{T}{\ell N}(-kNx) = \frac{kT}{\ell}x$$

spring constant $\propto T$. $x \propto 1/T$ for fixed f. For ideal gas, $V \propto T$ for fixed pressure.

Solution 5: Generating functions, cumulants, and the central limit theorem

a.) Generating functions for some distributions

$$\varphi_G(k) = e^{-k^2/2}, \varphi_C(k) = e^{-|k|}, \varphi_B(k) = \left(1 + \rho(e^{ik} - 1)\right)^N, \varphi_P(k) = \exp\left(\lambda(e^{ik} - 1)\right)$$

$$\varphi_B(k) = \left(1 + \rho(e^{ik} - 1)\right)^N \to \exp\left(\lambda(e^{ik} - 1)\right) = \varphi_P(k)$$

b.) moment

The proof is rather trivial. The Cauchy distribution has a singularity at $k = 0$, which means that the first moment (or average) is ill-defined. One may be tempted to say that the average is 0 because the Cauchy distribution is even. However, this is of no use not only because of the generating function and but also because of the law of large numbers; see Sol. 5-d.).

c.) cumulant

Since $\varphi = e^{\chi}$,

$$\frac{d\varphi}{dk} = \frac{d\chi}{dk}\varphi \to \frac{d^n\varphi}{dk^n} = \sum_{p=0}^{n-1}\binom{n-1}{p}\left(\frac{d}{dk}\right)^{p+1}\chi\left(\frac{d}{dk}\right)^{n-1-p}\varphi.$$

Now put $k = 0$, then we get

$$m_n = \sum_{p=0}^{n-1}\binom{n-1}{p}\kappa_{p+1}m_{n-1-p} = \kappa_n + \sum_{p=0}^{n-2}\binom{n-1}{p}\kappa_{p+1}m_{n-1-p} = \kappa_n + \sum_{p=1}^{n-1}\binom{n-1}{p-1}\kappa_p m_{n-p}$$

$$\kappa_1 = m_1, \quad m_1 = \kappa_1,$$

$$\kappa_2 = m_2 - m_1^2, \quad m_2 = \kappa_2 + \kappa_1^2,$$

$$\kappa_3 = m_3 - 3m_2m_1^2 + 2m_1^3, \quad m_3 = \kappa_3 + 3\kappa_2\kappa_1 + \kappa_1^3,$$

$$\kappa_4 = m_4 - 4m_3m_1 - 3m_2^2 + 12m_1^2m_2 - 6m_1^4 \quad m_4 = \kappa_4 + 4\kappa_3\kappa_1 + 3\kappa_2^2 + 6\kappa_2\kappa_1^2 + \kappa_1^4.$$

d.) central Limit theorem

Since

$$\begin{aligned}\left\langle \exp\left(ik\frac{X_i - \mu}{\sqrt{N}\sigma}\right)\right\rangle &= \exp\left(-i\frac{k\mu}{\sqrt{N}\sigma}\right)\varphi\left(\frac{k}{\sqrt{N}\sigma}\right) \\ &= \left(1 - i\frac{k\mu}{\sqrt{N}\sigma} - \frac{1}{2}\frac{k^2\mu^2}{N\sigma^2}\right)\left(1 + i\frac{k\mu}{\sqrt{N}\sigma} - \frac{1}{2}\frac{k^2(\sigma^2 + \mu^2)}{N\sigma^2}\right) + o\left(\frac{k^2}{2N}\right) \\ &= 1 - \frac{k^2}{2N} + o\left(\frac{k^2}{2N}\right)\end{aligned}$$

and all X_i are independent, we can obtain that

$$\langle e^{ikS_N} \rangle = \left(1 - \frac{k^2}{2N} + o\left(\frac{k^2}{2N}\right)\right)^N \to e^{-k^2/2}.$$

cf.) Law of large numbers.

If N is sufficiently large and μ is finite, $S_N = \dfrac{X_1 + \cdots + X_N}{N} \to \mu$ with probability 1.

$$\left\langle \exp\left(ik\frac{X_i}{N}\right)\right\rangle = 1 + i\mu\frac{k}{N} + o(k/N) \Rightarrow \left\langle e^{ikS_N}\right\rangle \to e^{ik\mu}.$$

For Cauchy distribution, $\langle e^{ikS_N}\rangle = e^{-|k|}$ regardless of N. Hence, it is better to say that the Cauchy distribution does not have a mean.

Solution 6: A Lévy flight on living polymers

$$p(r) = \int dlP(l)\frac{1}{\sqrt{4\pi D(l)\tau^*}}\exp\left(-\frac{r^2}{4D(l)\tau^*}\right) = \frac{1}{\sqrt{\pi D^*}}\int_0^\infty dyy^{(\alpha+2)/2}\exp\left(-\frac{r^2}{D^*}y^\alpha - y\right),$$

where $D^* = 4D_0\tau^* l_D^\alpha l_0^{-\alpha}$. If $\langle r^2\rangle$ is finite, a tracer particle moves diffusively thanks to the central limit theorem.

$$\langle r^2\rangle = 2\pi\tau^*\int D(l)P(l) \propto \int_0^\infty dyy^{1-\alpha}e^{-y} = \begin{cases}\text{finite} & \text{if } \alpha < 2,\\ \infty & \text{if } \alpha \geq 2.\end{cases}$$

To understand the *superdiffusive* motion, let us find out the asymptotic behavior of $p(r)$ when $r \gg 1$. Let $A^{\alpha-1} = r^2/D^*$ and set $Ay = z$, then

$$p(r) \propto A^{-(\alpha+4)/2}\int_0^\infty dzz^{(\alpha+2)/2}\exp\left(-\frac{1}{A}(z^\alpha + z)\right).$$

Since A is very large, the main contribution of the above integral happens when $z \leq z_0$ where z_0 is the solution of the equation $\dfrac{1}{A}(z_0^\alpha + z_0) = 1$. Since $\alpha \geq 2$, $z_0 \simeq A^{1/\alpha}$ approximately. Hence

$$p(r) \sim A^{-(\alpha+4)/2}\int_0^{z_0} dzz^{(\alpha+2)/2} \propto A^{-(\alpha+4)/2}A^{(\alpha+4)/(2\alpha)} = \left(A^{-(\alpha-1)}\right)^{(\alpha+4)/(2\alpha)} \propto r^{-(\alpha+4)/\alpha}.$$

The largest step size among N iid steps can be calculated as

$$N\int_{r_M}^\infty p(r)dr = 1 \Rightarrow r_M^2 \sim N^{\alpha/2}.$$