Math 254A Lecture 20 Notes

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May 12, 2021

1 Deriving van der Waal's Equation (Part 3)

1.1 Bound on α

Last time, we had a quantity α which depended on various factors. We bounded it by a term $\alpha(m, r, \varepsilon)$ which only depended on these 3 quantities. We will compare this to the integral $\int \varphi = \int \varphi^r$.

$$\left| \alpha(m, r, \varepsilon) - \int \varphi^r \right| = \left| (\varepsilon m)^3 \sum_{v \in \varepsilon m \mathbb{Z}^3} \varphi^r(v) - \int \varphi^r \right|$$

Let Q_v be the cube with side length εm and center v.

$$\begin{aligned}
&= \left| \sum_{v \in \varepsilon m \mathbb{Z}^3} \left((\varepsilon m)^3 \varphi^r(v) - \int_{Q_v} \varphi^r \right) \right| \\
&= \left| \sum_{v} \left(|Q_v| \varphi^r(v) - \int_{Q_v} \varphi^r \right) \right| \\
&\leq \sum_{v} \int_{Q_v} |\varphi^r(v) - \varphi^r(x)| \, dx \\
&\leq \sum_{v : Q_v \cap \overline{B_r} \neq \varnothing} (\varepsilon m)^3 \cancel{\frac{\sqrt{3}}{2}} \varepsilon m \cdot \frac{\overset{O(1)}{\cancel{\|\nabla \varphi\|}}}{r^4} \\
&= O\left(\frac{r^3}{(\varepsilon m)^3} \cdot \frac{(\varepsilon m)^4}{r^4} \right) \\
&= O\left(\frac{\varepsilon m}{r} \right).
\end{aligned}$$

So

$$\alpha(m, r, \varepsilon) = \alpha + O\left(\frac{\varepsilon m}{v} \right)$$

for some constant α.

1.2 Maximizing the entropy term

Now consider maximizing

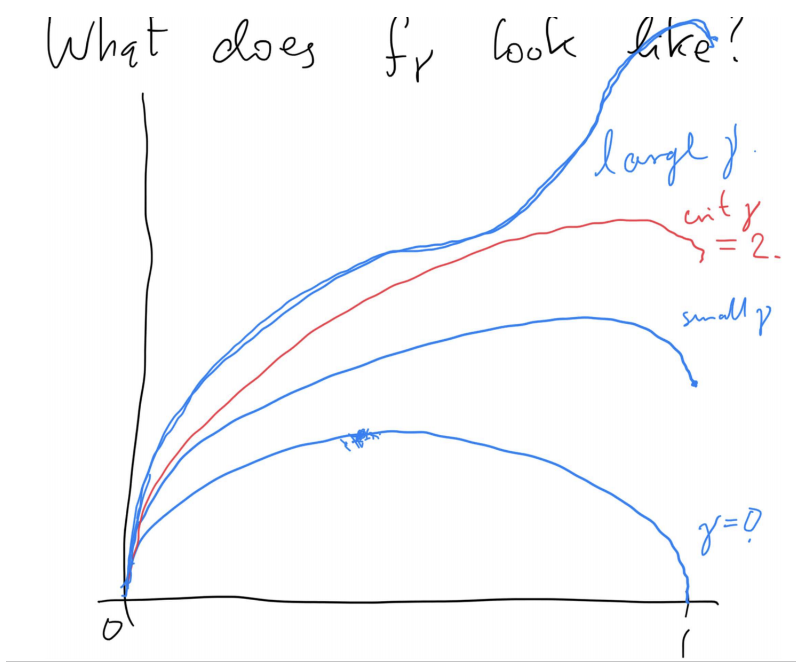
$$\frac{1}{(n/m^3)} \sum_{k \in \mathcal{C}_n} [H(\rho_k, 1-\rho_k) + \gamma \rho_k^2],$$

where $\gamma = \beta\alpha(m, \varepsilon, r)/\varepsilon^3 = (\beta/\varepsilon^3)(\alpha + O(\varepsilon m/r))$. Now, we want to try to maximize this over $\rho \in \widetilde{\Omega}_n$ with $|\rho| = N_n/m^3$ (recall $N_n/n^3 \to \varepsilon^3/v$ as $n \to \infty$). We can also write this expression as

$$\frac{1}{|\mathcal{C}_n|} \sum_{k \in \mathcal{C}_n} f_\gamma(\rho_k),$$

where $f_\gamma(x) = H(x, 1-x) + \gamma x^2$ for $0 \leq x \leq 1$.

What does f_γ look like? Here is a picture:



There is a critical value of γ which is the largest γ for which this is still concave. Check using calculus that the critical γ equals 2.

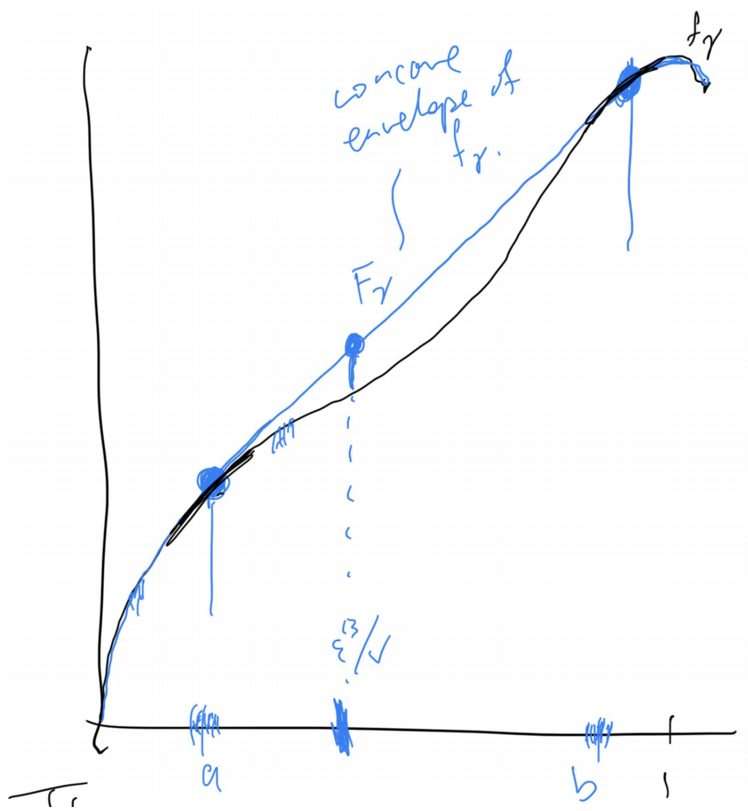
If $\gamma \leq 2$, f_γ is concave, so Jensen's inequality gives

$$\begin{aligned}\frac{1}{|\mathcal{C}_n|} \sum_{k \in \mathcal{C}_n} f_\gamma(\rho_k) &\leq f_\gamma\left(\frac{1}{|C_n|}\sum_k \rho_k\right) \\ &= f_\gamma\left(\frac{N_n}{m^3}\right)\end{aligned}$$

$$
\begin{aligned}
&= f_\gamma\left(\frac{N_n}{m^3}\right) \\
&\xrightarrow{n\to\infty} f_\gamma\left(\frac{\varepsilon^3}{v}\right).
\end{aligned}
$$

We can make this close to tight by taking $\rho_k \approx \varepsilon^3/v$ for all k.

What if $\gamma > 2$? Use the *concave envelope* F_γ of f_γ:



Then

$$
\begin{aligned}
\frac{1}{|\mathcal{C}_n|}\sum_{k\in\mathcal{C}_n} f_\gamma(\rho_k) &\le \frac{1}{|\mathcal{C}_n|}\sum_{k\in\mathcal{C}_n} F_\gamma(\rho_k) \\
&\le F_\gamma\left(\frac{1}{|\mathcal{C}_n|}\sum_{k\in\mathcal{C}_n} \rho_k\right) \\
&\approx F_\gamma\left(\frac{\varepsilon^3}{v}\right)
\end{aligned}
$$

as $n \to \infty$. This also can be brought as close as we like once $n \to \infty$ and m is large.

- If $\varepsilon^3/v \notin (a,b)$, then $F_\gamma(\varepsilon^3/v) = f_\gamma(\varepsilon^3/v)$. Then just take $\rho_k \approx \varepsilon^3/v$ for all k.
- If $a < \varepsilon^3/v < b$, then $\rho_k \approx \varepsilon^3/v$ for all k will give you

  $$\frac{1}{|\mathcal{C}_n|}\sum_{k \in \mathcal{C}_n} f_\gamma(\rho_k) = f_\gamma\left(\frac{\varepsilon^3}{v}\right) < F_\gamma\left(\frac{\varepsilon^3}{v}\right).$$

  Instead, express $\varepsilon^3/v = ta + (1-t)b$. Now choose the values ρ_k so that $\rho_k \approx a$ for $\approx t|\mathcal{C}_n|$ many ks and $\rho_k \approx b$ for $\approx (1-t)|\mathcal{C}_n|$ many ks. Then

  $$\frac{1}{|\mathcal{C}_n|}\sum_{k \in \mathcal{C}_n} f_\gamma(\rho_k) \approx t f_\gamma(a) + (1-t) f_\gamma(b) = F_\gamma\left(\frac{\varepsilon^3}{v}\right)$$

The conclusion is that

$$\frac{1}{|\mathcal{C}_n|}\sum_{k \in \mathcal{C}_n} f_\gamma(\rho_k) = F_\gamma\left(\frac{\varepsilon^3}{v}\right) + O\left(\frac{1}{m}\right)$$

as $n \to \infty$.

1.3 Maximizing the effective partition function

Is the maximization problem for $\log \widehat{Z}_n^r$ close to the same value? Yes!

Go back to

$$\max_{|\rho| = N_n/m^3} \left\{ W(\rho) - \frac{\beta}{n^3}\widetilde{\Phi}_n^r(\rho) \right\}.$$

Can we get this close to the same value? Yes. Since f_γ is strictly convex near a and b, we must have roughly a t fraction of ρ_ks close to a and roughly a $(1-t)$ fraction of ρ_ks close to b

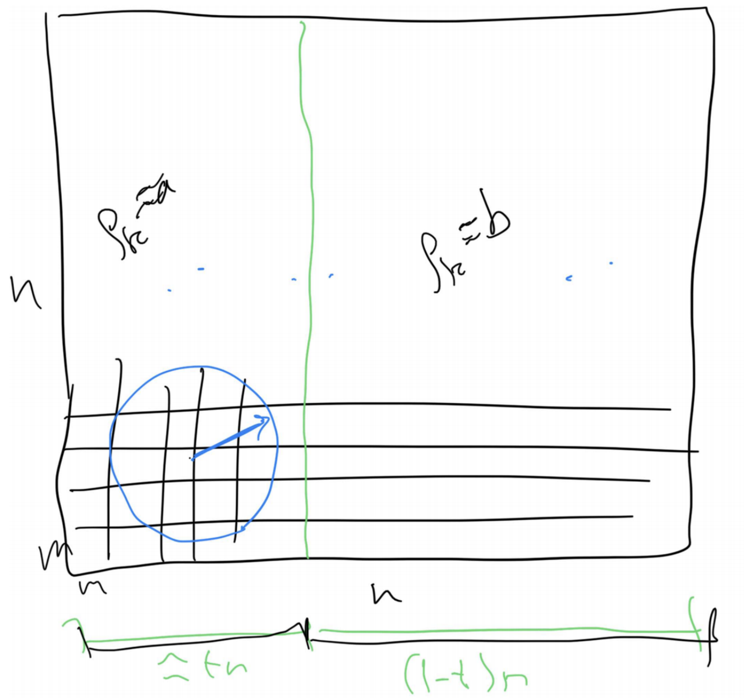
When is the above maximum close to the average of f_γ? We had the bound via AM-GM:

$$\sum_k H(\rho_k, 1-\rho_k) + \beta m^3 \sum_{k,\ell} \varphi^r(\varepsilon(k-\ell))\rho_k\rho_\ell \le \sum_k H(\rho_k, 1-\rho_k) + \beta m^3 \sum_{k,\ell} \varphi^r(\varepsilon(k-\ell))\frac{\rho_k^2 + \rho_\ell^2}{2}.$$

The difference equals

$$\beta m^3 \sum_{k,\ell} \varphi^r(\varepsilon(k-\ell))\frac{1}{2}(\rho_k - \rho_\ell)^2.$$

This is small if $\rho_k \approx \rho_\ell$ for most pairs (k,ℓ) where $\varphi^r(\varepsilon(k-\ell))$ is not negligible. What kinds of ρ achieve all these requirements? Choose it according to this picture:



Then we do get

$$W(\rho) - \frac{\beta}{n^3}\widetilde{\Phi}_n^r(\rho) \approx \frac{1}{|\mathcal{C}_n|}\sum_k f_\gamma(\rho_k) \approx F_\gamma\left(\frac{\varepsilon^3}{v}\right).$$

We will finish off this story next time.