Math 254A Lecture 19 Notes

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1 Deriving van der Waal's Equation (Cont.)

1.1 Recap+partitioning space into boxes lemma

In our current setting we have a box $B_n = \frac{1}{\varepsilon}(R_n \cap \varepsilon\mathbb{Z}^3) = \{1, \dots, n\}^n$. We have N_n particles in B_n, where $\frac{|B_n|}{N_n} \to \frac{v}{\varepsilon^3}$. The particles are located at $\omega \in \Omega_n = \{0,1\}^{B_n}$, where $|\omega| = N_n$. We have a "local density map" $D : \Omega_n \to \widetilde{\Omega}_n = \{0, 1/m^3, \dots, 1\}^{\mathcal{C}_n}$ with

$$D(\omega)_k = \frac{1}{m^3} \sum_{i \in C_k} \omega_i,$$

where $m \mid n$ and $\{C_k : k \in \mathcal{C}_n\}$ is a partition of B_n into $(m \times m \times m)$-boxes and $\mathcal{C}_n$ is the set of centers of boxes.

The original energy of $\omega \in \Omega_n$ is

$$\Phi_n^r(\omega) = -\sum_{i,j \in B_n} \varphi^r(\varepsilon(i-j))\omega_i\omega_j,$$

where $\varphi : \mathbb{R}^3 \to [0,\infty)$ is C^1, symmetric, has support $\subseteq \overline{B_1(0)}$, and $\varphi^r(x) = r^{-3}\varphi(x/r)$ is a dilation for $r > 0$.

The **effective energy** of $\omega \in \widetilde{\Omega}_n$ is

$$\widetilde{\Phi}_n^r(\rho) = -m^6 \sum_{k,\ell \in \mathcal{C}_n} \varphi^r(\varepsilon(k-\ell))\rho_k\rho_\ell.$$

We also had the following lemma:

Lemma 1.1. *If $D(\omega) = \rho$, then*

$$\Phi_n^r(\omega) = \widetilde{\Phi}_n^r(\rho) + O\left(\frac{n^3 m}{\varepsilon^2 r}\right).$$

Proof. Last time, we showed that

$$\left| \sum_{i \in C_k, j \in C_\ell} \varphi^r(\varepsilon(i-j))\omega_i\omega_j \right| \leq m^6 O\left(\frac{m^7\varepsilon}{r^4}\right).$$

Finally, we sum over $k, \ell \in \mathcal{C}_n$:

$$|\Phi_n^r(\omega) - \widetilde{\Phi}_n^r(\rho)| = \left| \sum_{k,\ell \in \mathcal{C}_n} \left[\sum_{i \in C_k, j \in C_\ell} \varphi^r(\varepsilon(i-j))\omega_i\omega_j - m^6\varphi^r(\varepsilon(k-\ell))\rho_k\rho_\ell \right] \right|.$$

Observe that if $\mathrm{dist}(C_k, C_\ell) > r/\varepsilon$, then the expression in the square braces equals 0. How many pairs (k,ℓ) are left? The number of k we can choose first is $(n/m)^3$. Then the number of ℓs that "hit" k equals $O(r^3/(\varepsilon m^3))$. The total number of nonzero terms is $O\left(\frac{n^3r^3}{\varepsilon^3m^6}\right)$. Now multiply by the previous bound on those terms to get

$$\leq O\left(\frac{n^3m}{\varepsilon^2 r}\right).$$ □

Note that we will let $n, r, m \to \infty$ (with $m = \sqrt{r}$), and then finally let $\varepsilon \to 0$.

1.2 Estimating the size of the partition

Now use this lemma to approximate the partition

$$\begin{aligned}
Z_n^r &= \sum_{\substack{\omega \in \Omega_n \\ |\omega| = N_n}} \exp(-\beta\Phi_n^r(\omega)) \\
&= \sum_{\substack{\rho \in \widetilde{\Omega}_n \\ |\rho| = N_n/m^3}} \sum_{D(\omega)=\rho} \exp(-\beta\Phi_n^r(\omega)) \\
&= \sum_{\substack{\rho \in \widetilde{\Omega}_n \\ |\rho| = N_n/m^3}} \sum_{D(\omega)=\rho} \exp(-\beta\widetilde{\Phi}_n^r(\omega)) \cdot \exp\left(O\left(\frac{n^3m}{\varepsilon^2r}\right)\right) \\
&= \underbrace{\sum_{\substack{\rho \in \widetilde{\Omega}_n \\ |\rho| = N_n/m^3}} |D^{-1}(\{\rho\})| \exp(-\beta\widetilde{\Phi}_n^r(\omega))}_{\widetilde{Z}_n^r} \cdot \exp\left(O\left(\frac{n^3m}{\varepsilon^2r}\right)\right).
\end{aligned}$$

Next, estimate $|D^{-1}(\rho)|$. This equals

$$\prod_{k \in \mathcal{C}_n} (\#\text{ ways to put } m^3\rho_k \text{ particles into } m^3 \text{ holes}) = \prod_{k \in \mathcal{C}_n} \binom{m^3}{m^3\rho_k}$$

$$= \prod_k e^{m^3 H(\rho_k, 1-\rho_k) + o(m^3)}$$
$$= e^{n^3[W(\rho)+o(1)]},$$

where
$$W(\rho) := \frac{1}{n^3} \sum_{k \in \mathcal{C}_n} m^3 H(\rho_k, 1-\rho_k) = \frac{1}{(n/m)^3} \sum_{k \in \mathcal{C}_n} H(\rho_k, 1-\rho_k).$$

Now insert this new approximation to get
$$\widetilde{Z}_n^r = e^{o(n^3)} \underbrace{\sum_{\substack{\rho \in \widetilde{\Omega}_n \\ |\rho| = N_n/m^3}} \exp(n^3 W(\rho) - \beta \widetilde{\Phi}_n^r(\rho))}_{\widehat{Z}_n^r}.$$

The key observation is that the number of terms here is $\leq (m^3+1)^{n^3/m^3} = \exp O(n^3 \cdot \frac{\log m}{m^3})$. We will use this via the following:

Lemma 1.2. *Let $a_i \geq 0$ for all $i \in I$ (with $|I| < \infty$). Then*
$$\max_i a_i \leq \sum_{i \in I} a_i \leq |I| \max_i a_i.$$

Corollary 1.1.
$$\begin{aligned} n^3 \max &\left\{ W(\rho) - \frac{\beta}{n^3} \widetilde{\Phi}_n^r(\rho) : \rho \in \widetilde{\Omega}_n, |\rho| = \frac{N_n}{m^3} \right\} \\ &\leq \log \widetilde{Z}_n^r \\ &\qquad \leq n^3 \max \left\{ W(\rho) - \frac{\beta}{n^3} \widetilde{\Phi}_n^r(\rho) : \rho \in \widetilde{\Omega}_n, |\rho| = \frac{N_n}{m^3} \right\} + O\left(n^3 \cdot \frac{\log m}{m^3} \right). \end{aligned}$$

Our main remaining task is to understand the maximum of
$$W(\rho) - \frac{\beta}{n^3} \widetilde{\Phi}_n^r(\rho)$$
for $\rho \in \widetilde{\Omega}_n$ such that $|\rho| = N_n/m^3$. Let's unpack this:
$$\begin{aligned} W(\rho) - \frac{\beta}{n^3} \widetilde{\Phi}_n^r(\rho) &= \frac{1}{(n/m)^3} \sum_k H(\rho_k, 1-\rho_k) + \frac{\beta m^6}{n^3} \sum_{k,\ell} \varphi^r(\varepsilon(k-\ell)) \rho_k \rho_\ell \\ &= \frac{1}{(n/m)^3} \left[\sum_k H(\rho_k, 1-\rho_k) + \beta m^3 \sum_{k,\ell} \varphi^r(\varepsilon(k-\ell)) \rho_k \rho_\ell \right] \end{aligned}$$

The key idea is to bound the right term above by something with no cross terms. Observe that $\rho_k \rho_\ell \leq \frac{1}{2}(\rho_k^2 + \rho_\ell^2)$ using the AM-GM inequality. Insert this into the second term above:

$$\begin{aligned} m \sum_{k,\ell} \varphi^r(\varepsilon(k-\ell))\rho_k \rho_\ell &\leq m \sum_{k,\ell} \varphi^r(\varepsilon(k-\ell)) \left[\frac{\rho_k^2 + \rho_\ell^2}{2}\right] \\ &= m^3 \sum_{k,\ell} \rho_k^2 \varphi^r(\varepsilon(k-\ell)) \\ &= \frac{1}{\varepsilon^3} \sum_{k \in \mathcal{C}_n} \rho_k^2 \underbrace{\left[(\varepsilon m)^3 \sum_{\ell \in \mathcal{C}_n} \varphi^r(\varepsilon(k-\ell))\right]}_{=:\alpha(n,m,r,\varepsilon,k)}. \end{aligned}$$

So we will try to maximize

$$\begin{aligned} &\frac{1}{(n/m)^3}\left[\sum_k H(\rho_k, 1-\rho_k) + \beta m^3 \sum_k \rho_k^2 \cdot \alpha(n,m,r,\varepsilon,k)\right] \\ &\qquad = \frac{1}{(n/m)^3} \sum_{k \in \mathcal{C}_n} \left[H(\rho_k, 1-\rho_k) + \beta m^3 \cdot \alpha(n,m,r,\varepsilon,k)\rho_k^2\right] \end{aligned}$$

Now consider

$$\alpha(n,m,r,\varepsilon,k) = (\varepsilon m)^3 \sum_{\ell \in \mathcal{C}_n} \varphi(\varepsilon(k-\ell))$$

Ignoring that some k can be on the boundary of the box,

$$\begin{aligned} &\leq (\varepsilon m)^3 \sum_{v \in \varepsilon m \mathbb{Z}^3} \varphi^r(v) \\ &= (\varepsilon m)^3 \sum_{v \in \varepsilon m \mathbb{Z}^3} \frac{1}{r^3}\varphi(v/r) \\ &= \frac{\varepsilon^3 m^3}{r^3} \sum_{v \in (\varepsilon m/r)\mathbb{Z}^3} \frac{1}{r^3}\varphi(v). \end{aligned}$$

As $r \to \infty$, this will give a Riemann sum for $\int \varphi$. We will plug this back into the previous expression next time.