

STATISTICAL MECHANICS: Problem Set 2

NAME: Stephen Iota (siota001@ucr.edu)
 COURSE: Physics 133 (Spring 2019), Prof. Kuhlman
 DATE: May 25, 2019

Sethna problems 2.6, 3.5 and 3.9. Painstakingly typeset using L^AT_EX. All final answers are boxed.

1 Fourier and Green

An initial density profile $\rho(x, t = 0)$ is perturbed slightly from ρ_0 . The density obeys the diffusion equation $\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2}$, where $D = 0.001 \text{ m}^2/\text{s}$.

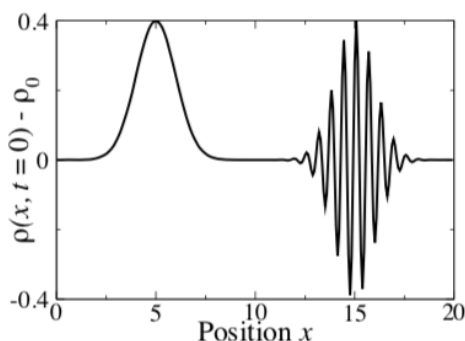


Figure 1: Initial profile density deviation from average.

(a) Fourier Consider just a cosine wave. If the initial wave were $\rho_{\cos}(x, 0) = \cos 10x$, what would it be at $t = 10\text{s}$?

Solution: We can decompose ρ into a superposition of complex plane wave solutions using the Fourier method. We expect the solution to look like $\rho_{\cos} = \rho_k e^{ikx}$. We can superimpose all different wave vectors to get a general solution.

$$\rho(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \rho_k(0) e^{ikx} e^{-Dk^2 t} dk$$

where the coefficients $\rho_k(0)$ are the Fourier transform of the initial density profile

$$\rho_k(0) = \int_{-\infty}^{\infty} \rho(x, 0) e^{-ikx} dx$$

Plugging in $\rho_{\cos}(x, 0) = \cos 10x$, we get

$$\begin{aligned} \rho_k &= \int_{-\infty}^{\infty} \cos 10x e^{-ikx} dx \\ &= \int_{-\infty}^{\infty} \frac{e^{i10x} + e^{-i10x}}{2} e^{-ikx} dx \\ &= \frac{1}{2} [\delta(k - 10) + \delta(k + 10)] \end{aligned}$$

So the initial distribution is composed of two frequencies. Now we solve for the time evolution in position

space.

$$\begin{aligned}
\rho(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{2} [\delta(k-10) + \delta(k+10)] e^{ikx} e^{-Dk^2 t} dk \\
&= \frac{1}{4\pi} \int_{-\infty}^{\infty} [\delta(k-10) e^{ikx} e^{-Dk^2 t} + \delta(k+10) e^{ikx} e^{-Dk^2 t}] dk \\
&= \frac{1}{4\pi} [(e^{i10x} + e^{-i10x}) e^{-D100t}] \\
&= \frac{1}{8\pi} \cos 10x e^{-D100t}
\end{aligned}$$

This is the general time evolution for ρ_{\cos} . Solving for $t = 0$ yields

$$\begin{aligned}
\rho(x, t = 10s) &= \frac{1}{8\pi} \cos 10x e^{-(.001 \cdot 100 \cdot 10)} \\
&= \boxed{\frac{1}{8\pi} \cos 10x e^{-1}}
\end{aligned}$$

(b) Green If a wave at some earlier time $-t_0$ were a δ -function at $x = 0$, such that $\rho(x, -t_0) = \delta(x)$, what choice of time elapsed t_0 would yield a Gaussian $\rho(x, 0) = \exp(-x^2/2)/\sqrt{2\pi}$ for the given diffusion constant D ?

Solution: We define Green's function $G(x, t)$ to be the time evolution of $G(x, t = -t_0) = \delta(x)$. We follow the same steps as in part a to solve for $G(x, t)$.

$$\begin{aligned}
G_k(-t_0) &= \int G(x, -t_0) e^{-ikx} dx \\
&= \int \delta(x) e^{-ikx} = 1
\end{aligned}$$

G_k is independent of k . The time evolved Fourier transform is $G_k(t) = e^{-Dk^2(t+t_0)}$. The time evolution in position space is

$$\begin{aligned}
G(x, t) &= \frac{1}{2\pi} \int e^{ikx} G_k(-t_0) e^{-Dk^2(t+t_0)} dk \\
&= \frac{1}{2\pi} \int e^{ikx} e^{-Dk^2(t+t_0)} dk
\end{aligned}$$

The answer to this integral is the well known Green's function for the diffusion equation

$$G(x, t) = \frac{1}{\sqrt{4\pi D(t+t_0)}} e^{-x^2/4D(t+t_0)}$$

We need to find a time $-t_0$ such that $G(x, 0)$ looks like a Gaussian function centered about the origin for the given diffusion constant D . By analysis, we see that a time of $\boxed{t_0 = 500 \text{ seconds}}$ will give a Gaussian at $t = 0$.

(c) Pictures Now consider time evolution for the next ten seconds. The initial density profile $\rho(x, t = 0)$ is as shown in fig. ???. What figure represents the density at $t = 10s$?

Solution: The density profile in fig. ?? is a Gaussian centered at $x = 5$ on the left, and a smooth envelope function multiplied by $\cos 10x$ centered at $x = 15$ on the right. From the previous two parts, we know that the Gaussian function takes a much longer time to diffuse than the cosine function. Thus, in 10 seconds, we expect the function on the left to remain fairly similar. The short wavelength parts of the cosine function will be suppressed. We expect the distribution at $t = 10 \text{ sec}$ to look like $\boxed{\text{fig. ?? (figure E from the text)}}$.

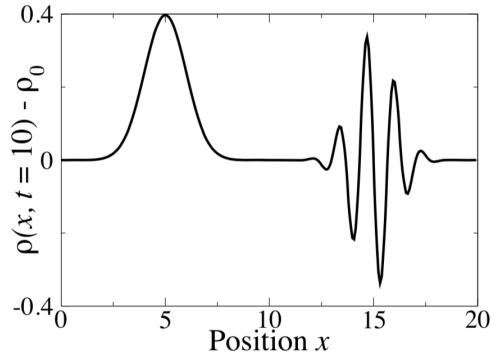


Figure 2: Profile density at $t = 10$ seconds.

2 Hard sphere gas

A 2D $L \times L$ box with hard walls contains a gas of N hard disks of radius $r \ll L$, as shown in fig. ???. The disks are dilute; the summed area $N\pi r^2 \ll L^2$. Let A be the effective area allowed for the disks in the box: $A = (L - 2r)^2$.

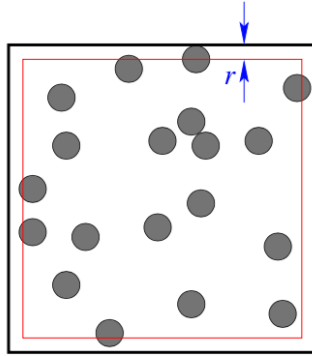


Figure 3: Hard sphere gas.

(a) The area allowed for the second disk is approximately $A - \pi(2r)^2$. What is the allowed $2N$ -dimensional volume in configuration space, of allowed zero-energy configurations of hard disks, in this dilute limit?

Solution: For $N = 2$, $A_2 = A(A - 4\pi r^2)$; for $N = 3$, $A_3 = A(A_2)(A_2 - 4\pi r^2)$, and so on. As N increases, each disk will have a smaller area by $4\pi r^2$ than the previous disk.

$$A_N = \frac{1}{N!} \prod_{n=0}^N A - n4\pi r^2$$

(b) What is the configuration entropy for the hard disks?

Solution: Let S denote configuration entropy. Using answer from part a:

$$\begin{aligned}
S &= k_B \log A_N \\
&= k_B \log \left(\frac{1}{N!} \prod_{n=0}^N A - n4\pi r^2 \right) \\
&= k_B \left(-\log N! + \sum_{n=1}^N \log (A - (n-1)4\pi r^2) \right)
\end{aligned}$$

where in the last step we changed the starting index. In the dilute limit, $N4\pi r^2 \ll A$. We Taylor expand $\log(A - n4\pi r^2)$:

$$\begin{aligned}
\log(A - (n-1)4\pi r^2) &= \log A + \log(1 - (n-1)4\pi r^2/A) \\
&\approx \log A - (n-1) \frac{4\pi r^2}{A}
\end{aligned}$$

Plugging in this approximation to the sum, we find a sum of the form $\sum_{n=1}^N = N(N-1)/2$. We use Stirling's approximation $\log N! \approx N \log N - N$.

$$S = k_B \left(-N \log N - N + \left(N \log A - \frac{N(N-1)4\pi r^2}{2A} \right) \right)$$

Simplifying, we reach our result

$$S = Nk_B \left(1 + \log \left(\frac{A}{N} - \frac{4\pi r^2}{N} \frac{N-1}{2} \right) \right)$$

where we might possibly be able to say $\frac{4\pi r^2}{N} \frac{N-1}{2}$ is about $2\pi r^2$.

3 Gauss and Poisson

Calculate the probability of having n particles in a subvolume V , for a box with total volume KV and a total number of particles $T = KN_0$.

(a) Find the exact formula for this probability; n particles fall in the subvolume V , with a total of T particles in KV .

Solution: Suppose n particles are in subvolume V and $T - n$ particles are outside of V , in subvolume $(K-1)V$, where the total volume is KV . In configuration space, the available volume is $V^n((K-1)V)^{T-n} = V^T(K-1)^{T-n}$, and the total volume is $(KV)^T$. The probability is given by the ratio of these two volumes, where we need to be mindful about the different ways to pick the n particles. The total probability is given by:

$$\begin{aligned}
P(n) &= \binom{T}{n} \frac{(K-1)^{T-n}}{K^T} \\
&= \boxed{\frac{T!}{n!(T-n)!} \frac{(K-1)^{T-n}}{K^T}}
\end{aligned}$$

(b) Show that the Poisson distribution is normalized: $\sum_n \rho_n = 1$. Calculate the mean of the distribution $\langle n \rangle$ in terms of a . Calculate the variance $\langle (n - \langle n \rangle)^2 \rangle$.

Solution: For normalization:

$$\begin{aligned}\sum_{n=0}^{\infty} \rho_n &= \exp\{-a\} \sum_{n=0}^{\infty} \frac{a^n}{n!} \\ &= \exp\{-a\} \exp\{a\} \\ &= \boxed{1}\end{aligned}$$

For mean of Poisson distribution:

$$\begin{aligned}\langle n \rangle &= \sum_{n=0}^{\infty} n \frac{a^n}{n!} e^{-a} \\ &= \sum_{n=1}^{\infty} n \frac{a^n}{n!} e^{-a} \\ &= \sum_{n=1}^{\infty} \frac{a a^{n-1}}{(n-1)!} e^{-a} \\ &= a \sum_{n=0}^{\infty} \frac{a^n}{n!} e^{-a} \\ &= a \sum_{n=0}^{\infty} \frac{a^n}{n!} e^{-a} \\ &= a \sum_{n=0}^{\infty} \rho_n\end{aligned}$$

which is equal to \boxed{a} because the distribution is normalized. For the variance, we have $\langle (n - \langle n \rangle)^2 \rangle = \langle n^2 \rangle - \langle n \rangle^2$.

$$\begin{aligned}\langle n \rangle^2 &= \sum_{n=0}^{\infty} n^2 \frac{a^n}{n!} e^{-a} \\ &= a \sum_{n=0}^{\infty} (n+1) \rho_n \\ &= a \langle n+1 \rangle \\ &= a^2 + a\end{aligned}$$

This gives us a variance of $(a^2 + a) - (a^2) = \boxed{a}$.

(c) As $K \rightarrow \infty$, show that the probability that n particles fall in the subvolume V has the Poisson distribution $\rho_n = a^n e^{-a} / n!$. What is a ?

Solution: Recall the answer to part a:

$$P(n) = \frac{T!}{n!(T-n)!} \frac{(K-1)^{T-n}}{K^T}$$

As we let K and $T \rightarrow \infty$, $(1 - 1/K)^{(T-n)} \approx e^{-\frac{T}{K}}$. Also $T! \approx (T/e)^T$. We simplify:

$$\begin{aligned}
\frac{T!}{n!(T-n)!} &\approx \frac{(T/e)^T}{((T-n)/e)^{T-n}} \\
&= \left(\frac{T-n}{T}\right)^{n-T} \left(\frac{T}{e}\right)^n \\
&\approx e^{\frac{n}{T}(T-n)} \left(\frac{T}{e}\right)^N \\
&\approx T^n
\end{aligned}$$

The final result is a Poisson distribution where $a = T/K$.

$$\boxed{P(n) = \frac{(T/K)^n}{n!} e^{-T/K}}$$