We discuss Maxwell, Boltzmann and $\delta$-function.

1 [Use of $\delta$-function]
Suppose we know how to compute the average $\langle \cdot \rangle_u$ over a random variable $u$. Then, the density distribution function $f$ for $x = \varphi(u)$ is given by

$$f(x) = \langle \delta(x - \varphi(u)) \rangle_u.$$  \hspace{1cm} (DH3.1)

This is the most important formula for density distribution functions.

(1) You must be able to explain why this is so.
(2) Now, we should be able to use $\delta$-functions. Compute the following integrals.

(i) $\int_0^2 dx \delta(x - 1)(x^2 + 2x - 3)$. \hspace{1cm} (DH3.2)
(ii) $\int_0^1 dx \delta(x - \pi/3) \cos x$. \hspace{1cm} (DH3.3)
(iii) $\int_0^2 dx \delta(3x - \pi) \cos x$. \hspace{1cm} (DH3.4)
(iv) $\int_0^\infty dx \delta(x^2 - 3x - 4)x^3$. \hspace{1cm} (DH3.5)
(v) $\int_{-\infty}^\infty dx \delta(x^3 + 2x^2 - x - 2)e^x$. \hspace{1cm} (DH3.6)

2 [2D ideal gas]$^1$

There is a 2D ideal gas in equilibrium at temperature $T$.

Let us introduce the following notations:
- $\bar{v}$: the root mean square velocity$^2$ of the particles.
- $v_p$: the mode (= the most probable) speed$^3$ of the particles.
- $v_m$: the median speed$^4$ of the particles.
- $\bar{v}_s$: the average speed$^5$ of the particles.

(1) Calculate all the quantities. [Calculate the density distribution for the speed; using the $\delta$-function is handy.]
(2) Show that generally $\bar{v} \geq \bar{v}_s$ (even if the gas is not in equilibrium).
(3) Is there any general inequality between $v_p$ and $v_m$ irrespective of the actual distribution?

Remark. You may use some software to perform integrals, BUT I strongly recommend you not to do so

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$^1$This is related to Q5-1.

$^2\sqrt{\langle v^2 \rangle}$.

$^3$the most frequent speed.

$^4$the speed such that the probability of a particle to have the speed less than that is 1/2.

$^5\langle |v| \rangle$. 
blindly. Use it sparingly. My solution will not use it.

**Partial solution to (1).**
Since all are wrt the speed (even $v = \sqrt{\langle v^2 \rangle} = \sqrt{\langle |v|^2 \rangle} = \sqrt{\langle v^2 \rangle}$), let us determine the density distribution function $f(v)$ for the speed $v = |v|$.

$$f(v) = \langle \delta(v - |v|) \rangle = \int_{v \in \mathbb{R}^2} dv \, \delta(v - |v|) \left( \frac{m}{2\pi k_B T} \right) e^{-mv^2/2k_BT} \quad (\text{DH3.7})$$

$$= \int_0^\infty 2\pi u du \, \delta(v - u) \left( \frac{m}{2\pi k_B T} \right) e^{-mu^2/2k_BT} \quad (\text{DH3.8})$$

$$= \frac{m}{k_B T} v e^{-mv^2/2k_BT}. \quad (\text{DH3.9})$$

This can also be obtained easily with an elementary change of variables. Confirm that this is indeed normalized.

Let us calculate a general formula:

$$\langle v^\alpha \rangle = \int_0^\infty dv \frac{m}{k_B T} v^{1+\alpha} e^{-mv^2/2k_BT} = \int_0^\infty dx \left( \frac{2k_B T}{m} \right)^{\alpha/2} e^{-x} \quad (\text{DH3.10})$$

$$= \left( \frac{2k_B T}{m} \right)^{\alpha/2} \Gamma(1 + \alpha/2), \quad (\text{DH3.11})$$

where $\Gamma$ is the Gamma function defined by

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt \quad (\text{DH3.12})$$

for $x$ whose real part is positive.\(^6\) $\Gamma(1/2) = \sqrt{\pi}$ (just a disguised Gaussian integral), $\Gamma(1) = 1$, and note that

$$\Gamma(x + 1) = x \Gamma(x), \quad (\text{DH3.13})$$

because

$$\Gamma(x + 1) = \int_0^\infty dt \, t^x e^{-t} = - \int_0^\infty dt \, t^x \frac{d}{dt} e^{-t} = t^x e^{-t} \bigg|_{t=0}^\infty + x \int_0^\infty dt \, t^{x-1} e^{-t} = x \Gamma(x). \quad (\text{DH3.14})$$

Therefore, for example, $\Gamma(5/2) = (3/2)\Gamma(3/2) = (3/4)\sqrt{\pi}$, and $\Gamma(N + 1) = N!$ for positive integer $N$.

As you see from the formula (DH3.10), if $\alpha$ is an even positive integer, we can perform the integral in an elementary fashion. Otherwise, I do not believe you can do it easily; you need an integral table (obsolete now) or some software. However, you should understand why the result is rather aesthetic with $\sqrt{\pi}$ instead of an ugly number. See


\(^6\)and then is analytically continued to the complex plane except for non-positive integers.

Since Phys 427 is a course taken by those who are graduating from physics, I take it for granted that you know elementary analysis (with multivariate functions), linear algebra, complex analysis and differential equations.
for a fairly quick study of the Gamma function, or the real reference http://dlmf.nist.gov/5. The latter is a NIST applied math site, useful for practitioners.

Beyond this point you must get all the required quantities explicitly.

3 [Boltzmann factor]

(1) There is a potential step of height 4.2 pN·nm as shown in Fig. DH3.1. The system is assumed to be uniform (within the walls parallel to the sheet of paper). The particles in the box barely interact with each other (i.e., as an ideal gas). What is the ratio of the number densities in A and in B: \( n_B/n_A \)? [See the summary of the Boltzmann constant at the end.]

![Figure DH3.1: A box with a potential step of height \( \epsilon = 4.2 \) pN·nm. The gray portion is with potential energy \( \epsilon \) higher relative to the white portion in the container.](image)

(2) There are two one-particle states the energy gap between which is 150 \( k_B \) (in K). We have two particles that do not energetically interact. What is the probability to find (the center of mass of) only one particle in the higher energy one-particle state at \( T = 300 \) K,

(i) if the particles are identical fermions?

(ii) if the particles are identical bosons?

(iii) if the particles are not identical?

(3) A typical intermolecular force (in 3-space) is described by the Lenard-Jone potential \( \varphi(r) \):

\[
\varphi(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right],
\]

which is illustrate in Fig. DH3.2.

![Figure DH3.2: Lenard-Jone potential](image)

Let us assume realistic values\(^7\) \( \epsilon/k_B = 150 \) (in K) and \( \sigma = 3.5 \times 10^{-10} \) m. Estimate the

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\(^7\)e.g., cf. E. Wilhelm and R. Battino, Estimation of Lennard-Jones (6,12) Pair Potential Parameters from
ratio of probabilities to find another particle (of the same chemical species) around $2\sigma$ and around $5\sigma$ from the origin. Here, ‘around’ means the shells of thickness $dr$. Do not forget that the particles are in 3-space.

4 [Harmonic potential]
A point mass of mass $m = 1.2$ pg is tethered at the origin with a harmonic spring with the spring constant $k = 3.2$ pN/nm.\(^8\)

(1) Find the (correctly normalized) density distribution function $f(r)$ of its location $r$ in 3-space.

(2) What is the density distribution function $g(\ell)$ of the length $\ell$ of the spring?

(3) What is the mean-square displacement of the point mass from the origin?

(4) What is the most probably $\ell$?

Summary of the Boltzmann constant $k_B$\(^9\)
It would be practical to have some sense of the magnitude of the Boltzmann constant.

$$k_B = 1.3806503 \times 10^{-23} \text{ J/K}$$
$$= 1.3806503 \times 10^{-2} \text{ pN \cdot nm/K}$$
$$= 8.617343 \times 10^{-5} \text{ eV/K}.$$

The gas constant $R$ is defined by

$$R \equiv N_A k_B = 8.314462 \text{ J/mol \cdot K} = 1.986 \text{ cal/mol \cdot K}.$$  \hspace{1cm} \text{(DH3.16)}

Here, $N_A = 6.02214076(18) \times 10^{23}$/mol is Avogadro’s constant and 1 cal = 4.18605 J.

It is convenient to remember that at room temperature (300 K):\(^{10}\)

$$k_B T = 4.14 \text{ pN \cdot nm}$$
$$= 0.026 \text{ eV},$$

$$R T = 2.49 \text{ kJ/mol} = 0.6 \text{ kcal/mol}.$$  

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\(^8\)These units are convenient ones for biomacromolecules.

\(^9\)\text{Representative energy scales}\:
5–10 pN is a typical force felt or exerted by molecular machines; a few nm is a typical displacement of molecular motors. Cf., the diameter of DNA is 2 nm (its pitch is 3.4 nm); the $\alpha$-helix pitch is 3.6 amino acid residues = 0.54 nm. To ionize an atom, a few electron volts are needed, so, if $T$ is the room temperature (300 K), it is about 100 $k_B T$. Note that even on the surface of the sun (with the temperature corresponding to the black body radiation of about 6000 K), hydrogen atoms are not significantly ionized.

\(^{10}\)Under physiological condition, hydrolysis of a single ATP molecule provides about $20 k_B T$. 

Homework 3 due at midnight on Feb 11 (M), 2019.
Submit to cfan11@illinois.edu

The file (single file) must not be more than 0.5 MB titled qqqHW3.pdf, where qqq must be your identifier, e.g., NetID.

You may discuss with your friends AFTER you have made due efforts of your own to solve the problems. I trust you. I wish you to fully understand the solutions when you submit your homeworks (and get the full credit).

No solution without your justification will get any credit.

1 [δ-function exercise]
Evaluate the following expressions

(1) \[ \int_{\pi/10}^{19\pi/10} d\theta \, \delta(\sin \theta) \cos \theta. \] (DH3.17)

(2) \[ \int_{-1/2}^{\infty} dx \, e^{-x} \delta(\sin(\pi x)). \] (DH3.18)

(3) \[ \int_{-\infty}^{\infty} dx \, |x| \delta(2x^2 - 5x - 3). \] (DH3.19)

2 [3-Harmonic potential energy]
Find the potential energy distribution \( F(U) \) for the 3-harmonic oscillator already described in Discussion 3, 4. Here, \( U = kr^2/2 \).

3 [Three levels]\(^{11}\)
There are three one-particle states with energies 0, \( \epsilon \) and 2\( \epsilon \), where \( \epsilon = 150k_B \) (in K). We have three particles that do not energetically interact.

(1) What is the probability to find only one particle in the energy 2\( \epsilon \) one-particle state,
   (i) if the particles are identical fermions?
   (ii) if the particles are identical bosons?

(2) What is the probability to find no particle in the one-particle ground state,
   (i) if the particles are identical fermions?
   (ii) if the particles are identical bosons?

\(^{11}\)Some questions are really trivial, or you may well say stupid.