AMSI (2017)

Stochastic Equations and Processes in Physics and Biology

Exercise sheet 1: Probability, transformation of random variables

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- 1. **Q1: Unbiased estimator for the variance**

  Show that if $X_i \sim$ iid with $E(X_i) = \mu$ and $\mathrm{Var}(X_i) = \sigma^2$, then

  $$s^2 = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \langle X \rangle)^2$$

  with $\langle X \rangle = (1/n) \sum_{i=1}^{n} X_i$, is an unbiased estimator for the variance σ^2.

- 2. **Q2: Gas of active particles in 3D**

  (a) Calculate the average number of hits per unit area and the pressure in the gas of active particles that move with a constant velocity V. The gas is completely homogeneous with a constant number density ρ.

  (b) Calculate the distribution of the relative velocity $U = |\boldsymbol{v}_1 - \boldsymbol{v}_2|$

- 3. **Q3:** Show that if $X_1 \sim N(0, \sigma_1^2)$ and $X_2 \sim N(0, \sigma_2^2)$ then $X_1 + X_2 \sim N(0, \sigma_1^2 + \sigma_2^2)$. Thus, show that the distribution of the relative velocity $\boldsymbol{V}_r = \boldsymbol{V}_1 - \boldsymbol{V}_2$ in an ideal gas of particles of mass m with Maxwell distribution of the velocities $\boldsymbol{V}_1$ and $\boldsymbol{V}_2$ is given by

  $$\rho(\boldsymbol{V}_r) = \left(\frac{m}{4\pi kT} \right)^{3/2} \exp\left(-\frac{m\boldsymbol{V}_r^2}{4kT} \right).$$

- 4. **Q4:** Derive the equation of state for an ideal gas of particles with Maxwell distribution of the velocities.

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Q1: Solution

We need to show that

$$E\left(\frac{1}{n-1}\sum_{i=1}^{n}(X_i - \langle X\rangle)^2\right) = \sigma^2$$

First we calculate

$$E\left(X_i\sum_{i=1}^{n}X_k\right) = E(X_i^2) + \sum_{i\neq k}E(X_iX_k) = \sigma^2 + \mu^2 + (n-1)\mu^2,$$

where we have used $E(X_i^2) = \sigma^2 + \mu^2$. In addition, we note

$$\begin{aligned}
E\left(\langle X\rangle^2\right) &= \frac{1}{n^2}E\left(\left[\sum_{i=1}^{n}X_i\right]^2\right) \\
&= \frac{1}{n^2}\left[E(X_1^2) + E(X_2^2) + \ldots + E(X_n^2) + 2\sum_{i\neq k}E(X_iX_k)\right] \\
&= \frac{1}{n^2}\left[n(\sigma^2+\mu^2) + 2\frac{n(n-1)}{2}\mu^2\right] = \frac{1}{n^2}(n\sigma^2 + n^2\mu^2).
\end{aligned}$$

Finally, we obtain

$$\begin{aligned}
E\left(\frac{1}{n-1}\sum_{i=1}^{n}(X_i - \langle X\rangle)^2\right) &= \frac{1}{n-1}\sum_{i=1}^{n}E\left[X_i^2 - 2X_i\langle X\rangle + \langle X\rangle^2\right] \\
&= \frac{1}{n-1}\left[n(\sigma^2+\mu^2) - 2\frac{n}{n}(\sigma^2 + n\mu^2) + \frac{1}{n}(n\sigma^2 + n^2\mu^2)\right] = \sigma^2.
\end{aligned}$$

Q2: Solution

To calculate the average number of hits per unit area, we need to know the distribution $f(v_z)$ of the projection of the velocity v_z onto any given direction, i.e. onto the z-axis. Then the average number of hits dN per time dt per unit area is given by

$$\frac{dN}{dt} = \rho \int_0^V dv_z \, v_z f(v_z),$$

where ρ is the number density (number of molecules per unit volume).

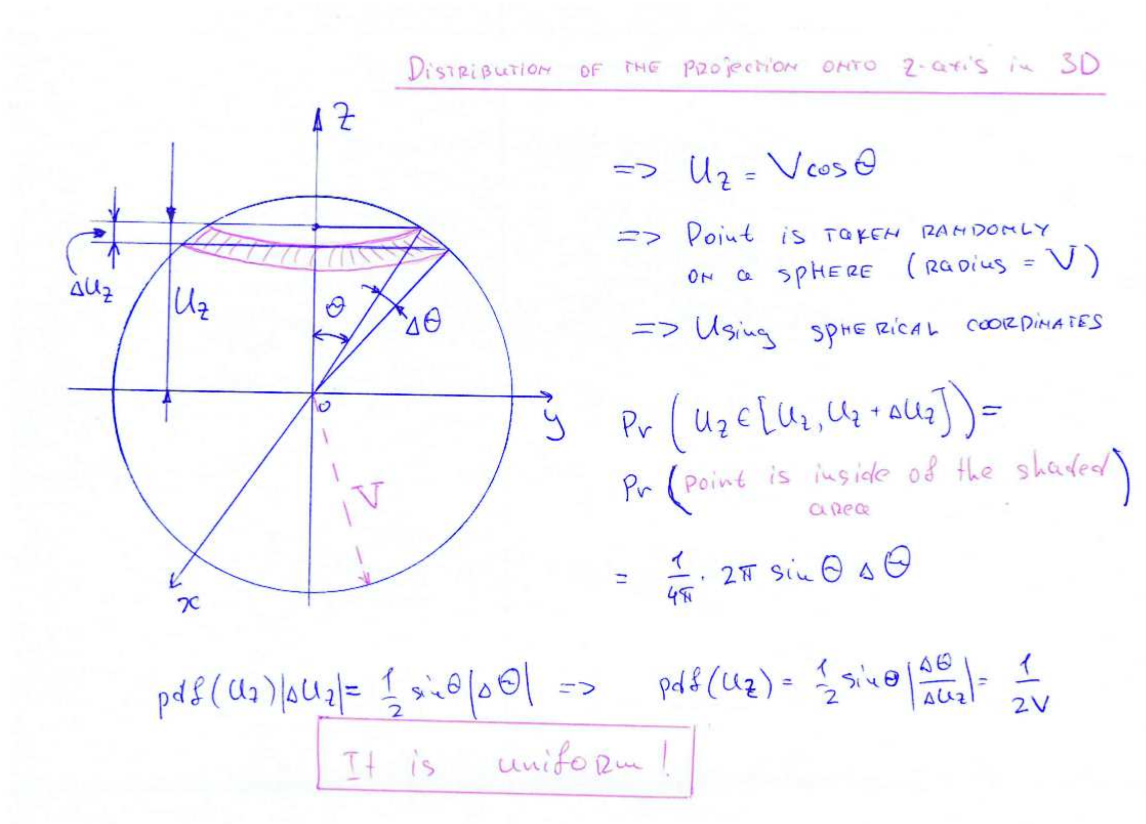

Figure 1: Distribution of the projection of the velocity of an active particle

As shown in the sketch in Fig.1, the projection v_z is dsitributed uniformly in 3D with

$$f(v_z) = \frac{1}{2V}, \qquad v_z \in [-V, +V].$$

Consequently,

$$\frac{dN}{dt} = \rho \int_0^V dv_z \, v_z f(v_z) = \frac{\rho V}{4}.$$

Pressure:

Assume elastic collisions with the wall, the pressure P is given by the rate of change of the momentum of molecules that hit the wall of a unit area

$$P = \rho \int_0^V dv_z \, (2mv_z) v_z f(v_z) = \frac{m\rho V^2}{3} = \frac{\rho_V V^2}{3},$$

where ρ_V is the mass density (kg/m^3).

Relative velocity: The magnitude of the relative velocity U can be found as the distance between two random points on a sphere with radius V (see sketch in Fig.2)

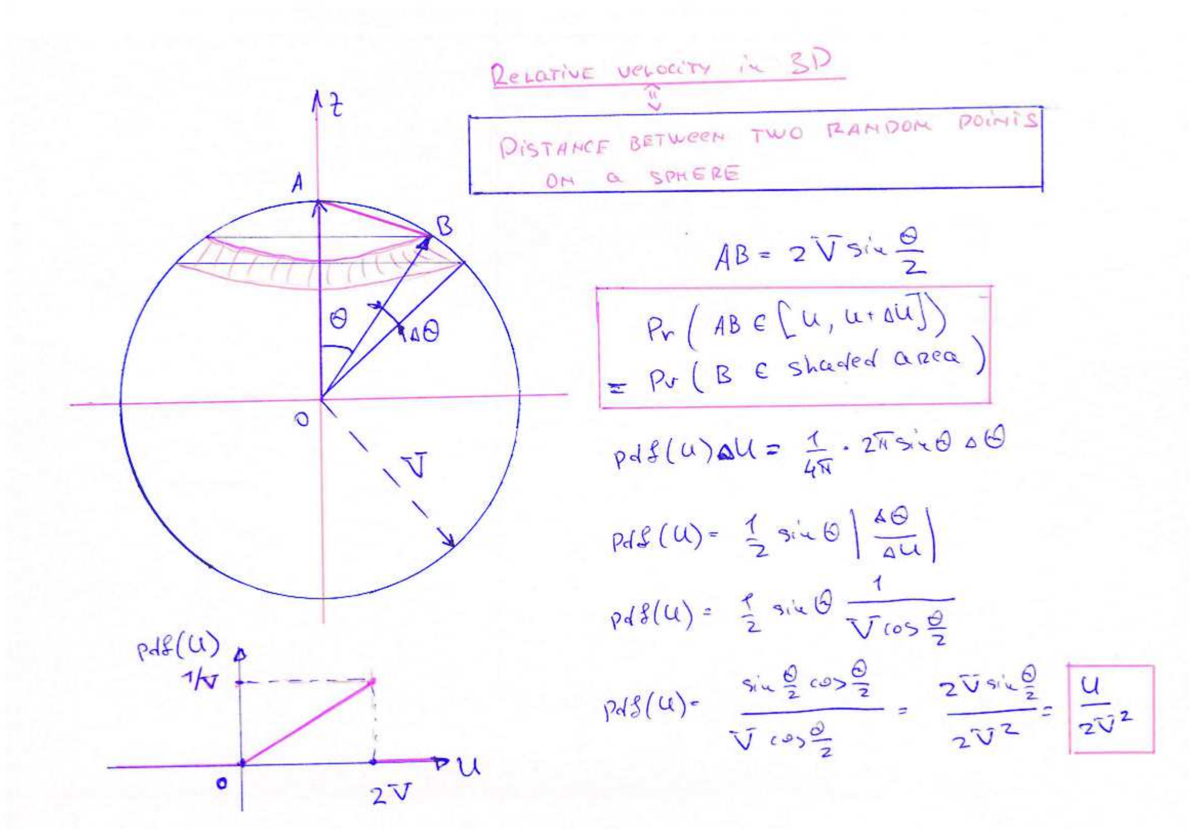

Figure 2: Realtive velocity in the gas of active particles.

The average of the magnitude of the relative velocity is given by

$$\langle U \rangle = \int_0^{2V} dU \, U \frac{U}{2V^2} = \frac{4}{3} V$$

Q3: Solution

We assume $X_i \sim N(0, \sigma_i^2)$ with the pdf

$$f_i(x) = \sqrt{\frac{1}{2\pi\sigma_i^2}} \exp\left(-\frac{x^2}{2\sigma_i^2}\right).$$

The pdf $\rho(z)$ of the sum $Z = X_1 + X_2$ is given by the convolution

$$\rho(z) = \int_{-\infty}^{\infty} dx\, f_1(x) f_2(z-x).$$

Taking into account the following result:

$$\frac{x^2}{2\sigma_1^2} + \frac{(z-x)^2}{2\sigma_2^2} = \frac{(\sigma_1^2+\sigma_2^2)}{2\sigma_1^2\sigma_2^2}\left(x - z\frac{\sigma_1^2}{\sigma_1^2+\sigma_2^2}\right)^2 + \frac{z^2}{2(\sigma_1^2+\sigma_2^2)}.$$

we obtain

$$\rho(z) = \sqrt{\frac{1}{4\pi^2\sigma_1^2\sigma_2^2}} \exp\left(-\frac{z^2}{2(\sigma_1^2+\sigma_2^2)}\right) \int_{-\infty}^{\infty} dx\, \exp\left(-\frac{(\sigma_1^2+\sigma_2^2)}{2\sigma_1^2\sigma_2^2}\left(x - z\frac{\sigma_1^2}{\sigma_1^2+\sigma_2^2}\right)^2\right).$$

Observing that

$$\int_{-\infty}^{\infty} dx\, \exp\left(-\frac{(x-A)^2}{2B^2}\right) = \sqrt{2\pi B^2},$$

we conclude

$$\rho(z) = \sqrt{\frac{1}{2\pi(\sigma_1^2+\sigma_2^2)}} \exp\left(-\frac{z^2}{2(\sigma_1^2+\sigma_2^2)}\right).$$

Relative velocity in an ideal gas:
The velocity $\boldsymbol{v}$ of particles in the gas follows Maxwell distribution

$$\boldsymbol{v} = (v_x, v_y, v_z), \quad \text{with} \quad v_x, v_y, v_z \sim N\left(0, \frac{kT}{m}\right).$$

we are looking for the distribution of

$$\boldsymbol{U} = \boldsymbol{v}_1 - \boldsymbol{v}_2 = \boldsymbol{v}_1 + (-\boldsymbol{v}_2)$$

Due to symmetry of the Maxwell distribution, the distribution of $-\boldsymbol{v}$ and $\boldsymbol{v}$ are identical. For each of the coordinates we have

$$U_x \sim N\left(0, \frac{kT}{m} + \frac{kT}{m}\right) = N\left(0, \frac{2kT}{m}\right)$$

So that

$$f(\boldsymbol{U}) = \left(\frac{m}{4\pi kT}\right)^{3/2} \exp\left(-\frac{m\boldsymbol{U}^2}{4kT}\right).$$

Q4: Solution

We need to calculate the pressure in the gas with Maxwell distribution of the velocities

$$f(\boldsymbol{v}) = \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m\boldsymbol{v}^2}{2kT}\right).$$

Similar to Q2, we assume elastic collisions of molecules with the wall and write

$$\begin{aligned} P &= \rho_0 \left(\frac{m}{2\pi kT}\right)^{3/2} \int_{-\infty}^{+\infty} dv_y \int_{-\infty}^{+\infty} dv_z \int_0^{\infty} dv_x \, 2mv_x^2 \exp\left(-\frac{m\boldsymbol{v}^2}{2kT}\right) \\ &= \rho_0 \frac{2m}{2}\frac{kT}{m} = \rho_0 kT, \end{aligned}$$

where ρ_0 is the number density.

Introducing the gas constant $R = kN_A = 8.31$ (J mol^{-1} K^{-1}), where $N_A = 6.022 \times 10^{23}$ (mol^{-1}) is the Avogadro constant, we obtain

$$P = \frac{\rho_v RT}{M},$$

where ρ_v is the mass density and M is the mass per one mol of gas.