Universität des Saarlandes
Fakultät 7 – Physik und Mechatronik

Fachrichtung 7.1 – Theoretische Physik
Prof. Dr. L. Santen
Dr. R. Shaebani (Mail: shaebani@lusi.uni-sb.de)
Dr. C. Chevalier (Mail: carole@lusi.uni-sb.de)
Web: http://santen.physik.uni-saarland.de

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Blatt 3 zur Theoretischen Physik IV, WS2023/2024

(Abgabe bis 24.11.2023, 8.30 Uhr)

Exercise 1 *Run & tumble (random walk and diffusion equation)* [1] [13 Points]

Purcell, in an essay *Life at low Reynolds number*, describes the strange physical world at the scale of bacteria. The bacterium E. coli swims using roughly five corkscrew-shaped propellers called flagella, which spin at 100 revolutions per second. These propellers mesh nicely into a bundle when they rotate counter-clockwise, causing the bacterium to run forward. But when they rotate clockwise, the bundle flies apart and the bacterium tumbles. Assume that during a tumble the bacterium does not change position, and after a tumble it is pointed in a random direction. Pretend the runs are of fixed duration $T \approx 1\,s$ and speed $V \approx 20\,\mu m/s$, and they alternate with tumbles of duration $\tau \approx 0.1\,s$.

a) What is the mean-square distance $\langle \mathbf{r}^2 \rangle$ moved by our bacterium after a time $t = N(T + \tau)$, in terms of V , T , t, and τ ? What is the formula for the diffusion constant? (Hint: Be careful, your formula for the diffusion constant should depend on the fact that the diffusion is in three dimensions.)

   Purcell tells us that the cell does not need to swim to get to new food after it has exhausted the local supply. Instead, it can just wait for food molecules to diffuse to it, with a rate he says is $4\pi aCD$ food molecules per second. Here a is the radius of the cell, C is the food concentration at infinity, and $D \approx 10^{-9}\,m^2/s$ is the food diffusion constant.

b) Solve the diffusion equation for the density of food molecules in the steady state, and confirm Purcell's formula for the rate at which food is eaten. We assume the food is eaten by the bacterium with perfect efficiency at the sphere of radius a ($\rho(a) = 0$).
   Hint: Use the Laplacian in spherical coordinates:

$$\nabla^2 \rho = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\frac{r^2 \partial \rho}{\partial r} \right)$$

   since the function $\rho(\mathbf{r}) = \rho(r)$ has spherical symmetry.

   The cell lives in an environment which varies in space. It swims to move toward regions with higher concentrations of food, and lower concentrations of poisons (a behavior called chemotaxis). Bacteria are too small to sense the concentration gradient from one side of the cell to the other. The run-and-tumble strategy is designed to move them far enough to tell if things are getting better. In particular, the cells run for longer times when things are getting better (but not shorter when things are getting worse).

[1] From the book of Sethna, James P., Statistical Mechanics: Entropy, Order Parameters, and Complexity, 2nd edn (Oxford, 2021; online edn, Oxford Academic, 22 Apr. 2021), https://doi.org/10.1093/oso/9780198865247.001.0001.

c) Model chemotaxis with a one-dimensional run-and-tumble model along a coordinate x. The velocity $\pm V$ is chosen with equal probability at each tumble, with the same velocity and tumble time τ as above. But now the duration T_+ of runs in the positive x direction is larger than the duration T of runs in the negative direction. Compare the run speed V to the average velocity $\langle \frac{dx}{dt} \rangle$ of the bacterium toward a better life.

Exercise 2 *Run & tumble simulation* [4 Points]

The given code (blatt3_bacterium.py) simulate the run & tumble kinetics of a bacterium described in the previous exercise. Change the code to calculate and draw the mean square distance $\langle \mathbf{r}^2 \rangle$ and verify the theoretical result $\langle \mathbf{r}^2 \rangle = NV^2T^2$.

Exercise 3 *Particles with two energy levels (microcanonical ensemble)* [10 Points]

In quantum mechanics, an energy level is degenerate if it corresponds to two or more different measurable states of a quantum system. Consider a system N of identical but distinguishable particles, each of which can assume one of the two energy values $\epsilon > 0$ and 0. The upper energy level should have a g-fold degeneracy, while the lower level is non-degenerate. The total energy of the system is denoted by E and the occupation numbers of the two levels by n_0 and n_+. Use the microcanonical ensemble in the following.

a) Show that the state sum is

$$\Omega(E, N) = \frac{N!\ g^{n_+}}{n_+!\ (N - n_+)!}$$

b) The entropy is defined as $S(E, N) = k_\mathrm{B} \ln \Omega(E, N)$ with the Boltzmann constant k_B. Calculate S, when N and E are large. (We fix $E/(\epsilon N) =: x$ constant for $N \longrightarrow \infty$.)
Hint: Use the Stirling formula in the form: $\ln N! \approx N \ln N - N$.

c) Find the population numbers n_+ and n_0 depending on the temperature T of the system, which is defined by $\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_N$.

d) Now determine n_+ and n_0 in the limit $T \longrightarrow 0$.

Exercise 4 *Hard sphere gas (microcanonical ensemble)* [2] [13 Points]

We can improve on the realism of the ideal gas by giving the atoms a small radius. If we make the potential energy infinite inside this radius (hard spheres), the potential energy is simple (zero unless the spheres overlap, which is forbidden). Let us do this in two dimensions; three dimensions is only slightly more complicated, but harder to visualize. A two-dimensional $L \times L$ box with hard walls contains a gas of N distinguishable hard disks of radius $r \ll L$ (Fig. 1). The disks are dilute; the summed area $N\pi r \ll L^2$. Let A be the effective area allowed for the disks in the box (Fig. 1): $A = (L - 2r)^2$.

a) The area allowed for the second disk is $A - \pi(2r)^2$ (Fig. 1), ignoring the small correction when the excluded region around the first disk overlaps the excluded region near the walls of the box. What is the allowed $2N$-dimensional volume in configuration space Ω_{HD} of allowed zero-energy configurations of hard disks, in this dilute limit? Leave your answer as a product of N terms.

Our formula in part (a) expresses Ω_{HD} strangely, with each disk in the product only feeling the excluded area from the former disks. For large numbers of disks and small densities, we can rewrite Ω_{HD} more symmetrically, with each disk feeling the same excluded area A_e .

b) Use $(1 - \epsilon) \approx e^{-\epsilon}$ and $\sum_{m=0}^{N-1} m = \frac{N(N-1)}{2}$ to approximate

$$\Omega_{HD} \approx (Ae^{-N\delta})^N,$$

solving for δ and evaluating any products and sums over disks.

[2] *Ibid.*

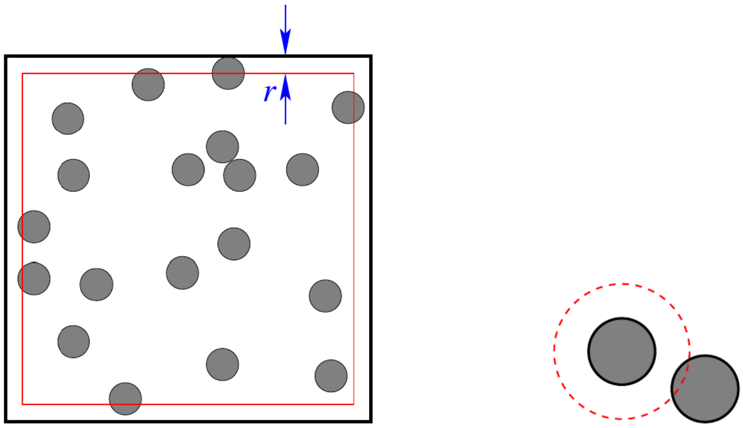

Figure 1: **Hard sphere gas.**

c) Show that

$$\Omega_{HD} \approx (A - A_e)^N.$$

Interpret your formula for the excluded area A_e, in terms of the range of excluded areas you found in part (a) as you added disks.

d) Find the pressure for the hard-disk gas in the large N approximation of part (c), as a function of temperature$T$, A, r, and N . Does it reduce to the ideal gas law if the disk radius $r = 0$?
Hint: Constant energy is the same as constant temperature for hard particles, since the potential energy is zero.