New York University
Physics Department
Class GA.2061 "Non-Equilibrium Statistical Physics", Fall 2021

Home Work 01 *Solutions*

1. Later in the class, we will heavily rely on understanding of random walks. This problem is to refresh you on this subject. Consider a random walk of some n steps, each step is $\vec{y}_i$; end-to-end vector of this random walk is $\vec{R} = \sum_i \vec{y}_i$. If different steps are statistically independent, each isotropically distributed, and all of them have the same length ℓ, then $\left\langle \vec{R} \right\rangle = 0$ and $\left\langle \vec{R}^2 \right\rangle = n\ell^2$; make sure you absolutely understand these two statements. Generalize these results for the following cases:

   (a) Steps are distributed isotropically and are independent, but their length is random, with distribution $g(|\mathbf{y}|)$;

   (b) Steps are all of the same length ℓ and independent, but distributed non-isotropically, with distribution $g(\mathbf{y})$;

   (c) Steps are distributed isotropically and all of the same length ℓ, but are not quite independent, steps i and j are correlated such that $\langle \vec{y}_i \cdot \vec{y}_j \rangle = \ell^2 e^{-|i-j|/m}$. In this case, consider $n \gg m$.

Solution

   (a) In this case $\left\langle \vec{R} \right\rangle = 0$ and $\left\langle \vec{R}^2 \right\rangle = n\ell_{\text{eff}}^2$, where $\ell_{\text{eff}}^2 = \int \vec{y}^2 g(\vec{y}) d^d y$. Thus, as before, $\left\langle R^2 \right\rangle \propto n$ albeit with modified "effective step" length.

   (b) If the distribution $g(\mathbf{y})$ is not isotropic, that means there (can be some) preferred direction such that $\langle \vec{y}_i \rangle \equiv \int g(\vec{y}) \vec{y} d^2 \vec{y} = \vec{a}$, with some vector $\vec{a}$. In this case $\left\langle \vec{R} \right\rangle = n\vec{a}$ and $\left\langle \vec{R}^2 \right\rangle = n\ell^2 + n(n-1)a^2$. Note that in this case, at sufficiently large n, the dominant contribution is $\left\langle \vec{R}^2 \right\rangle \Big|_{n\to\infty} = n^2 a^2$, which means, that drift wins against diffusion. In other words, systematic change wins over random.

   (c) In this case, $\left\langle \vec{R} \right\rangle = 0$ while $\left\langle \vec{R}^2 \right\rangle = \ell^2 \sum_{ij} e^{-|i-j|/m}$. Assuming $n \gg m$, we can say this double sum is n times the sum over the $k = i - j$: $\left\langle \vec{R}^2 \right\rangle = \ell^2 n \sum_{k=-\infty}^{\infty} e^{-|k|/m}$, where the summation can be pulled to infinity, because it is rapidly converging. If we replace the sum by the integral, it is then equal to $2m$. Thus $\left\langle \vec{R}^2 \right\rangle = n\ell_{\text{eff}}^2$, where $\ell_{\text{eff}}^2 = 2\ell^2 m$. Again, in this case, the "square-root-of-n-law" remains valid, albeit with a modified effective step length.

2. Consider an isolated statistical system. Its state of thermodynamic equilibrium corresponds to the maximal entropy. We now consider fluctuations around this state, and suppose these fluctuations are described by some variables $\{x_i\}$, defined for simplicity such that their averages are equal to zero in the state of thermodynamic equilibrium. For instance, you can imagine a little colloidal particle attached by a spring to an immobile pivot and submerged into a volume of liquid; in that case, there are six values of x, three coordinates and three components of velocity for this Brownian particle as it fluctuates around its equilibrium position. Along with $\{x_i\}$, it is useful to define also conjugate quantities $X_k = -\partial S / \partial x_k$, where S is entropy of the system. Prove that $\langle x_i X_k \rangle = \delta_{ik}$, where average is taken over equilibrium distribution.

   Hint: In equilibrium, probability distribution of $\{x\}$ is, up to a normalization factor, $P(\{x\}) \propto e^S$, where entropy close to its maximum can be expanded as $S = S_0 - (1/2) \sum_{lm} \beta_{lm} x_l x_m$.

Solution

   We need to compute the *equilibrium* average

$$\langle x_i X_k \rangle = \int A e^{-(1/2)\sum_{lm} \beta_{lm} x_l x_m} x_i \underbrace{\sum_j \beta_{kj} x_j}_{X_k} d\{x\} = A \sum_j \beta_{kj} \int e^{-(1/2)\sum_{lm} \beta_{lm} x_l x_m} x_i x_j d\{x\} \ , \tag{1}$$

   where A is the normalization factor which we don't need to specify right now. To evaluate the latter integral, the following trick is useful. We defined $\{x_i\}$ such that their equilibrium values are zero. Let us step back and imagine that there are some non-zero values $\{x_i^0\}$, then entropy reads $S = -(1/2)\sum_{lm}\left(x_l - x_l^0\right)\left(x_m - x_m^0\right)$, and then quite trivially the average for every x_i must be nothing else but x_i^0:

$$\overline{x}_i = \int Ae^{-(1/2)\sum_{lm}\beta_{lm}\left(x_l - x_l^0\right)\left(x_m - x_m^0\right)} x_i d\{x\} = x_i^0 \ . \tag{2}$$

What we do is we differentiate the above equality with respect to x_k^0, and then at the end return to our original notation in which $\{x_j^0\} = 0$. In the left hand side, we have exactly the integral of our interest, while the right hand side is 1 if $i = k$ and zero otherwise, yielding the expected

$$\langle x_i X_k \rangle = \delta_{ik} \ . \tag{3}$$