33-765 — Statistical Physics

Department of Physics, Carnegie Mellon University, Spring Term 2020, Deserno

Problem sheet #9

33. Statistical Physics of the N-dimensional quadratic Hamiltonian *(12 points)*

Consider a phase space with N degrees of freedom $\{x_i\}_{i=1,\ldots,N}$ and on it a quadratic Hamiltonian

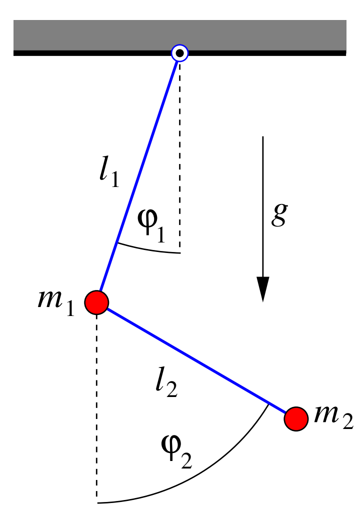
$$H = \frac{1}{2}\boldsymbol{x}^\top \mathsf{K}\,\boldsymbol{x} \quad , \quad \text{or in components:} \quad H = \frac{1}{2}\sum_{i,j=1}^{N} x_i K_{ij} x_j \stackrel{!}{=} \frac{1}{2} x_i K_{ij} x_j \quad \text{(Einstein summation convention!)}\,,$$

where the "kernel" K is symmetric and positive definite. To de-clutter the problem, we will ignore the beauty factor $\frac{1}{N!\,h^N}$.

1. Show that the canonical partition function is given by $Z := \mathrm{Tr}\,\mathrm{e}^{-\beta H} \stackrel{!}{:=} \int \mathrm{d}^N x\; \mathrm{e}^{-\frac{1}{2}\beta x_i K_{ij} x_j} = \Big(\det \frac{\beta \mathsf{K}}{2\pi}\Big)^{-1/2}$.
   Hint: transform to new coordinates $\boldsymbol{y} = \mathsf{T}\boldsymbol{x}$, or $y_i = T_{ij}x_j$ in which K is diagonal! What key property does T have?
2. Starting with the result from problem 31.1, show that the equipartition theorem in this case can be written as
$$\langle \boldsymbol{x}\otimes\boldsymbol{x}\rangle \equiv \langle \boldsymbol{x}\,\boldsymbol{x}^\top\rangle = k_{\mathrm{B}}T\,\mathsf{K}^{-1} \quad , \quad \text{or in components:} \quad \langle x_i x_j\rangle = k_{\mathrm{B}}T\,K^{-1}_{ij}\,.$$
3. We now amend the Hamiltonian by a "source term", $H = \frac{1}{2}\boldsymbol{x}^\top\mathsf{K}\,\boldsymbol{x} - \boldsymbol{J}\cdot\boldsymbol{x}$. This Hamiltonian is still quadratic, but it takes its minimum not at $\boldsymbol{x} = \boldsymbol{0}$ but at some displaced value $\boldsymbol{x}^*$. Find it!
4. Use your result from the previous part to *complete the square* of this shifted quadratic matrix expression.
   In other words: write $H = \frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}^*)^\top\mathsf{K}\,(\boldsymbol{x}-\boldsymbol{x}^*) +$ stuff, and then find "stuff".
5. Show that for a general $\boldsymbol{J} \neq \boldsymbol{0}$ the partition function is given by $Z = \mathrm{Tr}\,\mathrm{e}^{-\beta H} = \Big(\det\frac{\beta\mathsf{K}}{2\pi}\Big)^{-1/2}\mathrm{e}^{\frac{1}{2}\beta\boldsymbol{J}^\top\mathsf{K}^{-1}\boldsymbol{J}}$.
6. Prove that $\langle x_i x_j\rangle = \langle x_i x_j\rangle_{\boldsymbol{J}=\boldsymbol{0}} + \langle x_i\rangle\langle x_j\rangle$. Hence, unsurprisingly, the covariance $\mathrm{Cov}(x_i, x_j)$ does not depend on $\boldsymbol{J}$.
7. Verifying that $k_{\mathrm{B}}T\,\frac{\partial}{\partial J_k}\mathrm{e}^{-\beta H} = x_k\,\mathrm{e}^{-\beta H}$, re-derive the equipartition theorem by continuing the following calculation:
$$\mathrm{Cov}(x_i,x_j) = \langle x_i x_j\rangle_{\boldsymbol{J}=\boldsymbol{0}} = \frac{\mathrm{Tr}\big(x_i x_j\,\mathrm{e}^{-\beta H}\big)}{\mathrm{Tr}\big(\mathrm{e}^{-\beta H}\big)}\bigg|_{\boldsymbol{J}=\boldsymbol{0}} = \frac{\mathrm{Tr}\Big(\Big(k_{\mathrm{B}}T\,\frac{\partial}{\partial J_i}\Big)\Big(k_{\mathrm{B}}T\,\frac{\partial}{\partial J_j}\Big)\,\mathrm{e}^{-\beta H}\Big)}{\mathrm{Tr}\big(\mathrm{e}^{-\beta H}\big)}\bigg|_{\boldsymbol{J}=\boldsymbol{0}} = \cdots$$

34. Statistical Physics of the double pendulum *(8 points)*

Consider a planar double pendulum, as sketched in the figure on the right: two masses m_1 and m_2, two pendulum lengths l_1 and l_2, and two degrees of freedom φ_1 and φ_2.



1. Write down the Lagrangian $L(\varphi_1, \varphi_2, \dot\varphi_1, \dot\varphi_2)$ of the system.
2. Expand the Lagrangian to quadratic order. *We will henceforth continue with this!*
   Hint: adopting a vector-matrix notation will greatly simplify the rest of the problem!
3. Calculate the canonically conjugate momenta p_1 and p_2 belonging to φ_1 and φ_2.
4. Find the Hamiltonian $H(\varphi_1, \varphi_2, p_1, p_2)$ of the system.
5. Show that the kinetic energy has the form $\frac{1}{2}\boldsymbol{x}^\top\mathsf{K}\;\boldsymbol{x}$ that we have discussed in the previous problem. What is $\boldsymbol{x}$ and what is K?
6. Calculate K^{-1}.
7. Finally, let's turn up the heat: if this system is in contact with a heat bath at temperature T, *calculate the correlation coefficient between p_1 and p_2!*