33-765 Homework 9

Nathaniel D. Hoffman

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33. Statistical Physics of the N-dimensional Quadratic Hamiltonian

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

$$H = \frac{1}{2}\mathbf{x}^\top \mathbf{K}\mathbf{x}$$

or in components,

$$H = \frac{1}{2}x_i K_{ij} x_j$$

where the "kernel" $\mathbf{K}$ 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 $Z := \mathrm{Tr}\left(e^{-\beta H}\right) = \int \mathrm{d}^N x\, e^{-\frac{1}{2}\beta x_i K_{ij} x_j} = \left(\det \frac{\beta \mathbf{K}}{2\pi}\right)^{-1/2}$.

If we change bases to one in which K_{ij} is diagonal ($y_i = T_{ij}x_j$, $\det(T) = 1$ since $\mathbf{T}$ must be orthogonal),

$$\begin{aligned}
Z &= \int \mathrm{d}^N x\, e^{-\frac{1}{2}\beta x_i K_{ij} x_j} \\
&= \int \mathrm{d}^N y \det(T) e^{-\frac{1}{2}\beta y_i T^{-1}_{ij} K_{ij} T_{ij} y_j} \\
&= \int \mathrm{d}^N y\, e^{-\frac{1}{2}\beta y_i K_{ii} y_i} \\
&= \int \mathrm{d}^N y\, e^{\sum_{i=1}^N -\frac{1}{2}\beta K_{ii} y_i^2} \\
&= \int \mathrm{d}^N y \prod_{i=1}^N e^{-\frac{1}{2}\beta K_{ii} y_i^2} \\
&= \prod_{i=1}^N \int \mathrm{d}y_i\, e^{-\frac{1}{2}\beta K_{ii} y_i^2} \\
&= \prod_{i=1}^N \left(\sqrt{\frac{2\pi}{\beta K_{ii}}}\right)
\end{aligned}$$

$$= \left(\sqrt{\frac{2^N \pi^N}{\beta^N \prod_{i=1}^N K_{ii}}} \right)$$

where

$$\prod_{i=1}^N K_{ii} = \det(\mathbf{K})$$

since the diagonalized $\mathbf{K}$ has its eigenvalues on the diagonal and the determinant can be defined as the product of the eigenvalues.

$$\begin{aligned} Z &= \left(\sqrt{\frac{2^N \pi^N}{\beta^N \det(\mathbf{K})}} \right) \\ &= \left(\sqrt{\det\left(\frac{2\pi}{\beta \mathbf{K}}\right)} \right) \\ &= \left(\det \frac{\beta \mathbf{K}}{2\pi} \right)^{-1/2} \end{aligned}$$

We can bring the other constants in because they are multiplied N-times, and

$$\det(\alpha \mathbf{K}) = \alpha^N \det(\mathbf{K})$$

where N is the dimension of $\mathbf{K}$.

2. Starting with the result from problem 31.1, show that the equipartition theorem in this case can be written as

$$\langle \mathbf{x} \otimes \mathbf{x} \rangle \equiv \left\langle \mathbf{x}\mathbf{x}^\top \right\rangle = k_B T \mathbf{K}^{-1}$$

or, in components,

$$\langle x_i x_j \rangle = k_B T K_{ij}^{-1}.$$

From problem 31.1, we know that

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = k_B T \delta_{ij}$$

$$\begin{aligned} \frac{\partial H}{\partial x_k} &= \frac{1}{2} \partial_k \left(x_i K_{ij} x_j \right) = \frac{1}{2} \left(\delta_{ik} K_{ij} x_j + x_i K_{ij} \delta_{jk} \right) \\ &= \frac{1}{2} \left(K_{kj} x_j + K_{ik} x_i \right) \\ &= \frac{1}{2} \left(K_{kj} x_j + K_{ki} x_i \right) \\ &= \frac{1}{2} \left(K_{kj} x_j + K_{kj} x_j \right) \\ &= K_{kj} x_j \\ \frac{\partial H}{\partial x_j} &= K_{jk} x_k \end{aligned}$$

so

$$\begin{aligned} \langle x_i K_{jk} x_k \rangle &= k_B T \delta_{ij} \\ \langle x_i x_k \rangle &= k_B T \delta_{ij} K_{jk} \\ &= k_B T K_{ik} \\ \langle x_i x_j \rangle &= k_B T K_{ij} \end{aligned}$$

3. We now amend the Hamiltonian by a "source term", $H = \frac{1}{2}\mathbf{x}^\top \mathbf{K}\mathbf{x} - \mathbf{J}\cdot\mathbf{x}$. This Hamiltonian is still quadratic, but it takes its minimum not at $\mathbf{x} = \mathbf{0}$ but at some displaced value $\mathbf{x}^*$. Find it!

To minimize the Hamiltonian, we set its derivative to zero and solve:

$$\begin{aligned}\frac{\partial H}{\partial \mathbf{x}} &= \frac{1}{2}\left(\mathbf{x}^\top \cdot \mathbf{K} + \mathbf{K}^\top \cdot \mathbf{x}\right) - \mathbf{J} \\ 0 &= \mathbf{K}^\top \mathbf{x}^* - \mathbf{J} \\ \mathbf{x}^* &= \mathbf{K}^{-1}\cdot \mathbf{J}\end{aligned}$$

4. Use your result from the previous part to complete the square of this shifted quadratic matrix expression. In other words, write it in the form $H = \frac{1}{2}(\mathbf{x}-\mathbf{x}^*)^\top \mathbf{K}(\mathbf{x}-\mathbf{x}^*) + \text{stuff}$.

$$\begin{aligned}\frac{1}{2}(\mathbf{x}-\mathbf{x}^*)^\top \mathbf{K}(\mathbf{x}-\mathbf{x}^*) &= \frac{1}{2}\left(\mathbf{x}^\top\mathbf{K}\mathbf{x} + (\mathbf{x}^*)^\top \mathbf{K}\mathbf{x}^* - (\mathbf{x}^*)^\top\mathbf{K}\mathbf{x} - \mathbf{x}^\top\mathbf{K}\mathbf{x}^*\right) \\ &= \frac{1}{2}\left(\mathbf{x}^\top\mathbf{K}\mathbf{x} + (\mathbf{K}^{-1}\cdot\mathbf{J})^\top\mathbf{K}\mathbf{K}^{-1}\cdot\mathbf{J} - (\mathbf{K}^{-1}\cdot\mathbf{J})^\top\mathbf{K}\mathbf{x} - \mathbf{x}^\top\mathbf{K}\mathbf{K}^{-1}\cdot\mathbf{J}\right) \\ &= \frac{1}{2}\left(\mathbf{x}^\top\mathbf{K}\mathbf{x} + \mathbf{J}^\top\cdot(\mathbf{K}^{-1})^\top\mathbf{K}\mathbf{K}^{-1}\cdot\mathbf{J} - \mathbf{J}^\top\cdot(\mathbf{K}^{-1})^\top\mathbf{K}\mathbf{x} - \mathbf{x}^\top\mathbf{K}\mathbf{K}^{-1}\cdot\mathbf{J}\right) \\ &= \frac{1}{2}\left(\mathbf{x}^\top\mathbf{K}\mathbf{x} + \mathbf{J}^\top\mathbf{K}^{-1}\mathbf{J} - \mathbf{J}^\top\mathbf{x} - \mathbf{x}^\top\mathbf{J}\right) \\ &= \frac{1}{2}\mathbf{x}^\top\mathbf{K}\mathbf{x} + \frac{1}{2}\mathbf{J}^\top\mathbf{K}^{-1}\mathbf{J} - \mathbf{J}\cdot\mathbf{x} \\ &= H + \frac{1}{2}\mathbf{J}^\top\mathbf{K}^{-1}\mathbf{J}\end{aligned}$$

so

$$H = \frac{1}{2}(\mathbf{x}-\mathbf{x}^*)^\top\mathbf{K}(\mathbf{x}-\mathbf{x}^*) - \frac{1}{2}\mathbf{J}^\top\mathbf{K}^{-1}\mathbf{J}$$

5. Show that for a general $\mathbf{J} \neq \mathbf{0}$, the partition function is given by $Z = \operatorname{Tr} e^{-\beta H} = \left(\det \frac{\beta\mathbf{K}}{2\pi}\right)^{-1/2} e^{\frac{1}{2}\beta\mathbf{J}^\top\mathbf{K}^{-1}\mathbf{J}}$.

This follows easily from the first part of this problem along with the fact that the part we just added by completing the square doesn't depend on $\mathbf{x}$, so we can factor it out:

$$\begin{aligned}Z = \int \mathrm{d}^N x\, e^{-\frac{1}{2}\beta x_i K_{ij} x_j} e^{\frac{1}{2}\beta\mathbf{J}^\top\mathbf{K}^{-1}\mathbf{J}} &= e^{\frac{1}{2}\beta\mathbf{J}^\top\mathbf{K}^{-1}\mathbf{J}} \int \mathrm{d}^N x\, e^{-\frac{1}{2}\beta x_i K_{ij} x_j} \\ &= \left(\det\frac{\beta\mathbf{K}}{2\pi}\right)^{-1/2} e^{\frac{1}{2}\beta\mathbf{J}^\top\mathbf{K}^{-1}\mathbf{J}}\end{aligned}$$

6. Prove that $\langle x_i x_j\rangle = \langle x_i x_j\rangle_{\mathbf{J}=\mathbf{0}} + \langle x_i\rangle\langle x_j\rangle$. Hence, unsurprisingly, the covariance $\mathrm{Cov}(x_i, x_j)$ does not depend on $\mathbf{J}$.

$$\begin{aligned}\left\langle x_i \frac{\partial H}{\partial x_j}\right\rangle &= \langle x_i(x_k K_{kj} - J_j)\rangle \\ &= \langle x_i x_k K_{kj} - x_i J_j\rangle \\ &= K_{kj}\left\langle x_i x_k - x_i J_i K^{-1}_{kj}\right\rangle \\ k_B T\delta_{ij} &= K_{kj}\langle x_i x_k - x_i x^*_k\rangle \\ k_B T K^{-1}_{kj}\delta_{ij} &= \langle x_i x_k\rangle - \langle x_i\rangle x^*_j \\ k_B T K^{-1}_{kj} &= \langle x_i x_j\rangle - \langle x_i\rangle\langle x_j\rangle \\ \langle x_i x_j\rangle_{\mathbf{J}=\mathbf{0}} &= \langle x_i x_j\rangle - \langle x_i\rangle\langle x_j\rangle\end{aligned}$$

7. Verifying that $k_B T \frac{\partial}{\partial J_k} e^{-\beta H} = x_k e^{-\beta H}$, re-derive the equipartition theorem by continuing the following calculation:

$$\mathrm{Cov}(x_i, x_j) = \langle x_i x_j \rangle_{\mathbf{J}=\mathbf{0}} = \left.\frac{\mathrm{Tr}\big(x_i x_j e^{-\beta H}\big)}{\mathrm{Tr}(e^{-\beta H})}\right|_{\mathbf{J}=\mathbf{0}} = \left.\frac{\mathrm{Tr}\left(\left(k_B T \frac{\partial}{\partial J_i}\right)\left(k_B T \frac{\partial}{\partial J_j}\right) e^{-\beta H}\right)}{\mathrm{Tr}(e^{-\beta H})}\right|_{\mathbf{J}=\mathbf{0}} = \cdots$$

Looking at the numerator, we can pull the derivatives out of the trace because the trace is an integral over x and J does not depend on x. Ignoring the factors of $K_B T$ (for now), the numerator reads:

$$\partial_{J_i}\partial_{J_j}\,\mathrm{Tr}\,e^{-\beta H} = \partial_{J_i}\partial_{J_j}\left(\det \frac{\beta \mathbf{K}}{2\pi}\right)^{-1/2} e^{\frac{1}{2}\beta \mathbf{J}^\top \mathbf{K}^{-1}\mathbf{J}}$$

For brevity, I will define $A \equiv \left(\det \frac{\beta \mathbf{K}}{2\pi}\right)^{-1/2}$.

$$\begin{aligned}
\partial_{J_i}\partial_{J_j} A e^{\frac{1}{2}\beta J_k K^{-1}_{kl} J_l} &= \partial_{J_i} A \left(e^{\frac{1}{2}\beta J_k K^{-1}_{kl} J_l}\right) \frac{\beta}{2}\left(\delta_{jk} K^{-1}_{kl} J_l + J_k K^{-1}_{kl}\delta_{jl}\right)\\
&= \partial_{J_i} A \left(e^{\frac{1}{2}\beta J_k K^{-1}_{kl} J_l}\right) \frac{\beta}{2}\left(K^{-1}_{jl} J_l + J_k K^{-1}_{kj}\right)\\
&= \partial_{J_i} A \left(e^{\frac{1}{2}\beta J_k K^{-1}_{kl} J_l}\right) \beta (K^{-1}_{jl} J_l)\\
&= A \left(e^{\frac{1}{2}\beta J_k K^{-1}_{kl} J_l}\right) \partial_{J_i}\beta (K^{-1}_{jl} J_l) + A\partial_{J_i}\left(e^{\frac{1}{2}\beta J_k K^{-1}_{kl} J_l}\right) \beta (K^{-1}_{jl} J_l)\\
&= A \left(e^{\frac{1}{2}\beta J_k K^{-1}_{kl} J_l}\right) \left[\beta K^{-1}_{jl}\delta_{li} + K^{-1}_{jl} J_l \frac{\beta^2}{2}(\delta_{ik} K^{-1}_{kl} J_l + J_k K^{-1}_{kl}\delta_{il})\right]\\
&= A \left(e^{\frac{1}{2}\beta J_k K^{-1}_{kl} J_l}\right) \left[\beta K^{-1}_{jl}\delta_{li} + K^{-1}_{jl} J_l \frac{\beta^2}{2}(K^{-1}_{il} J_l + J_k K^{-1}_{ki})\right]\\
&= A \left(e^{\frac{1}{2}\beta J_k K^{-1}_{kl} J_l}\right) \left[\beta K^{-1}_{jl}\delta_{li} + K^{-1}_{jl} J_l \beta^2 K^{-1}_{il} J_l\right]\\
&= \mathrm{Tr}\,e^{-\beta H}\left[\beta K^{-1}_{jl}\delta_{li} + K^{-1}_{jl} J_l \beta^2 K^{-1}_{il} J_l\right]
\end{aligned}$$

However, this whole thing is being evaluated at $\mathbf{J} = \mathbf{0}$. If we reinsert this expression into the equation, the traces in the numerator and denominator cancel. I will write the factors of $k_B T k_B T \equiv \frac{1}{\beta^2}$:

$$\begin{aligned}
\langle x_i x_j \rangle &= \frac{1}{\beta^2}\left[\beta K^{-1}_{jl}\delta_{li} + \cancelto{0}{K^{-1}_{jl} J_l \beta^2 K^{-1}_{il} J_l}\right]\\
&= \frac{1}{\beta} K^{-1}_{ij}\\
&= k_B T K^{-1}_{ij}
\end{aligned}$$

34. Statistical Physics of the Double Pendulum

Consider a planar double pendulum: 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.

$$L = \mathrm{KE} - \mathrm{PE}$$

where

$$KE = \sum_i \frac{1}{2} m_i v_i^2 = \sum_i \frac{1}{2} m_i (\dot{x}_i^2 + \dot{y}_i^2)$$

and

$$PE = \sum_i m g y_i$$

Of course, this is in Cartesian coordinates, not the coordinates given by the problem. In the given coordinates,

$$\begin{aligned} x_1 &= l_1 \sin(\varphi_1) & y_1 &= -l \cos(\varphi_1) \\ x_2 &= l_1 \sin(\varphi_1) + l_2 \sin(\varphi_2) & y_2 &= -l_1 \cos(\varphi_1) - l_2 \cos(\varphi_2) \end{aligned}$$

In these coordinates, we find that

$$\text{KE} = \frac{m_1 + m_2}{2} l_1^2 \dot{\varphi}_1^2 + \frac{m_2}{2} l_2^2 \dot{\varphi}_2^2 + m_2 l_1 l_2 \dot{\varphi}_1 \dot{\varphi}_2 \cos(\varphi_1 - \varphi_2)$$

and

$$\text{PE} = -(m_1 + m_2) l_1 g \cos(\varphi_1) - m_2 l_2 g \cos(\varphi_2)$$

so

$$L = \frac{m_1 + m_2}{2} l_1^2 \dot{\varphi}_1^2 + \frac{m_2}{2} l_2^2 \dot{\varphi}_2^2 + m_2 l_1 l_2 \dot{\varphi}_1 \dot{\varphi}_2 \cos(\varphi_1 - \varphi_2 a) + (m_1 + m_2) l_1 g \cos(\varphi_1) + m_2 l_2 g \cos(\varphi_2)$$

2. Expand the Lagrangian to quadratic order.

To quadratic order, $\cos(\varphi) \to 1 - \frac{\varphi^2}{2}$ and $\cos(\varphi_1 - \varphi_2) \to 1 + \varphi_1 \varphi_2 - \frac{1}{2}\left(\varphi_1^2 - \varphi_2^2\right)$. When we put these substitutions into the Lagrangian and cancel anything else that is now of higher than quadratic order, we find that

$$\begin{aligned} \text{KE} &= \frac{m_1 + m_2}{2} l_1^2 \dot{\varphi}_1^2 + \frac{m_2}{2} l_2^2 \dot{\varphi}_2^2 + m_2 l_1 l_2 \dot{\varphi}_1 \dot{\varphi}_2 \\ &= \dot{\varphi}^\top \mathbf{A} \dot{\varphi} \end{aligned}$$

where

$$\mathbf{A} = \frac{1}{2} \begin{pmatrix} (m_1 + m_2) l_1^2 & m_2 l_1 l_2 \\ m_2 l_1 l_2 & m_2 l_2^2 \end{pmatrix}$$

The potential energy becomes

$$\begin{aligned} \text{PE} &= -(m_1 + m_2) l_1 g \left(1 - \frac{1}{2} \varphi_1^2\right) - m_2 l_2 g \left(1 - \frac{1}{2} \varphi_2^2\right) \\ &= -g l_1 (m_1 + m_2) - g l_2 m_2 + \frac{1}{2} g \left(l_1 (m_1 + m_2) \varphi_1^2 + l_2 m_2 \varphi_2^2\right) \\ &= \varphi^\top \mathbf{B} \varphi \end{aligned}$$

where

$$\mathbf{B} = \frac{g}{2} \begin{pmatrix} (m_1 + m_2) l_1 & 0 \\ 0 & m_2 l_2 \end{pmatrix}$$

and we can eliminate the two constant terms out in front because they will not effect the equations of motion. All together, the Lagrangian now reads as

$$L = \dot{\varphi}^\top \mathbf{A} \dot{\varphi} - \varphi^\top \mathbf{B} \varphi$$

3. Calculate the canonically conjugate momenta p_1 and p_2 belonging to φ_1 and φ_2.

The canonical conjugate momenta are defined as

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\varphi}} = \mathbf{A}^\top \dot{\varphi} + \dot{\varphi}^\top \mathbf{A} = 2\mathbf{A}\dot{\varphi}$$

so

$$\dot{\varphi} = \frac{1}{2}\mathbf{A}^{-1}\mathbf{p}$$

Note that one of the operations I did above was only possible because $\mathbf{A}$ is symmetric, so it is equal to its transpose.

4. Find the Hamiltonian $H(\varphi_1, \varphi_2, p_1, p_2)$ of the system.

The Hamiltonian is defined by

$$H = \mathrm{KE} + \mathrm{PE}$$

and substituting in the conjugate momenta from the previous problem, we find

$$H = \frac{1}{4}\mathbf{p}^\top \mathbf{A}^{-1}\mathbf{p} + \varphi^\top \mathbf{B}\varphi$$

5. Show that the kinetic energy has the form $\frac{1}{2}\mathbf{x}^\top \mathbf{K}\mathbf{x}$ that we discussed in the previous problem. What is $\mathbf{x}$ and what is $\mathbf{K}$?

The kinetic energy sure seems to have the same form with $\mathbf{x} = \mathbf{p}$ and $\mathbf{K} = \frac{1}{2}\mathbf{A}^{-1}$. We must determine if $\mathbf{A}^{-1}$ is positive definite and symmetric. We can write it as

$$\frac{1}{2}\mathbf{A}^{-1} = \frac{1}{4\det(\mathbf{A})}\begin{pmatrix} m_2 l_2^2 & -m_2 l_1 l_2 \\ -m_2 l_1 l_2 & (m_1 + m_2) l_1^2 \end{pmatrix} \equiv \mathbf{K}$$

By observation, it is symmetric. Additionally, it must be positive definite since all of it's eigenvalues

$$\lambda = \frac{1}{2}\,\mathrm{Tr}(\mathbf{K}) \pm \sqrt{\frac{1}{4}\,\mathrm{Tr}(\mathbf{K})^2 - \det(\mathbf{K})}$$

are positive, as a result of $\det(\mathbf{K}) = \frac{1}{m_1 m_2 l_1^2 l_2^2} > 0$.

6. Calculate $\mathbf{K}^{-1}$.

$$\mathbf{K}^{-1} = 2\mathbf{A} = \begin{pmatrix} (m_1 + m_2) l_1^2 & m_2 l_1 l_2 \\ m_2 l_1 l_2 & m_2 l_2^2 \end{pmatrix}$$

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!

The correlation can be written as

$$\begin{aligned} \rho_{p_i p_j} = \frac{\mathrm{Cov}(p_i, p_j)}{\sigma_{p_i}\sigma_{p_j}} &= \frac{\mathrm{Cov}(p_i, p_j)}{\sqrt{\mathrm{Cov}(p_i, p_i)\mathrm{Cov}(p_j, p_j)}} \\ &= \frac{\langle p_i p_j \rangle}{\sqrt{\langle p_i^2 \rangle \langle p_j^2 \rangle}} \\ &= \frac{\mathbf{K}_{ij}^{-1}}{\sqrt{\mathbf{K}_{ii}^{-1}\mathbf{K}_{jj}^{-1}}} \end{aligned}$$

$$
\begin{aligned}
\rho_{p_1p_2} &= \frac{m_2 l_1 l_2}{\sqrt{((m_1+m_2)l_1^2)(m_2 l_2^2)}} \\
&= \frac{m_2}{\sqrt{m_1+m_2^2}}
\end{aligned}
$$

In the limit of $m_2 >> m_1$, we see that $\rho_{p_1p_2} \to 1$, indicating that as the middle mass becomes less consequential, the momenta become directly correlated. When $m_2 << m_1$, $\rho_{p_ip_j} \to 0$, indicating that in this limit, the momenta will have no correlation at all.