

1. Properties of quantum systems in canonical equilibrium

Consider a closed quantum system and use the Heisenberg picture in which operators evolve in time.

- (a) Prove that

$$\langle \hat{A}(t) \rangle = \text{Tr}(\hat{A}(t)\hat{\rho}) = \text{constant} \quad (1)$$

if $\hat{\rho}(\hat{\mathcal{H}})$ and the evolution is the usual Heisenberg one, with the same Hamiltonian $\hat{\mathcal{H}}$.

- (b) Prove that

$$C_{AB}(t, t') \equiv \langle \hat{A}(t)\hat{B}(t') \rangle = \text{Tr}(\hat{A}(t)\hat{B}(t')\hat{\rho}) \quad (2)$$

is stationary, meaning that it is a function of $t - t'$ and not t and t' independently, if $\hat{\rho}(\hat{\mathcal{H}})$ and the evolution is the usual Heisenberg one, with the same Hamiltonian $\hat{\mathcal{H}}$.

- (c) Prove that the two-time correlation of the anti-commutator/commutator of $\hat{A}(t)$ and $\hat{B}(t')$ are also stationary, under the same conditions.
- (d) By using $\hat{\rho}(\hat{\mathcal{H}}) = e^{-\beta\hat{\mathcal{H}}}/\mathcal{Z}$, rewrite the two-time correlation function of $\hat{A}(t)$ and $\hat{B}(t')$ as

$$C_{AB}(t, t') = C_{BA}(t', t + i\beta\hbar) = C_{BA}(-t - i\beta\hbar, -t') \quad (3)$$

and, if one uses stationarity,

$$C_{AB}(t - t') = C_{BA}(t' - t - i\beta\hbar) = C_{BA}(-t - i\beta\hbar + t') \quad (4)$$

- (e) Fourier transform the two sides of the previous relation with respect to $t - t'$ and prove that

$$\tilde{C}_{AB}(\omega) = e^{i\beta\omega} \tilde{C}_{BA}(-\omega) \quad (5)$$

This is one of the **KMS relations**. They are consequences of the periodicity of the trace and the choice $\hat{\rho} = e^{-\beta\hat{\mathcal{H}}}/\mathcal{Z}$.

- (f) Using (5), show that

$$\tilde{C}_{[A,B]}(\omega) = \tanh\left(\frac{\beta\hbar\omega}{2}\right) \tilde{C}_{\{A,B\}}(\omega) \quad (6)$$

This is a way to express the **quantum FDT**, relating the time-dependent linear response and the correlation function. Indeed, one can show that $\tilde{C}_{[A,B]}(\omega)$ is proportional to the linear response function of $\hat{A}$ to a perturbation applied to $\hat{B}$ through the **Kubo relation** (one has to be careful about causality). While the Kubo relation is just linear response, the FDT needs Boltzmann equilibrium to hold. One can Fourier transform back to time, but then the FDT looks ugly.

(g) Assuming that (6) allows us to write

$$\hbar \text{Im} \tilde{R}_{AB}(\omega) = \tanh\left(\frac{\beta \hbar \omega}{2}\right) \tilde{C}_{\{A,B\}}(\omega) \quad (7)$$

thanks to the Kubo relation, take now the $\hbar \rightarrow 0$ limit of (7), and show

$$\text{Im} \tilde{R}_{AB}(\omega) = \beta \omega \tilde{C}_{AB}(\omega) \quad (8)$$

since $\tilde{C}_{\{A,B\}}(\omega) \rightarrow 2\tilde{C}_{AB}(\omega)$,

(h) We will not derive the classical time-dependent FDT from here (we need to use Kramers-Kronig to write the real part in terms of the imaginary one, etc., but the expression is

$$R(t - t') = -\beta \partial_t C(t - t') \quad \text{for } t - t' > 0 \quad (9)$$

You can find details of these derivations in Chapter 3 of
TEACHING/Master2025/quantum-out-of-equilibrium-25.pdf
in my webpage

2. The SSK model

Consider the Spherical Sherrington-Kirkpatrick model

$$\mathcal{H} = -\frac{1}{2} \sum_{i \neq j} J_{ij} s_i s_j \quad (10)$$

where each $-\infty < s_i < \infty$ but all of them are spherically constrained

$$\sum_i s_i^2 = N \quad (11)$$

The couplings J_{ij} are taken from a Gaussian pdf with zero mean and variance $[J_{ij}^2] = J^2/N$. We will impose the global constraint with a Lagrange multiplier and work with

$$\mathcal{H} = -\frac{1}{2} \sum_{i \neq j} J_{ij} s_i s_j - \frac{z}{2} \sum_i (s_i^2 - N) \quad (12)$$

- (a) Interpret this problem as one particle with position $\vec{s}$ constrained to be on a sphere with radius $\sqrt{N}$.
- (b) Use the basis of eigenvectors of the matrix $\mathbb{J}$, to diagonalize the Hamiltonian. Let us call λ_μ the eigenvalues and $\vec{v}_\mu$ the associated eigenvectors, with $\mu = 1, \dots, N$, and $s_\mu = \vec{s} \cdot \vec{v}_\mu$ the new variables. The spin-glass model has been mapped on the problem of a single particle, with position $\vec{s}$, on a sphere with radius $\sqrt{N}$, with orthonormal coordinate system $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_N$. There are harmonic potentials $-\frac{\lambda_\mu}{2} s_\mu^2$, in each of these directions. s_μ are the coordinates of the particle's position in each of these directions.
- (c) Identify the stationary points of the Hamiltonian. Hint: first work at fixed z , and then find the corresponding z in each case. Identify their index, say defined as the number of positive eigenvalues of the Hessian. Order them by the value of their energy density. Visualize the energy landscape.
- (d) Focus on $T = 0$. Write the Markovian Langevin equation in the original and the rotated basis. Solve it for generic initial conditions. Write the equation that fixes the Lagrange multiplier, which should be considered to be time-dependent.
- (e) Take $s_i(0) = 1$ for all i , which corresponds to a high temperature initial condition (uncorrelated with J_{ij}). Take for the λ_μ in the $N \rightarrow \infty$ limit a Wigner semi-circle law,

$$\rho(\lambda) = \frac{1}{2\pi J^2} (4J^2 - \lambda^2)^{1/2} \quad (13)$$

with finite support $[-2J, 2J]$.

The relation

$$\int d\lambda \rho(\lambda) e^{-\lambda x} = \frac{I_1(2Jx)}{Jx}, \quad (14)$$

where I_1 is the first Bessel function, will be useful, as well as the limit

$$\lim_{x \gg 1/J} I_1(2Jx) \sim \frac{e^{2Jx}}{\sqrt{2\pi Jx}} \quad (15)$$

Find the time-dependence of $z(t)$ and its asymptotic large t limit.

- (f) Relate $z(t)$ to the time-dependent energy density $e(t)$. Hint: multiply the Langevin equation by $s_\mu(t^-)$, sum over μ , and take the limit $t^- \rightarrow t$. Estimate the asymptotic limit $e_\infty = e(t \rightarrow \infty)$. Does it coincide with the minimal energy calculated in item (c)?
- (g) Calculate the two time correlation function. Is it stationary? How does it depend on the times?
- (h) Calculate the linear response function. Is it related to the correlation function through the FDT?

You can find details of these derivations in
LFC & Dean, *Ful J. Phys. A: Math. Gen.* 28, 4213-4234 (1995)

3. Derive the generalized Langevin equation from the coupled system

$$\mathcal{H} = \mathcal{H}_{\text{syst}} + \mathcal{H}_{\text{env}} + \mathcal{H}_{\text{int}} \quad (16)$$

integrating over the environmental degrees of freedom, assuming they are harmonic oscillators, and linear coupling to a generic function of the system's variable

$$H_{\text{int}} = \sum_{a=1}^{N_{\text{osc}}} c_a \mathcal{V}(x) q_a \quad (17)$$

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The quantum version can also be found there.