3.S: Summary

References

- R. Balescu, *Equilibrium and Nonequilibrium Statistical Mechanics* (Wiley, 1975) An advanced text with an emphasis on fluids and kinetics.
- R. Balian, *From Macrophysics to Microphysics* (2 vols., Springer-Verlag, 2006) A very detailed discussion of the fundamental postulates of statistical mechanics and their implications.)

Summary

• *Distributions*: Equilibrium statistical mechanics describes systems of particles in terms of time-independent statistical distributions. Where do these distributions come from? How does a system with a given set of initial conditions come to have time-independent properties which can be described in this way?

• *Master equation*: Let $P_i(t)$ be the probability that a system is in state $|\, i\,\rangle$ at time t. The evolution of the $P_i(t)$ is given by $\frac{dP_i}{dt} = \sum_j (W_{ij} P_j - W_{ji} P_i) = -\sum_j \Gamma_{ij}\, P_j$, where the rates $W_{ij} \geq 0$ are nonnegative. Conservation of probability means $\sum_i \Gamma_{ij} = 0$ for all j, hence $\psi^t = (1, 1, \ldots, 1)$ is a left eigenvector with eigenvalue zero. The corresponding right eigenvector is the equilibrium distribution: $\Gamma_{ij}\, P_j^{eq} = 0$. Detailed balance, $W_{ij}\, P_j^{eq} = W_{ji}\, P_i^{eq}$, is a more stringent condition than the requirement of a stationary distribution alone. Boltzmann's H-theorem: $\dot{\mathsf{H}} \leq 0$, where $\mathsf{H} = \sum_i P_i \ln(P_i / P_i^{eq})$. Thus, the ME dynamics are *irreversible*. But the underlying microscopic laws are reversible!

• *Hamiltonian evolution*: $\dot\varphi_i = J_{ij}\, \frac{\partial H}{\partial \varphi_j}$, where $\varphi = (q_1, \ldots, q_r, p_1, \ldots, p_r)$ is a point in $2r$-dimensional phase space, and $J = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix}$. Phase space flow is then incompressible: $\boldsymbol{\nabla} \cdot \dot\varphi = 0$, hence phase space densities $\varrho(\varphi, t)$ obey Liouville's equation, $\partial_t\, \varrho + \dot\varphi \cdot \boldsymbol{\nabla} \varrho = 0$ (follows from continuity and incompressibility). Any function $\varrho(\Lambda_1, \ldots, \Lambda_k)$, where each Λ_i is conserved by the phase space dynamics, will be a stationary solution to Liouville's equation. In particular, the microcanonical distribution, $\varrho_E(\varphi) = \delta\big(E - H(\varphi)\big) / D(E)$ is such a solution, where $D(E) = \mathsf{Tr}\ \delta\big(E - H(\varphi)\big)$ is the *density of states*.

• *Poincaré Recurrence*: Let $g_\tau \varphi(t) = \varphi(t + \tau)$ be the τ-advance mapping for a dynamical system $\dot\varphi = \mathbf{V}(\varphi)$. If (i) g_τ is invertible, (ii) g_τ preserves phase space volumes, and (iii) the volume of phase accessible given the dynamics and initial conditions is finite, then in any finite neighborhood $\mathcal{R}_0$ of phase space there exists a point $\varphi_0 \in \mathcal{R}_0$ such that $g_\tau^n \varphi_0 \in \mathcal{R}_0$ with n finite. This means all the perfume molecules eventually go back inside the bottle (if it is opened in a sealed room).

• *Kac ring model*: Normally the recurrence time is orders of magnitude greater than the age of the Universe, but for the Kac ring model, one can simulate the recurrence phenomenon easily. The model consists of a ring of N sites, and a quenched (fixed) random distribution of flippers on F of the links $(F \leq N)$. On each site lies a discrete spin variable which is polarized either up or down. The system evolves discretely by all spins advancing clockwise by one site during a given time step. All spins which pass through a flipper reverse their polarization. Viewed probabilistically, if p_n is the probability any given spin is up at time n, then under the assumptions of the *Stosszahlansatz* $p_{n+1} = (1 - x) p_n + x(1 - p_n)$, where $x = F/N$ is the flipper density. This leads to exponential relaxation with a time scale $\tau = -1/\ln|1 - 2x|$, but the recurrence time is clearly N (if F is even) or $2N$ (if F is odd).

• *Ergodicity and mixing*: A dynamical system is *ergodic* if

$$\big\langle f(\varphi) \big\rangle_T = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\ f\big(\varphi(t)\big) = \frac{\mathsf{Tr}\ f(\varphi)\, \delta\big(E - H(\varphi)\big)}{\mathsf{Tr}\ \delta\big(E - H(\varphi)\big)} = \big\langle f(\varphi) \big\rangle_S \,. \tag{3.S.1}$$

This means long time averages are equal to phase space averages. This does not necessarily mean that the phase space distribution will converge to the microcanonical distribution. A stronger condition, known as *mixing*, means that the distribution spreads out 'evenly' over the phase space hypersurface consistent with all conservation laws. Thus, if g is a phase space map, and if $\nu(A) \equiv D_A(E)/D(E)$ is the fraction of the energy hypersurface (assume no conserved quantities other than $H = E$) contained in A, then g is mixing if $\lim_{n\to\infty} \nu\left(g^n A \cap B\right) = \nu(A)\, \nu(B)$. An example of a mixing map on a two-dimensional torus is the Arnold 'cat map',

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} \ \mathrm{mod}\ \mathbb{Z}^2 \ . \tag{3.S.2}$$

• *Thermalization of quantum systems*: This is a current research topic. One proposal, due to Deutsch (1991) and Srednicki (1994) is the *eigenstate thermalization hypothesis* (ETH). This says that thermal information is encoded in each eigenstate, such that if $E_\alpha \in [E, E + \Delta E]$, then

$$\langle \Psi_\alpha \,|\, \mathcal{A} \,|\, \Psi_\alpha \rangle = \langle \mathcal{A} \rangle_{E_\alpha} \ , \tag{3.S.3}$$

the expectation value of some local, translationally-invariant, few-body operator $\mathcal{A}$ in the state $|\, \Psi_\alpha \,\rangle$, is given by its average over a small energy window containing E_α. If this is the case, then so long as we prepare an initial state such that the spread of energies is within ΔE of some value E, where $\Delta E \ll E - E_0$ with E_0 the ground state energy, then $\langle \mathcal{A} \rangle_T = \langle \mathcal{A} \rangle_E$, and time averages become energy averages. Equivalently, the *reduced density matrix* ρ_S corresponding to a system S which is a subset of a universe U, with $W \cup S = U$ (W is the 'world'), is a thermal density matrix: $\rho_S = Z_S^{-1} e^{-\beta \hat{H}_S}$, where $\hat{H}_S$ is the Hamiltonian restricted to S, and with temperature fixed by the requirement $\mathsf{Tr}\,(\rho_S \hat{H}_S) = E \cdot (V_S / V_U)$, where the last factor is a ratio of volumes. ETH does not hold for so-called *integrable models* with an extensive number of independent conserved quantities. But it has been shown, both perturbatively as well as numerically, to hold for certain model nonintegrable systems. An interesting distinction between classical and quantum thermalization: in the quantum case, time evolution does not create the thermal state. Rather, it *reveals* the thermal distribution which is *encoded in each eigenstate* after sufficient time that dephasing has occurred and all correlations between the different wavefunction expansion coefficients is lost.

Endnotes

1. Exceptions involve quantities which are conserved by collisions, such as overall particle number, momentum, and energy. These quantities relax to equilibrium in a special way called *hydrodynamics*.↩
2. 'Compact' in the parlance of mathematical analysis means 'closed and bounded'.↩
3. The equality $\ln det\, M = \mathsf{Tr}\, \ln M$ is most easily proven by bringing the matrix to diagonal form via a similarity transformation, and proving the equality for diagonal matrices.↩
4. Actually, the microscopic laws of physics are *not* time-reversal invariant, but rather are invariant under the product PCT, where P is parity, C is charge conjugation, and T is time reversal.↩
5. The natural numbers $\mathbb{N}$ is the set of non-negative integers $\{0, 1, 2, \ldots\}$.↩
6. In the nonrelativistic limit, $T = p^2/2m$. For relativistic particles, we have $T = (p^2c^2 + m^2c^4)^{1/2} - mc^2$.↩
7. Actually, what the recurrence theorem guarantees is that there is a configuration arbitrarily close to the initial one which recurs, to within the same degree of closeness.↩
8. Unfortunately, many important physicists were German and we have to put up with a legacy of long German words like *Gedankenexperiment*, *Zitterbewegung*, *Brehmsstrahlung*, *Stosszahlansatz*, *Kartoffelsalat*,↩
9. The cat map gets its name from its initial application, by Arnold, to the image of a cat's face.↩
10. There is something beyond mixing, called a K*-system*. A K-system has positive Kolmogorov-Sinai entropy. For such a system, closed orbits separate exponentially in time, and consequently the Liouvillian L has a Lebesgue spectrum with denumerably infinite multiplicity.↩
11. More generally, we could project onto a K-dimensional subspace, in which case there would be K eigenvalues of $+1$ and $N - K$ eigenvalues of 0, where N is the dimension of the entire vector space.↩
12. Recall that in systems with no disorder, eigenstates exhibit Bloch periodicity in space.↩
13. Since the probability $P_i(t)$ is real, if the eigenvalue with the smallest (largest negative) real part is complex, there will be a corresponding complex conjugate eigenvalue, and summing over all eigenvectors will result in a real value for $P_i(t)$.↩