

# Quantum ergodicity: fundamentals and applications.

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<b>I. CLASSICAL CHAOS. KICKED ROTOR MODEL AND THE CHIRIKOV STANDARD MAP.</b>	

Emergence of statistical description and thermodynamics in dynamical systems (aka thermalization) is closely related to the concept of chaos leading to the ergodic behavior. In classical systems

chaos implies strong usually exponential sensitivity of the trajectories to small perturbations. In

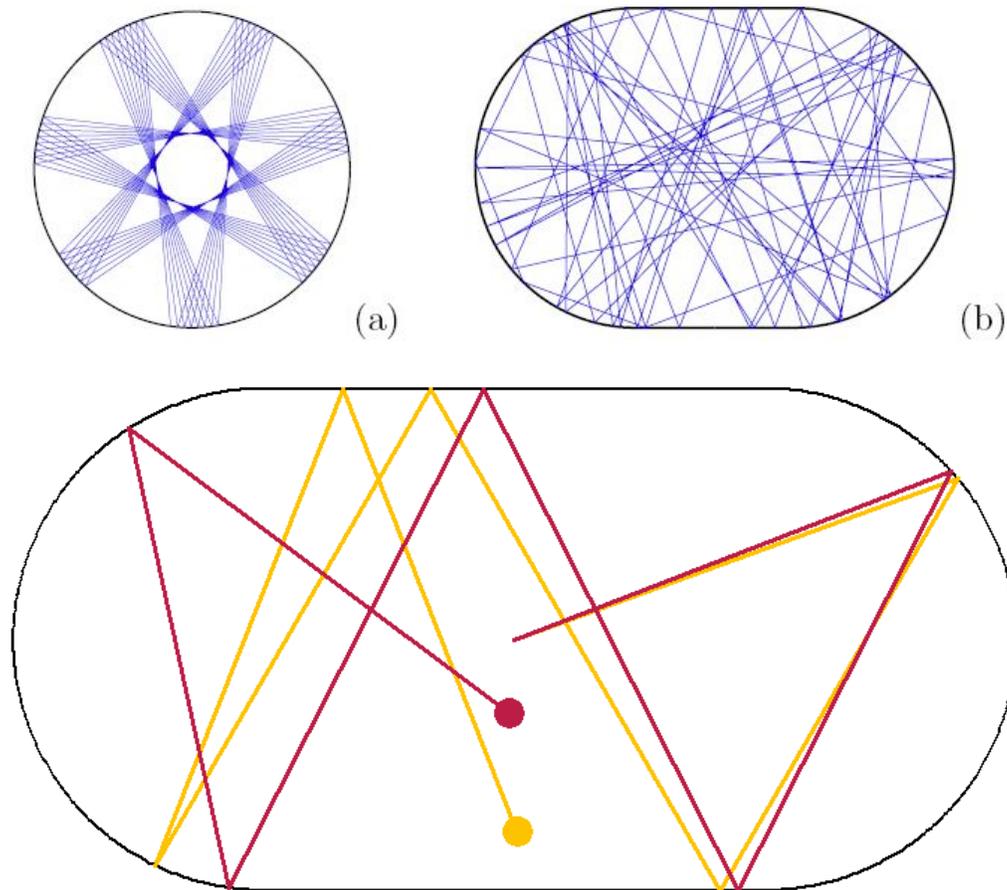


FIG. 1 Examples of trajectories of a particle bouncing in a cavity (i) non-chaotic circular (top left image) and (ii) chaotic Bunimovich stadium (top right image). The bottom panel shows evolution of two initially close trajectories in the chaotic regime. The images are taken from scholarpedia and wikimedia.

Fig. 1 we illustrate the motion of a particle in a regular and chaotic two-dimensional cavity. The top left panel illustrates long time trajectory of a particle in a regular circular cavity. It is visually clear that the motion of the particle is completely regular and thus non-ergodic. Indeed long time average is clearly not-equivalent to the micro-canonical ensemble average with all points in real space and all directions in the momentum space being equally probable. On the other hand the top right figure showing the trajectory chaotic Bunimovich stadium looks much less regular. Moreover in this chaotic regime if we compare two trajectories, which are initially close to each other then we see that after few bounces they become completely uncorrelated both in terms of positions and direction of motion (bottom graph). This is a consequence of the chaotic dynamics in the system.

There are many examples of dynamical systems exhibiting chaotic behavior. In this course we

will focus on Hamiltonian systems since our goal is connecting the microscopic laws of Nature and statistical physics. One of the simplest examples of Hamiltonian systems with a chaotic dynamics is the kicked rotor, analyzed in detail by Boris Chirikov in 1950th. The Hamiltonian of the system is very simple

$$\mathcal{H}(p, \phi, t) = \frac{p^2}{2m} - K \cos(\phi)\delta(t - nT) \quad (\text{I.1})$$

It essentially represents a freely rotating particle (it is easier to think about  $p$  as an angular momentum and  $\phi$  as a canonically conjugate angle) which periodically exhibits a momentum kick, which depends on the position (angle). We are choosing an opposite sign convention in front of  $K$  than usual because then the time averaged Hamiltonian reduces to the conventional pendulum with the energy minimum at  $\phi = 0$ . Clearly the sign of  $K$  is not important since one can always shift  $\phi \rightarrow \phi + \pi$ . Note that this is a problem with a time-dependent Hamiltonian not static as it was the case with billiards. We have to pay this price because in static problems with a single degree of freedom there is no chaos as the momentum is a unique function of the (conserved) energy and position. Let us write the equations of motion for our rotor

$$\frac{d\phi}{dt} = \frac{\partial \mathcal{H}}{\partial p} = \frac{p}{m}, \quad \frac{dp}{dt} = -\frac{\partial \mathcal{H}}{\partial \phi} = -K \sin(\phi)\delta(t - nT). \quad (\text{I.2})$$

These equations of motion can be easily integrated between the kicks. Let us denote by  $p_n$  and  $\phi_n$  the momentum and the angle of the particle just before the  $n$ -th kick, i.e. at time  $t = nT - \epsilon$ , where  $\epsilon \rightarrow 0$ . Then it is easy to see that the equations of motion result in the following recursion relation

$$\phi_{n+1} = \phi_n + Tp_{n+1} \quad (\text{I.3})$$

$$p_{n+1} = p_n - K \sin(\phi_n) \quad (\text{I.4})$$

These equations give us a discrete map (known as the standard Chirikov map) allowing one to uniquely determine the position (angle) and the momentum and arbitrary moment of time. Namely if  $nT < t < (n+1)T$  then clearly  $p(t) = p_{n+1}$ ,  $\phi(t) = \phi_n + p_{n+1}(t \bmod T)$ . It is clear that without loss of generality we can assume that the momentum is periodic function defined modulo  $2\pi/T$ . This immediately follows from the invariance of the equations of motion above under  $p_{n+1} \rightarrow p_{n+1} + 2\pi/T$  and  $\phi_{n+1} \rightarrow \phi_{n+1} + 2\pi$ .

Let us now qualitatively analyze the time evolution following from the Chirikov map. To simplify notations we assume  $m = T = 1$ , which can be always done by appropriately rescaling time units and  $K$ . Then the dynamics is determined by the value of  $K$  and the initial angle and

momentum. First we assume that  $K \ll 1$  and  $p_0 \ll 1$ . Then from equations (I.4) it is clear that both momentum and the angle change very little during each period so instead of solving discrete equations we can take the continuum limit with respect to the period and write

$$\frac{\partial \phi}{\partial n} \approx p, \quad \frac{\partial p}{\partial n} = -K \sin(\phi) \rightarrow \frac{\partial^2 \phi}{\partial n^2} \approx K \sin(\phi). \quad (\text{I.5})$$

This equation represents the motion of a pendulum in a cosine potential and is completely regular. Depending on the initial conditions there are two types of trajectories corresponding either to oscillations  $p \ll K$  or to full rotations if  $p \gg K$ . A more careful look shows that we even do not need to assume that the initial momentum is small, the only crucial assumption is that  $K \ll 1$ . Next we need to check the stability of the found trajectory. It might happen that if we include corrections to the continuum approximation we will immediately recover chaos. However, as proven by Kolmogorov, Arnold and Moser this does not happen. In particular, they formulated the KAM theorem, which states that regular motion is stable against small perturbations. We can check the stability of the above solution perturbatively. In particular, Eqs. (I.4) can be written as

$$\phi_{n+1} - 2\phi_n + \phi_{n-1} = -K \sin(\phi_n) \quad (\text{I.6})$$

If  $K$  is small we can assume that  $\phi$  is a nearly continuous variable and expand it into the Taylor series

$$\frac{d^2 \phi}{dn^2} + \frac{1}{12} \frac{d^4 \phi}{dn^4} \approx -K \sin(\phi) \quad (\text{I.7})$$

In general the second fourth derivative term in the equation above is quite dangerous. But our goal is to treat it perturbatively. From the unperturbed solution we see that (at least in the localized regime) the natural frequency of oscillations is  $\sqrt{K}$ . This means that each derivative with respect to  $n$  brings an extra factor of  $\sqrt{K}$  (*Check this by an explicit calculation.*) Thus the fourth derivative term is proportional to  $K^2$  and is small when  $K \ll 1$ .

When  $K$  is large continuum approximation for the map clearly fails. Momentum has large jumps from kick to kick and so does the phase. Because both are determined modulo  $2\pi$  it is intuitively clear that the motion will be random, i.e. chaotic. However, this property of global chaos is very hard to prove and the rigorous analytical proof does not exist even now. Let us follow much less ambitious goal and analyze stability of the fixed points of the map:

$$\phi_{n+1} = \phi_n + p_{n+1} = \phi_n, \quad p_{n+1} = p_n - K \sin(\phi_n) \quad (\text{I.8})$$

It is clear that there are only two possible solutions  $p_n = 0, \phi_n = 0$  and  $p_n = 0, \phi_n = \pi$ . Now let us perturb the trajectories a little bit and see whether they will remain stable. The linearized

equations then read

$$\delta\phi_{n+1} - 2\delta\phi_n + \delta\phi_{n-1} = -K \cos(\phi_0)\delta\phi_n = \mp K\delta\phi_n, \quad (\text{I.9})$$

where the plus and minus signs refer to the fixed points  $\phi = 0$  and  $\phi = \pi$ , respectively. We might recognize equations of motion for coupled harmonic oscillators where  $\pm K$  plays the role of the frequency squared. Because this is a translationally invariant system we will seek the solution in the following form

$$\phi_{n+1} = \lambda\phi_n = \lambda^n\phi_0 \quad (\text{I.10})$$

For a harmonic chain you might recognize standard procedure of going to normal Fourier modes if  $\lambda = \exp[iq]$ . But here we have to be careful because frequency  $\sqrt{\pm K}$  can be imaginary. After this substitution the system (I.9) reduces to a simple quadratic equation

$$\lambda^2 - (2 \mp K)\lambda + 1 = 0, \quad (\text{I.11})$$

which has two solutions

$$\lambda_{1,2} = 1 \mp \frac{K}{2} \pm \sqrt{\mp K + \frac{K^2}{4}}. \quad (\text{I.12})$$

Now let us analyze these two solutions separately for the two fixed points. We start from the  $\phi = 0$  point corresponding to the  $-$  sign. Then we have two solutions

$$\lambda_{1,2} = 1 - \frac{K}{2} \pm \sqrt{\frac{K^2}{4} - K} \quad (\text{I.13})$$

It is clear that for  $0 < K < 4$  the expression in the square root is negative leading to the imaginary contribution to  $\lambda$ . In the same range of  $K$  the absolute value of the real part of  $\lambda$  is less than one. This means that our solution is stable. Indeed if we introduce a small deviation in phase then as the discrete time  $n$  increases will not grow. Moreover in this range we can check that

$$|\lambda^2| = (1 - K/2)^2 + K - K^2/4 = 1 \quad (\text{I.14})$$

implying that  $\lambda = \exp[i\omega]$ , exactly like for a harmonic chain. So any small deviation will oscillate around the fixed point.

If  $K > 4$  then the situation changes completely. Now we are getting to real solutions for  $\lambda$  and the solution with the negative sign

$$\lambda_2 = 1 - \frac{K}{2} - \sqrt{\frac{K^2}{4} - K}$$

clearly gives  $|\lambda_2| > 1$  implying it is unstable: any small fluctuation exponentially grows without bound with time, at least in the linearized regime. This exponential growth does not prove the chaos yet but this is a strong indicator that the dynamics is chaotic. The exponent characterizing the rate of growth  $\log(\lambda)$  is called the Lyapunov exponent. In chaotic systems with many degrees of freedom there are many Lyapunov exponents and typically the largest of them determines the rate of divergence of nearby phase space trajectories.

The analysis of the other attractor with  $\phi = \pi$  is even simpler

$$\lambda_{1,2} = 1 + \frac{K}{2} \pm \sqrt{K + \frac{K^2}{4}}. \quad (\text{I.15})$$

Clearly for any positive  $K$  there are two real solutions with one larger than one. So this point is always unstable. This is not very surprising since this attractor corresponds to the situation, where a mass sits on top of the potential. It is interesting that if instead of  $\delta$  kicks one applies fast periodic motion of the pendulum:  $K = K_0 + a \sin(\nu t)$  then one can stabilize the top equilibrium  $\phi = \pi$ . This is known as the Kapitza effect (or Kapitza pendulum) and there are many demonstrations how it works. In Fig. 2 we show the phase space portrait of the kicked rotor at different values of  $K$ . It is clear that as  $K$  increases the system becomes more and more chaotic. At  $K = K_c \approx 1.2$  there is a delocalization transition, where the chaotic region becomes delocalized and the system increases its energy without bound.

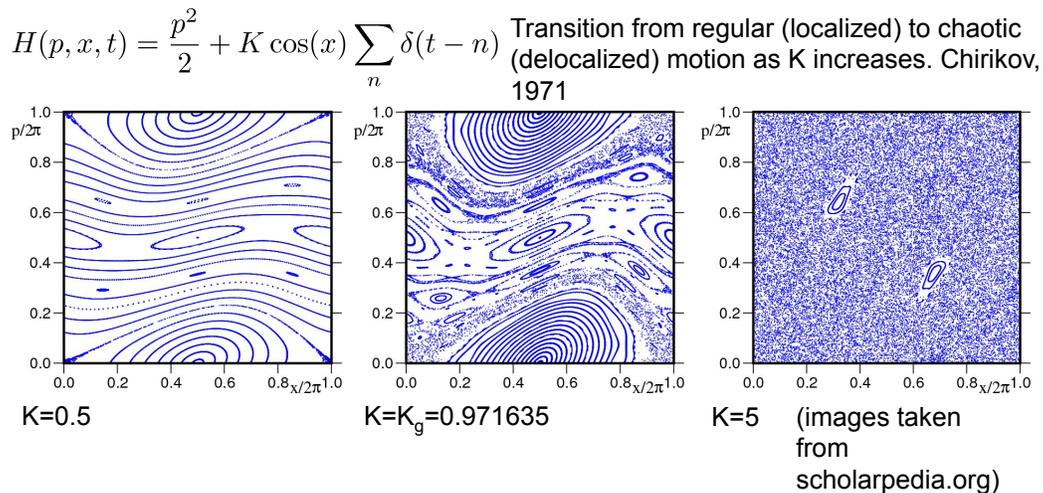


FIG. 2 Phase space portrait (Poincaré cross-section) for the kicked rotor at different values of the parameter  $K$ . Note that the opposite convention  $K \rightarrow -K$  or  $\theta \rightarrow \theta + \pi$  is used in the images.

To summarize this section we note that dynamics of Hamiltonian systems can be both regular and chaotic. Chaotic dynamics usually leads to ergodicity and thermalization. It is characterized by exponential sensitivity of the phase space trajectories to the initial conditions: small changes

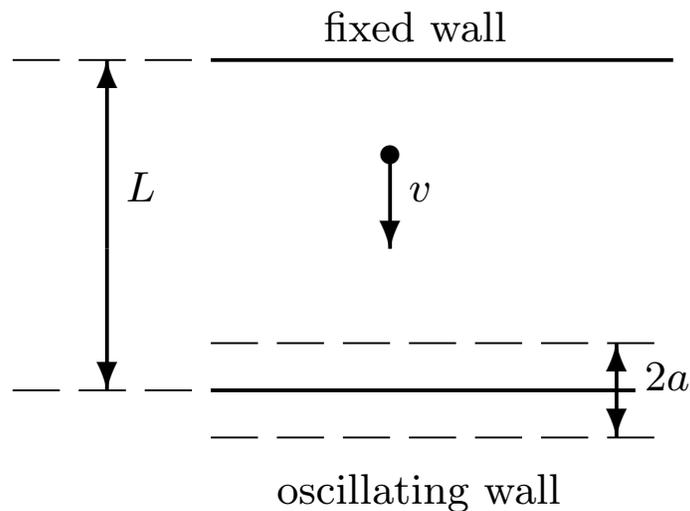


FIG. 3 Illustration of the setup for the Fermi-Ulam problem. See text for details.

exponentially grow in time. We saw that at least in some regimes regular dynamics is stable against small perturbations. There is a rigorous KAM theorem proving this. Then the transition to chaos occurs gradually (as we increase non-linearity in the system) through the overlapping resonances of the regular motion. The corresponding theory formulated by Chirikov has many implications to our understanding of chaotic systems. The situation is much less clear in thermodynamic limit, i.e. when we have infinitely many degrees of freedom. There is no analogue of the KAM theorem in this case and it is generally believed that infinitesimal non-linearity is sufficient to cause chaos and ergodicity. However, in the first part of the course, we mentioned an example of the Fermi-Pasta-Ulam problem, for which this is obviously not the case and the system remains non-ergodic even as one increases its size. Perhaps one-dimensional systems are really exceptional but until now the issue of ergodicity in the thermodynamic limit is not resolved.

### A. Problems

#### 1. Fermi-Ulam problem.

Consider the following Fermi-Ulam problem (do not confuse with the Fermi-Pasta-Ulam problem). The setup is shown in Fig. 3 A particle freely moves up or down without any force (there

is also a version of this problem with gravity) between two walls separated by the length  $L$ . The top wall is still so the collision of the particle with the wall is a simple reflection. The bottom wall undergoes small in amplitude fluctuations:  $z = a \cos(\omega t)$  where  $a \ll L$ . The goal of this exercise is to understand the motion of the particle in this setup.

- Write down the map describing the discretized dynamics of the momentum of the particle and the phase of the bottom wall between consequent collisions. Can you find any fixed points of this map? Use your intuition for guessing which trajectory should be time invariant.
- Analyze qualitatively fast and slow limits of the particle motion. In which limit can you anticipate the chaotic behavior and in which limit do you expect the regular motion? Perform the stability analysis of the fixed points and see if it supports with your qualitative reasoning.
- Using Mathematica or other software simulate the trajectories of this map in different regime (focus only on the points where the collision with the bottom wall occurs). Plot these points in a two-dimensional graph (if you have sufficiently many points this graph will give you the Poincar cross-section.)

## 2. Kapitza Pendulum

Kapitza pendulum is another famous example of a periodically driven system, which can have both periodic and chaotic behavior.

The setup for this pendulum is shown in Fig. 4. It represents a usual pendulum in the vertical gravitational field, where the top suspension point undergoes small amplitude oscillations of amplitude  $a \ll L$  and frequency  $\omega$ . Here is a link a short fragment of a video (in Russian) where the famous Russian mathematician Vladimir Arnold, one of the co-authors of the KAM theorem, makes his own experimental demonstration of stable motion of the Kapitza pendulum around inverted position: Kapitza pendulum. V. Arnold mathematically proved that this motion is stable for small perturbation. The full 8 minute video can be found on youtube: <http://www.youtube.com/watch?v=ZBSLK3Jbd2I>

- Write the Lagrangian for this system as a function of the angle  $\theta$  (counted from the average position of the suspension) and the velocity  $\dot{\theta}$
- Write the equations of motion for the Kapitza pendulum. Find the stationary points.

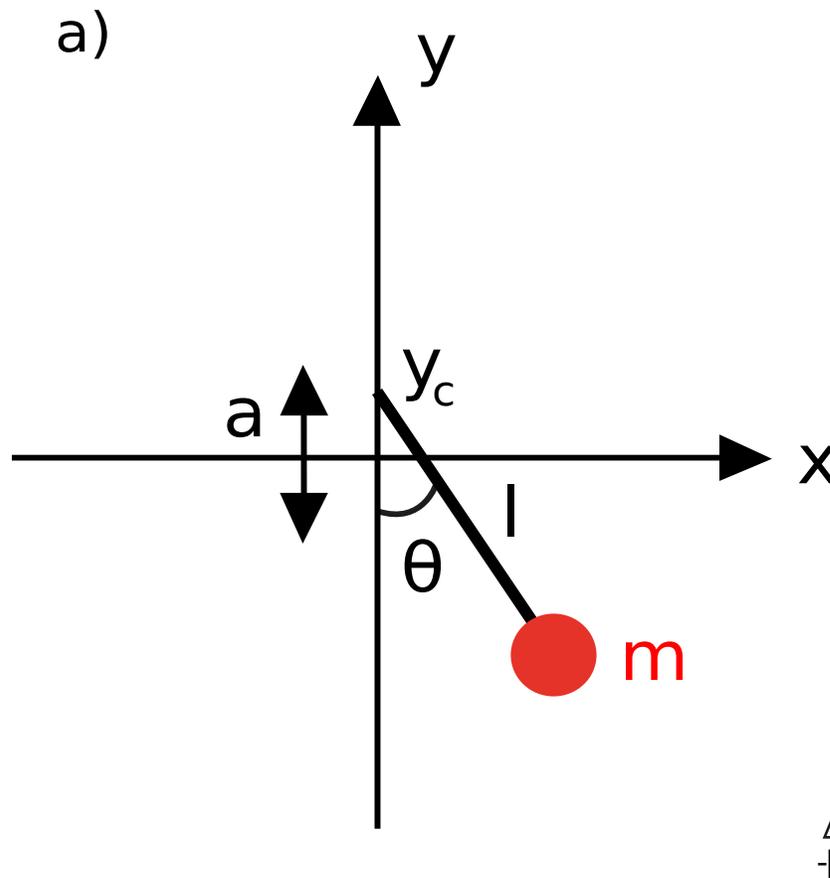


FIG. 4 Kapitza pendulum

- Analyze stability of these stationary points in the fast and slow limits. You should find that under certain conditions there is a new stable equilibrium near  $\theta = \pi$ .
- Using mathematica or other software analyze the phase portrait of this pendulum at different regimes. As in the previous problem you can use stroboscopic map analyzing the position and velocity at integer multiples of the oscillation period

## II. QUANTUM CHAOTIC SYSTEMS. RANDOM MATRIX THEORY.

From the early days of quantum mechanics (von Neumann 1929) it was clear that the classical concept of quantum chaos and quantum ergodicity does not directly apply to quantum mechanical systems. The main reason is that the Schrödinger equation is linear and for linear systems one can not have exponentially departing trajectories, at least in terms of distances between wave-functions. In 1950th E. Wigner suggested a general framework for describing equilibrium (stationary) prop-

erties of complex systems using the random matrix theory. His argument was that any complex Hamiltonian is an exponentially large matrix, which exact form is not important for understanding statistical properties of energy levels. Instead one should regard the Hamiltonian as a matrix with random coefficients, which satisfy general symmetries (for example the time reversal invariance). The success of this theory was tremendous and now predictions of this theory serve as one of the main indicators of quantum chaos.

To get a sense about the random matrix theory (RMT) let us first consider a simple  $2 \times 2$  Hamiltonian, which entries we treat as random numbers taken from some Gaussian distribution (for more details see V. Kravtsov, “Random matrix theory: Wigner-Dyson statistics and beyond”, arxiv:0911.0639, another good source for reading is T. Guhr, A. MüllerGroeling, H. A. Weidenmüller “Random-matrix theories in quantum physics: common concepts”, Physics Reports **299**, 189-425 (1998):

$$\mathcal{H} = \begin{bmatrix} \varepsilon_1 & V/\sqrt{2} \\ V^*/\sqrt{2} & \varepsilon_2 \end{bmatrix} \quad (\text{II.1})$$

Here we wrote the factor  $1/\sqrt{2}$  in the off-diagonal matrix elements for convenience. If the system is invariant under time reversal (there is no external magnetic field or other similar terms in the original Hamiltonian) then the eigenstates of the Hamiltonian can be all chosen to be real and hence  $V = V^*$ . Otherwise  $\Re[V]$  and  $\Im[V]$  are treated as independent random entries. This matrix can be easily diagonalized and the eigenvalues are

$$E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \frac{1}{2} \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2|V|^2} \quad (\text{II.2})$$

We can now compute the statistics of level separation. For simplicity we assume that we deal with real matrices and that the individual entries in this matrix have the Gaussian distribution with zero mean and the same variance  $\sigma$

$$P(E_1 - E_2 = \omega) = \frac{1}{(2\pi)^{3/2}\sigma^3} \int \dots \int d\varepsilon_1 d\varepsilon_2 dV \delta(\sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2V^2} - \omega) \exp\left[-\frac{\varepsilon_1^2 + \varepsilon_2^2 + V^2}{2\sigma^2}\right]. \quad (\text{II.3})$$

This integral can be evaluated in steps. First let us change variables  $\varepsilon_2 = \varepsilon_1 + \sqrt{2}\xi$ . Then the integral over  $\varepsilon_1$  is a simple Gaussian and we are left with

$$P(E_1 - E_2 = \omega) \equiv P(\omega) = \frac{1}{\pi\sigma^2} \int \int d\xi dV \delta(\sqrt{2\xi^2 + 2V^2} - \omega) \exp\left[-\frac{\xi^2 + V^2}{2\sigma^2}\right]. \quad (\text{II.4})$$

Then we go to the cylindrical coordinates:  $V = r \cos(\phi)$ ,  $\xi = r \sin(\phi)$ . The remaining integrals are very simple and we obtain

$$P(\omega) = \frac{\omega}{2\sigma^2} \exp\left[-\frac{\omega^2}{4\sigma^2}\right] \quad (\text{II.5})$$

This distribution has a characteristic property of the repulsion between levels at small separation (probability of having the levels very close to each other linearly vanishes with  $\omega$ ) and Gaussian decay at large level separation. It turns out that these two features survive level statistics in larger systems and the level distribution is well described by the approximate expressions (Wigner Surmise)

$$P(\omega) = A_\beta \omega^\beta \exp[-B_\beta \omega^2], \quad (\text{II.6})$$

where  $\beta = 1$  if we have time reversal invariance (orthogonal ensemble) and  $\beta = 2$  if we do not have time reversal symmetry (unitary ensemble). The coefficients  $A_\beta$  and  $B_\beta$  are found from the normalization and from fixing the mean level spacing. The exact Wigner-Dyson distributions do not have a closed analytic form but they are qualitatively (and even quantitatively) close to the Wigner Surmise (especially for the unitary ensemble  $\beta = 2$ ). In particular, for  $\beta = 1$  the normalized distribution with average spacing being equal to one is well approximated by

$$P(\omega) = \frac{\pi}{2} \omega \exp\left[-\frac{\pi}{4} \omega^2\right]. \quad (\text{II.7})$$

Before checking how this distribution works in different situation let us contrast it with our expectations in non-ergodic situations. Of course for small single-particle systems the statistics of levels is well described by the details of the potential. Like in the harmonic potential the levels are equidistant, in a square well the levels spacing grows with energy and so on. But we always keep in mind systems with many degrees of freedom. The simplest example of such non-ergodic system is an array of harmonic oscillators with some incommensurate frequencies. Then different many-body energy levels can be expressed as

$$E = \sum_j n_j \omega_j, \quad (\text{II.8})$$

where  $n_j$  are the occupation numbers and  $\omega_j$  are frequencies. If we look into large energies with large occupation numbers nearby energy levels (which are very closely spaced) can come from very different sets of  $\{n_j\}$ . This means that they are effectively uncorrelated with each other. It is also intuitively clear that at large  $E$  there is no particular pattern in the number of levels entering the interval  $[E, E + \delta E]$  thus we are essentially dealing with uncorrelated random numbers. As we know from the first part of the course we expect that the distribution of these numbers is well described by the Poisson statistics, i.e. the probability of having  $n$  energy levels in a particular interval  $\delta E$  is given by

$$P_n = \frac{\lambda^n}{n!} \exp[-\lambda], \quad (\text{II.9})$$

where  $\lambda$  is the average number of these levels in this interval (e.g. averaged over many nearby intervals). This Poisson statistics is very different from the Wigner - Dyson statistics. In particular, there is no level repulsion since the Hamiltonian is completely diagonal in the single-particle basis. The probability that within the given interval  $\delta E = \omega$  there are no levels is simply expressed by

$$P_0(\omega) = \exp[-\omega], \quad (\text{II.10})$$

which is very different from the Wigner Surmize (II.7). This statement is in fact known in literature as the Berry-Tabor conjecture (1977), which states that in the "generic" case the quantum energy eigenvalues behave like a sequence of independent random variables (i.e. have Poisson statistics) provided that the underlying classical dynamics is completely integrable. In Fig. 5 we show level

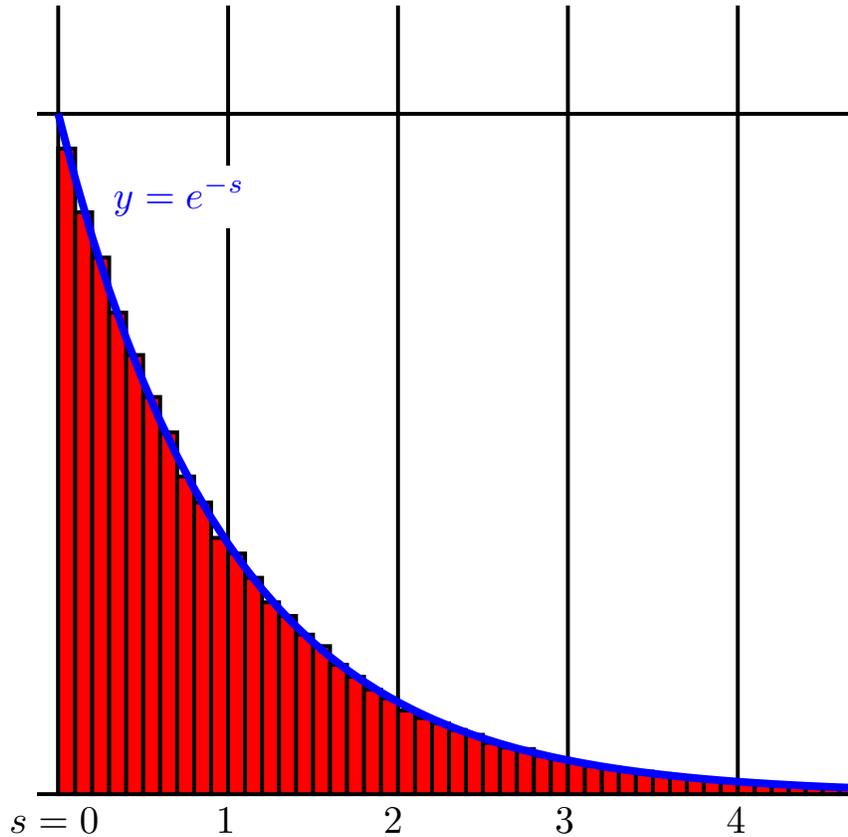


FIG. 5 Level statistics in a rectangular cavity with the ratio of sides  $a/b = \sqrt[4]{5}$  (Z. Rudnick, What Is Quantum Chaos?, Notices of the AMS 55, 32 (2008)). The levels are given by a simple formula:  $E_{n,m} = \pi^2(m^2/a^2 + n^2/b^2)$ .

statistics for a rectangular cavity with sides  $a$  and  $b$ , which have the following ratio:  $a/b = \sqrt[4]{5}$ . Clearly they agree perfectly well with the Poisson statistics. Yet the Berry-Tabor conjecture is not

proven in general and there are notorious exceptions. For example level statistics in a square well  $a = b$  is not given by the Poisson distribution because of commensurability of the spectra. Usually commensurate frequencies result from additional symmetries (like e.g. in a hydrogen atom) and lead to extra degeneracies. In quantum systems level statistics (Poisson vs. Wigner-Dyson) is used as one of the main indicators for the quantum chaos.

### A. Examples of the Wigner-Dyson distribution.

Random matrix statistics found many applications, which extend much beyond the framework of the original derivation. Let us illustrate this with several examples. Fig. 6 illustrates statistics

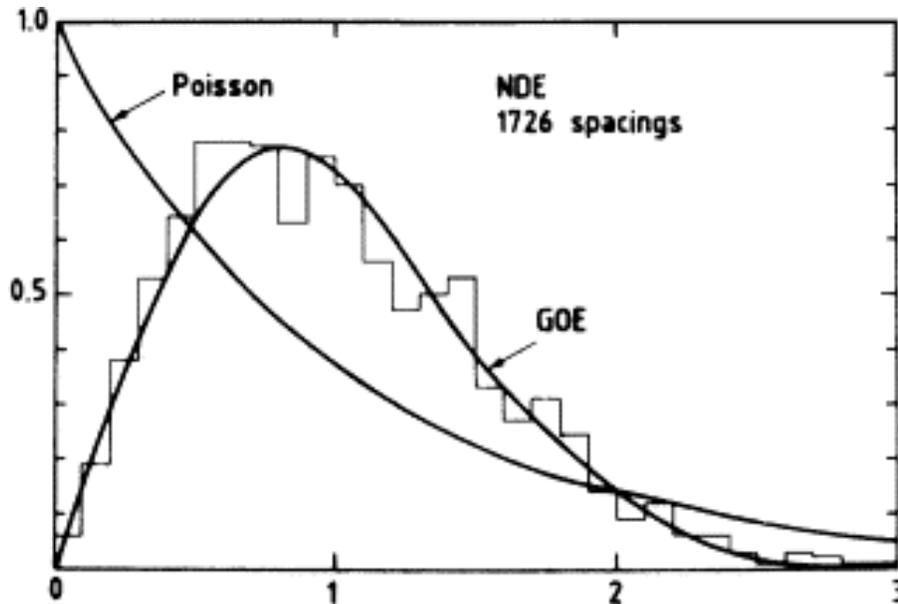


FIG. 6 Level statistics of 1726 level spacings taken from absorption spectra of different heavy nuclei. The data is taken from K.H. Bchhoff (Ed.), Nuclear Data for Science and Technology, Reidel, Dordrecht (1983)

of nearby level spacings of heavy nuclei. The data shows distribution of 1726 level spacings taken from different nuclei. The figure also shows the Poisson and the Wigner-Dyson distributions (for an orthogonal ensemble). It is clear from the figure that the latter works much better, while the Poisson statistics is completely off.

Next let us consider level statistics in a classical chaotic system. We will choose a Sinai billiard: a square (rectangle) with a circle in the middle Fig. 7 indicates close statistics between classical chaos and the random matrix theory. Clearly the statistics of level spacings in the Sinai billiard perfectly agrees with the Wigner-Dyson ensemble. At the same time this billiard together with Bunimovich stadium is one of the classical examples of chaotic systems. This situation is generic:

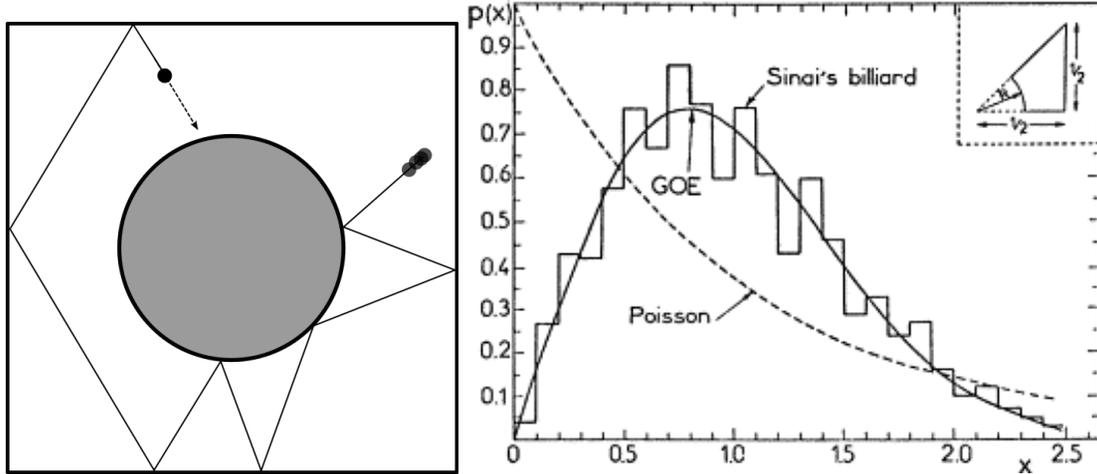


FIG. 7 Sinai billiard, which is a classical chaotic systems, similar to the Bunimovich stadium considered earlier. Left panel illustrates the Billiard and the classical trajectory (image source Wikipedia). Right panel shows level spacing statistics for the same billiard together with the Poisson and the Wigner-Dyson distributions (image source O. Bohigas, M.J. Giannoni, C. Schmit Phys. Rev. Lett. **52**, 1 (1984)).

energy levels in classical chaotic systems are typically well described by the Wigner-Dyson statistics. In Fig. 8 we show another example of the level statistics for a classical chaotic system also analyzed

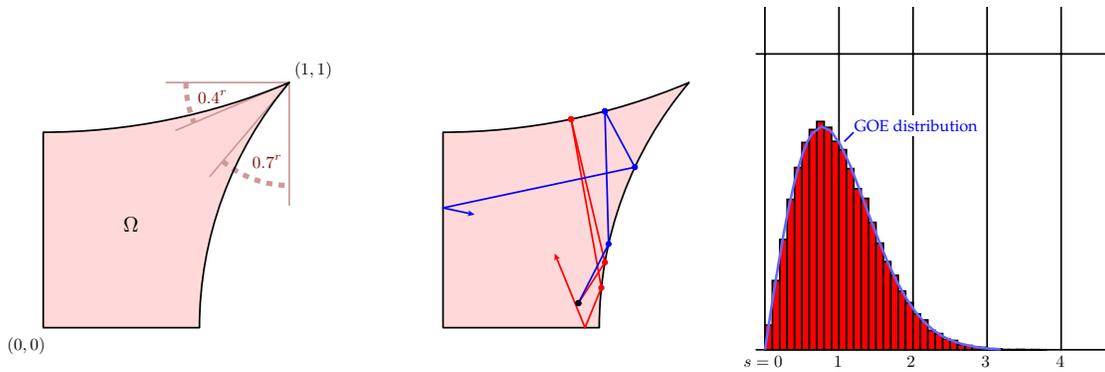


FIG. 8 Another chaotic system analyzed by Sinai (left panel) and illustration of classical trajectories (middle panel). Right panel shows level spacing statistics, which again perfectly agrees with the Wigner-Dyson ensemble (Z. Rudnick, What Is Quantum Chaos?, Notices of the AMS 55, 32 (2008)).

by Sinai.

As a next example we illustrate statistics of the level spacing of the high energy hydrogen atom in a magnetic field. Fig. 9 shows statistics of calculated level spacings in a hydrogen atom in strong external magnetic field. The top panel describes low energy spectra where the classical motion is regular and the level statistics is Poissonian. The bottom panels shows the high energy region corresponding to the classical chaotic motion. The plot clearly illustrates the crossover from the

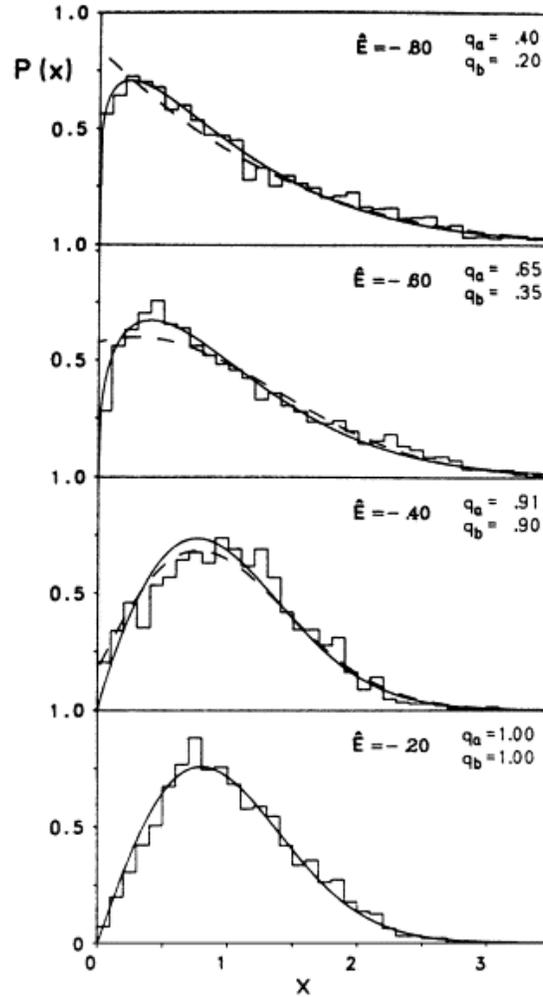


FIG. 9 Statistics of calculated highly excited energy levels in a hydrogen atom in external magnetic field. Energy  $\tilde{E}$  increases from the top to the bottom panel, meaning that the bottom panel describes higher excited states. The transition from the Poisson to the Wigner-Dyson statistics is clearly visible on this plot. The data is taken from Ref. D. Wintgen, H. Friedrich, Phys. Rev. A, **35**, 1464 (1987)

Poisson statistics to the Wigner dyson statistcis as the system become more chaotic.

Our next example will be more somewhat more exotic. In Fig. 10 we show statistics of time intervals between bus arrival times in the city of Cuernavaca (Mexico). The crosses illustrate the actual data and the solid curve is the Dyson-Wigner distribution for the Gaussian unitary ensemble. The agreement is very good. Of course this does not yet imply that there is an underlying linear model (though this is not impossible) describing arrival times. But this illustration shows something generic about Wigner-Dyson statistics: level repulsion (driven maximizing the ridership in a given bus or other reasons) and a Gaussian or exponential tail at long times. Just to demystify things a little bit, the Maxwell-Boltzmann distribution of the magnitude of the velocity in three-dimensions

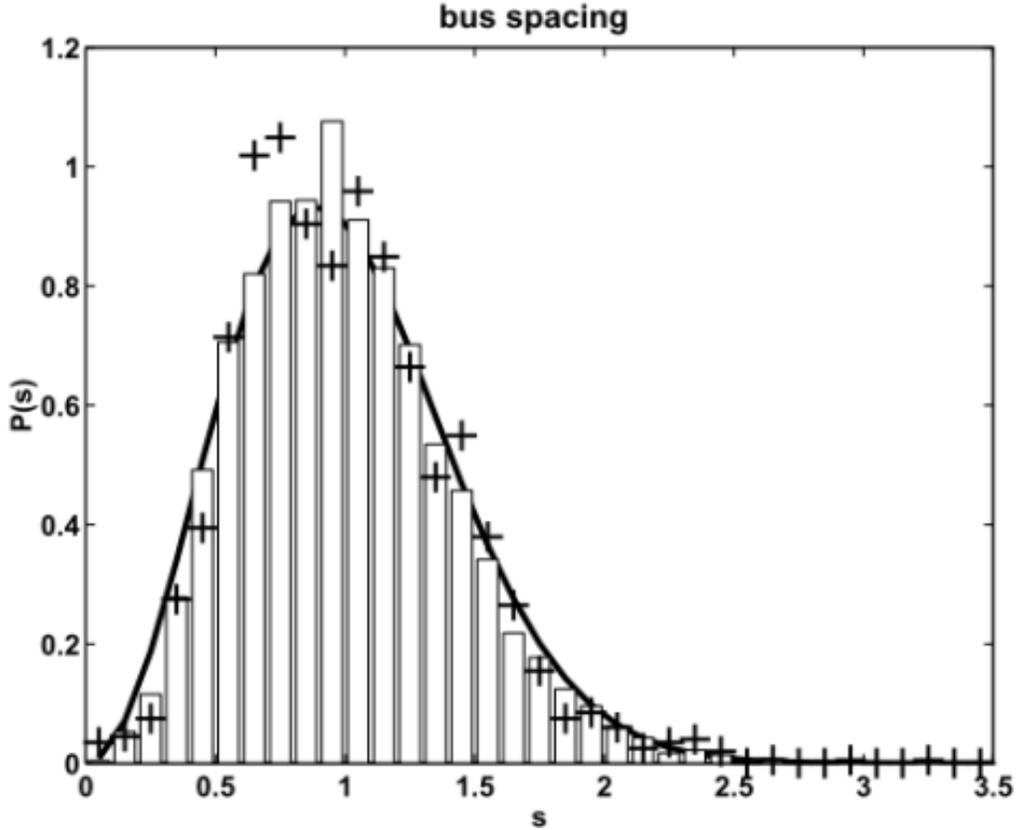


FIG. 10 A histogram of spacings between bus arrival times in Cuernavaca (Mexico), in crosses; the solid line is the prediction from random matrix theory. (M. Krbálek and P. Seba, *J. Phys. A: Math. Gen.* **33**, L229 (2000)).

also looks very similar to the Dyson-Wigner ensemble.

As a final example of the situation where the random matrix statistics naturally emerges let us mention the distribution of zeros of the Riemann zeta-function. For  $\Re(s) > 1$  the latter is formally defined as

$$\zeta(s) = \sum_{n \geq 1} \frac{1}{n^s} \quad (\text{II.11})$$

and for other values of  $s$  by an appropriate analytic continuation. As was proven by Euler the Riemann zeta function is related to the prime numbers again for  $\Re(s) > 1$ :

$$\zeta(s) = \prod_{p=\text{prime}} \frac{1}{1 - p^{-s}}. \quad (\text{II.12})$$

The proof of this result is very simple and elegant. Notice that

$$\frac{\zeta(s)}{2^s} = \frac{1}{2^s} + \frac{1}{4^s} + \frac{1}{6^s} + \dots$$

is a sum of inverse powers of all even integers, i.e. integers multiple of two. Thus

$$\zeta(s) - \frac{1}{2^s}\zeta(s) = I_2(s) = 1 + \frac{1}{3^s} + \frac{1}{5^s} + \dots$$

Then let us do a similar exercise and analyze  $I_2(s)/3^s$ . It is very easy to see that

$$I_3(s) = I_2(s) - \frac{1}{3^s}I_2(s) = \zeta(s) \left(1 - \frac{1}{2^s}\right) \left(1 - \frac{1}{3^s}\right) = 1 + \frac{1}{5^s} + \frac{1}{7^s} + \frac{1}{11^s} + \dots \quad (\text{II.13})$$

is a sum of inverse powers of all integers which are neither a multiple of two nor three. Continuing this exercise and using the fundamental theorem of arithmetic, stating that any number has a unique decomposition in prime numbers, we prove Eq. (II.12).

This product representation of the Riemann's zeta-function allows us to map it to the partition function of the non-interacting harmonic chain with the frequencies of the normal modes related to the prime numbers. Recall that the partition function for a single oscillator is

$$z_p(\beta) = \sum_n \exp[-\beta\omega_p n] = \frac{1}{1 - \exp[-\beta\omega_p]}, \quad (\text{II.14})$$

where we set the units  $\hbar = 1$ . If we associate prime numbers with different modes and require that

$$\omega_p = \log(p), \quad \beta = s$$

then we will see that

$$Z(\beta) = \prod_p z_p(\beta) = \zeta(\beta) \quad (\text{II.15})$$

The (complex) zeros of the zeta function are thus the complex zeros of the partition function of this model. As we will discuss later the structure of complex zeros of the partition function (also known as Lee-Yang or Fisher zeros) contains the information about phases and phase transitions.

The Riemann's zeta function has many fascinating properties. One of them that the non-trivial zeros of  $\zeta(s)$ , i.e. zeros which are not negative integers, lie on the line  $\Re(s) = 1/2$ . This conjecture is called the Riemann's hypothesis and it remains one of the greatest unsolved problems in mathematics. By now it was checked for the zeros up to the first  $10^{22}$ . In Fig. (11) we show the distribution of the normalized spacings of the  $10^9$  zeros of the Riemann's zeta function centered around the zero number  $1.3 \cdot 10^{16}$ . This distribution is astonishingly well described by the Wigner-Dyson statistics of the unitary ensemble. This agreement shows that there is some deep connection between prime and random numbers.

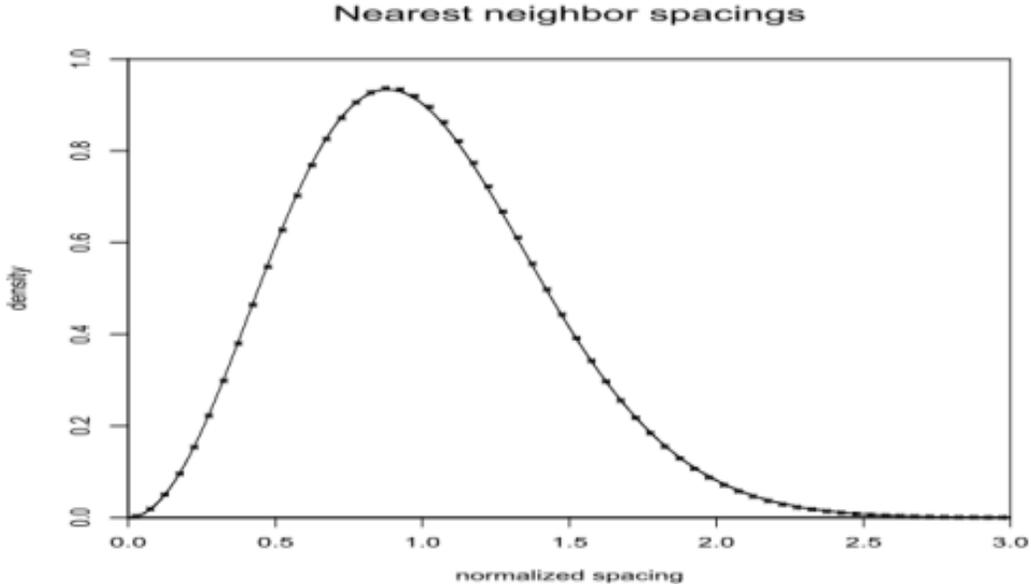


FIG. 11 Distribution of the spacings between one billion zeros of the Riemann's zeta function near zero number  $1.3 \cdot 10^{16}$  and the Wigner-Dyson statistics for the unitary ensemble. A. M. Odlyzko, "Dynamical, Spectral, and Arithmetic Zeta Functions", Amer. Math. Soc., Contemporary Math. series **290**, 139 (2001)

### III. QUANTUM DYNAMICS IN PHASE SPACE. ERGODICITY NEAR THE CLASSICAL LIMIT.

Before moving our discussion to many-particle interacting systems to which laws of statistical mechanics and thermodynamics apply we will try to reconcile two apparently different languages for describing chaotic systems: classical, where we rely on the sensitivity of the time evolution to small perturbations and the quantum, where we look into the statistics of the energy levels. In general this task remains unresolved, but at least we will try to formulate quantum dynamics in the way, which is similar to the classical one, understand quantum dynamics in the semiclassical limit and formulate a very powerful Berry's conjecture for the semiclassical eigenstates.

#### A. Quick summary of classical Hamiltonian dynamics in phase-space.

We will generally deal with Hamiltonian systems, which are defined by specifying a set of canonical variables  $p_j, q_j$  satisfying canonical relations

$$\{p_i, q_j\} = \delta_{ij}, \quad (\text{III.1})$$

where  $\{\dots\}$  denotes the Poisson bracket.

$$\{A(\vec{p}, \vec{q}), B(\vec{p}, \vec{q})\} = \sum_j \frac{\partial A}{\partial p_j} \frac{\partial B}{\partial q_j} - \frac{\partial B}{\partial p_j} \frac{\partial A}{\partial q_j} = B \Lambda A, \quad (\text{III.2})$$

where

$$\Lambda = \sum_j \overleftarrow{\partial} \frac{\partial}{\partial p_j} \frac{\partial}{\partial q_j} - \overleftarrow{\partial} \frac{\partial}{\partial q_j} \frac{\partial}{\partial p_j}$$

is the symplectic skew symmetric operator. It is easy to check that any orthogonal transformation

$$Q = R(\lambda)q, P = R(\lambda)p \quad (\text{III.3})$$

preserves both the Poisson brackets and the symplectic operator. A general class of transformations which preserve the Poisson brackets are known as canonical transformations and can be expressed through the generating functions (see e.g. L. Landau and E. Lifshitz, Classical Mechanics). It is easy to check that infinitesimal canonical transformations can be generated by gauge potentials

$$q_j(\lambda + \delta\lambda) = q_j(\lambda) - \frac{\partial A(\lambda, \vec{p}, \vec{q})}{\partial p_j} \delta\lambda, \quad (\text{III.4})$$

$$p_j(\lambda + \delta\lambda) = p_j(\lambda) + \frac{\partial A(\lambda, \vec{p}, \vec{q})}{\partial q_j} \delta\lambda, \quad (\text{III.5})$$

where  $\lambda$  parametrizes the canonical transformation and the gauge potential  $A$  is some function of canonical variables and parameters. Then up to the terms of the order of  $\delta\lambda^2$  the transformation above preserves the Poisson brackets

$$\{p_i(\lambda + \delta\lambda), q_j(\lambda + \delta\lambda)\} = \delta_{ij} + \delta\lambda \left( \frac{\partial^2 A}{\partial p_j \partial q_i} - \frac{\partial^2 A}{\partial p_i \partial q_j} \right) + O(\delta\lambda^2) = \delta_{ij} + O(\delta\lambda^2). \quad (\text{III.6})$$

Hamiltonian dynamics is a particular canonical transformation parametrized by time

$$\frac{\partial q_j}{\partial t} = \{H, q_j\} = \frac{\partial H}{\partial p_j}, \quad \frac{\partial p_j}{\partial t} = \{H, p_j\} = -\frac{\partial H}{\partial q_j} \quad (\text{III.7})$$

Clearly these Hamiltonian equations are equivalent to Eqs. (III.5) with the convention  $A_t = -H$ .

One can extend canonical transformations to the complex variables. Instead of doing this in all generality we will focus on particular phase space variables which are complex wave amplitudes. E.g. for Harmonic oscillators for each normal mode with the Hamiltonian

$$H_k = \frac{p_k^2}{2m} + \frac{m\omega_k^2}{2} q_k^2 \quad (\text{III.8})$$

we can define new linear combinations

$$p_k = i\sqrt{\frac{m\omega_k}{2}}(a_k^* - a_k), \quad q_k = \sqrt{\frac{1}{2m\omega_k}}(a_k + a_k^*) \quad (\text{III.9})$$

or equivalently

$$a_k^* = \frac{1}{\sqrt{2}} \left( q_k \sqrt{m\omega_k} - \frac{i}{\sqrt{m\omega_k}} p_k \right), \quad a_k = \frac{1}{\sqrt{2}} \left( q_k \sqrt{m\omega_k} + \frac{i}{\sqrt{m\omega_k}} p_k \right). \quad (\text{III.10})$$

It is clear that in new variables the Hamiltonian reads

$$H_k = \omega_k a_k^* a_k. \quad (\text{III.11})$$

Let us now compute the Poisson brackets of the complex wave amplitudes

$$\{a_k, a_k\} = \{a_k^*, a_k^*\} = 0, \{a_k, a_k^*\} = i. \quad (\text{III.12})$$

To avoid dealing with the imaginary Poisson brackets it is convenient to introduce new coherent state Poisson brackets

$$\{A, B\}_c = \sum_k \frac{\partial A}{\partial a_k} \frac{\partial B}{\partial a_k^*} - \frac{\partial B}{\partial a_k} \frac{\partial A}{\partial a_k^*} = A \Lambda_c B, \quad (\text{III.13})$$

where

$$\Lambda_c = \sum_k \frac{\overleftarrow{\partial}}{\partial a_k} \frac{\partial}{\partial a_k^*} - \frac{\overleftarrow{\partial}}{\partial a_k^*} \frac{\partial}{\partial a_k}. \quad (\text{III.14})$$

As for the coordinate momentum case, the coherent symplectic operator  $\Lambda_c$  is preserved under the canonical transformations. From this definition it is immediately clear that

$$\{a_k, a_q^*\}_c = \delta_{kq}. \quad (\text{III.15})$$

Comparing this relation with Eq. (III.12) we see that standard and coherent Poisson brackets differ by the factor of  $i$ :

$$\{\dots\} = i\{\dots\}_c. \quad (\text{III.16})$$

Let us write the Hamiltonian equations of motion for the new coherent variables. Using that

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} - \{A, H\} = \frac{\partial A}{\partial t} - i\{A, H\}_c \quad (\text{III.17})$$

and using that our variables do not explicitly depend on time (such dependence would amount to going to a moving frame, which we will not consider here) we find

$$i \frac{da_k}{dt} = \{a_k, H\}_c = \frac{\partial H}{\partial a_k^*}, \quad i \frac{da_k^*}{dt} = \{a_k^*, H\}_c = -\frac{\partial H}{\partial a_k} \quad (\text{III.18})$$

These equations are also known as Gross-Pitaevskii equations. Note that these equations are arbitrary for arbitrary Hamiltonians and not restricted to Harmonic systems.

And finally let us write down the Liouville equations of motion for the probability distribution  $\rho(q, p, t)$  or  $\rho(a, a^*, t)$ . The latter just express incompressibility of the probability flow, which directly follows conservation of the phase space volume  $d\Gamma = dqdp$  or  $d\Gamma = da da^*$  for arbitrary

canonical transformations including time evolution and from the conservation of the total probability  $\rho d\Gamma$ :

$$0 = \frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} - \{\rho, H\} = \frac{\partial\rho}{\partial t} - i\{\rho, H\}_c, \quad (\text{III.19})$$

or equivalently

$$\frac{\partial\rho}{\partial t} = \{\rho, H\}, \quad i\frac{\partial\rho}{\partial t} = -\{\rho, H\}_c \quad (\text{III.20})$$

### 1. Exercises

1. Show that the generator of translations  $\vec{q}(X) = \vec{q}_0 - \vec{X}$  is the momentum operator:  $\vec{A}_{\vec{X}}(\vec{q}, \vec{p}) = \vec{p}$ . You need to treat  $\vec{X}$  as a three component parameter  $\vec{\lambda}$ . Note that the number of particles (and thus phase space dimension) can be much higher than three.
2. Show that the generator of the rotations around z-axis:

$$q_x(\theta) = \cos(\theta)q_{x0} - \sin(\theta)q_{y0}, \quad q_y(\theta) = \cos(\theta)q_{y0} + \sin(\theta)q_{x0},$$

$$p_x(\theta) = \cos(\theta)p_{x0} - \sin(\theta)p_{y0}, \quad p_y(\theta) = \cos(\theta)p_{y0} + \sin(\theta)p_{x0},$$

is the angular momentum operator:  $A_\theta = p_x q_y - p_y q_x$ .

3. Find the gauge potential  $A_\lambda$  corresponding to the orthogonal transformation (III.3).
4. Check that any unitary transformation  $\tilde{a}_k = U_{k,k'} a'_{k'}$ , where  $U$  is a unitary matrix, preserves the coherent state Poisson bracket, i.e.  $\{\tilde{a}_k, \tilde{a}_q^*\}_c = \delta_{k,q}$ . Verify that the Bogoliubov transformation

$$\gamma_k = \cosh(\theta_k) a_k + \sinh(\theta_k) a_{-k}^*, \quad \gamma_k^* = \cosh(\theta_k) a_k^* + \sinh(\theta_k) a_{-k}, \quad (\text{III.21})$$

with  $\theta_k = \theta_{-k}$  also preserves the coherent state Poisson bracket, i.e.

$$\{\gamma_k, \gamma_{-k}\}_c = \{\gamma_k, \gamma_{-k}^*\}_c = 0, \quad \{\gamma_k, \gamma_k^*\}_c = \{\gamma_{-k}, \gamma_{-k}^*\}_c = 1. \quad (\text{III.22})$$

### B. Quantum systems in first and second quantized forms. Coherent states.

Now we move to quantum systems. As for the classical systems let us first define the language. We will use two different representations of the operators using either coordinate-momentum (first

quantized picture) or creation-annihilation operators (second quantized picture). In the second quantized form we will be only considering bosons because finding semiclassical limit for fermions is still an open question. These phase space variables satisfy canonical commutation relations:

$$[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}, [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \quad (\text{III.23})$$

Throughout these notes we introduce “hat”-notations for the operators to avoid confusion with the phase space variables. From this relations it is clear that in the classical limit the commutator should reduce to the coherent state Poisson bracket. As in the classical systems any Unitary transformation of the canonical variables preserves their commutation relations.

Since we will be always keeping in mind the classical limit we will be predominantly working in the Heisenberg representation where the operators are time dependent and satisfy canonical equations of motion

$$i\hbar\frac{d\hat{q}_i}{dt} = [\hat{q}_i, \hat{H}], \quad i\hbar\frac{d\hat{p}_i}{dt} = [\hat{p}_i, \hat{H}], \quad (\text{III.24})$$

$$i\hbar\frac{d\hat{a}_i}{dt} = [\hat{a}_i, \hat{H}], \quad i\hbar\frac{d\hat{a}_i^\dagger}{dt} = [\hat{a}_i^\dagger, \hat{H}]. \quad (\text{III.25})$$

As in the classical case these equations can be thought of as continuous canonical transformations parametrized by time. Next let us define representation of these operators. For canonical coordinate and momentum the natural representation, which is most often used in literature is coordinate, where

$$\hat{q}_j \rightarrow x_j, \quad \hat{p}_j = -i\hbar\frac{\partial}{\partial x_j} \quad (\text{III.26})$$

This representation is realized using coordinate eigenstates  $|\vec{x}\rangle = |x_1, x_2, \dots, x_M\rangle$  such that any state  $|\psi\rangle$  is written as

$$|\psi\rangle = \int D\vec{x} \psi(\vec{x})|\vec{x}\rangle. \quad (\text{III.27})$$

Here  $M$  denotes the total number of independent coordinate components, e.g. in the three-dimensional space  $M$  is equal to three times the number of particles.

In a similar fashion the natural representation for creation and annihilation operators is given by coherent states:

$$\hat{a}_j \rightarrow \alpha_j, \quad \hat{a}_j^\dagger \rightarrow -\frac{\partial}{\partial \alpha_j} \quad (\text{III.28})$$

Clearly in this form the creation and annihilation operators satisfy canonical commutation relations (III.23). Coherent states can be created from the vacuum state by exponentiating the creation

operator:

$$|\alpha_1, \alpha_2, \dots, \alpha_M\rangle = \prod_{j=1}^M e^{-|\alpha_j|^2/2} e^{\alpha_j a_j^\dagger} |0\rangle, \quad (\text{III.29})$$

where  $|0\rangle$  is the global particle vacuum annihilated by all operators  $\hat{a}_j$ <sup>1</sup>. One can check that these coherent states are properly normalized:

$$\int D\alpha D\alpha^* \langle \alpha_1, \alpha_2, \dots, \alpha_M | \alpha_1, \alpha_2, \dots, \alpha_M \rangle = 1, \quad (\text{III.30})$$

where we use the integration measure  $d\alpha d\alpha^* = d\Re(\alpha) d\Im(\alpha) / \pi$ . Unlike the coordinate states they are not orthogonal, which means that the coherent state basis is over-complete.

### C. Wigner-Weyl quantization

#### 1. Coordinate-Momentum representation

We are now ready to formulate phase space representation of quantum operators and the density matrix. To simplify notations we suppress component index in phase space variables except when extensions to multiple components is not straightforward. For any Hermitian operator  $\hat{\Omega}(\hat{q}, \hat{p})$  we define the Weyl symbol, which depends on the corresponding phase space variables  $q, p$ :

$$\Omega_W(q, p) = \int d\xi \left\langle q - \frac{\xi}{2} \left| \hat{\Omega}(\hat{q}, \hat{p}) \right| q + \frac{\xi}{2} \right\rangle e^{ip\xi/\hbar}. \quad (\text{III.31})$$

The Weyl symbol is clearly uniquely defined for any operator with off-diagonal elements in the coordinate space decaying to zero. We will consider only such operators. In the classical limit the exponential term  $\exp[ip\xi/\hbar]$  very rapidly oscillates unless  $\xi$  is very close to zero. Thus we see that the Weyl symbol becomes equal to the classical function  $\Omega(q, p)$ . Before proceeding let us point that there is some ambiguity in defining quantum classical correspondence in this way. In particular, instead of Eq. (III.31), one could define a continuous range of functions characterized by some real number  $\epsilon$ :

$$\Omega_\epsilon(q, p) = \int d\xi \langle q - \epsilon\xi | \hat{\Omega}(\hat{q}, \hat{p}) | q + (1 - \epsilon)\xi \rangle e^{ip\xi/\hbar}. \quad (\text{III.32})$$

This transform is always well defined and one can show that it is possible to build complete and unique phase-space representation of any quantum-mechanical operator for any  $\epsilon$ . For coherent

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<sup>1</sup> Note that there is a sign mismatch between  $\hat{a}^\dagger|\alpha\rangle = \partial_\alpha|\alpha\rangle$  and the representation (III.28). This is because the derivative operator acting on the basis vector is opposite in sign to the derivative operator acting on the wave function  $|\psi\rangle = \int d\alpha\psi(\alpha)|\alpha\rangle$ .

states such freedom is well understood leading to  $P$  and  $Q$  (Husimi) representations (for more details see the text books: C.W. Gardiner and P. Zoller. Quantum Noise. Springer-Verlag, Berlin Heidelberg, third edition, 2004; D.F. Walls and G.J. Milburn. Quantum Optics. Springer-Verlag, Berlin, 1994). Clearly the Weyl symbol corresponds to the symmetric choice  $\epsilon = 1/2$ . In these lectures we will stick only to the Weyl quantization.

Let us now compute the Weyl symbol for some simple operators. First let  $\Omega(\hat{q}, \hat{p}) = V(\hat{q})$  depends only on the coordinate. Then obviously

$$V_W(q) = \int d\xi V(q) \delta(\xi) e^{ip\xi/\hbar} = V(q), \quad (\text{III.33})$$

i.e. the Weyl symbol amounts to the substitution the operator  $\hat{q}$  by the number  $q$ . One can check that the same is true for any operator depending only on momentum

$$\Omega_W(p) = \Omega(p) \quad (\text{III.34})$$

The easiest way to see this is to note that the definition of the Weyl symbol is symmetric with respect to  $q \leftrightarrow p$ .

Now let us consider a slightly more complicated operator  $\hat{\Omega}(\hat{q}, \hat{p}) = \hat{q}\hat{p}$ . Then

$$(\hat{q}\hat{p})_W = \int d\xi (q - \xi/2) \langle q - \xi/2 | \hat{p} | q + \xi/2 \rangle e^{ip\xi/\hbar} = \int d\xi \int \frac{dk}{2\pi\hbar} (q - \xi/2) k e^{i(p-k)\xi/\hbar} = pq + \frac{i\hbar}{2} \quad (\text{III.35})$$

To get the last result we inserted the resolution of identity

$$I = \int \frac{dk}{2\pi\hbar} |k\rangle \langle k|$$

inside the matrix element appearing in the integral. In the same way we can find that

$$(\hat{p}\hat{q})_W = pq - \frac{i\hbar}{2}. \quad (\text{III.36})$$

For a general “normal” ordered operator  $\hat{\Omega}(\hat{q}, \hat{p})$  such that the coordinate operators appear on the left of momentum operators the Weyl symbol (III.31) can be written as

$$\Omega_W(q, p) = \int \frac{d\xi d\eta}{4\pi\hbar} \Omega\left(q - \frac{\xi}{2}, p + \frac{\eta}{2}\right) e^{-i\xi\eta/2\hbar}. \quad (\text{III.37})$$

The equivalence of Eqs. (III.37) and (III.31) can be established by the same trick of inserting the identity (III.C.1) into Eq. (III.31).

While the integral expressions for finding the Weyl symbol are very general, it is very useful to introduce the representation of the canonical coordinate and momentum operator, which gives the Weyl symbol right away. This is known as the Bopp representation:

$$\hat{q} = q + \frac{i\hbar}{2} \frac{\partial}{\partial p}, \quad \hat{p} = p - \frac{i\hbar}{2} \frac{\partial}{\partial q}. \quad (\text{III.38})$$

This representation clearly respects the canonical commutation relations (III.23) and is symmetric with respect to coordinate and momentum. Then the Weyl symbol of the arbitrary operator  $\hat{\Omega}(\hat{q}, \hat{p})$  is given by

$$\Omega_W(q, p) = \hat{\Omega}\left(q + i\hbar/2 \partial_p, p - i\hbar/2 \partial_q\right) 1, \quad (\text{III.39})$$

We wrote unity on the right of this expression showing that derivatives acting on unity give zero. For example

$$(\hat{q}\hat{p})_W = \left(q + \frac{i\hbar}{2} \partial_p\right) \left(p - \frac{i\hbar}{2} \partial_q\right) 1 = \left(q + \frac{i\hbar}{2} \partial_p\right) p = pq + \frac{i\hbar}{2}, \quad (\text{III.40})$$

which is the correct result. Similarly

$$(\hat{q}^2 \hat{p}^2)_W = \left(q + \frac{i\hbar}{2} \partial_p\right)^2 p^2 = q^2 p^2 + 2q \frac{i\hbar}{2} \partial_p p^2 - \frac{\hbar^2}{4} \partial_p^2 p^2 = p^2 q^2 + 2i\hbar qp - \frac{\hbar^2}{2}. \quad (\text{III.41})$$

One can check that this is also the correct result by e.g. explicitly performing integration in Eq. (III.37).

Let us prove Eq. (III.39). First note that if we prove this statement for a normal ordered operator  $\hat{\Omega}_{mn} \hat{q}^m \hat{p}^n$  then we will automatically prove this statement for any operator, which is analytic in  $\hat{q}$  and  $\hat{p}$ . Indeed obviously any analytic function can be represented as a sum of normal ordered polynomials of  $\hat{q}$  and  $\hat{p}$ . Thus if we prove the statement for  $\hat{\Omega}_{mn}$  we prove it for any operator. Since the latter is normal ordered we can use Eq. (III.37)

$$\begin{aligned} (\hat{q}^m \hat{p}^n)_W &= \int \int \frac{d\xi d\eta}{4\pi\hbar} \left(q - \frac{\xi}{2}\right)^m \left(p + \frac{\eta}{2}\right)^n e^{-i\xi\eta/(2\hbar)} = \int \int \frac{d\xi d\eta}{4\pi\hbar} \left(p + \frac{\eta}{2}\right)^n (q - i\hbar\partial_\eta)^m e^{-i\xi\eta/(2\hbar)} \\ &= \int d\eta \left(p + \frac{\eta}{2}\right)^n (q - i\hbar\partial_\eta)^m \delta(\eta) = (q + i\hbar\partial_\eta)^m \left(p + \frac{\eta}{2}\right)^n \Big|_{\eta=0} = \left(q + \frac{i\hbar}{2} \partial_p\right)^m p^n \end{aligned} \quad (\text{III.42})$$

Thus we proved that the representation of  $\hat{q}$  is indeed given by the Bopp operator. Bopp representation of  $\hat{p}$  e.g. immediately follows from the commutation relation. Alternatively it follows from the symmetry of the representation of the Weyl symbol with respect to the change  $p \leftrightarrow q, \xi \leftrightarrow -\eta$ .

Let us note that there is an alternative Bopp representation expressed through the left derivatives:

$$\hat{q} = q - \frac{i\hbar}{2} \overleftarrow{\partial}_p, \quad \hat{p} = p + \frac{i\hbar}{2} \overleftarrow{\partial}_q, \quad (\text{III.43})$$

where the left derivative now acts on the operator on the left. While for now left and right representations are equivalent as we will see later causality uniquely defines the correct representation when we consider non-equal time correlation functions.

As a next ingredient of the Weyl quantization we will establish rules for addition and multiplication of operators. The former are trivial

$$(\hat{\Omega}_1 + \hat{\Omega}_2)_W = \Omega_{1W} + \Omega_{2W}, \quad (\text{III.44})$$

The Weyl symbol of the product of two operators is much less trivial; it is given by the Moyal product:

$$(\Omega_1 \Omega_2)_W(q, p) = \Omega_{1,W}(q, p) \exp \left[ -\frac{i\hbar}{2} \Lambda \right] \Omega_{2,W}(q, p), \quad (\text{III.45})$$

where  $\Lambda$  is the symplectic operator introduced earlier (III.A). As earlier, before proving this relation let us first check that it agrees with simple results

$$(\hat{q}\hat{p})_W = q \exp \left[ -\frac{i\hbar}{2} \Lambda \right] p = qp - q \frac{i\hbar}{2} \left[ \overleftarrow{\frac{\partial}{\partial p}} \frac{\partial}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q} \frac{\partial}{\partial p} \right] p + 0 = pq + \frac{i\hbar}{2}, \quad (\text{III.46})$$

where we used that all higher order terms in the expansion of the exponent give zero because they contain higher order derivatives with respect to  $q$  and  $p$ . Clearly we got the correct result.

Similarly

$$\begin{aligned} (\hat{q}^2 \hat{p}^2)_W &= q^2 \exp \left[ -\frac{i\hbar}{2} \Lambda \right] p^2 = qp - q^2 \frac{i\hbar}{2} \left[ \overleftarrow{\frac{\partial}{\partial p}} \frac{\partial}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q} \frac{\partial}{\partial p} \right] p^2 - q^2 \frac{\hbar^2}{8} \left[ \overleftarrow{\frac{\partial}{\partial p}} \frac{\partial}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q} \frac{\partial}{\partial p} \right] p^2 \\ &= p^2 q^2 + 2i\hbar pq - \frac{\hbar^2}{2}, \end{aligned} \quad (\text{III.47})$$

which is again the correct result (cf. Eq. (III.41)). The proof of the Moyal product relation is straightforward, but somewhat lengthy. It can be found e.g. in Ref. (M. A. Hillery, R. F. OConnell, M. O. Scully, and E. P. Wigner. Phys. Rep., 106: 121, 1984). Another way to prove this relation is to consider the Bopp representation and check manually that

$$(\hat{q}^n \hat{p}^m)_W \exp \left[ -\frac{i\hbar}{2} \Lambda \right] \Omega_{2,W}(q, p) = \left( q + \frac{i\hbar}{2} \partial_p \right)^n \left( p - \frac{i\hbar}{2} \partial_q \right)^m \Omega_2(\hat{q}, \hat{p}). \quad (\text{III.48})$$

The Moyal product obviously satisfies the following relation

$$\Omega_{1,W} \exp \left[ -\frac{i\hbar}{2} \Lambda \right] \Omega_{2,W} = \Omega_{2,W} \exp \left[ +\frac{i\hbar}{2} \Lambda \right] \Omega_{1,W}. \quad (\text{III.49})$$

From this relation we immediately derive the Weyl symbol of the commutator

$$[\hat{\Omega}_1, \hat{\Omega}_2]_W = -2i\Omega_{1,W} \sin \left( \frac{\hbar}{2} \Lambda \right) \Omega_{2W} = -i\hbar \{ \Omega_{1,W}, \Omega_{2,W} \}_{MB}, \quad (\text{III.50})$$

where ‘‘MB’’ stands for the Moyal bracket:

$$\{A, B\}_{MB} = \frac{2}{\hbar} A \sin \left( \frac{\hbar}{2} \Lambda \right) B.$$

Obviously in the classical limit  $\hbar \rightarrow 0$  the Moyal bracket reduces to the Poisson bracket (cf. Eq. (III.2)).

Weyl symbol of the density matrix  $\hat{\rho}$  is known as the Wigner function:

$$W(q, p) = \int d\xi \langle q - \xi/2 | \hat{\rho} | q + \xi/2 \rangle e^{ip\xi/\hbar} = \int d\xi \rho(q - \xi/2, q + \xi/2) e^{ip\xi/\hbar}. \quad (\text{III.51})$$

In particular, if the density matrix represents a pure state:  $\hat{\rho} = |\psi\rangle\langle\psi|$  then

$$W(q, p) = \int d\xi \psi^*(q + \xi/2) \psi(q - \xi/2) e^{ip\xi/\hbar}. \quad (\text{III.52})$$

The Wigner function is normalized and in this sense it is similar to the classical probability distribution

$$\int \frac{dqdp}{2\pi\hbar} W(q, p) = \int dq d\xi \rho(q - \xi/2, q + \xi/2) \delta(\xi) = \text{Tr}[\hat{\rho}] = 1. \quad (\text{III.53})$$

Unlike probability distribution, the Wigner function is not necessarily positive (as we see later considering explicit examples). Therefore it is often referred to as the quasi-probability distribution.

Now let us prove that the expectation value of any operator is given by the average of the corresponding Weyl symbol over the Wigner function:

$$\langle \hat{\Omega}(\hat{q}, \hat{p}) \rangle \equiv \text{Tr}[\hat{\rho} \hat{\Omega}(\hat{q}, \hat{p})] = \int \frac{dqdp}{2\pi\hbar} W(q, p) \Omega_W(q, p) \quad (\text{III.54})$$

This statement proves that the Wigner-Weyl quantization, i.e. representation of quantum systems through the Weyl symbols and the Wigner function, is complete. The proof of this statement is straightforward:

$$\begin{aligned} \int \frac{dqdp}{2\pi\hbar} W(q, p) \Omega_W(q, p) &= \int \frac{dqdp}{2\pi\hbar} \int d\xi \int d\xi' \langle q - \xi/2 | \hat{\rho} | q + \xi/2 \rangle \langle q - \xi'/2 | \hat{\Omega} | q + \xi'/2 \rangle \exp[ip(\xi + \xi')/\hbar] \\ &= \int dq \int d\xi \langle q - \xi/2 | \hat{\rho} | q + \xi/2 \rangle \langle q + \xi/2 | \hat{\Omega} | q - \xi/2 \rangle = \int dq \langle q | \hat{\rho} \hat{\Omega} | q \rangle = \text{Tr}[\hat{\rho} \hat{\Omega}]. \end{aligned} \quad (\text{III.55})$$

Let us consider an example of a harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2} \hat{q}^2. \quad (\text{III.56})$$

First consider the zero temperature density matrix corresponding to the ground state wave function

$$|\psi_0\rangle = \frac{1}{(2\pi a_0^2)^{1/4}} e^{-q^2/(4a_0^2)}, \quad a_0 = \sqrt{\frac{\hbar}{2m\omega}}. \quad (\text{III.57})$$

Then the Wigner function

$$W(q, p) = \int d\xi \frac{1}{\sqrt{2\pi a_0^2}} \exp\left[-\frac{(q + \xi/2)^2}{4a_0^2} - \frac{(q - \xi/2)^2}{4a_0^2}\right] e^{ip\xi/\hbar} = 2 \exp\left[-\frac{q^2}{2a_0^2} - \frac{p^2}{2p_0^2}\right], \quad p_0 = \frac{\hbar}{2a_0}. \quad (\text{III.58})$$

Thus the Wigner function is positive Gaussian function for the Harmonic oscillators in the ground state. It is easy to realize that this is true for any harmonic system in the ground state since the latter can be always represented as a product of the ground state for each normal mode. This simple Gaussian structure persists to finite temperature states. In particular for a thermal density matrix

$$\hat{\rho} = \frac{1}{Z} \sum_n e^{-\beta\hbar\omega(n+1/2)} |n\rangle\langle n| \quad (\text{III.59})$$

the Wigner function reads:

$$W(q, p) = 2 \tanh(\hbar\omega/2T) \exp \left[ -\frac{q^2}{2a_0^2 \coth(\hbar\omega/2T)} - \frac{p^2}{2p_0^2 \coth(\hbar\omega/2T)} \right] \quad (\text{III.60})$$

This result clearly reduces to Eq. (III.58) in the zero temperature limit. In the high temperature regime  $\hbar\omega \ll T$  we can approximate  $\coth(\hbar\omega/2T)$  by  $2T/\hbar\omega$  and thus

$$W(q, p) \approx \frac{\hbar\omega}{T} \exp \left[ -\frac{p^2/2m + m\omega^2 q^2/2}{T} \right], \quad (\text{III.61})$$

which is exactly the classical Boltzmann's distribution of the Harmonic oscillator up to the factor of  $\hbar$ , which is due to the integration measure  $dqdp/(2\pi\hbar)$ .

#### D. Coherent state representation.

All results in the momentum representation immediately translate to the coherent state representation. Since the proofs are almost identical we will simply list the main results and show several examples.

First let us define the Weyl symbol of an arbitrary operator written in the second quantized form  $\hat{\Omega}(\hat{a}, \hat{a}^\dagger)$ . As earlier we suppress the single-particle state index in the operators  $\hat{a}$  and  $\hat{a}^\dagger$  to simplify notations.

$$\Omega_W(a, a^*) = \int \int d\eta^* d\eta \left\langle a - \frac{\eta}{2} \left| \hat{\Omega}(\hat{a}, \hat{a}^\dagger) \right| a + \frac{\eta}{2} \right\rangle e^{\frac{1}{2}(\eta^* a - \eta a^*)}. \quad (\text{III.62})$$

Here  $|\alpha\rangle$  denote coherent states. As in the coordinate momentum representation the Weyl symbol of a symmetrically ordered operator can be obtained by simple substitution  $\hat{a} \rightarrow a$  and  $\hat{a}^\dagger \rightarrow a^*$ .

For normally ordered operators, where all  $\hat{a}^\dagger$  terms appear on the left of  $\hat{a}$  terms, Eq. (III.62) implies

$$\Omega_W(a, a^*) = \int \int d\eta d\eta^* \Omega(a^* - \eta^*/2, a + \eta/2) e^{-|\eta|^2/2}. \quad (\text{III.63})$$

As in the coordinate representation Weyl quantization is naturally associated with the coherent state Bopp representation

$$\hat{a}^\dagger = a^* - \frac{1}{2} \frac{\partial}{\partial a} = a^* + \frac{1}{2} \overleftarrow{\frac{\partial}{\partial a}}, \quad (\text{III.64})$$

$$\hat{a} = a + \frac{1}{2} \frac{\partial}{\partial a^*} = a - \frac{1}{2} \overleftarrow{\frac{\partial}{\partial a^*}}. \quad (\text{III.65})$$

The complex derivatives here are understood in the standard way through the derivatives with respect to real and imaginary parts of  $a$ :

$$\frac{\partial}{\partial a} = \frac{1}{2} \frac{\partial}{\partial \Re a} - \frac{i}{2} \frac{\partial}{\partial \Im a}, \quad \frac{\partial}{\partial a^*} = \frac{1}{2} \frac{\partial}{\partial \Re a} + \frac{i}{2} \frac{\partial}{\partial \Im a}. \quad (\text{III.66})$$

The choice of the representation with the conventional (right) derivatives and the one with left derivatives is arbitrary. However, as we discuss below, for time dependent problems it is dictated by causality. This representation of creation and annihilation operators is clearly symmetric and preserves the correct commutation relations. It also automatically reproduces the Weyl symbol of any operator. Let us illustrate this representation with a couple of simple examples. First consider the number operator  $\hat{n} = \hat{a}^\dagger \hat{a}$  and its normal ordered square:  $:n^2 := a^\dagger a^\dagger a a$ . First we evaluate the Weyl symbol using Eq. (III.73):

$$\begin{aligned} n_W &= \int d\eta d\eta^* (a^* - \eta^*/2)(a + \eta/2) \exp[-|\eta|^2/2] = a^* a - \frac{1}{2}, \\ (:n^2:)_W &= \int d\eta d\eta^* (a^* - \eta^*/2)^2 (a + \eta/2)^2 \exp[-|\eta|^2/2] = |a|^4 - 2|a|^2 + \frac{1}{2}. \end{aligned} \quad (\text{III.67})$$

Next we do the same calculation using the Bopp representation

$$\begin{aligned} n_w &= \left( a^* - \frac{1}{2} \partial_a \right) a = a^* a - \frac{1}{2}, \\ (:n^2:)_W &= \left( a^* - \frac{1}{2} \partial_a \right)^2 a^2 = |a|^4 - a^* \partial_a a^2 + \frac{1}{4} \partial_a^2 a^2 = |a|^4 - 2|a|^2 + \frac{1}{2}. \end{aligned} \quad (\text{III.68})$$

For simple polynomial operators Bopp representation gives the simplest way to evaluate the Weyl symbols of the operators.

Again by a close analogy to the coordinate-momentum representation it is straightforward to show that the Weyl symbol of the product of two operators is given by the Moyal product (cf. Eq. (III.45)):

$$(\hat{\Omega}_1 \hat{\Omega}_2)_W = \Omega_{1,W} \exp \left[ \frac{\Lambda_c}{2} \right] \Omega_{2,W}, \quad (\text{III.69})$$

where the symplectic coherent state operator  $\Lambda_c$  is defined in Eq. (III.14). From this result we immediately derive that the Weyl symbol of the commutator of the two operators is

$$[\hat{\Omega}_1, \hat{\Omega}_2] = 2\Omega_{1,W} \sinh \left[ \frac{\Lambda_c}{2} \right] \Omega_{2,W}, \quad (\text{III.70})$$

which can be termed as the coherent state Moyal bracket.

Let us check that in this way we can reproduce the Weyl symbol of the operators considered before

$$\begin{aligned}(\hat{a}^\dagger \hat{a})_W &= a^* \exp[\Lambda_c/2] a = a^* a + \frac{1}{2} a^* \Lambda_c a + 0 = a^* a - \frac{1}{2}, \\(\hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a})_W &= (a^*)^2 [1 + \Lambda_c/2 + \Lambda_c^2/8 + 0] a^2 = |a|^4 - 2|a|^2 + \frac{1}{2},\end{aligned}\tag{III.71}$$

which are identical to Eq. (III.68).

The Wigner function is again defined as the Weyl symbol of the density matrix:

$$W(a, a^*) = \int \int d\eta^* d\eta \left\langle a - \frac{\eta}{2} \left| \hat{\rho} \right| a + \frac{\eta}{2} \right\rangle e^{\frac{1}{2}(\eta^* a - \eta a^*)}.\tag{III.72}$$

The expectation value of any operator is given by averaging the corresponding Weyl symbol weighted with the Wigner function:

$$\langle \hat{\Omega}(\hat{a}, \hat{a}^\dagger) \rangle = \int \int da da^* W(a, a^*) \Omega_W a, a^*.\tag{III.73}$$

So the Wigner function again plays the role of the quasi-probability distribution of the complex amplitudes.

Let us consider few simple examples of Wigner functions. We start from the vacuum state:  $\hat{\rho} = |0\rangle\langle 0|$ . Note that the overlap of the ground state and the coherent state is

$$\langle 0|a\rangle = \exp[-|a|^2/2].\tag{III.74}$$

Thus

$$W_0(a^*, a) = \int \int d\eta^* d\eta \exp[-|a|^2 - |\eta|^2/4] e^{\frac{1}{2}(\eta^* a - \eta a^*)} = 2 \exp[-2|a|^2]\tag{III.75}$$

Similarly the Wigner function of any coherent state is a shifted Gaussian. If  $\hat{\rho} = |\alpha\rangle\langle \alpha|$  then

$$W_\alpha(a^*, a) = 2 \exp[-2|a - \alpha|^2]\tag{III.76}$$

The proof of this result is essentially the same using that:

$$\langle \alpha|a\rangle = \exp[-|a|^2/2 - |\alpha|^2/2 + \alpha^* a].\tag{III.77}$$

Another important example is the Wigner function of the Fock state

$$|N\rangle = \frac{(a^\dagger)^N}{\sqrt{N!}} |0\rangle\tag{III.78}$$

The overlap of the Fock state and coherent state is obviously

$$\langle N|a\rangle = \frac{a^N \exp[-|a|^2/2]}{\sqrt{N!}} \quad (\text{III.79})$$

Therefore

$$\begin{aligned} W_N(a^*, a) &= \frac{1}{N!} \int \int d\eta d\eta^* \left(a^* - \frac{\eta^*}{2}\right)^N \left(a + \frac{\eta}{2}\right)^N e^{-|a|^2 - |\eta|^2/4} e^{\frac{1}{2}(\eta^* a - \eta a^*)} \\ &= \frac{4}{N!} \int \int d\tilde{\eta} d\tilde{\eta}^* (2a^* - \tilde{\eta}^*)^N (2a + \tilde{\eta})^N e^{-2|a|^2 - |\tilde{\eta}|^2} = 4e^{-2|a|^2} \sum_{m=0}^N (-1)^{N-m} |2a|^{2m} \frac{N!}{(m!)^2 ((N-m)!)^2} \\ &\int \int d\tilde{\eta} d\tilde{\eta}^* |\tilde{\eta}|^{2(N-m)} e^{-|\tilde{\eta}|^2} = 4(-1)^N e^{-2|a|^2} \sum_{m=0}^N (-1)^m |2a|^{2m} \frac{N!}{(m!)^2 (N-m)!} = 2e^{-2|a|^2} L_N(4|a|^2), \end{aligned} \quad (\text{III.80})$$

where  $L_N(x)$  is the Laguerre polynomial:

$$L_N(x) = (-1)^N \sum_{m=0}^N (-1)^m \frac{N!}{(m!)^2 (N-m)!} x^m.$$

Unlike previous examples involving coherent states, the Wigner function for the Fock state is very non-local, especially at large  $N$ . It highly oscillates at  $|a|^2 < N$  and then rapidly decays at  $|a|^2 > N$ . Due to these oscillations it is e.g. very hard to use this Wigner function for Monte-Carlo sampling so one can try to find approximate Wigner functions which correctly reproduce the lowest moments of the true distribution. The simplest example of an approximate Wigner function would be a Gaussian  $Wg(n)$ , where  $n = a^*a$ :

$$Wg(n) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(n-n_0)^2}{2\sigma^2}}. \quad (\text{III.81})$$

Because we will be interested in large  $N$  we can extend the range of  $n$  to the full real axis. Unphysical negative values of  $n$  will occur with vanishingly small probability. We will require that this function correctly reproduces the first two moments of the number operator:

$$N = \langle \hat{n} \rangle = \int_{-\infty}^{\infty} dn n_w Wg(n) = \bar{n} - \frac{1}{2} = n_0 - \frac{1}{2} \quad (\text{III.82})$$

and

$$N^2 = \langle \hat{n}^2 \rangle = \langle : \hat{n}^2 : + \hat{n} \rangle = \overline{n^2 - 2n + 1/2 + n - 1/2} = n_0^2 + \sigma^2 - n_0, \quad (\text{III.83})$$

where the over-line implies averaging with respect to the approximate Wigner function  $Wg(n)$ .

The first equation implies  $n_0 = N + 1/2$  and the second gives

$$N^2 = N^2 + N + \frac{1}{4} - N - \frac{1}{2} + \sigma^2 \Rightarrow \sigma = \frac{1}{2}. \quad (\text{III.84})$$

Thus the best Gaussian approximation to the Wigner function for the Fock state is

$$Wg(n) = \frac{2}{\sqrt{2\pi}} e^{-2(n-N-\frac{1}{2})^2}. \quad (\text{III.85})$$

### E. Coordinate-momentum versus coherent state representations.

To summarize the discussion above we will contrast the two phase-space pictures in Table I. This

TABLE I Coherent state versus coordinate momentum phase space

Representation	coordinate-momentum	coherent
Phase space variables	$\mathbf{q}, \mathbf{p}$	$\mathbf{a}, \mathbf{a}^*$
Quantum operators	$\hat{\mathbf{q}}, \hat{\mathbf{p}}$	$\hat{\mathbf{a}}, \hat{\mathbf{a}}^\dagger$
Standard representation	$\hat{\mathbf{q}} \rightarrow \mathbf{q}, \hat{\mathbf{p}} \rightarrow -i\hbar\partial_{\mathbf{q}}$ (coordinate basis)	$\hat{\mathbf{a}} \rightarrow \mathbf{a}, \hat{\mathbf{a}}^\dagger \rightarrow -\partial_{\mathbf{a}}$ (coherent state basis)
Canonical commutation relations	$[\hat{q}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha,\beta}$ ( $\alpha, \beta$ refer to different particles)	$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$ ( $i, j$ refer to single-particle states)
Quantum-classical correspondence	$\hat{\mathbf{q}} \rightarrow \mathbf{q}, \hat{\mathbf{p}} \rightarrow \mathbf{p}, [\hat{A}, \hat{B}] \rightarrow -i\hbar\{A, B\}$ $\{A, B\} = \sum_\alpha \frac{\partial A}{\partial p_\alpha} \frac{\partial B}{\partial q_\alpha} - \frac{\partial A}{\partial q_\alpha} \frac{\partial B}{\partial p_\alpha}$	$\hat{\mathbf{a}} \rightarrow \mathbf{a}, \hat{\mathbf{a}}^\dagger \rightarrow \mathbf{a}^*, [\hat{A}, \hat{B}] \rightarrow \{A, B\}_c$ $\{A, B\}_c = \sum_j \frac{\partial A}{\partial a_j} \frac{\partial B}{\partial a_j^*} - \frac{\partial A}{\partial a_j^*} \frac{\partial B}{\partial a_j}$
Wigner function	$W(\mathbf{q}, \mathbf{p}) = \int d\xi \left\langle \mathbf{q} - \frac{\xi}{2} \left  \hat{\rho} \right  \mathbf{q} + \frac{\xi}{2} \right\rangle e^{i\mathbf{p}\xi/\hbar}$	$W(\mathbf{a}, \mathbf{a}^*) = \int \int d\eta^* d\eta \left\langle \mathbf{a} - \frac{\eta}{2} \left  \hat{\rho} \right  \mathbf{a} + \frac{\eta}{2} \right\rangle \times e^{\frac{1}{2}(\eta^* \mathbf{a} - \eta \mathbf{a}^*)}$
Weyl symbol	$\Omega_W(\mathbf{q}, \mathbf{p}) = \int d\xi \left\langle \mathbf{q} - \frac{\xi}{2} \left  \hat{\Omega} \right  \mathbf{q} + \frac{\xi}{2} \right\rangle e^{i\mathbf{p}\xi/\hbar}$	$\Omega_W(\mathbf{a}, \mathbf{a}^*) = \int \int d\eta^* d\eta \left\langle \mathbf{a} - \frac{\eta}{2} \left  \hat{\Omega} \right  \mathbf{a} + \frac{\eta}{2} \right\rangle \times e^{\frac{1}{2}(\eta^* \mathbf{a} - \eta \mathbf{a}^*)}$
Moyal product	$(\Omega_1 \Omega_2)_W = \Omega_{1,W} \exp \left[ -\frac{i\hbar}{2} \Lambda \right] \Omega_{2,W},$ $\Lambda = \sum_\alpha \frac{\overleftarrow{\partial}}{\partial p_\alpha} \frac{\overrightarrow{\partial}}{\partial q_\alpha} - \frac{\overleftarrow{\partial}}{\partial q_\alpha} \frac{\overrightarrow{\partial}}{\partial p_\alpha}$	$(\Omega_1 \Omega_2)_W = \Omega_{1,W} \exp \left[ \frac{\Lambda_c}{2} \right] \Omega_{2,W},$ $\Lambda_c = \sum_j \frac{\overleftarrow{\partial}}{\partial a_j} \frac{\overrightarrow{\partial}}{\partial a_j^*} - \frac{\overleftarrow{\partial}}{\partial a_j^*} \frac{\overrightarrow{\partial}}{\partial a_j}$
Moyal bracket	$\{\Omega_1, \Omega_2\}_{MB} = \frac{2}{\hbar} \Omega_1 \sin \left[ \frac{\hbar}{2} \Lambda \right] \Omega_2$	$\{\Omega_1, \Omega_2\}_{MBC} = 2\Omega_1 \sinh \left[ \frac{1}{2} \Lambda_c \right] \Omega_2$
Bopp operators	$\hat{\mathbf{q}} = \mathbf{q} + \frac{i\hbar}{2} \frac{\partial}{\partial \mathbf{p}} = \mathbf{q} - \frac{i\hbar}{2} \frac{\overleftarrow{\partial}}{\partial \mathbf{p}},$ $\hat{\mathbf{p}} = \mathbf{p} - \frac{i\hbar}{2} \frac{\partial}{\partial \mathbf{q}} = \mathbf{p} + \frac{i\hbar}{2} \frac{\overleftarrow{\partial}}{\partial \mathbf{q}}$	$\hat{\mathbf{a}}^\dagger = \mathbf{a}^* - \frac{1}{2} \frac{\partial}{\partial \mathbf{a}} = \mathbf{a}^* + \frac{1}{2} \frac{\overleftarrow{\partial}}{\partial \mathbf{a}},$ $\hat{\mathbf{a}} = \mathbf{a} + \frac{1}{2} \frac{\partial}{\partial \mathbf{a}^*}, = \mathbf{a} - \frac{1}{2} \frac{\overleftarrow{\partial}}{\partial \mathbf{a}^*}$

table highlights close analogy between particle and wave pictures. While the two representations are formally equivalent one can build different approximation schemes using these representations as starting points, e.g. expanding around different classical limits one representing classical particles evolving according to the Newton's laws and another classical waves evolving according to Gross-Pitaevskii (or Ginzburg-Landau) equations.

## F. Spin systems.

The machinery developed above allows one to extend the Weyl quantization to spin systems. The spin operators satisfy the canonical commutation relations:

$$[\hat{s}_a, \hat{s}_b] = i\epsilon_{abc}\hat{s}_c, \quad (\text{III.86})$$

where  $\epsilon_{abc}$  is the fully antisymmetric tensor. The classical limit corresponds to the spin quantum number  $S \gg 1$  so we expect that quantum-classical correspondence will be exact in the large  $S$ -limit. Formally spin systems can be mapped to boson systems using the Schwinger representation:

$$\hat{s}_z = \frac{\hat{\alpha}^\dagger \hat{\alpha} - \hat{\beta}^\dagger \hat{\beta}}{2}, \quad \hat{s}_+ = \hat{\alpha}^\dagger \hat{\beta}, \quad \hat{s}_- = \hat{\beta}^\dagger \hat{\alpha}. \quad (\text{III.87})$$

This representation allows us to apply results from the previous section directly to the spin systems without need to introduce spin-coherent states. The bosonic fields  $\alpha$  and  $\beta$  in Eq. (III.87) should satisfy an additional constraint  $\hat{n} = \hat{\alpha}^\dagger \hat{\alpha} + \hat{\beta}^\dagger \hat{\beta} = 2S$ . Note that any spin-spin interactions commute with this constraint for each spin, therefore if the constraint is satisfied by the initial state, spin dynamics is equivalent to the dynamics of bosons.

Using Eqs. (III.64) and (III.65) we can find an analogue of the Bopp operators for the spin systems:

$$\hat{s}_z = \frac{\alpha^* \alpha - \beta^* \beta}{2} - \frac{1}{8} \left( \frac{\partial^2}{\partial \alpha^* \partial \alpha} - \frac{\partial^2}{\partial \beta^* \partial \beta} \right) - \frac{1}{4} \left( \alpha^* \frac{\partial}{\partial \alpha^*} - \alpha \frac{\partial}{\partial \alpha} - \beta^* \frac{\partial}{\partial \beta^*} + \beta \frac{\partial}{\partial \beta} \right), \quad (\text{III.88})$$

$$\hat{s}_+ = \alpha^* \beta + \frac{1}{2} \left( \alpha^* \frac{\partial}{\partial \beta^*} - \beta \frac{\partial}{\partial \alpha} \right) - \frac{1}{4} \frac{\partial^2}{\partial \alpha \partial \beta^*}, \quad (\text{III.89})$$

$$\hat{s}_- = \alpha \beta^* + \frac{1}{2} \left( \alpha \frac{\partial}{\partial \beta} - \beta^* \frac{\partial}{\partial \alpha^*} \right) - \frac{1}{4} \frac{\partial^2}{\partial \alpha^* \partial \beta}. \quad (\text{III.90})$$

These equations can be also written using compact notations:

$$\hat{\mathbf{s}} = \mathbf{s} - \frac{i}{2} [\mathbf{s} \times \vec{\nabla}] - \frac{1}{8} \left[ \vec{\nabla} + (\mathbf{s} \cdot \vec{\nabla}) \vec{\nabla} - \frac{1}{2} \mathbf{s} \nabla^2 \right], \quad (\text{III.91})$$

or equivalently

$$\hat{s}_z = s_z - \frac{i}{2} \left( s_x \frac{\partial}{\partial s_y} - s_y \frac{\partial}{\partial s_x} \right) - \frac{1}{8} \frac{\partial}{\partial s_z} - \frac{s_z}{16} \left( \frac{\partial^2}{\partial s_z^2} - \frac{\partial^2}{\partial s_x^2} - \frac{\partial^2}{\partial s_y^2} \right) - \frac{s_x}{8} \frac{\partial^2}{\partial s_x \partial s_z} - \frac{s_y}{8} \frac{\partial^2}{\partial s_y \partial s_z}. \quad (\text{III.92})$$

and similarly for other components. Here  $\vec{\nabla} = \partial/\partial \mathbf{s}$  and

$$s_z = \frac{\alpha^* \alpha - \beta^* \beta}{2}, \quad s_x = \frac{\alpha^* \beta + \beta^* \alpha}{2}, \quad s_y = \frac{\alpha^* \beta - \beta^* \alpha}{2i} \quad (\text{III.93})$$

are the Schwinger representation of the classical spins. One can check that these momentum variables satisfy standard angular momentum relations:

$$\{s_\alpha, s_\beta\} = \epsilon_{\alpha,\beta,\gamma} s_\gamma. \quad (\text{III.94})$$

These expressions can be used in constructing Weyl symbols for various spin operators. Let us give a few specific examples:

$$(\hat{s}_z)_W = s_z, (\hat{s}_z^2)_W = s_z^2 - \frac{1}{8}, (\hat{s}_z \hat{s}_x)_W = s_z s_x + \frac{i}{2} s_y. \quad (\text{III.95})$$

In principle, the mapping (III.87) is sufficient to express the Wigner function of any initial state in terms of the bosonic fields  $\alpha$  and  $\beta$ . General expressions can be quite cumbersome, however, one can use a simple trick to find a Wigner transform of any pure single spin state and generalize it to any given density matrix. Assume that a spin is pointing along the  $z$ -axis. This can always be achieved by a proper choice of a coordinate system. Then in terms of bosons  $\hat{\alpha}$  and  $\hat{\beta}$  the initial state is just  $|2S, 0\rangle$ . In other words the wave function is a product of two Fock states one having  $2S$  particles and one 0 particles. The corresponding Wigner function is then (see Eq. (III.80):

$$W(\alpha, \alpha^*, \beta, \beta^*) = 4e^{-2|\alpha|^2 - 2|\beta|^2} L_{2S}(4|\alpha|^2). \quad (\text{III.96})$$

At large  $S$  the Laguerre polynomial is a rapidly oscillating function and very inconvenient to deal with. So instead of the exact expression to a very good accuracy (up to  $1/S^2$ ) we can use a Gaussian approximation (cf. Eq. (III.85) one can use

$$W(\alpha, \beta) \approx 2\sqrt{2}e^{-2|\beta|^2} e^{-2(|\alpha|^2 - 2S - 1/2)^2}. \quad (\text{III.97})$$

Then the best Gaussian approximation for the Wigner function reads

$$W(s_z, \vec{s}_\perp) \approx \frac{2}{\pi\sqrt{\pi}S} e^{-s_\perp^2/S} e^{-4(s_z - S)^2}. \quad (\text{III.98})$$

The Wigner function is properly normalized using the integration measure  $ds_x ds_y ds_z = 2\pi s_\perp ds_\perp ds_z$ . This Wigner function has a transparent interpretation. If the quantum spin points along the  $z$  direction, because of the uncertainty principle, the transverse spin components still fluctuate due to zero-point motion so that

$$\langle s_x^2 \rangle = \langle s_y^2 \rangle = \frac{S}{2}. \quad (\text{III.99})$$

This is indeed the correct quantum-mechanical result. It also correctly reproduces the second moment of  $s_z$ :

$$\langle s_z^2 \rangle = \overline{s_z^2} - 1/8 = S^2 + \frac{1}{8} - \frac{1}{8} = S^2, \quad (\text{III.100})$$

where we used Eq. (III.95) for the Weyl symbol for  $s_z^2$ . Clearly from Eq. (III.96) one can derive the Wigner function for a spin with an arbitrary orientation by the appropriate rotation of the coordinate axes.

## 1. Exercises

1. Write down an explicit expression for the Weyl symbol of a general operator (III.31) as an integral in the momentum space.
2. Complete the proof of Eq. (III.36).
3. Consider a fully symmetrized polynomial of  $\hat{p}$  and  $\hat{q}$  of degree  $n$ , which can be represented either as

$$\hat{\Omega}_n(\hat{p}, \hat{q}) = \hat{p}\Omega_{n-1}(\hat{p}, \hat{q}) + \hat{\Omega}_{n-1}(\hat{p}, \hat{q})\hat{p}$$

or as

$$\hat{\Omega}_n(\hat{p}, \hat{q}) = \hat{q}\Omega_{n-1}(\hat{p}, \hat{q}) + \hat{\Omega}_{n-1}(\hat{p}, \hat{q})\hat{q},$$

where  $\hat{\Omega}_{n-1}(\hat{p}, \hat{q})$  is the symmetrized polynomial of degree  $n-1$ . Prove that the Weyl symbol of the fully symmetrized polynomial is simply obtained by substituting  $\hat{p} \rightarrow p$  and  $\hat{q} \rightarrow q$ . For example

$$(\hat{p}\hat{q} + \hat{q}\hat{p})_W = 2pq, \quad (\hat{p}^2\hat{q} + 2\hat{p}\hat{q}\hat{p} + \hat{q}\hat{p}^2)_W = 4p^2q. \quad (\text{III.101})$$

4. Considering polynomial functions or otherwise prove the equivalence of two Bopp representations (III.38) and (III.43).
5. Prove the relation (III.48) starting from  $m = 0$  and arbitrary  $n$  and then generalizing the proof to arbitrary  $m$ .
6. Prove Eq. (III.60). Hint. One possibility is to expand both the Wigner function and the final result in powers of  $\exp[-\beta\hbar\omega]$ . Another possibility is to use coherent state representation of the Wigner function discussed below, where all calculations are much simpler since they do not require using Hermite polynomials.
7. Using definition of the Weyl symbol (III.62) prove that  $(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger)_W = 2aa^*$ .
8. Prove the result (III.75) by completing the square.
9. Complete calculations to prove Eq. (III.80). Visualize this distribution for various  $N$ .

10. Prove that for finite temperature density matrix of the non-interacting system  $H = \hbar\omega a^\dagger a$  the Wigner function is a Gaussian:

$$W_T(a^*, a) = 2 \coth\left(\frac{\hbar\omega}{2T}\right) \exp\left[-2|a|^2 \tanh\left(\frac{\hbar\omega}{2T}\right)\right]. \quad (\text{III.102})$$

11. Verify Eqs. (III.95).

### G. Quantum dynamics in phase space. Truncated Wigner approximation (Liouvillian dynamics)

Next we move to time-dependent systems. In this section we will focus on coherent state phase space since it found more applications to interacting systems. All results immediately translate to the coordinate-momentum picture using Table I. We will explicitly quote only final expressions where necessary. Time evolution of the density matrix for an arbitrary Hamiltonian system is given by the von Neumann equation:

$$i\hbar\dot{\rho} = [\hat{\mathcal{H}}, \rho]. \quad (\text{III.103})$$

Taking the Weyl transform of both sides of the equation and using Eq. (III.70) for the coherent state Moyal bracket we find:

$$i\hbar\dot{W} = 2H_W \sin\left[\frac{1}{2}\Lambda_c\right] W. \quad (\text{III.104})$$

This equation in the coordinate-momentum representation reads

$$\dot{W} = \frac{2}{\hbar} W \sin\left(\frac{\hbar}{2}\Lambda\right) H_W \quad (\text{III.105})$$

If we expand the Moyal bracket in the powers of the symplectic operator  $\Lambda_c$  (or  $\Lambda$ ) and stop at the leading order then the Moyal bracket reduces to the Poisson bracket and the von Neumann's equation (III.105) reduces to the classical Liouville equations (III.20) with the Wigner function replacing the classical probability distribution. It is interesting that in the coordinate-momentum picture the classical limit is formally recovered as  $\hbar \rightarrow 0$  as expected. In the coherent state picture the classical limit is found when the occupation number of relevant modes becomes large  $N = a^*a \rightarrow \infty$ . The Planck's constant merely sets the time units and can be completely rescaled. Of course the mode occupation number in e.g. harmonic equilibrium systems is given by the ratio  $T$  and  $\hbar\omega$  and diverges as  $\hbar \rightarrow 0$  so there is no inconsistency.

This leading order approximation where the Wigner function satisfies the classical Liouville equations is known in literature as the truncated Wigner approximation (TWA). Formally it is

obtained by truncating the expansion of the von Neumann's equation

$$i\dot{W} = 2H_W \sin \left[ \frac{1}{2} \Lambda_c \right] W = H_W \Lambda_c W + \frac{1}{4} H_W \Lambda_c^3 W + \dots \approx H_W \Lambda_c W \quad (\text{III.106})$$

at the leading order in  $1/N$  ( $\hbar$ ). Let us make a few comments about TWA. First we observe that it is exact for non-interacting systems which involve particles in a harmonic potential, non-interacting particles in arbitrary time-dependent potential, arbitrary non-interacting spin systems in time-dependent magnetic fields and others. This observation immediately follows from noticing that for such systems all terms involving third and higher order derivatives of the Hamiltonian identically vanish. Second we observe that the Liouville equation can be solved by characteristics, i.e. the probability distribution is conserved along the classical trajectories. Thus classical trajectories have the same interpretation within TWA: they conserve the Wigner function. This implies that within TWA the expectation value of an arbitrary observable can be written as

$$\langle \hat{O}(t) \rangle = \int da da^* W_0(a_0, a_0^*) O_W(a(t), a^*(t), t), \quad (\text{III.107})$$

where  $W_0(a_0, a_0^*)$  is the initial Wigner function and  $a(t)$  and  $a^*(t)$  are solutions of the classical Gross-Pitaevski (Newton's in the corpuscular case) equations satisfying the initial conditions  $a(t) = a_0$ ,  $a^*(t) = a_0^*$ . Finally let us point that TWA is asymptotically exact at short times. We will present the formal proof in the next section when we discuss the structure of quantum corrections. But heuristically this statement relies on noting that formally  $\hbar$ , divided by an energy scale, sets the time unit and thus the classical limit  $\hbar \rightarrow 0$  is equivalent to looking into very short times.

In many-particle systems one rarely considers interactions higher than two body, i.e. involving more than four creation and annihilation operators. This means that the expansion of the Moyal bracket always stops at the third order and the exact evolution equation for the Wigner function is

$$i\dot{W} = \sum_j \frac{\partial H_W}{\partial a_j} \frac{\partial W}{\partial a_j^*} - \frac{\partial H_W}{\partial a_j^*} \frac{\partial W}{\partial a_j} + \frac{1}{8} \sum_{i,j,k} \frac{\partial^3 \mathcal{H}_W}{\partial a_i \partial a_j^* \partial a_k^*} \frac{\partial^3 W}{\partial a_i^* \partial a_j \partial a_k} - \frac{\partial^3 \mathcal{H}_W}{\partial a_i^* \partial a_j \partial a_k} \frac{\partial^3 W}{\partial a_i \partial a_j^* \partial a_k^*}, \quad (\text{III.108})$$

where for completeness we inserted all single-particle indices. This third order Fokker-Planck equation is relatively simple looking. However, there are no available methods to solve it for complex systems. In particular, it can not be solved by the methods of characteristics, i.e. there is no well defined notion of trajectories. In the next section we will show how one can solve this equation perturbatively using the notion of quantum jumps.

Quantum jumps also appear in the context of finding non-equal time correlation functions. Intuitively such jumps are expected from basic uncertainty principle. E.g. measuring the position

of a particle at time  $t$  necessarily induces uncertainty in its momentum and affects the outcome of the second measurement at a later time. It turns out that the Bopp representation is most suitable to analyze the non-equal time correlation function. We simply understand derivatives appearing in Eqs. (III.38), (III.43), (III.64), (III.65) as a response to an infinitesimal jumps in phase space variable, which can be calculated either instantaneously for equal time-correlation functions or at a later time for non-equal time correlation functions. E.g. for  $t_1 < t_2$

$$\langle \hat{a}^\dagger(t_1)\hat{a}(t_2) \rangle = \int \int da_0 da_0^* W(a_0, a_0^*) \left( a^*(t_1)a(t_2) - \frac{1}{2} \frac{\partial a(t_2)}{\partial a(t_1)} \right) \quad (\text{III.109})$$

The last term is understood as a linear response of the function  $a(t_2)$  to infinitesimal jump in  $a$  at the moment  $t_1$ :  $a(t_1) \rightarrow a(t_1) + \delta a$ . This representation is valid even if  $t_1 > t_2$  but then it becomes not casual because the response of  $a(t_2)$  is evaluated to the jump, which will occur in the future. Here it is much more convenient to restore causality by using the left Bopp representation (III.43). Then e.g. again assuming that  $t_1 < t_2$

$$\langle \hat{a}(t_2)a^\dagger(t_1) \rangle = \int \int da_0 da_0^* W(a_0, a_0^*) \left( a(t_2)a^*(t_1) + \frac{1}{2} \frac{\partial a(t_2)}{\partial a(t_1)} \right) \quad (\text{III.110})$$

In the classical limit the two expressions clearly coincide but in general the two responses are different. In particular, the non-equal time commutator, which is up to a factor is the retarder Green's function appearing in standard Kubo linear response theory, is given purely by the response to the jump:

$$\langle [\hat{a}^\dagger(t_1), \hat{a}(t_2)] \rangle = - \int \int da_0 da_0^* W(a_0, a_0^*) \frac{\partial a(t_2)}{\partial a(t_1)} \quad (\text{III.111})$$

Clearly as  $t_2 \rightarrow t_1 + 0$  we recover standard bosonic commutation relations. Conversely the symmetric correlation function, which appears e.g. in dissipative response of the systems, does not contain quantum jumps:

$$\langle [\hat{a}^\dagger(t_1), \hat{a}(t_2)]_+ \rangle = 2 \int \int da_0 da_0^* W(a_0, a_0^*) a^*(t_1)a(t_2). \quad (\text{III.112})$$

While this representation of the non-equal time correlation functions is completely general, it is most useful within TWA, where response at a later time can be easily computed as a difference between two classical trajectories: the original one and the one infinitesimally shifted at time  $t_1$ .

TWA is a very powerful tool for analyzing quantum dynamics in the semiclassical limit, where quantum fluctuations are responsible for initial seed triggering the dynamics but the consequent evolution is nearly classical. There are many applications to quantum optics, physics of ultracold gases, simulation of kinetics of chemical reactions, evolution of early universe and others. In

these notes we will only consider simple applications to simple systems. Further more complicated examples can be found e.g. in Refs. (P. B. Blakie, A. S. Bradley, M. J. Davis, R. J. Ballagh, and C. W. Gardiner, 2008, *Advances in Physics* 57, 363, A. Polkovnikov, Phase space representation of quantum dynamics, *Annals of Phys.* 325, 1790 (2010)).

### 1. Single particle in a harmonic potential.

As a first illustration of the phase space methods for studying quantum dynamics let us consider a particle moving in a harmonic potential. Here all the calculations can be done analytically without any approximations. The Hamiltonian of a single harmonic oscillator is

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2 = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2), \quad (\text{III.113})$$

where the coordinate and momentum operators  $\hat{q}$  and  $\hat{p}$  are related to creation and annihilation operators  $\hat{a}$  and  $\hat{a}^\dagger$  in a standard way:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left( \hat{q} + \frac{i}{m\omega}\hat{p} \right), \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left( \hat{q} - \frac{i}{m\omega}\hat{p} \right). \quad (\text{III.114})$$

Now suppose that the particle is prepared in the ground state and we are suddenly applying a linear potential  $V(q) = -\lambda q$ . So that the Hamiltonian becomes

$$\hat{H} = \hat{H}_0 - \lambda\hat{q} \quad (\text{III.115})$$

Next we compute various observables as a function of time.

*Coordinate-momentum representation.* First we will solve this problem using the coordinate-momentum representation. The corresponding Wigner function is a Gaussian computed earlier (III.58). Next we need to solve the classical equations of motion:

$$\frac{dp}{dt} = -m\omega^2 q + \lambda, \quad \frac{dq}{dt} = \frac{p}{m} \quad (\text{III.116})$$

satisfying the initial conditions  $q(0) = q_0$ ,  $p(0) = p_0$ . Clearly the solution is

$$q(t) = q_{\text{cl}}(t) + q_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t), \quad (\text{III.117})$$

where  $q_{\text{cl}}(t) = \lambda/m\omega^2(1 - \cos(\omega t))$  is the classical trajectory describing the motion of the particle, which is initially set to rest. Then we need to substitute this solution to the observable corresponding to the quantum operator of interest and find the average over the initial conditions.

For the expectation value of the position we trivially find  $\langle \hat{q}(t) \rangle = q_{cl}(t)$ , which is just a particular case of the Ehrenfest's principle. Similarly we find

$$\langle \hat{q}^2 \rangle = \overline{q^2(t)} = q_{cl}^2(t) + a_0^2. \quad (\text{III.118})$$

This is of course also the correct result, which can be easily obtained from the solution of the Schrödinger equation.

Next let us show how to compute a non-equal time correlation function. In particular,  $\langle \hat{q}(t)\hat{q}(t') \rangle$  with  $t < t'$ . For this we will use the time-dependent Bopp representation (III.38)

$$\hat{q}(t) = q(t) + \frac{i\hbar}{2} \frac{\partial}{\partial p(t)} \quad (\text{III.119})$$

and interpret this derivative as a response to the infinitesimal jump in momentum at time  $t$ . Then

$$\begin{aligned} \langle \hat{q}(t)\hat{q}(t') \rangle &= \overline{\left( q_{cl}(t) + q_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) + \frac{i\hbar}{2} \frac{\partial}{\partial \delta p} \right)} \\ &\quad \times \overline{\left( q_{cl}(t') + q_0 \cos(\omega t') + \frac{p_0}{m\omega} \sin(\omega t') + \frac{\delta p}{m\omega} \sin(\omega(t' - t)) \right)} \\ &= q_{cl}(t)q_{cl}(t') + a_0^2 \cos(\omega(t - t')) + ia_0^2 \sin(\omega(t' - t)). \end{aligned} \quad (\text{III.120})$$

Note that this correlation function is complex because it does not correspond to the expectation value of a Hermitian operator. Similarly for the correlation function with the opposite ordering of  $t$  and  $t'$  we find

$$\langle \hat{q}(t')\hat{q}(t) \rangle = q_{cl}(t)q_{cl}(t') + a_0^2 \cos(\omega(t - t')) - ia_0^2 \sin(\omega(t' - t)) \quad (\text{III.121})$$

Therefore the symmetric part of the correlation function is simply given by

$$\left\langle \frac{\hat{q}(t')\hat{q}(t) + \hat{q}(t)\hat{q}(t')}{2} \right\rangle = q_{cl}(t)q_{cl}(t') + a_0^2 \cos(\omega(t - t')) \quad (\text{III.122})$$

and the expectation value for the commutator is

$$\langle \hat{q}(t)\hat{q}(t') - \hat{q}(t')\hat{q}(t) \rangle = 2ia_0^2 \sin(\omega(t' - t)). \quad (\text{III.123})$$

This commutator vanishes at  $t \rightarrow t'$  and rapidly oscillates if  $\omega(t' - t) \gg 1$ .

*Coherent state representation.* For illustration purposes we repeat this calculation in the coherent state representation. In the second quantized form the Hamiltonian of the system reads

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2) - \lambda a_0(\hat{a} + \hat{a}^\dagger). \quad (\text{III.124})$$

The classical (Gross-Pitaevski) equation for the oscillator reads:

$$i\hbar \frac{\partial \alpha}{\partial t} = \hbar\omega\alpha - \lambda a_0. \quad (\text{III.125})$$

We use  $\alpha(t)$  and  $\alpha^*(t)$  to denote phase space variables to avoid confusion with the notation  $a_0$  for the oscillator length. This equation has the following solution

$$\alpha(t) = \frac{\lambda a_0}{\hbar\omega} (1 - e^{-i\omega t}) + \alpha_0 e^{-i\omega t}. \quad (\text{III.126})$$

Using the explicit form of the Wigner function of the vacuum state (III.75) we immediately find

$$\langle \hat{q}^2(t) \rangle = a_0^2 \overline{(\alpha(t) + \alpha^*(t))} = \frac{2a_0^2\lambda}{\hbar\omega} (1 - \cos(\omega t)) = q_{\text{cl}}(t). \quad (\text{III.127})$$

Similarly

$$\langle \hat{q}^2(t) \rangle = a_0^2 \overline{(\alpha^2(t) + (\alpha^*(t))^2 + 2\alpha(t)\alpha^*(t))} = q_{\text{cl}}^2(t) + a_0^2. \quad (\text{III.128})$$

We obviously got the same answers as before. Similarly one can verify the result for the non-equal time correlation function. Of course it is not surprising that both methods give identical exact results for harmonic systems. However, it is important to realize that once we deal with more complicated interacting models the correct choice of the phase space can significantly simplify the problem. Moreover the expansions around the two possible classical limits are very different. Thus for a system of noninteracting particles moving in some external potential TWA in the coordinate-momentum representation is only approximate unless the potential is harmonic. At the same time TWA in the coherent state representation is exact.

## 2. Collapse (and revival) of a coherent state

Next consider a slightly more complicated case of an initial single-mode coherent state evolving according to the quartic interacting Hamiltonian

$$\hat{H} = \frac{U}{2} \hat{a}^\dagger \hat{a} (\hat{a}^\dagger \hat{a} - 1). \quad (\text{III.129})$$

Clearly the eigenstates of this Hamiltonian are the Fock states  $|n\rangle$  with eigen energies

$$\epsilon_n = \frac{U}{2} n(n-1).$$

This problem is closely related to the collapse-revival experiment by M. Greiner et. al. (M. Greiner, O. Mandel, T. W. Haensch, and I. Bloch, *Nature* **419**, 51, 2002). Because the problem does

not have kinetic term it can be easily solved analytically. In particular, the expectation value of the annihilation operator can be found by expanding the coherent state in the Fock basis and propagating it in time

$$|\psi(t)\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle e^{-i\epsilon_n t}. \quad (\text{III.130})$$

Then we find

$$\begin{aligned} \langle \psi(t) | \hat{a} | \psi(t) \rangle &= e^{-|\alpha|^2} \sum_{n,m} \frac{(\alpha^*)^n (\alpha^m)}{\sqrt{n!m!}} e^{i(\epsilon_n - \epsilon_m)t} \langle n | a | m \rangle = e^{-|\alpha|^2} \sum_n \frac{(\alpha^*)^n \alpha^{n+1}}{\sqrt{n!(n+1)!}} \sqrt{n+1} e^{i(\epsilon_n - \epsilon_{n+1})t} \\ &= \alpha e^{-|\alpha|^2} \sum_n \frac{|\alpha|^2^n}{n!} e^{-iUn} = \alpha \exp [|\alpha|^2 (e^{-iUt} - 1)]. \end{aligned} \quad (\text{III.131})$$

Qualitatively at larger  $N = |\alpha|^2$  this solution gives first rapid decay of the coherence, where  $\langle \hat{a}(t) \rangle$  decays to an exponentially small number at a characteristic time  $\tau = UN$  and then at a much later time  $t_0 = 2\pi/U$  there is a complete revival of the state. The classical limit here corresponds to  $N \rightarrow \infty$ ,  $U \rightarrow 0$  and  $UN = \lambda$  fixed. Clearly in the classical limit there is still collapse of the state by no revival since  $t_0 \sim 2\pi N/\lambda \rightarrow \infty$ .

Next we solve the problem using TWA. For doing this we first compute the Weyl symbol of the Hamiltonian (III.129):

$$H_W(a^*, a) = \frac{U}{2} |a|^2 (|a|^2 - 2) + \frac{U}{4}. \quad (\text{III.132})$$

Note that there is an extra  $-1$  in the first term Hamiltonian as compared to the naive substitution  $\hat{a} \rightarrow a$  due to the Weyl ordering. Using this Hamiltonian we find classical Gross-Pitaveski equations of motion for the complex amplitudes:

$$i \frac{\partial a(t)}{\partial t} = U(|a|^2 - 1)a(t). \quad (\text{III.133})$$

This equation can be trivially solved using that  $|a(t)|^2 = |a_0|^2$  is the integral of motion:

$$a(t) = a_0 e^{-iU(|a_0|^2 - 1)t} \quad (\text{III.134})$$

The solution should be supplemented by random initial conditions distributed according to the Wigner function:

$$W(a_0, a_0^*) = 2 \exp[-2|a_0 - \alpha|^2]. \quad (\text{III.135})$$

Using the explicit analytic solution of Eq. (III.133) and the Wigner function above we can calculate the expectation value of the coherence  $\langle \hat{a}(t) \rangle$  within TWA by Gaussian integration

$$a(t) \approx \alpha \exp \left[ -\frac{iU|\alpha|^2 t}{1 + iUt/2} \right] \exp[iUt] \frac{1}{(1 + iUt/2)^2}, \quad (\text{III.136})$$

This expression is more complicated than the simple exact quantum results. Let us discuss its qualitative features. First of all we can see that at a characteristic time  $\tau = 1/(UN)$  there is a collapse of the coherence as in the quantum case. One can check that for times much shorter than the revival time the TWA solution very closely matches the exact solution. However the TWA result completely misses revivals, which are thus intrinsically quantum related to discreteness of the Fock basis.

This example highlights important potential issue with TWA: it can miss long time behavior. One can imagine that if there is some small dephasing in the system e.g. due to decoherence such that revivals are destroyed then TWA solution will be accurate at all times.

Let us make a remark concerning Weyl ordering in simulations of bosonic systems using TWA. Most commonly one deals with two-body density-density interactions so typical Hamiltonian is

$$H(\hat{a}_j, \hat{a}_j^\dagger) = \sum_{ij} \left[ V_{ij} \hat{a}_i^\dagger \hat{a}_j + U_{ij} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_i \right]. \quad (\text{III.137})$$

where  $V_{ij}$  includes both kinetic part and the single particle potential and  $i$  and  $j$  can be either discrete or continuous indexes. Using the Bopp representation we find that the Weyl symbol for the Hamiltonian is

$$H_W(a_j^*, a_j) = \sum_{ij} [V_{ij} \alpha_i^* \alpha_j + U_{ij} |\alpha_i|^2 |\alpha_j|^2] - \frac{1}{2} \sum_i V_{ii} - \sum_{ij} |\alpha_i|^2 U_{ij} - \sum_i |\alpha_i|^2 U_{ii} + \frac{1}{2} \sum_i U_{ii} \quad (\text{III.138})$$

The constant terms are clearly non-important since they only give an energy shift. The only two important terms, which distinguish between Weyl symbol and naive classical Hamiltonian are

$$- \sum_{ij} |\alpha_i|^2 (U_{ij} + \delta_{ij} U_{ii}).$$

In general these terms can be very important for accurate description of dynamics using TWA. But in the most common case of translationally invariant interactions  $U_{ij} = U_{|i-j|}$  it is clear that this contribution is simply proportional to the number of particles and thus has no effect on dynamics in isolated systems since the latter is conserved. If we are dealing with e.g. two different species of bosons like a two-component system then this correction can become very important.

### 3. Spin dynamics in a linearly changing magnetic field: multi-level Landau-Zener problem.

As a final simple illustrative example we consider another situation where TWA is exact. In particular, we will analyze dynamics of an arbitrary spin  $S$  in a linearly changing magnetic field:

$$\hat{H} = 2h_z(t) \hat{s}^z + 2g \hat{s}^x, \quad (\text{III.139})$$

where  $h_z(t) = \delta t$ . We assume that the system is initially prepared in some way at  $t = -t_0$  and will be interested in finding expectation values of various observables at  $t = t_0$ , where  $t_0$  is large so that  $h_z(t_0) \gg g$ .

As we discussed in Sec. III.F one can map the time evolution of noninteracting spins to the evolution of noninteracting bosons using the Schwinger representation. Therefore TWA is exact in this case. Using Eqs. (III.87) the Hamiltonian (III.139) becomes:

$$\hat{H} = h_z(t)(\hat{\alpha}^\dagger \hat{\alpha} - \hat{\beta}^\dagger \hat{\beta}) + g(\hat{\alpha}^\dagger \hat{\beta} + \hat{\beta}^\dagger \hat{\alpha}). \quad (\text{III.140})$$

The Weyl symbol of this Hamiltonian is obtained by simply replacing quantum operators  $\hat{\alpha}, \hat{\beta}, \hat{\alpha}^\dagger, \hat{\beta}^\dagger$  by complex amplitudes  $\alpha, \beta, \alpha^*, \beta^*$ . Then the corresponding equations of motion are

$$i \frac{d\alpha}{dt} = \delta t \alpha + g \beta, \quad (\text{III.141})$$

$$i \frac{d\beta}{dt} = g \alpha - \delta t \beta. \quad (\text{III.142})$$

These equations should be supplemented by the initial conditions distributed according to the Wigner transform of the initial density matrix.

Note that Eqs. (III.141) and (III.142) map exactly to the equations describing the conventional Landau-Zener problem. Then the evolution can be described by a unitary  $2 \times 2$  matrix:

$$\alpha_\infty = T\alpha_0 + Re^{i\phi}\beta_0, \quad \beta_\infty = -Re^{-i\phi}\alpha_0 + T\beta_0, \quad (\text{III.143})$$

where (see e.g. J. Keeling and V. Gurarie, Phys. Rev. Lett. **101**, 033001 (2008))

$$T = e^{-\pi\gamma}, \quad R = \sqrt{1 - T^2}, \quad \phi = \gamma [\ln(\gamma) - 1] - 2\gamma \ln(\sqrt{2\delta T}), \quad (\text{III.144})$$

and  $\gamma = g^2/(2\delta)$  is the Landau-Zener parameter.

Using this result we can re-express different spin components at  $t \rightarrow \infty$  through the initial values:

$$\begin{aligned} s_\infty^z &= (T^2 - R^2) \frac{\alpha_0^* \alpha_0 - \beta_0^* \beta_0}{2} + \alpha_0^* \beta_0 R T e^{i\phi} + \alpha_0 \beta_0^* R T e^{-i\phi} \\ &= (T^2 - R^2) s_0^z + 2RT \cos(\phi) s_0^x - 2RT \sin(\phi) s_0^y, \\ s_\infty^x &= -2RT \cos(\phi) s_0^z + (T^2 - R^2 \cos(2\phi)) s_0^x + R^2 \sin(2\phi) s_0^y, \\ s_\infty^y &= 2RT \sin(\phi) s_0^z + R^2 \sin(2\phi) s_0^x + (T^2 + R^2 \cos(2\phi)) s_0^y. \end{aligned} \quad (\text{III.145})$$

Now using these expressions and the Weyl symbols of spin operators and their bilinears derived in Sec. III.F we can compute expectation values of various operators. This can be done for any

initial state but for concreteness we choose initial stationary state polarized along the  $z$ -direction. In the language of Schwinger bosons this is a Fock state  $|S - n, n\rangle$ , where a particular value of  $n$  corresponds to the initial polarization  $s_0^z = S - n$ .

$$\begin{aligned}\langle \hat{s}_\infty^z \rangle &= (T^2 - R^2)s_0^z \\ \langle (\hat{s}_\infty^z)^2 \rangle &= [T^4 + R^4 - 4T^2R^2] (s_0^z)^2 + 2T^2R^2s(s+1), \\ \langle \hat{s}_\infty^z \hat{s}_\infty^x + \hat{s}_\infty^z \hat{s}_\infty^x \rangle &= 2RT(T^2 - R^2) \cos(\phi) [s(s+1) - 3\langle (\hat{s}_0^z)^2 \rangle].\end{aligned}\quad (\text{III.146})$$

Note that for the conventional Landau-Zener problem corresponding to the spin  $s = 1/2$  the last two equations become trivial:  $\langle (\hat{s}_\infty^z)^2 \rangle = 1$  and  $\langle \hat{s}_\infty^z \hat{s}_\infty^x + \hat{s}_\infty^z \hat{s}_\infty^x \rangle = 0$ . But for larger values of spin these correlation functions are nontrivial with e.g.  $\langle \hat{s}_\infty^z \hat{s}_\infty^x + \hat{s}_\infty^z \hat{s}_\infty^x \rangle$  being an oscillating function of the rate  $\delta$  and the Landau-Zener parameter  $\gamma$ .

#### 4. Exercises

1. For the example 2: collapse and revivale of the coherent state, using Mathematica or other software, plot the dependence  $\langle \hat{a}(t) \rangle$  both using the exact result and TWA approximation. Choose  $N$  of the order of 10 and fix  $U$  at one (this can be always done by choosing appropriate time units). Check that TWA very accurately reproduces collapse already for  $N \sim 4, 5$ . Check that if you use naive classical Hamiltonian as opposed to the Weyl symbol  $H = \frac{U}{2}|a|^2(|a|^2 - 1)$  the agreement even at short times will be much worse.

#### H. Path integral derivation.

In the final section of these notes we will see how all the concepts introduced earlier: Wigner function, Weyl symbol, Bopp operators etc. naturally emerge from the Feynmann's path integral representation of the evolution operator. Using this approach it is also possible to understand structure of the quantum corrections beyond TWA and understand potential extension of this formalism to other setups: open systems, quantum tunneling problems (as possible non-classical saddle points). The derivation itself is very similar to the formalism used in the Keldysh approach to dynamics of quantum systems (see e.g. A. Kamenev and A. Levchenko, *Advances in Physics* **58**, 197 (2009)). The main difference is that we will be focusing on expansion of dynamics in the effective Planck's constant, while in the Keldysh technique the expansion parameter is usually the interaction strength. So the two approaches are rather complimentary to each other despite many

similarities. As in the previous section we will concentrate on the coherent state representation and only quote final results in the coordinate-momentum space.

Our starting point will be expectation value of some operator  $\hat{\Omega}(\hat{a}, \hat{a}^\dagger, t)$ . We assume that this operator is written in the normal ordered form. To shorten notations we will skip the single-particle indices in the bosonic fields and reinsert them only when needed.

$$\Omega(t) \equiv \langle \hat{\Omega}(\hat{a}, \hat{a}^\dagger, t) \rangle = \text{Tr} \left[ \rho T_\tau e^{i \int_0^t \hat{H}(\tau) d\tau} \hat{\Omega}(\hat{a}, \hat{a}^\dagger, t) e^{-i \int_0^t \hat{H}(\tau) d\tau} \right], \quad (\text{III.147})$$

Because in the coherent state picture the Planck's constant plays the mere role of conversion between time and energy units we set  $\hbar = 1$  throughout this section to simplify notations. Here time ordering symbol  $T_\tau$  implies that in both exponents later times appear closer to the middle, i.e. closer to the  $\hat{\Omega}$ . Next we split the exponent of the time ordered integral over time into a product:

$$T_\tau e^{i \int_0^t \hat{H}(\tau) d\tau} = \prod_{j=1}^M e^{i \Delta\tau \hat{H}(\tau_j)} \approx \prod_{j=1}^M (1 + i \Delta\tau \hat{H}(\tau_j)), \quad T_\tau e^{-i \int_0^t \hat{H}(\tau) d\tau} = \prod_{j=M}^1 e^{-i \Delta\tau \hat{H}(\tau_j)},$$

where  $\tau_j = j \Delta\tau$  is the discretized time (we assume that initial time is zero),  $\Delta\tau = t/M$  and  $M$  is a large number. We will eventually take the limit  $M \rightarrow \infty$ . Next we insert the resolution of identity

$$I = \int d\alpha_j d\alpha_j^* |\alpha_j\rangle \langle \alpha_j|$$

between each of the terms in the product. Because we have two exponents on the left and on the right of the operator  $\hat{\Omega}$  we need to distinguish two different  $\alpha$  fields. The one, which corresponds to the positive exponent we term forward field  $\alpha_{fK}$  and the one which corresponds to the negative exponent backward field  $\alpha_{b,j}$ . This notation is conventional in Keldysh technique and comes from the ordering in the Schwinger-Keldysh contour. Loosely speaking as we move from left to right we first increase time from 0 to  $t$  and then decrease it backward to zero. Then we find

$$\Omega(t) = \int \dots \int D\alpha_f D\alpha_f^* D\alpha_b D\alpha_b^* \langle \alpha_{b0} | \hat{\rho} | \alpha_{f0} \rangle e^{-\alpha_{f0}^* \alpha_{f0}/2 + \alpha_{f0}^* \alpha_{f1} + iH(\alpha_{f0}, \alpha_{f1}) \Delta\tau} \dots e^{-\alpha_{fM}^* \alpha_{fM}} \Omega(\alpha_{fM}^*, \alpha_{bM}, t) e^{\alpha_{fM}^* \alpha_{bM}} e^{-\alpha_{bM}^* \alpha_{bM} + \alpha_{bM}^* \alpha_{bM-1} - iH(\alpha_{bM}, \alpha_{bM-1}) \Delta\tau} \dots e^{-\alpha_{b0}^* \alpha_{b0}/2}. \quad (\text{III.148})$$

Next let us change the variables:

$$\alpha_j = \frac{\alpha_{fj} + \alpha_{bj}}{2}, \quad \eta_j = \alpha_{fj} - \alpha_{bj}, \quad \Leftrightarrow \quad \alpha_{fj} = \alpha_j + \frac{\eta_j}{2}, \quad \alpha_{bj} = \alpha_j - \frac{\eta_j}{2}.$$

As we will see below this choice of variables automatically leads to the Weyl quantization. Other choices e.g.  $\alpha_b = \alpha$ ,  $\alpha_f = \alpha + \eta$  will naturally lead to other representations. Physically the symmetric field  $\alpha$  corresponds to the classical field and  $\eta$  is a quantum field. It is intuitively clear

that in the classical limit there is a unique classical trajectory satisfying fixed initial conditions and thus the forward and backward fields should be essentially the same. Performing this change of variables and taking the continuum  $M \rightarrow \infty$  limit we find

$$\begin{aligned} \Omega(t) = & \int D\eta D\eta^* D\alpha D\alpha^* \left\langle \alpha_0 - \frac{\eta_0}{2} \middle| \hat{\rho} \middle| \alpha_0 + \frac{\eta_0}{2} \right\rangle \Omega \left[ \alpha^*(t) + \frac{\eta^*(t)}{2}, \alpha(t) - \frac{\eta(t)}{2} \right] e^{-\frac{1}{2}|\eta(t)|^2} e^{\frac{1}{2}(\eta_0^* \alpha_0 - \eta_0 \alpha_0^*)} \\ & \exp \left\{ \int_0^t d\tau \left[ \eta^*(\tau) \frac{\partial \alpha(\tau)}{\partial \tau} - \eta(\tau) \frac{\partial \alpha^*(\tau)}{\partial \tau} \right. \right. \\ & \left. \left. + iH_W \left( \alpha(\tau) + \frac{\eta(\tau)}{2}, \alpha^*(\tau) + \frac{\eta^*(\tau)}{2}, \tau \right) - iH_W \left( \alpha(\tau) - \frac{\eta(\tau)}{2}, \alpha^*(\tau) - \frac{\eta^*(\tau)}{2}, \tau \right) \right] \right\}, \quad (\text{III.149}) \end{aligned}$$

One can recognize that the integrals over boundary quantum fields  $\eta_0$  and  $\eta_t$  automatically give the Wigner function and the Weyl symbol of the operator  $\hat{\Omega}$  so that the expression above becomes

$$\begin{aligned} \Omega(t) = & \int D\eta D\eta^* D\alpha D\alpha^* W(\alpha_0, \alpha_0^*) \exp \left\{ \int_0^t d\tau \left[ \eta^*(\tau) \frac{\partial \alpha(\tau)}{\partial \tau} - \eta(\tau) \frac{\partial \alpha^*(\tau)}{\partial \tau} \right. \right. \\ & \left. \left. + iH_W \left( \alpha(\tau) + \frac{\eta(\tau)}{2}, \alpha^*(\tau) + \frac{\eta^*(\tau)}{2}, \tau \right) - iH_W \left( \alpha(\tau) - \frac{\eta(\tau)}{2}, \alpha^*(\tau) - \frac{\eta^*(\tau)}{2}, \tau \right) \right] \right\} \Omega_W(\alpha(t), \alpha^*(t), t), \quad (\text{III.150}) \end{aligned}$$

Before deriving TWA from this expression let us give a few comments on details of the derivation of Eq. (III.149), which is quite subtle.

First we analyze all the terms appearing in the path integral, which do not involve Hamiltonian:

$$\begin{aligned} S_1 = & \alpha_{f0}^* \alpha_{f0} / 2 + \alpha_{b0}^* \alpha_{b0} / 2 + \sum_{i=1}^{M-1} [\alpha_{fi}^* (\alpha_{fi+1} - \alpha_{fi}) - \alpha_{bi}^* (\alpha_{bi} - \alpha_{bi-1})] \\ & + \alpha_{f0}^* (\alpha_{f1} - \alpha_{f0}) - \alpha_{bM}^* (\alpha_{bM} - \alpha_{bM-1}) - \alpha_{b0}^* \alpha_{b0} + \alpha_{fM}^* (\alpha_{bM} - \alpha_{fM}). \quad (\text{III.151}) \end{aligned}$$

The first sum in the continuum limit becomes an integral:

$$\sum_{i=1}^{M-1} \alpha_{fi}^* (\alpha_{fi+1} - \alpha_{fi}) - \alpha_{bi}^* (\alpha_{bi} - \alpha_{bi-1}) \rightarrow \int_0^t d\tau \left( \alpha_f^*(\tau) \frac{\partial \alpha_f(\tau)}{\partial \tau} - \alpha_b^*(\tau) \frac{\partial \alpha_b(\tau)}{\partial \tau} \right), \quad (\text{III.152})$$

which under the substitutions  $\alpha_f \rightarrow \alpha + \eta/2$ ,  $\alpha_b \rightarrow \alpha - \eta/2$  and after integrating by parts becomes:

$$\int_0^t d\tau \left( \eta^*(\tau) \frac{\partial \alpha(\tau)}{\partial \tau} - \eta(\tau) \frac{\partial \alpha^*(\tau)}{\partial \tau} \right) + \alpha^*(t) \eta(t) - \alpha_0^* \eta_0. \quad (\text{III.153})$$

In the continuum limit the first and the second terms after the sum in (III.151) clearly go to zero and the last two read:

$$\alpha_{fM}^* (\alpha_{bM} - \alpha_{fM}) - \alpha_{b0}^* \alpha_{b0} = -|\alpha_0|^2 - |\eta_0|^2 / 4 + \frac{1}{2} (\alpha_0^* \eta_0 + \eta_0^* \alpha_0) - \alpha^*(t) \eta(t) - |\eta(t)|^2 / 2. \quad (\text{III.154})$$

Combining Eqs. (III.151) - (III.154) we derive:

$$S_1 = \int_0^t d\tau \left( \eta^*(\tau) \frac{\partial \psi(\tau)}{\partial \tau} - \eta(\tau) \frac{\partial \psi^*(\tau)}{\partial \tau} \right) - \frac{|\eta(t)|^2}{2} + \frac{1}{2}(\eta_0^* \alpha_0 - \alpha_0^* \eta_0). \quad (\text{III.155})$$

This immediately leads to the correct Hamiltonian independent part in Eq. (III.149). The part involving the Hamiltonian in that equation is very straightforward, essentially this is just the difference of Hamiltonians evaluated on forward and backward trajectory. A more subtle result is the emergence of the Weyl ordering. Formally it appears because the fields  $\alpha$  and  $\alpha^*$  appear at slightly different times. As we will see below quantum field  $\eta$  plays the role of the derivative with respect to the classical field  $\alpha$ . Thus the normal ordered Hamiltonian is actually evaluated at Bopp operators giving the Weyl symbol  $H_W$ .

In the leading order in quantum fluctuations we expand the integrand in Eq. (III.163) up to the linear terms in  $\eta$ . Then the functional integral over  $\eta(t)$  enforces the  $\delta$ -function Gross-Pitaevskii constraint on the classical field  $\alpha(t)$ :

$$i\partial_t \alpha = \frac{\partial H_W(\alpha(t), \alpha^*(t), t)}{\partial \alpha^*(t)} \equiv \{\alpha(t), H_W(\alpha(t), \alpha^*(t), t)\}_c \quad (\text{III.156})$$

and we recover TWA (III.107).

Next let us move to discussion of non-equal time correlation functions. The simplest one will be

$$\langle \hat{a}^\dagger(t_1) \hat{a}(t_2) \rangle. \quad (\text{III.157})$$

First we assume  $t_1 < t_2$ . We proceed in the same way as in the equal-time case by writing this expression in the path integral form inserting forward and backward coherent states. The only new ingredient is an extra term we encounter on the forward path

$$a_f^*(t) = a^*(t) + \frac{\eta^*(t)}{2} \quad (\text{III.158})$$

Note that in the path integral  $\eta^*$  couples to  $d\alpha = \alpha(t + \Delta t) - \alpha(t)$ . This implies that

$$\frac{\eta^*(t_1)}{2} = -\frac{i}{2} \frac{\partial}{\partial \delta \alpha} e^{i[\alpha(t_1 + \Delta t) + \delta \alpha - \alpha(t_1)] \eta^*} = -\frac{i}{2} \frac{\partial}{\partial \delta \alpha} e^{i[\alpha(t_1 + \Delta t) + \delta \alpha - \alpha(t_1)] \eta^*},$$

where we understand the partial derivative as infinitesimal response to the jump in  $\alpha$  at the moment  $t_1$ . Thus we recover that in order to measure the non-equal time correlation functions we simply need to make the substitution

$$\hat{a}^\dagger(t) = \alpha^*(t) - \frac{i\hbar}{2} \frac{\partial}{\partial \alpha(t)} \quad (\text{III.159})$$

In the same way we can see that

$$\hat{a}(t) = \alpha(t) + \frac{i\hbar}{2} \frac{\partial}{\partial \alpha^*(t)} \quad (\text{III.160})$$

This is nothing but the Bopp representation of the creation and annihilation operators. As we already know for equal time correlation functions they automatically generate the Weyl symbol of the observable. But for non-equal time correlation function the Bopp operators give very nice interpretation of the response which occurs at a later time. It is remarkable that like the Wigner function and the Weyl symbol the Bopp operators automatically appear in the path integral formalism.

For the opposite ordering  $t_1 > t_2$  we hit earlier time on the backward contour so the same analysis as above holds except that we change  $a_f \rightarrow a_b$ . But this results in change in sign in  $\eta$  and thus in change in sign in derivatives. So we immediately recover the left Bopp representation with the same interpretation for non-equal time correlation functions

$$\hat{a}^\dagger(t) = \alpha^*(t) + \frac{i\hbar}{2} \frac{\overleftarrow{\partial}}{\partial \alpha(t)} \quad \hat{a}(t) = \alpha(t) - \frac{i\hbar}{2} \frac{\overleftarrow{\partial}}{\partial \alpha^*(t)} \quad (\text{III.161})$$

While as we discussed earlier for equal time correlation functions both representations are equivalent and give the Weyl symbol, for non-equal time correlation functions there is an important difference. Namely the correct representation is dictated by causality so that we always evaluate the response to a jump, which occurred at an earlier time.

Interpretation of Bopp operators as a response to quantum jumps is particularly simple within TWA. Then the time evolution is essentially classical before and after the jump. Thus the response of a Weyl symbol  $\Omega_2(t_2)$  to say a jump in  $\alpha$  at moment  $t_1$  is literary a difference of  $\Omega_2$  evaluated on two trajectories with and without jump divided over this jump:

$$\frac{\partial \Omega_2(\alpha(t_2), \alpha^*(t_2), t_2)}{\partial a(t_1)} = \frac{\Omega(\alpha'(t_2), \alpha'^*(t_2), t_2) - \Omega(\alpha(t_2), \alpha^*(t_2), t_2)}{\delta \alpha},$$

where  $\alpha'(t_2)$  is the classical trajectory corresponding to an infinitesimal jump in  $\alpha(t_1)$ :  $\alpha(t_1) = \alpha(t_1) + \delta\alpha$  and  $\alpha(t_2)$  is the same trajectory without this jump. From the Bopp representation it is clear that for fully symmetric operators (equal or non-equal time) the quantum jump contributions drop and we can evaluate them by substituting operators  $\hat{a}$  by phase space variables  $\alpha$ . Conversely for commutators the only surviving contribution is the one containing at least one quantum jump.

While we focused our discussion on two-point correlation functions, derivation of the Bopp representation was completely general and extends to arbitrary number of creation and annihilation operators e.g. to three-point functions like

$$\langle \hat{a}^\dagger(t_1) \hat{a}(t_2) \hat{a}(t_3) \rangle \quad (\text{III.162})$$

Note, however, there is an important subtlety when we have three or more times involved. Namely not all correlation functions have causal representation. In particular, if  $t_2 < t_1, t_3$  there is no casual representation of the three-point function above. This implies that these functions are not physical and can not appear in any response. In functions, which have casual representation later times should always occur closer to the middle.

Another advantage in the path formulation of the evolution is that it allows us to go beyond the TWA and represent quantum corrections to dynamics as stochastic quantum jumps. We will be quite sketchy here, further details of derivation can be found in (A. Polkovnikov, Phase space representation of quantum dynamics, *Annals of Phys.* 325, 1790 (2010)). In our previous discussion leading to TWA we neglected third order terms in quantum fluctuations coming from the difference

$$iH_W \left( \alpha(\tau) + \frac{\eta(\tau)}{2}, \alpha^*(\tau) + \frac{\eta^*(\tau)}{2}, \tau \right) - iH_W \left( \alpha(\tau) - \frac{\eta(\tau)}{2}, \alpha^*(\tau) - \frac{\eta^*(\tau)}{2}, \tau \right)$$

in Eq. (III.163). To stay more focused consider the Hubbard model where (up to unimportant quadratic in  $\alpha$  and  $\alpha^*$  terms

$$H_W(\alpha, \alpha^*) = \sum_j \frac{U}{2} |\alpha_j|^4.$$

Thus the difference above becomes

$$i \sum_j \left( \eta_j^*(\tau) \frac{\partial H_w(\tau)}{\partial \alpha_j^*(\tau)} + \eta_j(\tau) \frac{\partial H_w(\tau)}{\alpha_j(\tau)} \right) + \frac{i}{4} U \sum_j |\eta_j(\tau)|^2 [\eta_j(\tau) \alpha_j^*(\tau) + \eta_j^*(\tau) \alpha_j(\tau)].$$

So the exact path integral representation of the evolution given by Eq. III.163 becomes

$$\begin{aligned} \Omega(t) = \int D\eta D\eta^* D\alpha D\alpha^* W(\alpha_0, \alpha_0^*) \exp \left\{ \int_0^t d\tau \sum_j \left[ \eta_j^*(\tau) \left( \frac{\partial \alpha_j(\tau)}{\partial \tau} + i \frac{\partial H_w(\tau)}{\partial \alpha_j^*(\tau)} \right) \right. \right. \\ \left. \left. - \eta_j(\tau) \left( \frac{\partial \alpha_j^*(\tau)}{\partial \tau} - i \frac{\partial H_w(\tau)}{\alpha_j(\tau)} \right) \right] + i \frac{U}{4} |\eta_j(\tau)|^2 (\eta_j^*(\tau) \alpha_j(\tau) + \eta_j(\tau) \alpha_j^*(\tau)) \right\} \Omega_W(\alpha_j(t), \alpha_j^*(t), t), \end{aligned} \quad (\text{III.163})$$

Before we were ignoring these cubic in  $\eta$  terms so that functional integration over the quantum field  $\eta(\tau)$  becomes trivial essentially enforcing the constraint of the classical Gross-Pitaevski equations of motion for the classical field  $\alpha$ . This was the TWA. With the cubic term we can no longer evaluate this path integral. Let us treat this cubic term perturbatively by expanding the exponent:

$$\begin{aligned} e^{i \sum_j \int_0^t d\tau \frac{U}{4} |\eta_j(\tau)|^2 [\eta_j(\tau) \alpha_j^*(\tau) + \eta_j^*(\tau) \alpha_j(\tau)]} = 1 + i \frac{U}{4} \sum_j \int_0^t d\tau \frac{U}{4} |\eta_j(\tau)|^2 [\eta_j(\tau) \alpha_j^*(\tau) + \eta_j^*(\tau) \alpha_j(\tau)] \\ - \frac{U^2}{16} \int \int_{0 < \tau_1 < \tau_2 < t} |\eta_j(\tau_1)|^2 [\eta_j(\tau_1) \alpha_j^*(\tau_1) + \eta_j^*(\tau_1) \alpha_j(\tau_1)] |\eta_j(\tau_2)|^2 [\eta_j(\tau_2) \alpha_j^*(\tau_2) + \eta_j^*(\tau_2) \alpha_j(\tau_2)] + \dots \end{aligned} \quad (\text{III.164})$$

Now let us recall that when we discussed non-equal time correlation functions we realized that

$$\eta_j^*(\tau) = -i \frac{\partial}{\partial \alpha_j(\tau)}, \quad \eta_j^*(\tau) = i \frac{\partial}{\partial \alpha_j^*(\tau)}$$

with the interpretation of derivatives as a response. Thus the expression for the expectation value including the first quantum correction reads:

$$\begin{aligned} \langle \hat{\Omega}(\hat{\alpha}, \hat{\alpha}^\dagger, t) \rangle &\approx \int \int d\alpha_0 d\alpha_0^* W_0(\alpha_0, \alpha_0^*) \\ &\left( 1 - i \frac{U}{4} \int_0^t d\tau \sum_j \left[ \alpha_j^*(\tau) \frac{\partial^3}{\partial \alpha_j(\tau) \partial \alpha_j^*(\tau) \partial \alpha_j^*(\tau)} - c.c. \right] \right) \Omega_W(\alpha(t), \alpha^*(t), t). \end{aligned} \quad (\text{III.165})$$

The interpretation of this expression is very straightforward. The first quantum correction to TWA represents a third order response of our observable to an infinitesimal jump in the classical field during the evolution  $\alpha(\tau) \rightarrow \alpha(\tau) + \delta\alpha$ ,  $\alpha^*(\tau) \rightarrow \alpha^*(\tau) + \delta\alpha^*$ . This jump can occur at any time during the evolution and at any space location and we need to sum over these jumps. Further corrections appear as multiple quantum jumps. It is clear that each quantum correction carries extra factor of  $1/N^2$  ( $\hbar^2$  in the coordinate momentum representation) thus we have a well defined expansion parameter.

It is interesting to note that this nonlinear response can be expressed through stochastic quantum jumps with non-positive probability distribution:

$$\begin{aligned} \langle \hat{\Omega}(\hat{a}, \hat{a}^\dagger, t) \rangle &\approx \int \int d\alpha_0 d\alpha_0^* W_0(a_0, a_0^*) \\ &\left[ 1 - i \frac{U}{4} \sum_n \sum_j \int d\xi_j d\xi_j^* \left( \alpha_j^*(\tau_n) F(\xi_j, \xi_j^*) - \alpha_j(\tau_n) F^*(\xi_j, \xi_j^*) \right) \right]_{\delta\alpha_j(\tau_n)=\xi_j} \frac{\Omega_W(\alpha'(t), \alpha'^*(t), t)}{\sqrt[3]{\Delta\tau}}, \end{aligned} \quad (\text{III.166})$$

Here we discretized time and introduced stochastic variable  $\xi_j$ . At time  $\tau_n$  we randomly choose  $\xi_j$  according to the (quasi)probability distribution  $F(\xi, \xi^*)$  and shift the classical fields  $\alpha_j$ : and  $\alpha_j^*$  by the amounts  $\delta\alpha_j = \xi_j \sqrt[3]{\Delta\tau}$  and  $\delta\alpha_j^* = \xi_j^* \sqrt[3]{\Delta\tau}$  (e.g.  $\alpha'_j = \alpha_j + \delta\alpha_j$ ). This procedure is very similar to the mapping of ordinary Fokker-Planck equation describing diffusion to the Langevin dynamics with two important differences: (i) In the Langevin dynamics the jumps are proportional to  $\sqrt{\Delta\tau}$  while here to  $\sqrt[3]{\Delta\tau}$ . (ii) In Langevin dynamics the function  $F$  can be chosen as a Gaussian with the second moment given by the diffusion constant. Here the (quasi)probability distribution can not be chosen as a positive function. Indeed in order for Eq. (III.166) to be equivalent to (III.165) we need to ensure that the first two moments of  $\xi_j$  and  $\xi_j^*$  vanish and the third moment gives non-vanishing contribution

$$\int \int d\xi_j d\xi_j^* \xi_j^2 \xi_j^* F(\xi_j, \xi_j^*) = 2 \quad (\text{III.167})$$

One can see this equivalence by expanding  $\Omega_W$  in terms of  $\delta\alpha$  (for simplicity we suppress spatial indexes):

$$\begin{aligned} \Omega_W(\alpha'(t), \alpha^*(t), t) &= \Omega_W(\alpha(t), \alpha^*(t), t) + \frac{\partial\Omega_W}{\partial\delta\alpha}\delta\alpha + \frac{\partial\Omega_W}{\partial\delta\alpha^*}\delta\alpha^* \\ &\quad + \frac{1}{2} \left( \frac{\partial^2\Omega_W}{\partial\delta\alpha\partial\delta\alpha}\delta\alpha^2 + \frac{\partial^2\Omega_W}{\partial\delta\alpha^*\partial\delta\alpha^*}(\delta\alpha^*)^2 + 2\frac{\partial^2\Omega_W}{\partial\delta\alpha\partial\delta\alpha^*}\delta\alpha\delta\alpha^* \right) \\ &\quad + \frac{1}{8} \left( \frac{\partial^3\Omega_W}{\partial(\delta\alpha)^3}\delta\alpha^3 + 4\frac{\partial^3\Omega_W}{\partial\delta\alpha^*(\delta\alpha)^2}\delta\alpha^*(\delta\alpha)^2 + 4\frac{\partial^3\Omega_W}{\partial(\delta\alpha^*)^2\delta\alpha}(\delta\alpha^*)^2\delta\alpha + \frac{\partial^3\Omega_W}{\partial(\delta\alpha^*)^3}(\delta\alpha^*)^3 \right) + \dots \end{aligned} \quad (\text{III.168})$$

Now if we use that  $\delta\alpha = \xi\sqrt[3]{\Delta\tau}$  and integrate over  $\xi$  we see that the first two terms in the expansion vanish because  $F$  is chosen such that  $\xi$  has vanishing first and second moments and the requirement (III.167) gives non-zero third order response, which is precisely equivalent to Eq. (III.165). All higher order derivative terms clearly vanish in the limit  $\Delta\tau \rightarrow 0$ . Let us give an example of such a function, which all the requirements:

$$F(\xi_j, \xi_j^*) = \xi_j^* (|\xi_j|^2 - 2) e^{-|\xi_j|^2}. \quad (\text{III.169})$$

Thus we get equivalent representation of the quantum corrections either in the form of the nonlinear response or in the form of stochastic quantum jumps. Note that because these jumps have non-positive probability distribution full simulation of stochastic dynamics results in a severe sign problem. However, if one is interested in leading order quantum corrections one needs to take into account only a few jumps and the sign problem is not very severe. But at the moment there are no known optimization schemes to simulate the dynamics even with few jumps.

## 1. Exercises

1. Repeat derivation of Eq. (III.149). Complete missing calculations.

### I. Ergodicity in the semiclassical limit. Berry's conjecture

The phase space formalism allows us to immediately draw conclusions about the ergodicity in quantum systems as they approach classical limit. Let us take e.g. the exact von Neumann's equation in the coherent state picture (Eq. (III.108)). For systems with two-body interactions the classical limit is formally taken by rescaling  $a_j \rightarrow \sqrt{N}a_j$ , the interaction coupling  $U \rightarrow U/N$  and taking the limit  $N \rightarrow \infty$ . Under this transformation the Weyl symbol of the Hamiltonian (III.138) has a well defined classical limit (the overall prefactor  $N$  in the classical Hamiltonian precisely plays

the role of the inverse Planck's constant). In the coordinate-momentum representation the classical limit is taken in a standard fashion by sending  $\hbar \rightarrow 0$  keeping all couplings in the Hamiltonian fixed. In this limit the truncated Wigner approximation (Liouvillian dynamics) is guaranteed to work at least for the times less than  $t^*(N)$ . Where  $t^*(N)$  diverges as  $N \rightarrow \infty$ . The reason for this statement is that the difference between the Liouvillian time evolution and the exact von Neumann's dynamics is contained in the last term in Eq. (III.108) is suppressed by a larger factor  $1/N$  ( $\hbar^2$  in the coordinate-momentum basis). So this term can play a significant role at most at long times. At the moment there are no analytic estimates of the time  $t^*(N)$  or even its scaling with  $N$  except for specific cases, where it is shown that it diverges as a power law of  $N$ . But clearly divergence of  $t^*(N)$  is required by the very existence of the classical limit.

On the other hand if the corresponding classical system is ergodic there is a finite ( $N, \hbar$ -independent) relaxation time  $\tau$  after which the system approaches the microcanonical ensemble. Thus in the regime  $\tau \ll t^*(N)$  it is essentially guaranteed that the Wigner function for any generic initial condition will approach the microcanonical distribution, which width is dictated by initial fluctuations of the total energy:

$$W(\alpha^*, \alpha, t) \rightarrow \rho_{mc}(\alpha^*, \alpha). \quad (\text{III.170})$$

The initial conditions can be fairly arbitrary with the exception of e.g. the ground state, where in the limit  $N \rightarrow \infty$  the system is completely localized in the phase space. As soon as there are some fluctuations present in the initial condition this statement should work.

The statement that the Wigner function should relax to the microcanonical distribution is very similar to the Berry's conjecture (M. Berry, 1977). This conjecture states that if we take the Wigner function of the microcanonical ensemble, which defined as an ensemble with the microcanonical width vanishing in the limit  $\hbar \rightarrow 0$  but still containing exponentially many energy levels, then we will get the usual Boltzmann's distribution. Or equivalently

$$\overline{|\psi^*(\vec{x} - \vec{\xi}/2)\langle\psi(\vec{x} + \vec{\xi}/2)|} = \frac{1}{\Sigma} \int d\vec{p} e^{-i\vec{p}\vec{\xi}/\hbar} \delta(E - H(\vec{x}, \vec{p})), \quad (\text{III.171})$$

where the over line implies the averaging over the microcanonical ensemble. This conjecture does not say anything about dynamics and approaching this ensemble, but it establishes how one can recover classical statistical mechanical limit from the quantum microcanonical ensemble. This conjecture thus does not require ergodicity of the system. Because as we know the Wigner function plays the role of the (quasi)probability distribution for any observable this conjecture immediately implies that in the classical limit  $\hbar \rightarrow 0$  one recovers classical statistical mechanics for all observables. By showing that the Wigner function of a Harmonic oscillator in the classical limit becomes

the Boltzmann's distribution and using the equivalence of statistical ensemble we basically proved this conjecture for any harmonic system, like coupled oscillators. However, there is no general proof of this conjecture for interacting systems.

#### IV. QUANTUM ERGODICITY IN MANY-PARTICLE SYSTEMS.

##### A. Eigenstate thermalization hypothesis (ETH)

As we discussed earlier in simple single-particle systems quantum ergodicity is reflected in the complex structure of the Hamiltonian. In particular, in the fact that the spectrum of the Hamiltonian is essentially described by random matrices. This should also imply that the eigenstates of the quantum chaotic systems should look like the eigenstates of a random matrix, i.e. they should essentially look like random vectors in the Hilbert space. Of course, because these eigenstates correspond to well defined energy this statement has to be refined. E.g. low energy states can not contain many high momentum plane waves. So we would rather expect that these eigenstates are random superpositions of plane waves taken from a narrow energy shell. For non-interacting particles this statement is precisely equivalent to the Berry's conjecture. This motivates us to suggest that similar situation should persist in many-particle ergodic systems, i.e. we might expect that the energy spectrum of such systems can be well represented by an appropriate random matrix ensemble and the corresponding eigenstates are random superpositions of simple states (like plane waves) taken from the energy shell. There is no proof for this statement but there is a lot of numerical evidence that this is true. Let us demonstrate this point using a particular Hamiltonian representing spin one half chain with an open boundary conditions (A. Gubin and L. Santos, Am. J. Phys. 80, 246 (2012)) described by the Hamiltonian:

$$H_{XXZ} = \frac{J_{XX}}{2} \sum_{i=1}^{L-1} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + \frac{J_{ZZ}}{2} \sum_{i=1}^{L-1} \sigma_i^z \sigma_{i+1}^z, \quad (\text{IV.1})$$

where  $\vec{\sigma}_i$  are the Pauli matrices describing spin one half degree of freedom on the site  $i$ . It is known that this so called XXZ chain is integrable, i.e. it is not ergodic, though the exact structure of eigenstates is quite complex. Following the work by A. Gubin and L. Santos let us introduce a single impurity into the chain by adding a local magnetic field in the  $z$ -direction

$$H_j = \epsilon \sigma_j^z. \quad (\text{IV.2})$$

Note that there is no summation over the sites in this term. In the case, when impurity is placed at the age  $j = 1$  or  $j = L$  this term effectively corresponds to changing boundary conditions

and does not break integrability of the system. While if the impurity is placed somewhere away from the edge of the system it makes it non-integrable, i.e. ergodic. Note that the Hamiltonian  $H = H_{XXZ} + H_j$  conserves the total magnetization along the  $z$ -direction, so the Hilbert space effectively splits into separate sectors with fixed  $S_z$ . In Fig. 12 we show the results of numerical

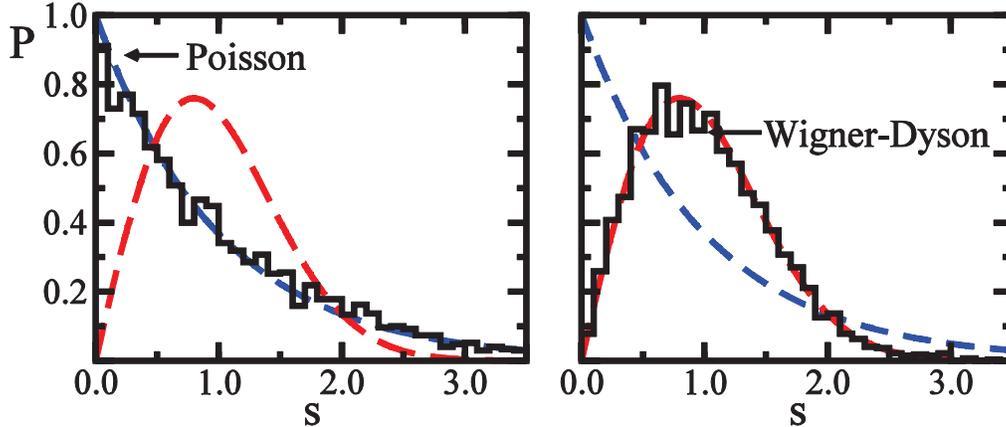


FIG. 12 Distribution of the levels spacings for the spin chain Hamiltonian  $H = H_{XXZ} + H_j$  (see text for details). The total magnetization is fixed at  $S^z = 1/2 \sum_j \sigma_j^z = 5$  and the couplings are  $J_{XX} = 1$ ,  $J_{ZZ} = 0.5$ , and  $\epsilon = 0.5$ . Left panel describes the integrable case with the impurity on site  $j = 1$  and the right panel corresponds to the non-integrable case with the impurity in the middle. Red and black lines are the Wigner-Dyson and the Poisson distributions respectively. The figure is taken from A. Gubin and L. Santos, Am. J. Phys. 80, 246 (2012)

simulations of the level spacing statistics for the two situations where the impurity is at the edge (left panel) and in the middle of the chain (right panel). The first (integrable) situation is perfectly described by the Poisson distribution in agreement with the Berry-Tabor conjecture. The second non-integrable case is conversely in the perfect agreement with the Wigner-Dyson statistics for the orthogonal ensemble. It is interesting that a single impurity seems to be sufficient to make the whole system completely chaotic.

While there is no general proof that many-body ergodic systems are always described by the random matrix ensembles there are no known counterexamples. Therefore we will use the conjecture that the eigenstates of an ergodic Hamiltonian are essentially random vectors in the Hilbert space subject to the macroscopic constraints (like fixed energy, momentum, magnetization or any other conserved quantity) as a starting point for our discussion and see how far we can go. Let us first check how this assumption works for a gas of weakly interacting particles. Namely, let us

assume that the eigenfunctions of the gas are given by random superpositions of the plane waves:

$$|\psi_n\rangle = \sum_{p_1, p_2, \dots, p_N} \alpha_{p_1, p_2, \dots, p_N} |p_1, p_2, \dots, p_N\rangle \quad (\text{IV.3})$$

where the coefficients  $\alpha_{p_1, \dots, p_N}$  are properly normalized random amplitudes (real or complex depending on whether the Hamiltonian respects time reversal symmetry):

$$\overline{|\alpha_{p_1, p_2, \dots, p_N}|^2} \sim \frac{1}{\mathcal{N}}, \quad (\text{IV.4})$$

where  $\mathcal{N}$  is the (exponentially big) Hilbert space size;  $\{p_j\}$  are the set of single-particle momenta satisfying the energy constraint:

$$\sum_j \frac{p_j^2}{2m} = E_n. \quad (\text{IV.5})$$

It is easy to check that in the limit of large number of particles this wavefunction yields the Gibbs distribution. Indeed the probability of say particle number one to have momentum  $p_1$  is

$$P(p_1) = \sum_{p_2, p_3, \dots, p_N} |\alpha_{p_1, p_2, \dots, p_N}|^2 \delta \left( \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \dots + \frac{p_N^2}{2m} - E_n \right) \quad (\text{IV.6})$$

Averaging this distribution over random amplitudes  $\alpha_{\{p_j\}}$  we find that

$$\overline{P(p_1)} = C \sum_{p_2, \dots, p_N} \delta \left( \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \dots + \frac{p_N^2}{2m} - E_n \right), \quad (\text{IV.7})$$

where  $C$  is the normalization constant and  $\delta(x)$  stands for the discrete delta-function of  $x$ . This expression is nothing as the averaging over the microcanonical ensemble. From the basic statistical ensemble we know that the microcanonical distribution in the limit  $N \gg 1$  results in the Maxwell-Boltzmann distribution of the individual particles. So we have proven that on average the random eigenstates on average correctly reproduce equilibrium density matrix.

Next let us ask the question how representative the average is. In order to do this we compute that statistical fluctuations of the momentum distribution for different random states. I.e. we compute

$$\begin{aligned} \overline{P^2(p_1)} - \left( \overline{P(p_1)} \right)^2 &= \sum_{p_2, \dots, p_N} \sum_{q_2, \dots, q_N} \overline{|\alpha_{p_1, p_2, \dots, p_N}|^2 |\alpha_{p_1, q_2, \dots, q_N}|^2} \\ &\times \delta \left( \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \dots + \frac{p_N^2}{2m} - E_n \right) \delta \left( \frac{p_1^2}{2m} + \frac{q_2^2}{2m} + \dots + \frac{q_N^2}{2m} - E_n \right) - \left( \overline{P(p_1)} \right)^2 \end{aligned} \quad (\text{IV.8})$$

Because the amplitudes are uncorrelated by the assumption of randomness the expression above reduces to the single sum

$$\overline{P^2(p_1)} - \left( \overline{P(p_1)} \right)^2 = \sum_{p_2, \dots, p_N} \left( \overline{|\alpha_{\{p_j\}}|^4} - \overline{|\alpha_{\{p_j\}}|^2}^2 \right) \delta \left( \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \dots + \frac{p_N^2}{2m} - E_n \right) \propto \frac{1}{\mathcal{N}}. \quad (\text{IV.9})$$

Here we used the assumption that the variance of each random coefficient is of the order of the mean. This will be the case e.g. if we take a random unit vector in the  $\mathcal{N}$  dimensional hyper-space and project it to orthogonal axes. From this simple example (another example is considered in *Exercises*) we see that the assumption about the random nature of eigenstates leads to the Gibbs distribution of individual degrees of freedom with exponential accuracy (note that  $\mathcal{N} \sim \exp[DN]$ , where  $D$  is roughly the available Hilbert space size per degree of freedom). The physical reason for this result is that the Hilbert space size  $\mathcal{N}$  is immensely big. Therefore for any random distribution of coefficients in this space any observable, which can be represented over the sum over these coefficients, will be essentially non-fluctuating. This property of the random states is called *typicality* and it was first noted by von Neumann in 1929.

These arguments can be generalized to arbitrary interacting systems under the statement of the Eigenstate Thermalization Hypothesis or simply ETH (J. Deutsch, 1991; M. Srednicki, 1994). This hypothesis postulated that the energy eigenstates of many-particle quantum ergodic systems are practically indistinguishable from each other within a narrow energy window and that from the point of view of physical observables each eigenstate is equivalent to the microcanonical ensemble:

$$\langle n|\mathcal{O}|n\rangle \approx \text{Tr}[\rho_{\text{micro}}\mathcal{O}], \quad (\text{IV.10})$$

where  $\rho_{\text{micro}}$  is the microcanonical density matrix centered around the energy  $E_n$ . The qualitative justification of this statement is essentially the same as in the simple example considered above: Eigenstates are complex random superpositions of many simple states like plane waves or Fock states. This hypothesis is consistent with the ideas we discussed before that ergodic quantum Hamiltonians essentially look like random matrices. As we will be discussing later the ETH is a very powerful conjecture from which many results of equilibrium and non-equilibrium thermodynamics can be obtained.

### 1. ETH and ergodicity. Fluctuation-dissipation relations from ETH.

First let us demonstrate that ETH leads to ergodicity in large systems. Let us consider the situation where an isolated system was prepared in some non-equilibrium initial state  $|\psi_0\rangle$ , e.g. by changing parameters of the Hamiltonian in time. We will assume that the system is isolated and its time evolution is described by some many-body Hamiltonian  $H$  with the eigenstates  $|n\rangle$ ,  $n = 1, 2, \dots, \mathcal{N}$  and the corresponding eigen energies  $E_n$ . Then the time evolved wave function will

be

$$|\psi(t)\rangle = \sum_n \alpha_n(t)|n\rangle = \sum_n \alpha_n(0)e^{-iE_n t}|n\rangle. \quad (\text{IV.11})$$

Now let us compute an expectation value of some observable  $\mathcal{O}$  in the long time limit:

$$\langle\psi(t)|\mathcal{O}|\psi(t)\rangle = \sum_{n,m} \alpha_n^* \alpha_m e^{i(E_n - E_m)t} \langle n|\mathcal{O}|m\rangle \xrightarrow{t \rightarrow \infty} \sum_n |\alpha_n|^2 \mathcal{O}_{nn}, \quad (\text{IV.12})$$

where  $\mathcal{O}_{nn} = \langle n|\mathcal{O}|n\rangle$  and we used that in the long time limit the oscillating terms in the sum above average to zero. More accurately we proved that

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle\psi(t)|\mathcal{O}|\psi(t)\rangle = \sum_n |\alpha_n|^2 \mathcal{O}_{nn}. \quad (\text{IV.13})$$

If the assumption of ETH work, i.e. if the matrix elements  $\mathcal{O}_{nm}$  are identical between eigenstates taken from the energy window then owing to  $\sum_n |\alpha_n|^2 = 1$  the sum above reduces to statistical average of  $\mathcal{O}$  taken from the microcanonical ensemble centered around mean energy of the system, i.e.

$$\sum_n |\alpha_n|^2 \mathcal{O}_{nn} \approx \langle\mathcal{O}\rangle_{\text{micro}} \quad (\text{IV.14})$$

Note that these considerations do not rely on the assumption of system being described by a pure state. Indeed we can think about an ensemble of pure states described by some initial density matrix

$$\rho_{mn}(t=0) = \overline{\alpha_n^*(0)\alpha_m(0)}. \quad (\text{IV.15})$$

Then clearly instead of Eq. (IV.12) we get

$$\langle\mathcal{O}(t)\rangle = \sum_{mn} \rho_{mn}(0) \mathcal{O}_{nm} e^{i(E_n - E_m)t} \xrightarrow{t \rightarrow \infty} \sum_n \rho_{nn} \mathcal{O}_{nn} \quad (\text{IV.16})$$

As long as the energy of the system is not too spread (which is always the case due to its additivity and the central limit theorem) the ETH ( $\mathcal{O}_{nn} \approx \text{const}(n)$ ) immediately implies equivalence of this long time average and the micro-canonical ensemble centered around the mean energy. Note that since probabilities to occupy energy eigenstates  $\rho_{nn}$  are time independent there is no need to specify at which time they are computed.

We see that the picture of the thermalization in the quantum language seems to be quite different than the corresponding classical picture. Time evolution in the basis of the (many-particle) eigenstates is trivial, it is just dephasing. The chaos, ergodicity and thermalization are hidden in

the nature of these eigenstates and time evolution slowly projects the initial non-equilibrium state of the system into the statistical mixture of these states. Later we will see that the same process of thermalization we can still view as a delocalization in the Hilbert space.

Let us now make an important remark distinguishing statements of typicality of random eigenstates and the ETH. Typicality arguments tell us that if we take a wave function, which is a random superposition of some basis states satisfying some macroscopic constraints like energy conservation then from the point of view of local few body observables this wave function will be identical to a microcanonical ensemble. Essentially typicality is a law of large numbers telling us that all fluctuations between different wave functions drawn from such a distribution of observables are suppressed in the size of the Hilbert space. In the top panel of Fig. 13 we illustrate a typical state

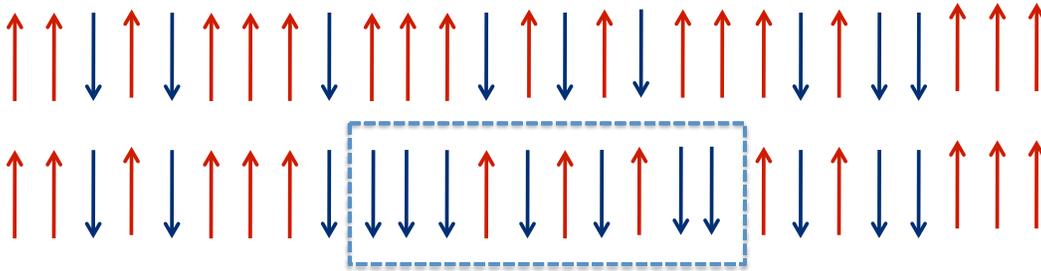


FIG. 13 Typical state of the noninteracting Ising model at fixed magnetization (top panel). The same state after the local quench where spins in the middle region are flipped by an external pulse (bottom panel).

of the Ising model with a fixed magnetization (in fact the typical state will be a random superposition of such states). For such state local magnetization will be well described by the Gibbs distribution. Note that this statement does not rely in any way on the ergodicity of the underlying Hamiltonian. Let us emphasize, however, that if we apply some external perturbation like flipping spins in a localized region of space, we will create a very atypical state, where the magnetization in the flipped region will have very different properties than the magnetization in the rest of the system. If the system is non-ergodic, e.g. it represents non-interacting spins in an external field, then this state can remain atypical for essentially infinitely long times. In other words if we project the atypical state after pulse to the eigenstates of the integrable Hamiltonian we will select very special states, which need not be thermal. On the other hand ETH states that in ergodic systems all eigenstates of the Hamiltonian are typical. Therefore projecting this non-equilibrium state to the eigenstates and dephasing restores typicality. In a way all states we create in a lab by applying various local perturbations to the system are atypical. This is precisely the reason why these states are non-equilibrium. It is the dephasing or projecting such non-equilibrium states to the

equilibrium eigenstates of the new Hamiltonian which restores typicality and leads to ergodicity.

ETH is, however, more than the simple statement about the equivalence of the diagonal matrix elements of local operators to the micro-canonical averages. ETH puts strong restrictions on off-diagonal matrix elements. Let us consider the expectation value of the variance of the local operator in some eigenstate  $|n\rangle$

$$\delta O_n^2 = \langle n|\mathcal{O}^2|n\rangle - \langle n|\mathcal{O}|n\rangle^2 = \sum_{m \neq n} |\mathcal{O}_{mn}|^2 \quad (\text{IV.17})$$

If ETH works for arbitrary local observables it should apply to their fluctuations too, which are also local observables. This means that  $\delta O_n^2$  should be equivalent to the fluctuations of  $\mathcal{O}$  computed withing the microcanonical ensemble. For the simple setup of the weakly interacting gas we saw that the whole distribution function of the momentum of each particle was given by the Maxwell-Boltzmann form. Thus indeed all the moments of the kinetic energy of finite number of particles will be identical to the statistical averages. But the sum above contains exponentially many terms, which implies that the off-diagonal elements  $|\mathcal{O}_{mn}|$ ,  $m \neq n$  are exponentially small. One possibility is that most of the off-diagonal elements are equal to zero and very few are non-zero. But this will be clearly inconsistent with the assumptions that the eigenstates are random superpositions of the simple states. So the more natural ansatz is to assume that (M. Srednicki, 1996) the all the matrix elements are exponentially small and that the following ansatz holds

$$O_{nm} = \langle n|\mathcal{O}|m\rangle = e^{-S(\bar{E})/2} f_O(\bar{E}, \omega) \sigma_{nm}, \quad (\text{IV.18})$$

where  $\bar{E} = (E_n + E_m)/2$ ,  $\omega = E_n - E_m$ ,  $S(E)$  is the equilibrium entropy of the system,  $f_O(\bar{E}, \omega)$  is some observable-dependent function, which slowly depends on the average energy  $\bar{E}$  but can change quite fast with the energy separation  $\omega$  and  $\sigma_{nm}$  is some random variable with zero mean and unit variance. Because for any Hermitean operator  $O_{nm} = O_{mn}^*$  it is clear that the function  $f(\bar{E}, \omega)$  satisfies the following relation

$$f_O(\bar{E}, \omega) = f_O^*(\bar{E}, -\omega). \quad (\text{IV.19})$$

Such an assumption about the off-diagonal matrix elements are dictated by requirements of finite fluctuations of the observable. Substituting the expression for the off-diagonal matrix elements into the expression for fluctuations (IV.17) and averaging over  $\sigma_{nm}^2$  we find that

$$\begin{aligned} \delta O_n^2 &= \int_{-\infty}^{\infty} d\omega \Omega(E_n + \omega) e^{-S(E_n + \omega/2)} |f_O(E_n + \omega/2, \omega)|^2 \\ &= \int_{-\infty}^{\infty} d\omega e^{\beta\omega/2} |f_O(E_n + \omega/2, \omega)|^2 \approx \int_{-\infty}^{\infty} d\omega e^{\beta\omega/2} |f_O(E_n, \omega)|^2 = 2 \int_0^{\infty} \cosh(\beta\omega/2) |f_O(E_n, \omega)|^2, \end{aligned} \quad (\text{IV.20})$$

where we used the assumption that the function  $f_O(E, \omega)$  slowly depends on the mean energy  $E$  and that we can expand the entropy to the linear order in  $\omega$ :  $S(E + \omega) \approx S(E) + \beta\omega$ . We see that in order for fluctuations being finite the function  $f_O$  should decay sufficiently fast with  $\omega$ . We can extend the calculation above and in similar way compute non-equal time correlation functions

$$\begin{aligned} \langle n|O(t)O(0)|n\rangle_c &\equiv \langle n|O(t)O(0)|n\rangle - \langle n|O|n\rangle^2 \\ &= \int_{-\infty}^{\infty} d\omega e^{\beta\omega/2 - i\omega t} |f_O(E + \omega/2, \omega)|^2 \approx \int_{-\infty}^{\infty} d\omega e^{-i\omega(t - i\beta/2)} |f_O(E, \omega)|^2. \end{aligned} \quad (\text{IV.21})$$

We thus see that  $|f_O(E, \omega)|^2$  is related to the spectral function:

$$|f_O(E, \omega)|^2 = e^{-\beta\omega/2} \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t} \langle n|O(t)O(0)|n\rangle_c. \quad (\text{IV.22})$$

This function, for example, appears in the Kubo response relations. Suppose that the operator  $O_\lambda$  is conjugate to some parameter  $\lambda$ , i.e.  $O_\lambda = -\partial_\lambda H$ . For example, if  $\lambda$  is the magnetic field then  $O_\lambda$  is the magnetization, if  $\lambda$  is a component of the vector potential then  $O_\lambda$  is the current and so on. Then the Kubo relation states that (see e.g. G. D. Mahan, Many-particle physics, third edition, 2000) the linear response to a time periodic modulation of  $\lambda$  at frequency  $\omega$  is described by the susceptibility  $\chi_\lambda(\omega)$ :

$$\begin{aligned} \chi_\lambda(\omega) &= i \int_0^\infty dt e^{i\omega t} \langle [O_\lambda(t), O_\lambda(0)] \rangle \\ &= 2\pi i |f_\lambda(\bar{E}, \omega)|^2 \sinh(\beta\omega/2) + \int_{-\infty}^{\infty} d\omega_1 \frac{2\omega_1}{\omega_1^2 - \omega^2} |f_\lambda(|\bar{E}, \omega_1)|^2 \sinh(\beta\omega_1/2), \end{aligned} \quad (\text{IV.23})$$

where the dashed integral stands for the principal value and we used the notation  $f_\lambda$  as a short hand for the  $f_{O_\lambda}$ . To derive the result above we used the ansatz for the off-diagonal matrix elements (IV.18) and the identity:

$$\int_0^\infty dt e^{i\nu t} = \pi\delta(\nu) + iP \frac{1}{\nu}.$$

So we see that the absolute value of function  $f$  can be expressed through the imaginary part of the susceptibility

$$|f_\lambda^2(\bar{E}, \omega)|^2 \approx \frac{\chi_\lambda''(\bar{E}, \omega)}{2\pi \sinh(\beta\omega/2)}. \quad (\text{IV.24})$$

Substituting this into the expression for the fluctuations of  $O_\lambda$  (IV.20) we find

$$\delta O_n^2 = \frac{1}{\pi} \int_0^\infty d\omega \chi_\lambda''(E, \omega) \coth \frac{\beta\omega}{2}. \quad (\text{IV.25})$$

This relation is nothing but the fluctuation-dissipation theorem, which as we see directly follows from the ETH.

We saw that the ETH following from the random matrix assumptions about the structure of the ergodic Hamiltonians essentially amount to the indistinguishability between expectation values of observables evaluated at different eigenstates with similar energies. The same assumptions lead to the relaxation of expectation values of physical observables to the appropriate microcanonical ensemble. We understood this relaxation in the sense that the time average of the expectation value of an arbitrary observable approaches the so called diagonal ensemble (Eq. (IV.16)), which in turn is equivalent to the microcanonical assumptions by the ETH. Next we want to understand how representative this average is, i.e. whether this relaxation is not just the statement about the average. In order to answer this question let us consider the average distance between the instantaneous expectation value of the observable and its time average:

$$\sigma^2 = \overline{\left(\langle \mathcal{O}(t) \rangle - \overline{\langle \mathcal{O} \rangle}\right)^2}, \quad (\text{IV.26})$$

where as before the over-line denotes the time average. By substituting the expression (IV.16) for the expectation value of  $\mathcal{O}(t)$  and its time average we find

$$\sigma^2 = \sum_{n,m,p,q} \rho_{mn}^0 \rho_{qp}^0 \mathcal{O}_{nm} \mathcal{O}_{pq} \overline{e^{i(E_n - E_m + E_p - E_q)t}} - \sum_{n,p} \rho_{nn} \mathcal{O}_{nn} \rho_{pp} \mathcal{O}_{pp} \quad (\text{IV.27})$$

Because the levels repel each other and there are no degeneracies the time average in the first term above is non-zero essentially only if either  $n = m$  and  $p = q$  or  $n = q$  and  $m = p$ . In principle, there are can be accidental degeneracies where  $E_n + E_p = E_m + E_q$  with all four indexes being different, but we will assume that they do not play a role. It is clear that the terms with  $n = m$  and  $p = q$  will be exactly canceled by the second term in the expression above so the terms, which will be left are those where  $n = q \neq m = p$  and thus

$$\sigma^2 = \sum_{n \neq p} \rho_{pn} \rho_{np} |\mathcal{O}_{np}|^2 \lesssim C e^{-S} \sum_{n \neq p} |\rho_{np}|^2 \leq C e^{-S} \text{Tr}(\rho^2) \leq C e^{-S}, \quad (\text{IV.28})$$

where we used the expression for the off-diagonal matrix elements of  $\mathcal{O}$  (IV.18) and  $C$  stand for the upper bound for the function  $|f_{\mathcal{O}}|^2$ , which is at most extensive in the system size. We thus see that if our ETH assumptions are correct then the observable  $\mathcal{O}$  relaxes to the statistical average given by the diagonal ensemble not only in the sense of time average but that it actually stays exponentially close to this average at almost all times. We emphasize that this statement does not imply that the observable  $\mathcal{O}$  does not fluctuate. For example by  $\mathcal{O}$  we can understand energy or particle number fluctuations. We proved that ETH implies that from the point of view of any local observable the

quantum system behaves ergodically, i.e. differences between taking into statistical properties of local observables with respect to the true time-dependent density matrix and its time average are exponentially small. Therefore like in classical ergodic systems we can say that quantum ergodicity implies relaxation of the isolated system to the microcanonical ensemble.

To demonstrate how ETH works numerically let us show results of the simulations from the work by M. Rigol et. al. (M. Rigol, V. Dunjko and M. Olshanii, Nature **452**, 854 (2008)). They considered so called hard core-bosons in a two-dimensional lattice with the Hamiltonian

$$H = -J \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i), \quad (\text{IV.29})$$

where  $\langle ij \rangle$  are the links connecting different sites of the lattice (see the top panel Fig. (14)),  $a_i^\dagger, a_i$  are creation and annihilation operators for bosonic particles, which satisfy additional constraint on each site  $a_i^\dagger a_i + a_i a_i^\dagger = 1$ . This constraint implies that on each site there can be either one or zero bosons. Physically this constraint can be realized by assuming that particles have very strong repulsive two-body interactions. It is interesting to point that the hard core constraint generates anti-commutation relations for bosons belonging the same site. This suggests that these bosons acquire some fermionic properties. And indeed in one-dimension this is the case. By performing the Jordan-Wigner transformation one can map exactly the hard core bosons to free fermions. However, in higher dimensions this is not the case and the bosons are always different from fermions. In particular, hard core bosons in 2D form non-integrable (ergodic) system. Let us also point that hard core bosons are exactly equivalent to spin one half particles. By performing the mapping

$$\sigma_i^z = 1 - 2a_i^\dagger a_i, \quad \sigma_i^+ = a_i^\dagger, \quad \sigma_i^- = a_i \quad (\text{IV.30})$$

it is easy to check that the operators  $\vec{\sigma}_i$  are the Pauli matrices in the Fock space with the state with zero bosons corresponding to a spin pointing along the  $z$ -direction (spin up) and the one-boson state maps to the spin down. Then the hopping term maps to the in-plane spin spin interaction  $a_i^\dagger a_j + a_j^\dagger a_i \rightarrow 2(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y)$ .

The middle panel of this figure shows results of numerical simulation of the zero momentum component of the density of hard core bosons along the  $x$ -direction as a function of time. For the initial condition Rigol et. al. used the state where all the bosons (there were five particles overall) were placed in the blue sector of the lattice, which was initially disconnected from the white sector. Then at time  $t = 0$  they turned on the tunneling and observed the dynamics. This middle panel shows the actual numerical data compared to three ensembles: canonical (in which the temperature

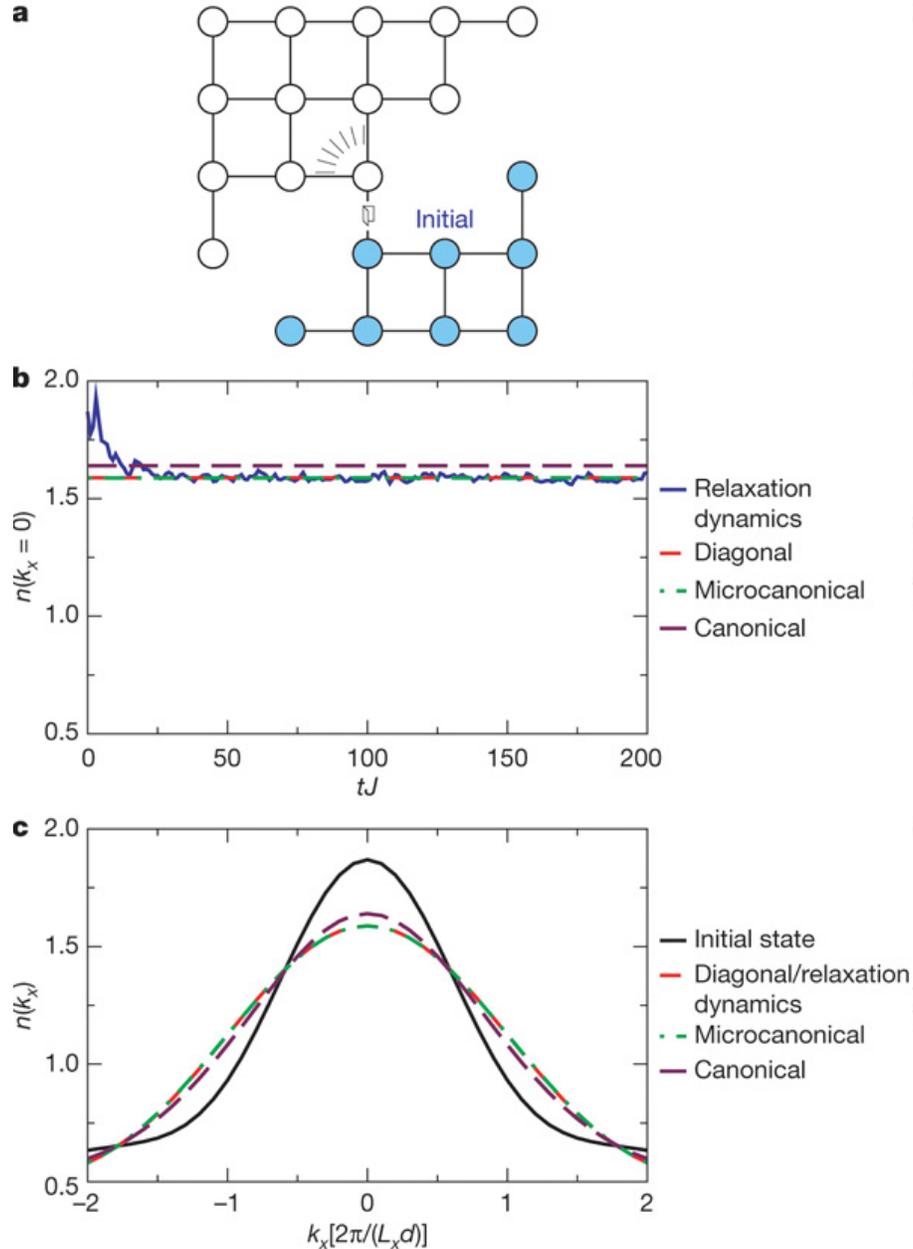


FIG. 14 Top panel: Geometry describing a two-dimensional lattice gas of hard core bosons. The links describe the bonds with non-zero tunnel coupling. Initially five bosons were placed in the blue region of the lattice, disconnected from the white region. Then at time  $t = 0$  the tunnel coupling connecting blue and white regions was turned on and thermalization dynamics was studied numerically. (Image taken from M. Rigol, V. Dunjko and M. Olshanii, *Nature* **452**, 854 (2008)). The middle panel shows time evolution of the zero component of the momentum distribution of the density of hard core bosons along the x-direction after quenching the link connecting blue and white regions and comparison with diagonal ensemble and two statistical ensembles (see text for more details). The bottom panel illustrates the whole momentum distribution for the initial state, diagonal ensemble and two statistical ensembles.

was chosen to match the mean energy), diagonal or time averaged and microcanonical (consisting of a single eigenstate of the final Hamiltonian with the energy closest to the mean). As we see from the figure the diagonal and micro-canonical ensembles give basically identical results and after initial transient dynamics the true time-dependent expectation value of the observable stays very closely to these two values. The canonical ensemble is slightly offset, which is not surprising for small systems. From the ensemble equivalence it is expected that in the thermodynamic limit all three ensembles will be identical. The bottom panel shows the whole momentum distribution for the initial time as well as for the diagonal, microcanonical and canonical ensembles. Again we see that the diagonal ensemble perfectly agrees with the microcanonical ensemble consisting of a single eigenstate. Canonical ensemble is again slightly off due to the finite size effects.

## 2. ETH and localization in the Hilbert space.

There is another complimentary view of the ETH, which is much closer to the classical interpretation of ergodicity as effectively the process of delocalization in the phase space. In quantum systems we usually deal with the Hilbert space instead of phase space and therefore we can think about the process of delocalization in the Hilbert space. In general in information theory and in equilibrium statistical physics a good measure of such delocalization is Shannon or statistical entropy

$$S = - \sum_n \rho_n \log(\rho_n), \quad (\text{IV.31})$$

where  $\rho_n$  are frequencies (probabilities) to occupy particular microstates, which are the energy eigenstates. Because in equilibrium statistical mechanics the density matrix is diagonal in the energy basis the statistical entropy is equal to the von Neumann's entropy  $S_{vn} = -\text{Tr}[\rho \log(\rho)]$ . It is clear that the entropy is measure of delocalization: if  $\rho_n = \delta_{nm}$ , i.e. if only one state is occupied then the entropy is zero and if  $\rho_n = 1/\mathcal{N}$ , i.e. all states are occupied with the same probability the entropy is maximum  $S = \log(\mathcal{N})$ . Because  $\mathcal{N}$  is typically exponential in the volume of the system the entropy is a very convenient measure of delocalization because it is extensive. Of course we also know that the concept of the entropy is the cornerstone of the Statistical physics.

One can expect that the entropy can also serve a measure of delocalization in the dynamical processes. it is clear that for isolated systems the von Neumann's entropy does not change for any dynamical processes even in ergodic systems. Thus we see that it is not a good measure for ergodicity. However, the entropy of the diagonal ensemble or the diagonal entropy (Eq. (IV.31)) is.

This entropy basically measures delocalization of the system in the eigenstates of the Hamiltonian, higher entropy implies that more states are occupied.

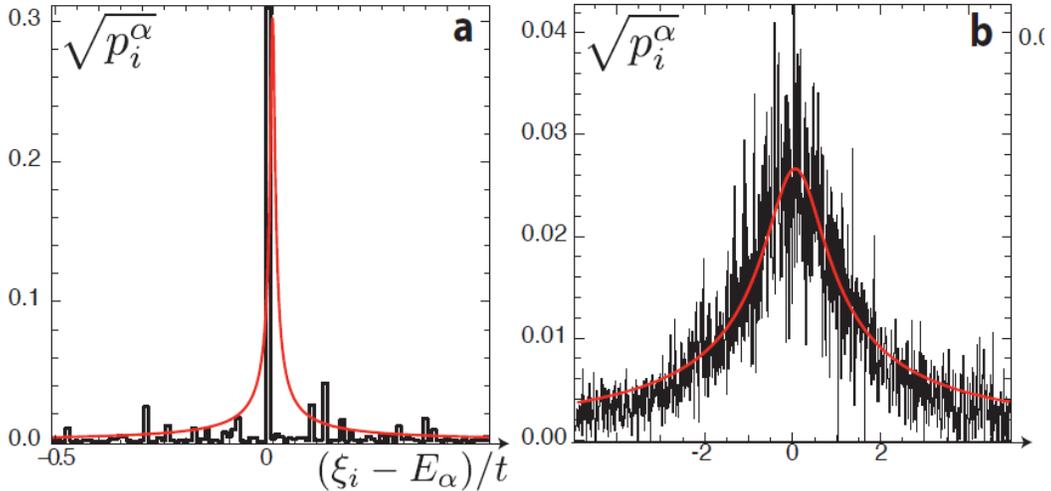


FIG. 15 Probability distribution of occupying the eigenstates of the Hamiltonian describing one-dimensional fermions with second nearest neighbor interactions breaking integrability (see text for details). The left panel corresponds to a weak interaction, which is very close to the integrable case. The right panel corresponds to the quench to the non-integrable case. It is clear that the probability distribution near the integrable case is very sparse with only few states occupied. While in the ergodic case essentially all eigenstates within any narrow energy window are occupied with similar probabilities. The plot is taken from Ref. C. Neuenhahn and F. Marquardt, Phys. Rev. E **85**, 060101(R) (2012).

Before discussing the expectations for the behavior of the entropy in ergodic and non-ergodic regimes let us look into numerical results for a specific systems obtained by C. Neuenhahn and F. Marquardt (Phys. Rev. E, **85**, 060101(R) (2012).) The system they analyzed were one dimensional spinless fermions with second nearest neighbor interactions:

$$H = -t \sum_j (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + V(n_i - 1/2)(n_{i+2} - 1/2), \quad (\text{IV.32})$$

where  $n_i = c_i^\dagger c_i$  is the density operator. Second nearest interaction is required to break integrability in this model, i.e. to induce ergodicity. They start from a Fock state with the mean energy  $\xi_i = \langle \psi_0 | H | \psi \rangle$ , where the initial wave function is a Slater determinant of different momentum states then switch on the interaction  $V$  and project the initial state to the eigenstates of the interacting Hamiltonian. Then they analyze (the square root of) the probability to occupy these eigenstates. The results of the numerical simulations are shown in Fig. (15). The left panel shows the distribution for quench to a small value of  $V$  where the system is nearly integrable and the right

panel shows the large amplitude quench. It is visually clear that in the former (nearly integrable case) the system is strongly localized, i.e. the distribution function is highly inhomogeneous with only few states occupied. On the contrary in the ergodic nonintegrable case corresponding to large value of  $V$  the distribution function is much more homogeneous with the states within any narrow energy window being occupied with roughly the same probability.

These numerical results are actually quite consistent with ETH and allow us to understand quantum ergodicity from yet another angle. The state created by the quench of a local perturbation does not distinguish nearby energy eigenstates because they are very similar to each other (this is the essence of ETH). For example, if we consider a small perturbation  $\epsilon V$ , where  $\epsilon$  is a small number characterizing the amplitude of the perturbation, then the corrections to the eigenstates of the Hamiltonian can be computed using the perturbation theory:

$$|\tilde{n}\rangle = |n\rangle + \epsilon \sum_{m \neq n} \frac{\langle n|V|m\rangle}{E_m - E_n} |m\rangle + \dots \quad (\text{IV.33})$$

Thus the transition probability from the state  $|n\rangle$  of an old Hamiltonian to some other state  $|m\rangle$  of the new Hamiltonian is approximately given by

$$p_{nm} \approx \epsilon^2 |\langle n|\partial_\epsilon|m\rangle|^2 = \epsilon^2 \frac{|\langle n|V|m\rangle|^2}{(E_n - E_m)^2} \sim \epsilon^2 e^{-S} \frac{|f_V(\bar{E}, \omega)|^2}{\omega^2}, \quad (\text{IV.34})$$

where we used Eq. (IV.18) for the representation of the off-diagonal matrix elements and substituted the square of the fluctuating variable  $\sigma_{nm}$  by its square. Since the overlap of two states is always bounded by unity we see that the function  $f_V(\bar{E}, \omega)$  should vanish at least linearly with  $\omega$ . Therefore the expression for the transition probability is free of divergences in the limit  $\omega \rightarrow 0$ . Then from ETH we see that the transition probability should be a smooth function of  $|m\rangle$  possibly multiplied by some positive random fluctuating variable encoded in  $\sigma_{nm}^2$ . It is easy to see that the similar situation persists in higher order perturbation theory. Essentially because all excitations are created by a local operator we can not distinguish nearby eigenstates and thus can not selectively occupy them. We thus come to an interesting conclusion that while ETH tells us that a single eigenstate is sufficient to define the microcanonical ensemble, we can never selectively excite the system in a single eigenstate but rather we always excite (exponentially) many of them.

These considerations immediately suggest that the entropy of the system should coincide with the thermodynamic entropy. Indeed by writing  $\rho_n = \bar{\rho}(E_n)\sigma_n$ , where  $\bar{\rho}(E)$  is the smooth part of the probability distribution and  $\sigma_n$  are fluctuating component with the mean equal to unity we find

$$S = - \sum_n \bar{\rho}(E_n)\sigma_n \log(\bar{\rho}(E_n)) - \sum_n \rho_n \log(\sigma_n) = - \sum_n \bar{\rho}(E_n) \log(\bar{\rho}(E_n)) + O(1). \quad (\text{IV.35})$$

The latter follows from the fact that  $\sum_n \rho_n = 1$  and  $\log(\sigma_n)$  is always of the order of unity unless we are dealing with pathological distributions. The first term in this sum is the von Neumann's entropy of the smooth ensemble, which is always extensive because the probability is distributed over exponentially many states. Conversely in integrable non-ergodic setups the probability distribution is localized in very few states and we expect that the corresponding entropy will be significantly less than the equilibrium thermodynamic value. This was indeed confirmed in several numerical simulations (see e.g. L. F. Santos, A. Polkovnikov, M. Rigol, *Phys. Rev. Lett.* **107**, 040601 (2011)). Thus we see that ETH allows one to understand quantum ergodicity as delocalization in the Hilbert space, which is much closer to the classical picture where ergodicity is understood as delocalization in phase space. We will return to this issue one more time when we discuss ergodicity in disordered interacting systems in the context of many-body localization.

### 3. ETH and quantum information

ETH also allows us to make important conclusions for information theory. The standard measure of information suggested by C. Shannon in 1948 is precisely given by the entropy

$$I = - \sum_n p_n \log(p_n), \quad (\text{IV.36})$$

where  $p_n$  are the relative frequencies of the outcomes of different events like particular letters appearing in words. Normally in information theory one uses log base two but we will ignore this subtlety. In quantum systems one usually extends the Shannon's definition to quantum information using the von Neumann's entropy

$$I = -\text{Tr}[\rho \log(\rho)]. \quad (\text{IV.37})$$

In the basis where the density matrix is diagonal clearly the quantum information reduces to the classical definition. Information theory is a very active field of research in the context of quantum computing, quantum cryptography, information and black holes, informational thermodynamics etc.

In these notes we will emphasize only one aspect related to the quantum ergodicity and ETH. Let us assume that the system is in the pure state so that the quantum entropy is zero. Now suppose we want to perform a series of measurements on the system to find out that this entropy is indeed zero. For simplicity we assume that we deal with projective measurements. Such measurements project the system to the measurement basis. From mathematical point of view this is equivalent

to the quench to a measurement Hamiltonian and relaxation to the diagonal ensemble. Thus if we want to measure the spin orientation along a particular axis, say  $z$  we apply a strong local magnetic field  $h_z$  along the  $z$ -axis, such that the Hamiltonian becomes

$$H \rightarrow H - h_z \sigma_j^z, \quad (\text{IV.38})$$

where  $j$  is the location of the measured spin and  $h_z$  is large compared to all other energy scales in the problem. Then the eigen-basis of this Hamiltonian factorizes into a direct product of the spin  $j$  pointing to the up and the rest of the system and the direct product of the spin  $j$  pointing down and the rest of the system with the energy separation to the first approximation  $2h_z$ . Then very quickly the spin  $j$  dephases so that the density matrix becomes diagonal with the entries proportional to the probabilities of occupying the spin up and spin down states, which are conserved in time. Because the measurement is done with the local operator according to ETH it projects the original state to all the states within the energy uncertainty with roughly the same probability. For local measurements the energy uncertainty is non-extensive because it corresponds to a quench by a local operator. However, the number of states within non-extensive energy shell is exponential. So we see that a single act of measurement, even if we measure orientation of a single spin in the whole Universe, immediately induces extensive entropy into the system and thus loss of the quantum information. Thus in ergodic systems pure states and quantum information associated with them are extremely fragile. If one builds any kind of quantum information device, it has to be non-ergodic.

#### 4. ETH and the Many-Body Localization

So far we discussed that quantum ergodicity can be understood as de-localization in the energy eigen basis. There is a strong numerical evidence that in disordered systems ergodicity is also directly related to the localization in real space in many-particle systems, or so called many-body localization (D. Basko, I. Aleiner, B. Altshuller, 2007). Before doing this let us briefly review single particle localization following ideas by Edwards and Thouless (1972) formulated later as a scaling theory of localization by the ‘‘gang of four’’ (E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, 1979).

Let us consider a single particle in a weakly disordered system. In other words we assume that disorder leads to isolated scattering events, which classically will correspond to a diffusive motion. Let us now take the volume of linear size  $L$  and analyze qualitatively conductivity through this

system, i.e. response of a particle to an infinitesimal linear potential. To do this we will look into two energy scales. The first is the so called Thouless energy, which counts the energy uncertainty due to finite time of a particle traversing the boundary. In diffusive, unlike ballistic systems, this time scales quadratically with the linear size:

$$\tau_D \sim \frac{L^2}{D}, \quad (\text{IV.39})$$

where  $D$  is the diffusion constant. Thus the energy uncertainty of any wave-packet is

$$E_T = \frac{\hbar}{\tau_D} = \frac{\hbar D}{L^2}. \quad (\text{IV.40})$$

This energy is precisely the Thouless energy. The other energy scale is the energy spacing between single particle states:

$$\Delta E = \frac{1}{\omega(E)} L^{-d}, \quad (\text{IV.41})$$

where  $\omega(E)$  is the single-particle density of states per unit volume. Comparing these two scales we see that in dimensions above two  $d > 2$  the Thouless energy scales down to zero slower with the system size implying that as  $L$  increases more and more levels appear within the single-particle energy shell. In turn this justifies the classical analysis and thus we expect that above two dimensions wave packets centered around high energy (classical) states propagate diffusively through the system, thus they are delocalized. This argument of course does not imply that all states are delocalized. We can always have bound localized states in the system. Conversely in dimensions below two the Thouless energy goes to zero faster than level spacing. Thus even if at short distances the system looks like diffusive once we reach long distances energy quantization becomes crucial. The argument by the ‘‘gang of four’’ elegantly formulated in terms of renormalization group transformation essentially states that diffusive transport persists in the system as long as the number of levels within the Thouless energy remains greater than one. If the Thouless energy flows to zero faster than level spacing then eventually this condition gets violated and then the system crosses over to the localized regime, where the localization length is given by

$$E_T(\xi) = \Delta E(\xi). \quad (\text{IV.42})$$

In two dimensions the two energies scale in the same way so the argument is more subtle. Essentially the result is that in two dimensions all states remain localized but the localization length can be exponentially large in the dimensionless parameter  $\hbar D \omega(E)$ .

For a long time it was believed that the phenomenon of localization only applies only applies to zero temperature non-interacting systems. The argument essentially follows from the schematic

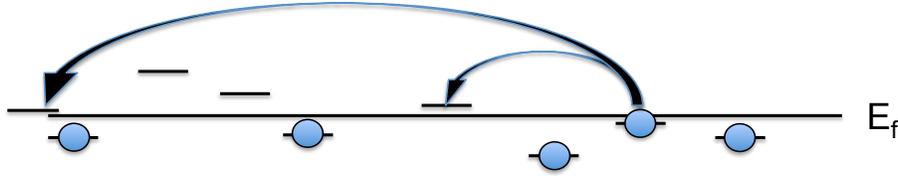


FIG. 16 A figure illustrating the hopping conductivity at finite temperature for fermions coupled to phonons. Even if the ground state of fermions is localized at finite temperatures there is always a nonzero probability of finding another localized state at slightly higher energy and move the Fermion there by absorbing a phonon.

figure 16. Assume that at zero temperature all single-particle states are localized (to be specific we assume that we are dealing with fermions). At zero temperature all states below the Fermi energy will be occupied and all states above Fermi energy will be empty. As soon as temperature becomes finite there is a non-vanishing probability within the Fermi-Golden rule for a fermion to absorb energy from the phonon bath and jump to another site. The smaller the temperature the smaller the chance since particles have to go to longer distances to find an empty state with nearly the same energy. But as soon as the temperature is finite we will always get finite conductivity (which is called hopping conductivity in this case). This argument has one implicit assumption that the Fermi-Golden rule can be applied. In the case of phonons this is justified because there are no coherent revivals and collapses since e.g. the emitted phonon simply disappears to the continuum.

For a long time it was assumed that this situation is generic for any type of interactions, e.g. particle-particle interactions will also immediately allow for transport at any finite temperature. However B. Altshuller (1997) presented arguments, later refined by D. Basko, I. Aleiner and B. Altshuller (2005) that this is not always the case. Essentially they argued that with local interactions it is not sufficient to move one particle (this will cost too much energy), one also needs to rearrange nearby particles, which is only possible in higher order perturbation theory. But as one goes to higher orders in interaction strength the transition probabilities are getting more and more suppressed. Using self consistent approximations they argued that this perturbation theory has finite radius of convergence (in interaction coupling) and thus finite threshold for delocalization. Moreover they argued that this threshold is extensive in volume and therefore finite temperature is not going to lead to immediate delocalization (see Fig. 17). These ideas were tested numerically numerically by several groups, in particular by A. Pal, V. Oganesyan, D. Huse in 2007. They considered a familiar to us one-dimensional spin one-half chain, which can be mapped to hard core

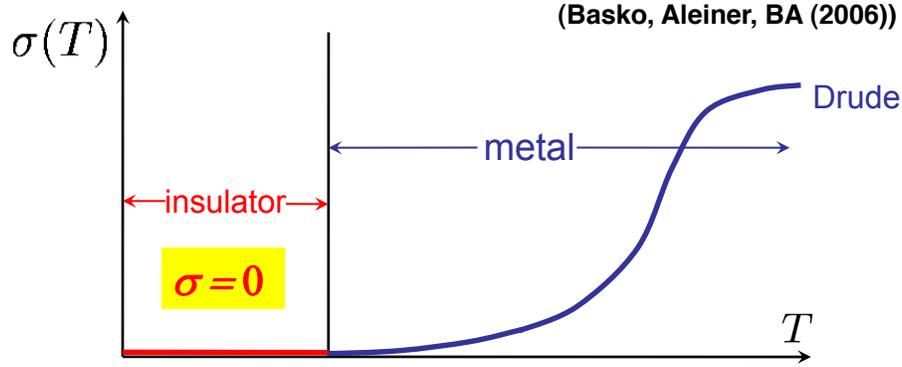


FIG. 17 Schematic phase diagram for the many-body localization proposed by D. Basko, I. Aleiner and B. Altshuller (2005). The plot is taken from B. Altshuller talk at KITP, UCSB (2012).

bosons, with an extra disordered magnetic field

$$H = \sum_{j=1}^L h_j s_j^z + J \vec{s}_j \vec{s}_{j+1}, \quad (\text{IV.43})$$

where  $h_j$  are uniformly and independently distributed random variables in the interval  $[-h, h]$ . This model does not have any known local integrals of motion other than energy for any  $h > 0$ . A. Pal and collaborators focused on the infinite temperature state where all spin configurations are equally probable. What they found numerically was consistent with the scenario of many-body localization. Fig. (18) shows numerically obtained phase diagram for this Hamiltonian, which

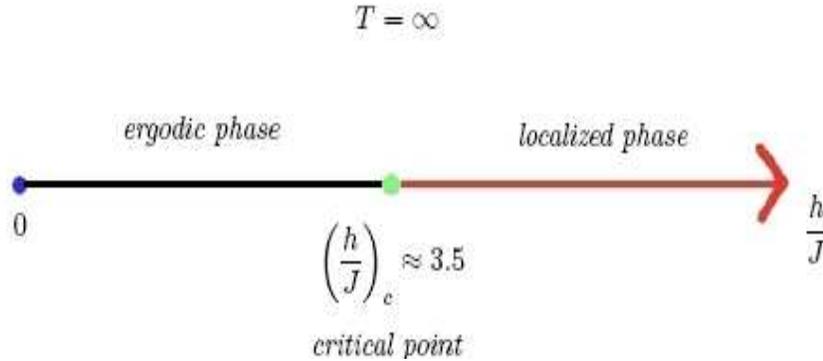


FIG. 18 Numerically obtained infinite temperature phase diagram for the disordered spin chain (see Eq. (IV.43).) As the disorder increases the system becomes localized even at infinite temperature. Fig. taken from A. Pal's, PhD Thesis, Princeton (2012).

shows transition from delocalized to localized phase at infinite temperature as disorder increases. These results were obtained by exact diagonalization in small systems and therefore they do not prove existence of the transition in the thermodynamic limit but they show very strong indications.

The authors determined this transition by several means. The first is they looked into mean square difference of the local magnetization between adjacent eigenstates (Fig. (19).) The results of this

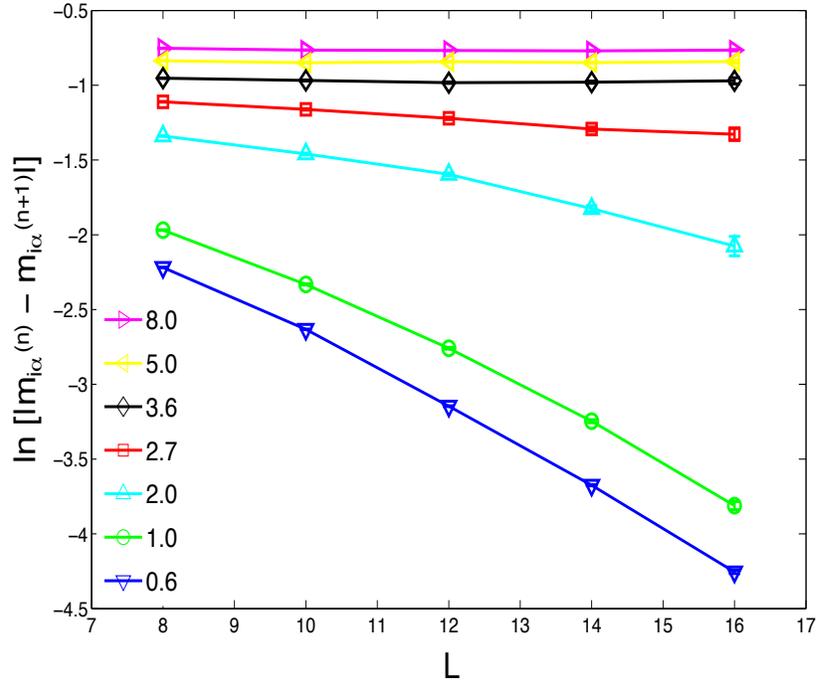


FIG. 19 Mean absolute value of the difference of the local magnetization between adjacent eigenstates as a function of the system size in the log scale. At strong disorder the difference stays finite even if the system size increases implying that nearby eigenstates correspond to very different spin configurations. At small disorder this difference, on the other hand, exponentially goes to zero indicating that nearby eigenstates are nearly identical from the point of view of local observables. This regime is fully consistent with ETH. Fig. taken from A. Pal's, PhD Thesis, Princeton (2012).

numerical analysis supports existence of the transition between ergodic and non-ergodic phases. At strong disorder the magnetization difference remains finite even if the system size increases. This means that nearby energy eigenstates come from completely different spin configurations. This clearly violates the assumptions of quantum ergodicity and ETH. In the weak disorder regime, on the other hand, this difference goes down exponentially with the system size. This means that nearby eigenstates from the point of view of local observables (a particular local observable) look indistinguishable. This is in turn precisely the statement of quantum ergodicity. Note that the transition happens at infinite temperature and that there are no obvious integrals of motion in the system. Based on our earlier discussion we can anticipate that in the former (non-ergodic) case the statistics of energy levels will be Poissonian and in the latter (ergodic) case it will be

Wigner-Dyson. And this is indeed what was observed (Fig. 20). This Figure shows the measure of

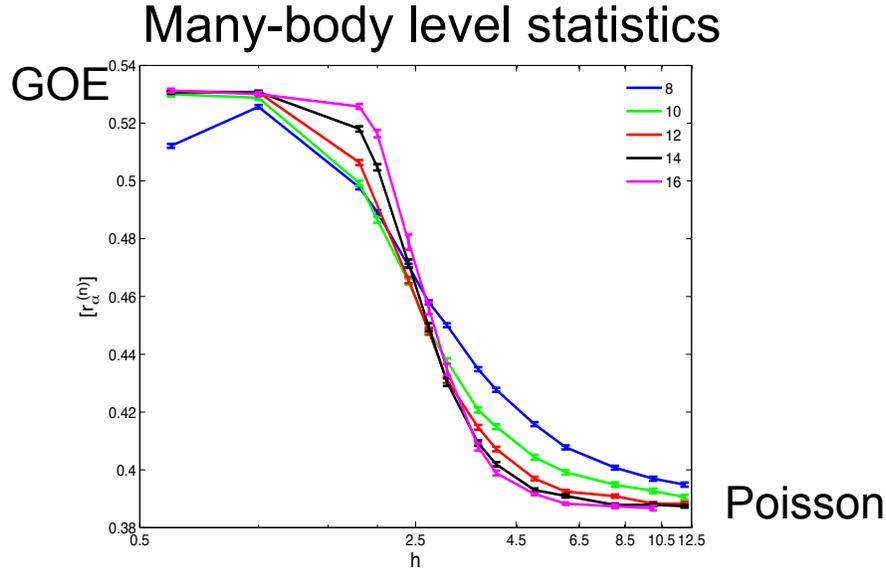


FIG. 20 Mean ratio of adjacent energy gaps  $r_\alpha^{[n]}$  (see text for details). This ratio shows a clear crossover between the two values expected for the Poisson statistics 0.39 at strong disorder and the Wigner-Dyson statistics at weak disorder 0.53. Fig. taken from A. Pal's, PhD Thesis, Princeton (2012).

the level statistics (Poisson or Wigner-Dyson) encoded in a single number defined as

$$r_\alpha^{[n]} = \frac{\min(E_n - E_{n-1}, E_{n+1} - E_n)}{\max(E_n - E_{n-1}, E_{n+1} - E_n)}. \quad (\text{IV.44})$$

and averaged over  $n$ . This number can be computed both for the Poisson statistics  $\langle r_\alpha^{[n]} \rangle = 2\ln(2) - 1 \approx 0.39$  and the Wigner-Dyson statistics  $\langle r_\alpha^{[n]} \rangle = 0.53$ . From the figure it is clear that as the system goes from ergodic to non-ergodic phase this number changes from the value consistent with the random matrix statistics to the Poisson statistics. So we see that even at infinite temperature and despite lack of existence of any obvious integrals of motion other than the energy disordered systems can undergo phase transitions between ergodic and non-ergodic phases in perfect agreement with general definitions of quantum ergodicity based on the random matrix theory and ETH.

It is interesting that in this case the transition from ergodic to non-ergodic phase, which as we discussed can be described as the localization transition in the energy space also coincided with localization in real space (or equivalently phase space). Fig. (21) illustrates memory of the magnetization about the initial state in the long time limit. Specifically the authors start from the

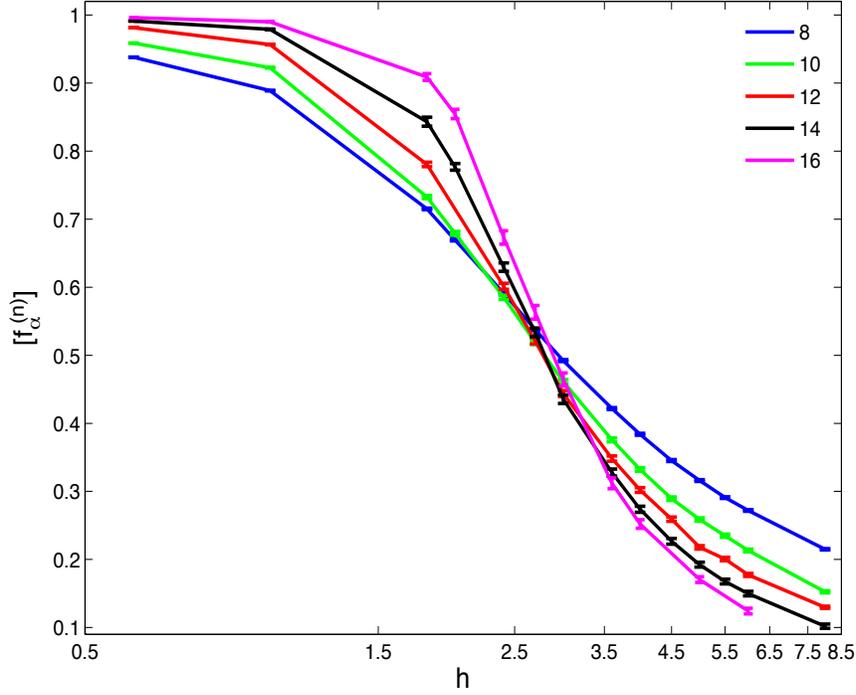


FIG. 21 Fraction of initial magnetization in the long time limit for the state prepared with initial long wave modulation of the magnetization along the  $z$  axis. In the ergodic phase the memory rapidly disappears with the system size, while in the non-ergodic phase the memory remains finite. Fig. taken from A. Pal's, PhD Thesis, Princeton (2012).

initial density matrix

$$\rho_0 = \frac{1}{Z} \exp[\epsilon M_1] \approx \frac{1 + \epsilon M_1}{Z},$$

where

$$M_1 = \sum_j s_j^z e^{2\pi i j/L}$$

and  $\epsilon$  is a small number. I.e. they start with a density matrix corresponding to a weak long-wavelength modulation of the magnetization along the  $z$ -axis. Then initially the mean magnetization is

$$\langle M_1(t=0) \rangle = \text{Tr}[\rho_0 M_1] = \frac{\epsilon}{Z} \sum_n \langle n | M_1^2 | n \rangle. \quad (\text{IV.45})$$

In the infinite time limit the system relaxes to the diagonal ensemble (this statement is unrelated to the ergodicity) so the magnetization relaxes to

$$\langle M_1(t) \rangle = \frac{\epsilon}{Z} \sum_{m,n} |\langle n | M_1 | m \rangle|^2 e^{i(E_n - E_m)t} \xrightarrow{t \rightarrow \infty} \frac{\epsilon}{Z} \sum_n |\langle n | M_1 | n \rangle|^2. \quad (\text{IV.46})$$

Thus a good measure of the memory plotted in Fig. 21 is the following function

$$f^{(n)} = 1 - \frac{|\langle n|M_1|n\rangle|^2}{\langle n|M_1^2|n\rangle}. \quad (\text{IV.47})$$

In the localized regime this function is close to unity while in the delocalized regime this function becomes exponentially small. This example highlights that at least in disordered systems quantum ergodicity, which is understood as delocalization in energy space of the Hamiltonian, also coincides with delocalization of the system in real space (or more generally phase space).

## B. Exercises

1. Consider a gas of weakly spin one half particles in the external magnetic field with the Hamiltonian

$$H = \sum_j h\sigma_j^z + H_{int}, \quad (\text{IV.48})$$

where  $H_{int}$  includes weak spin-spin interactions. Let us assume that the energy eigenstates are random superpositions of spins pointing in arbitrary direction:

$$|\psi_n\rangle = \sum_{s_1, s_2, \dots, s_N} \alpha_{s_1, s_2, \dots, s_N} |s_1\rangle |s_2\rangle \dots |s_N\rangle, \quad (\text{IV.49})$$

where  $s_j = \uparrow, \downarrow$  and  $\alpha_{\{s_j\}}$  are random amplitudes taken from a uniform distribution as long as the spin states satisfy the constraint  $-h \sum_j s_j = E_n$ . Show that under this assumption the probability distribution for a single spin is exponentially in  $N$  close to the Gibbs distribution.

2. Consider a square two dimensional lattice  $N \times N$  with incommensurate hoppings along the  $x$  and  $y$  directions such that the single particle Hamiltonian is

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j} \left[ J_x (a_{i,j}^\dagger a_{i+1,j} + a_{i+1,j}^\dagger a_{i,j}) + J_y (a_{i,j}^\dagger a_{i,j+1} + a_{i,j+1}^\dagger a_{i,j}) \right] \quad (\text{IV.50})$$

Here  $i, j = 1, \dots, N$  are the coordinates of the sites of the lattice along  $x$  and  $y$  directions respectively. You can consider either open or periodic boundary conditions. You can choose e.g.  $J_x = 1$  and  $J_y = \sqrt{2}$  or something like that.

- Choosing  $N$  sufficiently large analyze statistics of energy levels. You may split the entire energy spectrum into blocks of energy  $\Delta E$ , find average level spacing within each block and normalize level spacings to this average value.

- Now consider disordered array (still single particle), where on each link  $J_x$  and  $J_y$  are drawn from some distribution, e.g. drawn with a uniform probability in the interval  $[J - \delta J, J + \delta J]$  where  $\delta J \leq J$ . Instead of this disorder you can consider all  $J$  to be the same but some random bonds missing. If too many bonds are removed the system should be split into isolated clusters. Now analyze statistics again. Is it Wigner Dyason or Poissonian? Can you explain your answer.
- Now assume that you have two particles in the system with or without disorder. You can consider hard-core bosons. Find the energy spectrum in this system and analyze the statistics of the energy levels. If you consider periodic boundary conditions without disorder it is important to work in the sector of fixed (e.g. zero) center of mass lattice momentum since this is an additional conserved quantity.

## V. QUANTUM ERGODICITY AND EMERGENT THERMODYNAMIC RELATIONS

We now turn our attention to deriving macroscopic thermodynamic relations from microscopic dynamics. We will be using essentially only two assumptions: (i) systems relax to the diagonal ensemble and (ii) all many-body eigenstates with close energies are identical from the point of view of local observables. The first assumption agrees with our discussion that in ergodic systems the density matrix approaches the diagonal form in a sense that for all local observables the difference between diagonal ensemble expectation value and true expectation value becomes exponentially small at long times (see Eq. (IV.28)). The second assumption is the essence of the ETH. As we will see next using just these two assumptions alone is sufficient to recover most of the thermodynamic relations. Very often instead of these two assumptions it will be enough to start from the Gibbs distribution. Recall that the latter automatically follows from (i) and (ii) if we are dealing with subsystems of a larger, ergodic system. Indeed in this case from equivalence of a single eigenstate of the whole system to a microcanonical ensemble we immediately conclude that small subsystems must be described by the Gibbs distribution.

### A. Entropy and the fundamental thermodynamic relation

Let us start our discussion from the fundamental thermodynamic relation:

$$dE = TdS - \mathcal{F}_\lambda d\lambda, \tag{V.1}$$

where  $\lambda$  is a macroscopic parameter like volume, magnetic or electric field and  $\mathcal{F}_\lambda$  is the conjugate generalized force like pressure magnetization or polarization. We first assume that the initial density matrix is described by the Gibbs distribution

$$\rho_{nm}(\lambda) = \frac{1}{Z(\lambda)} e^{-\beta E_n(\lambda)} \delta_{nm}. \quad (\text{V.2})$$

Next we assume that there is some dynamical process resulting in infinitesimal energy change in the system and possibly infinitesimal change in the parameter  $\lambda$ . The system can be either open or closed during this process. After this process we let the system to relax to the diagonal ensemble, i.e. reach new equilibrium state. Then the infinitesimal energy change is given by

$$\begin{aligned} dE &= d \left( \sum_n \rho_{nn} E_n(\lambda) \right) = \sum_n \left[ E_n(\lambda) d\rho_{nn} + \rho_{nn} \frac{dE_n}{d\lambda} d\lambda \right] \\ &= \sum_n E_n d\rho_{nn} + \left. \frac{\partial E}{\partial \lambda} \right|_S d\lambda = \sum_n E_n d\rho_{nn} - F_\lambda d\lambda. \end{aligned} \quad (\text{V.3})$$

Here we used the fact that energy levels are only sensitive to the external parameter  $\lambda$  and do not depend on the details of the process (e.g. slow vs. fast, isolated vs. open etc.). Thus the last term in the first line can be written as the full derivative at a constant entropy, which is by definition is the (minus) generalized force:  $F_\lambda = -\partial_\lambda E|_S$ . Next let us compute the entropy change in the system, i.e. entropy difference between the final and the initial equilibrium states:

$$dS = -d \left[ \sum_n \rho_{nn} \log(\rho_{nn}) \right] = - \sum_n d\rho_{nn} \log(\rho_{nn}^0) - \sum_n d\rho_{nn} \quad (\text{V.4})$$

Note that the last term drops due to the conservation of probability. In the first term we use the explicit form of the Gibbs distribution (V.2) and get

$$dS = \beta \sum_n E_n(\lambda) d\rho_{nn} \quad (\text{V.5})$$

Comparing the two expressions for the energy and the entropy change (V.3), (V.5) we immediately recover the fundamental thermodynamic relation (V.1). Note that this derivation did not rely explicitly on ETH and thus are valid whether the system is ergodic or not. As we discussed above this is because the Gibbs ensemble implies equilibrium state whether we are dealing with a system of non-interacting spins or the complex many-particle systems. But what if the system is not described by the Gibbs ensemble? In this case ergodicity is crucial. Instead of repeating the derivation above for an arbitrary ensemble let us look carefully into the entropy of the relaxed system following some dynamical process

$$S(E) = - \sum_n \rho_{nn} \log(\rho_{nn}) \quad (\text{V.6})$$

Let us define some continuous function of energy  $\rho(E)$  such that  $\rho(E_n) = \rho_{nn}$ . This function can be e.g. simple interpolating function. Then the sum above can be formally written as the integral over energy

$$S(E) = - \int dE \rho(E) \Omega(E) \log(\rho(E)), \quad (\text{V.7})$$

where

$$\Omega(E) = \sum_n \delta(E - E_n)$$

is the many-particle density of states (we can also assume that it is continuous between energy levels by taking an appropriate interpolation procedure). Now let us note that the product  $\rho(E)\Omega(E) = W(E)$  is the probability distribution function for the energy. Indeed expectation value of any function of energy is

$$\langle f(E) \rangle = \sum_n \rho_{nn} f(E_n) = \int dE \Omega(E) \rho(E) f(E) = \int dE W(E) f(E). \quad (\text{V.8})$$

It is also obvious from the definition that

$$\int dE W(E) = \sum_n \rho_{nn} = 1,$$

i.e. this probability distribution is properly normalized. Representing  $\rho(E)$  as  $W(E)/\Omega(E)$  in Eq. (V.7) for the entropy we find that

$$S(E) = \int dE W(E) S_m(E) - \int dE W(E) \log(W(E)) \quad (\text{V.9})$$

The first term is simply the average of the microcanonical entropy  $S_m(E) = \log(\Omega(E))$  over the true energy distribution. As long as the latter is peaked around the mean value, i.e. as long as the fluctuations of the energy are subextensive, this term simply reduces to the standard thermodynamic entropy, which is extensive in the system size. The second term is more subtle. To analyze it let us split the energy distribution into the product of the smooth and the fluctuating parts:

$$W(E) = \bar{W}(E) \sigma(E),$$

where  $\bar{W}(E)$  is e.g. an averaged distribution over a non-extensive energy window containing exponentially many energy levels and  $\sigma(E)$  is the fluctuating variable with unit mean. Then the expression for the entropy can be further rewritten as

$$\begin{aligned} S(E) &= \int dE W(E) \sigma(E) S_m(E) - \int dE \bar{W}(E) \sigma(E) \log(\bar{W}(E)) - \int dE \bar{W}(E) \sigma(E) \log(\sigma(E)) \\ &\approx \int dE \bar{W}(E) S_m(E) - \int dE \bar{W}(E) \log(\bar{W}(E)) - \int dE \bar{W}(E) \sigma(E) \log(\sigma(E)) \end{aligned} \quad (\text{V.10})$$

We used the fact that if the integrand is  $\sigma(E)$  times arbitrary smooth function than  $\sigma(E)$  can be substituted by mean, which is unity. Here the first two terms define the smooth contribution to the entropy:

$$S_{sm} = \int dE \bar{W}(E) [S_m(E) - \log(\bar{W}(E))] \quad (\text{V.11})$$

and the last term is the fluctuating contribution

$$S_{fluct} = - \int dE \bar{W}(E) \sigma(E) \log(\sigma(E)). \quad (\text{V.12})$$

Unless the smooth part of the energy distribution in energy exponentially wide, which is impossible unless the mean energy is also exponentially large, the second term in the expression for  $S_{sm}$  is non-extensive, so the smooth entropy in the thermodynamic limit approaches the average microcanonical entropy. To be more specific let us recall that according to the central limit theorem total energy, which is always approximately equal to sum of energies of subsystems, should have the Gaussian distribution. This is true whether we are talking about ergodic or non-ergodic systems as long as we deal with local interactions. Thus writing

$$\bar{W}(E) = \frac{1}{\sqrt{2\pi}\delta E} \exp \left[ -\frac{(E - \bar{E})^2}{2\delta E^2} \right],$$

and expanding the microcanonical entropy  $S_m(E)$  near the mean energy  $\bar{E}$

$$S_m(E) = S_m(\bar{E}) + \beta(E - \bar{E}) + \frac{1}{2} \frac{\partial \beta}{\partial E} (E - \bar{E})^2 + \dots = S_m(\bar{E}) + \beta(E - \bar{E}) - \frac{(E - \bar{E})^2}{\delta E_c^2} + \dots$$

where  $\delta E_c^2 = -\partial_\beta E$  are the energy fluctuations in the canonical ensemble, we find

$$S_{sm} \approx S_m(\bar{E}) - \frac{1}{2} \frac{\delta E^2}{\delta E_c^2} + \log(\sqrt{2\pi}\delta E) + \frac{1}{2} = S_c(\bar{E}) - \frac{1}{2} \left( \frac{\delta E^2}{\delta E_c^2} - 1 \right) + \log \left( \frac{\delta E}{\delta E_c} \right), \quad (\text{V.13})$$

where

$$S_c(E) = \log \left( \sqrt{2\pi}\delta E_c \Omega(\bar{E}) \right) \quad (\text{V.14})$$

is the entropy of the canonical ensemble (up to corrections, which vanish in the thermodynamic limit). The remaining correction to the entropy is usually non-extensive. It is easy to see that it is always non-positive. This correction is zero precisely when the width of the energy distribution coincides with the width of the canonical ensemble  $\delta E = \delta E_c$ . This is expected since at given mean energy canonical distribution maximizes the entropy of the system.

Now let us look into the fluctuating part of the entropy

$$S_{fluct} = - \int dE W(E) \log(\sigma(E)). \quad (\text{V.15})$$

If the distribution of  $\sigma(E)$  is bounded and independent of the system size then clearly the integral above converges to a non-extensive number. This simply follows from the normalization of the probability distribution  $W(E)$ . This is precisely the situation arising in ergodic systems. Indeed as we argued in the previous section ETH implies that all eigenstates with nearby energies are similar to each other so in any dynamical process mediated by local interactions the states are occupied with similar probabilities. The precise distribution of  $\sigma(E)$  is not known at the moment, most likely it is a Gaussian centered around unity. In any case independent of the details of  $\sigma(E)$  we recover that the entropy of the system is always given by the smooth part of the entropy up to non-extensive corrections. The situation changes dramatically for non-ergodic systems. As we discussed if the system is excited by some dynamical process the energy occupation is very sparse such that only exponentially small subset of eigenstates is occupied. We will discuss this point in more detail later, when we analyze integrable (non-ergodic) systems. This means that the function  $\sigma(E)$  consists essentially of exponentially (in the system size) sparse and exponentially large peaks. Then the fluctuating entropy can become extensive giving negative extensive correction to the total entropy. In this case clearly the total entropy is not described by any thermodynamic ensemble.

The fact that for ergodic systems  $S(E) \approx S_{sm}(E) \approx S_c(E)$  immediately implies that the fundamental relation applies for any dynamical process even if the assumptions about the Gibbs distribution are not valid. One can also check this explicitly. In fact we have proven a more general statement that in ergodic systems the von Neumann's entropy of the relaxed density matrix (we can term it as the diagonal entropy since this is the entropy of the diagonal density matrix) is equivalent (up to non-extensive corrections) to the canonical entropy.

## **B. Doubly stochastic evolution in closed systems. Fluctuation relations.**

We now proceed with a more detailed analysis of consequences of ETH to dynamics in closed systems. I.e. in this section we will assume that the system is initially prepared in some initial stationary state, i.e. on a diagonal ensemble with respect to the initial Hamiltonian. Then this system is taken off equilibrium by some dynamical process, like an external pulse, which can be either fast or slow. Then the system is allowed to relax to the new diagonal ensemble in the sense we discussed before. This whole process can be described by some unitary evolution of the density matrix

$$\rho(t) = U^\dagger \rho_0 U, \tag{V.16}$$

where  $\rho_0$  is the initial density matrix and

$$U = T_t \exp \left[ -i \int_0^t dt' H(t') \right] = \prod_{t_i} e^{-iH(t_i)\Delta t} \quad (\text{V.17})$$

is the evolution operator. The time ordering symbol implies that earlier times appear on the right. In our analysis the precise form of the evolution operator will not be important. As we discussed after dynamical process the system relaxes to the diagonal ensemble so that expectation values of all observables are determined in the diagonal basis of the new Hamiltonian  $H(\lambda_1)$ , i.e. the Hamiltonian after the evolution. We denote the eigenstates of this Hamiltonian as  $|n_1\rangle$ . The initial density matrix by the assumption is diagonal in the eigenbasis of the old Hamiltonian  $H(\lambda_0)$ :  $|m_0\rangle$ . Then from Eq. (V.16) we find

$$\rho_{nn}(t) = \sum_m \langle n_1 | U^\dagger | m_0 \rangle \rho_{mm}^0 \langle m_0 | U | n_1 \rangle = \sum_m |U_{mn}|^2 \rho_{mm}^0, \quad (\text{V.18})$$

where we used that for unitary matrices  $U_{nm}^\dagger = \langle n | U^\dagger | m \rangle = \langle m | U | n \rangle^* = U_{mn}^*$ . Note that indexes  $n$  and  $m$  correspond to eigenstates of different Hamiltonians: initial ( $m$ ) and final ( $n$ ). Physically the squares of the matrix elements  $|U_{mn}|^2$  are the transition rates, i.e. probabilities of the transition from the eigenstate  $|m\rangle$  of the initial Hamiltonian to the eigenstate  $|n\rangle$  of the final Hamiltonian as a result of the dynamical process. Thus we can introduce the new notation

$$p_{m \rightarrow n} = |U_{mn}|^2 \quad (\text{V.19})$$

We use the terminology transition rate to reserve transition probability for the product of the transition rate and the probability to occupy the state  $|m\rangle$ . Using these notations we can rewrite Eq. (V.18) in the form of the many-body master equation

$$\rho_{nn}(t) = \sum_m p_{m \rightarrow n} \rho_{mm}^0. \quad (\text{V.20})$$

The transition rates are very familiar to us since we are routinely computing them e.g. within the Fermi-Golden rule calculations. Here we are not making any assumptions about the validity of the perturbation theory. Thus these rates  $p_{m \rightarrow n}$  are some complicated functions, which depend on the details of the system and the dynamical process. These rates, however, satisfy two very important property. The first one is the conservation of probability

$$\sum_n p_{m \rightarrow n} = \sum_n \langle n | U^\dagger | m \rangle \langle m | U | n \rangle = \langle m | U U^\dagger | m \rangle = 1. \quad (\text{V.21})$$

Indeed from this equation we see that

$$\sum_n \rho_{nn}(t) = \sum_m \rho_{mm}^0 \sum_n p_{m \rightarrow n} = \sum_m \rho_{mm}^0 = 1. \quad (\text{V.22})$$

It is clear that conservation of probability is fundamental property of any evolution whether it is unitary or not, so the property (V.21) must be always satisfied. The second important property of the transition rates is

$$\sum_m p_{m \rightarrow n} = \sum_m \langle n|U^\dagger|m\rangle \langle m|U|n\rangle = \langle n|U^\dagger U|n\rangle = 1 \quad (\text{V.23})$$

This property of the transition rates is much less intuitive. It tells that for the unitary evolution the sum of the transition rates to any state is the same. Clearly this property is violated for spontaneous emission, which is not a unitary process. Indeed for a two-level system the rate to go from the higher energy state to the lower energy state is generally nonzero if spontaneous emission is allowed, while the opposite rate is zero. On the other hand for stimulated processes, which can be described by unitary dynamics of a two-level system in an external electro-magnetic field the emission and absorption probabilities are the same. In mathematics the matrices satisfying the condition

$$\sum_m T_{mn} = \sum_n T_{nm} = 1 \quad (\text{V.24})$$

are called doubly stochastic. Thus for unitary process the transition rate matrix is doubly stochastic. Note that product of two doubly stochastic matrices  $T$  and  $R$  is again doubly stochastic, e.g.

$$\sum_n (TR)_{mn} = \sum_{n,q} T_{nq} R_{qn} = \sum_q T_{nq} = 1. \quad (\text{V.25})$$

This immediately implies that unitary dynamics is sufficient but not necessary condition for double-stochasticity of the transition rates. E.g. we can add arbitrary projection operators (perform projective measurements) to the dynamics, which break unitarity. The transition rate matrix will remain doubly-stochastic. The simplest non-unitary process can be described by some unitary dynamical process then waiting for a random time (which is equivalent to the time averaging of the density matrix) and then another dynamical process.

We can rewrite the master equation (V.20) in a more convenient form

$$\rho_{nn}(t) = \rho_{nn}^0 + \sum_m (p_{m \rightarrow n} \rho_{mm}^0 - p_{n \rightarrow m} \rho_{nn}^0) = \rho_{nn}^0 + \sum_m p_{m \rightarrow n} (\rho_{mm}^0 - \rho_{nn}^0) \quad (\text{V.26})$$

The first equality simply follows from the conservation of probability and has a standard form for any type of master or kinetic equations that the change in the probability of occupying state  $n$  increases due to transitions from other states  $m$  to  $n$  and decreases due to transitions from the

state  $n$  to other states  $m$ . The second equality is less intuitive and it relies on the doubly-stochastic nature of the transition rates.

The master equation describes evolution of the density matrix between two stationary states as a result of some dynamical process (pulse). A natural question to ask is what will happen if we repeatedly drive the system allowing it relax between the pulses. This will be an analogue of the quasi-static process with the important difference that we do not need to assume that the system is coupled to some external heat reservoir. The first question to understand is existence of the stationary distribution under this evolution, i.e. the distribution which does not change under the doubly stochastic evolution, i.e.

$$\rho_{nn} = \rho_{nn} + \sum_m p_{m \rightarrow n} (\rho_{nn} - \rho_{mm}) \quad (\text{V.27})$$

Looking carefully into this equation we see that there is indeed an attractor, which is constant probability distribution  $\rho_{nn} = \text{const}$ , which is simply the infinite temperature state. This result means, for example, that if we start from a 3-level isolated system with  $1/3$  occupation probability for each level then this distribution can not be changed by applying an arbitrary external pulse or sequence of pulses. Let us also note that the infinite temperature state is also the maximum entropy state. Next let us show that this uniform distribution is an attractor (and generically the only attractor) for the doubly-stochastic dynamics. In order to prove this let us introduce the distance between the uniform distribution  $\rho_{nn}^\infty = 1/\mathcal{N}$ , where  $\mathcal{N}$  is the Hilbert space size, and the current distribution  $\rho_{nn}$  and show that this distance can not increase. It is convenient to define the distance between the two distributions using the language of the information theory, known as the Kullback - Leibler (KL) divergence (also known as the relative entropy):

$$D(p||q) = \sum_n p_n \log \left( \frac{p_n}{q_n} \right). \quad (\text{V.28})$$

The KL divergence is non-negative ( $D(p||q) \geq 0$ ) and it is equal to zero only if  $q_n = p_n$ . This statement is known as the Gibbs inequality. To prove this statement we can extremize the function

$$D(p||q) + \lambda \sum_n (q_n - 1) \quad (\text{V.29})$$

with respect to  $q_n$ , where we introduced the Lagrange multiplier  $\lambda$  to enforce the probability conservation. Then we find

$$-\frac{p_n}{q_n} + \lambda = 0, \quad (\text{V.30})$$

which immediately implies that  $q_n = p_n$ . The fact that this is the minimum, not the maximum, trivially follows from e.g. observing the second derivatives of Eq. (V.29) are non-negative.

Let us now prove that the KL divergence between the distribution  $\rho_n$ <sup>2</sup>. Note that for the infinite temperature distribution this KL divergence or the relative entropy is also the entropy difference between that of the infinite temperature state and of the distribution  $\rho_n$ . Indeed

$$D(\rho||\rho^\infty) = \sum_n \rho_n \log(\rho_n \mathcal{N}) = \log(\mathcal{N}) - S(\rho) \quad (\text{V.31})$$

So the statement that the distance between  $\rho$  and  $\rho^\infty$  decreases is simply equivalent to the second law of thermodynamics for an isolated system stating that as a result of arbitrary dynamical processes its entropy should either increase or stay constant. To proof of the entropy increase relies on the Jensen's inequality that for any convex function  $\phi(x)$  such that

$$\frac{d^2\phi(x)}{dx^2} \geq 0 \quad (\text{V.32})$$

we have

$$\phi\left(\sum_n p_n x_n\right) \leq \sum_n p_n \phi(x_n), \quad (\text{V.33})$$

where  $p_j$  are arbitrary non-negative numbers satisfying  $\sum_n p_n = 1$ . Basically the Jensen's inequality states that for arbitrary probability distribution the function of the mean is less than the mean of the function. Let us sketch the proof of the Jensen's inequality. First assume that the probability distribution  $p_{\{n\}}$  has only two entries  $p_1$  and  $p_2 = 1 - p_1$ . Then Jensen's inequality can be trivially seen from plotting the convex function and observing that it is always below the straight line connecting the points  $x_1$  and  $x_2$ . For higher number of entries we can easily extend this proof

$$\begin{aligned} \phi\left(p_1 x_1 + (1 - p_1) \sum_{n \geq 2} \frac{p_n}{1 - p_1} x_n\right) &\leq p_1 \phi(x_1) + (1 - p_1) \phi\left(\sum_{n \geq 2} \frac{p_n}{1 - p_1} x_n\right) \\ &\leq p_1 \phi(x_1) + (1 - p_1) \frac{p_2}{1 - p_1} \phi(x_2) + (1 - p_1 - p_2) \phi\left(\sum_{n \geq 3} \frac{p_n}{1 - p_1 - p_2} x_n\right) \leq \dots \end{aligned} \quad (\text{V.34})$$

Now let us apply this inequality to the function  $\phi(x) = x \log(x)$ , which is clearly convex, using  $x_m = \rho_m^0$  and  $p_m = p_{m \rightarrow n}$  for fixed  $n$ . Note we need double-stochasticity to satisfy  $\sum_m p_m = 1$ . Then from the Jensen's inequality we find

$$\rho_n \log(\rho_n) = \sum_m p_{m \rightarrow n} \rho_m^0 \log\left(\sum_l p_{l \rightarrow n} \rho_l^0\right) \leq \sum_m p_{m \rightarrow n} \rho_m^0 \log(\rho_m^0) \quad (\text{V.35})$$

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<sup>2</sup> To shorten notations we denote  $\rho_n \equiv \rho_{nn}$

Summing this relation over  $n$  we find that

$$-S(\rho) = \sum_n \rho_n \log(\rho_n) \leq \sum_m \rho_m^0 \log(\rho_m^0) = -S(\rho^0) \Rightarrow S(\rho) \geq S(\rho^0), \quad (\text{V.36})$$

which is exactly the statement that under the doubly-stochastic evolution the entropy can not decrease. This means that the stationary flat distribution corresponding to the maximum entropy is the attractor of such evolution. Moreover it is the only attractor unless transition rates  $p_{m \rightarrow n}$  to certain states are identically equal to zero due to e.g. symmetry reasons. Note that in this proof we never relied on ergodicity or ETH, the entropy increase is a general property of any double-stochastic evolution.

From this result we immediately recover the famous Boltzmann's H-theorem for weakly interacting particles. Indeed assume that between collisions the particles are allowed to relax to the diagonal ensemble of the noninteracting Hamiltonian:

$$H_{kin} = \sum_j \frac{p_j^2}{2m} \quad (\text{V.37})$$

In this ensemble the eigenstates factorize  $|\psi^{(n)}\rangle = \prod_j |\psi_j^{(n)}\rangle$  and hence the entropy is the sum of entropies of individual particles (this is true whether particles are fermions, bosons or distinguishable classical particles). Then if we turn on interactions for a period of time and then let the particles to relax again in the non-interacting basis as we just proved the entropy increases. But these assumptions about relaxation (loss of phase memory) are precisely the assumptions of the kinetic theory within which H-theorem is proven. So we proved the H-theorem even without need to write down explicit kinetic equations. I.e. we proved it for any type of interactions as long as collisions between particles are uncorrelated.

Now let us exploit another property of the unitary evolution: the existence of the time reversal transformation. Recall that for time independent Hamiltonians from the Schrödinger equation

$$i\hbar\partial_t|\psi\rangle = H|\psi\rangle \quad (\text{V.38})$$

it follows that  $t \rightarrow -t$  is equivalent to  $|\psi\rangle \rightarrow |\psi^*\rangle$  and  $H \rightarrow H^*$ . We are considering in general a time dependent process, where  $H(t)$  changes according to some protocol in the interval  $t \in [0, t_0]$ . Then by the time reversal Hamiltonian we will understand  $H_T(t) = H^*(t_0 - t)$ . It is then clear that the complex conjugate of the wave function evolves under the time reversal Hamiltonian  $\tilde{H}$ . In particular, this implies that

$$\langle n(t_0)|U|m(0)\rangle^* = \langle m(0)|\tilde{U}|n(t_0)\rangle, \quad (\text{V.39})$$

where  $\tilde{U}$  is the evolution operator with the time-reversal Hamiltonian  $\tilde{H}$ . The arguments  $t$  and  $0$  in the basis vectors imply that they are taken with respect to the initial and final Hamiltonians. Note that if in each moment of time the Hamiltonian  $H(t)$  respects time-reversal symmetry then one can formally change the time propagation direction  $t \rightarrow -t$  without changing the transition probability (this amounts to the reverse process to occur in the interval  $[-t_0, 0]$  with the forward moving time). Also in this case time reversal of the Hamiltonian is simply time reversal of the quench protocol  $\tilde{H}(t) = H(t_0 - t)$ . From the equation above we find a very important property of the transition probabilities

$$p_{m \rightarrow n} = \tilde{p}_{n \rightarrow m}, \quad (\text{V.40})$$

where tilde implies the transition probability for the time-reversal process (as before we imply that indexes  $m$  and  $n$  correspond to the initial and final Hamiltonians). In particular, for systems with the time reversal symmetry and the time symmetric protocols:  $H(t) = H(t_0 - t)$  we have  $p_{m \rightarrow n} = p_{n \rightarrow m}$ . This equality also holds for the transition probabilities computed within the first order of the time-dependent perturbation theory (e.g. within the Fermi-Golden rule) even if the protocol is not symmetric. Mathematically the result (V.40) states that the transpose of the doubly stochastic matrix is also a doubly stochastic matrix. Thus the transpose of the transition rate matrix can be viewed as the rate matrix of some other process, which for unitary evolution is the time reversal process.

### 1. Jarzynski and Crooks relations.

The microscopic detailed balance (V.40) leads to very powerful fluctuation theorems. As earlier we first consider initial Gibbs distribution and then show how one can generalize the results to arbitrary initial states using the assumptions of ETH. The fluctuation theorems deal with the probability of doing work during some dynamical process during which the system can be considered isolated. By definition in this case the work is equal to the total energy change during this process so the probability of doing work  $W$  is

$$\begin{aligned} P(W) &= \sum_{n,m} \frac{1}{Z(\lambda_i)} e^{-\beta E_m(\lambda_i)} p_{m \rightarrow n} \delta(E_n(\lambda_f) - E_m(\lambda_i) - W) \\ &= \frac{Z(\lambda_f)}{Z(\lambda_i)} \sum_{n,m} \frac{1}{Z(\lambda_f)} e^{-\beta E_n(\lambda_f) + \beta W} \tilde{p}_{n \rightarrow m} \delta(E_m(\lambda_i) - E_n(\lambda_f) + W) = \frac{Z(\lambda_f)}{Z(\lambda_i)} e^{\beta W} \tilde{P}(-W). \end{aligned} \quad (\text{V.41})$$

Using that by definition  $Z(\lambda) = \exp[-\beta F(\lambda)]$ , where  $F(\lambda)$  is the Free energy of the system we rewrite the result above in the form known as the Crooks relation (G. Crooks, 1998):

$$P(W)e^{-\beta W} = \tilde{P}(-W)e^{-\beta \Delta F}, \quad (\text{V.42})$$

where  $\Delta F \equiv F(\lambda_f) - F(\lambda_i)$  is the equilibrium free energy difference between the final and initial Hamiltonians. Clearly for the cyclic processes  $\lambda_f = \lambda_i$  we have  $\Delta F = 0$  and the Crooks relation has a particularly simple form. In words, the Crooks relations states that the probability of doing a work  $W$  during some dynamical process is related to the probability of doing the negative of the same work (starting from the Gibbs distribution with the same temperature) in the time reversal process times the factor  $\exp[\beta W - \beta \Delta F]$ . Integrating the Crooks relation we find the Jarzynski relation or the Jarzynski equality (C. Jarzynski, 1997):

$$\langle \exp[-\beta W] \rangle = \exp[-\beta \Delta F]. \quad (\text{V.43})$$

This simple relation is one of few known non-equilibrium relations. It states that the expectation value of exponent of the product of the negative work multiplied and the inverse temperature gives essentially an exponential of the free energy difference. I.e. the Jarzynski relation connects the dynamical quantity, work, which depends on the details of the protocol and the equilibrium quantity, which is the free energy. In particular, this relation can be used to measure free energy differences in small systems by measuring the work. In large systems the Jarzynski relation is typically not very useful because the function  $\exp[-\beta W]$  will be dominated by very rare events where the work is small.

Now let us derive similar relations without making assumptions about the Gibbs distribution. Specifically we analyze the work rate,  $R(w)$ , which is defined as the probability of doing the work  $W$  starting from a given energy eigenstate  $|m\rangle$ . By definition the latter is given by

$$R(E_m, W) = \sum_{n \neq m} p_{m \rightarrow n} \delta(E_n - E_m - W) = \int dE_n \Omega_{\lambda_f}(E_n) p_{m \rightarrow n} \delta(E_n - E_m - W) = \bar{p}_{m \rightarrow n} \Omega_{\lambda_f}(E_m + W), \quad (\text{V.44})$$

where  $\bar{p}_{m \rightarrow n}$  is the mean transition rate between the energy levels. According to ETH in ergodic systems the transition rates between nearby levels are very similar to each other and thus  $\bar{p}_{m \rightarrow n}$  is a typical microscopic transition rate. Now let us analyze the work rate for the time reversal process where we start at energy  $E_m + W$  and do the negative work  $-W$ . Using similar considerations we find

$$\tilde{R}(E_m + W, -W) = \bar{p}_{n \rightarrow m} \Omega(E_m) = \bar{p}_{m \rightarrow n} \Omega(E_m) \quad (\text{V.45})$$

Comparing these two relations we find that

$$\begin{aligned} R(E_m, W)\Omega_{\lambda_i}(E_m) &= \tilde{R}(E_m + W, -W)\Omega_{\lambda_f}(E_m + W) \\ \Rightarrow R(E_m, W)e^{S(\lambda_i, E_m) - S(\lambda_f, E_m + W)} &= \tilde{R}(E_m + W, -W). \end{aligned} \quad (\text{V.46})$$

If we apply this relation to an infinitesimal process where  $W$  is small and  $\lambda_f - \lambda_i = \Delta\lambda$  is also small then we can expand the entropy difference in the expression above and find

$$R(E_m, W)\exp[-\beta\mathcal{F}_\lambda\Delta\lambda - \beta W] = \tilde{R}(E_m + W, -W) \quad (\text{V.47})$$

Integrating both parts with respect to  $W$  and using that  $R(E, W)$  only weakly depends on  $E$  we find

$$\langle \exp[-\beta W] \rangle \approx \exp[-\beta\Delta F], \quad (\text{V.48})$$

where we used that

$$\Delta F = -S\Delta T - \mathcal{F}_\lambda\Delta\lambda \quad (\text{V.49})$$

so that at constant temperature  $\Delta F = -\mathcal{F}_\lambda\Delta\lambda$ . Essentially we got the Jarzynski relation dropping the assumption about the Gibbs distribution. Instead we had to rely on the ETH assumptions that the transition rates to all the levels within a narrow energy shell are very close to each other. Also now this relation only holds approximately for processes where work and changes in the coupling constant are small. Nevertheless, as we will see in the next section, this relation is very powerful allowing us to find fundamental drift diffusion relations (Einstein relations) for driven isolated systems.

### C. Energy drift and diffusion in driven systems. Fokker-Planck equation and Einstein relations.

Fluctuation theorems outlined in the previous section can be used to understand energy flow in a system subject to an external noise, i.e. to external uncorrelated (in time) external drive. This setup is very analogous to the heating in a microwave oven. The heating there occurs not due to the coupling to external heat reservoir (like in conventional oven) but rather due to applying time-dependent electro-magnetic field. Even though this field is periodic in time, typical relaxation time in the systems is much faster than the pulse frequency so our assumption about uncorrelated perturbations is valid there. We will assume that this process is quasi-static, i.e. the system relaxes to the diagonal ensemble between the pulses and that the energy change (i.e. work on the system)

within each pulse is small (see Fig. 22). Thus we effectively consider a quasi-static process, where at each moment of time the system is described by a local equilibrium (diagonal ensemble), which does not have to be canonical. We can anticipate that the heating of the system should be described by the drift-diffusion equation, where the drift corresponds to the average energy flow and the diffusion to the energy spread. In general drift and diffusion are uncorrelated, but as we will see the fluctuation theorems put strong constraints between the two.

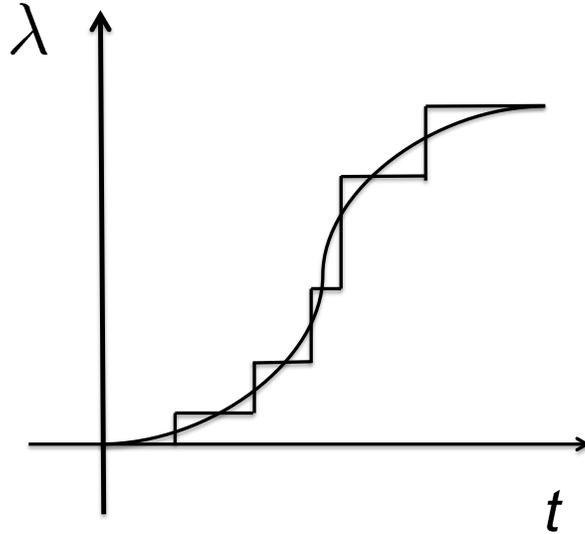


FIG. 22 Schematic representation of a continuous process as a series of jumps following relaxation. This approximation can be rigorously justified within the (adiabatic) time-dependent perturbation theory if the relaxation time (to the diagonal ensemble) in the system is short compared to the characteristic time scale associated with change in  $\lambda$

### 1. Derivation of the Fokker-Planck equation.

Now let us use the fluctuation theorems to derive the evolution of the energy distribution in a closed system, which undergoes the quasi-static process. To simplify the derivation we will assume that the process is cyclic. For the non-cyclic process one simply needs to split the energy change into the adiabatic deterministic part, which reflects the possible shift of energy levels with  $\lambda$  and the heating, which will be described by the same equation as in the cyclic process. For this purpose we rewrite the master equation

$$\rho_n(t + \delta t) = \sum_m p_{m \rightarrow n} \rho_m(t) \quad (\text{V.50})$$

as an equation for the energy distribution. For small enough  $\delta t$  the transition rates  $p_{m \rightarrow n}$  should scale as  $\delta t$ . We will implicitly use the fact that the probabilities to occupy energy states  $\rho_n$  are the smooth functions of  $n$ . Multiplying both sides of the equation by  $\Omega(E)$  and using that  $\rho_n(E)\Omega(E) = P(E)$  we find

$$P(E, t + \delta t) = \int dW R(E - W, W) P(E - W, t) \quad (\text{V.51})$$

where  $W = E_n - E_m$  is the work and  $R(E - W, W) = p_{m \rightarrow n} \Omega(E_n)$  is the transition rate introduced earlier. Because by the assumptions of the quasi-static process the work at each step is small  $W \propto \delta t$  we can utilize the fact that  $P(E)$  and  $R(E, W)$  are very slow functions of  $W$  and perform the Taylor expansion:

$$P(E - W, t) \approx P(E) - W \partial_E P(E) + \frac{W^2}{2} \partial_{EE}^2 P(E) + \dots, \quad R(E - W, W) \approx R(E) - W \partial_E R(E, W) + \dots$$

Then we find

$$\begin{aligned} \partial_t P(E, t) = & -\langle \delta W \rangle \partial_E P(E) - P(E) \partial_E \langle \delta W \rangle \\ & + \frac{1}{2} \langle \delta W^2 \rangle \partial_{EE}^2 P(E) + \partial_E P(E) \partial_E \langle \delta W^2 \rangle + \frac{1}{2} P(E) \partial_{EE}^2 \langle \delta W^2 \rangle + \dots, \end{aligned} \quad (\text{V.52})$$

where we use  $\langle \delta W \rangle$  instead of  $\langle W \rangle$  to emphasize that the average work is small, proportional to  $\delta t$ . And finally let us note that

$$\langle \delta W^2 \rangle = \langle \delta W^2 \rangle_c + \langle \delta W \rangle^2$$

Because  $\langle \delta W \rangle \propto \delta t$  the last term is of the order of  $\delta t^2$  and can be skipped. Introducing the standard notations

$$A(E) = \frac{\langle \delta W \rangle}{\delta t}, \quad B(E) = \frac{\langle \delta W^2 \rangle_c}{\delta t}, \quad (\text{V.53})$$

which play the role of the energy drift and diffusion we rewrite the equation for  $P$  in the following form

$$\partial_t P(E) = -\partial_E [A(E)P(E)] + \frac{1}{2} \partial_{EE}^2 [B(E)P(E)]. \quad (\text{V.54})$$

This equation is precisely the Fokker-Planck equation for the energy distribution. In general the drift and diffusion coefficients are independent functions of energy, but as we will see next, fluctuation relations put strong constraints on these coefficients.

## 2. Einstein relations between drift and diffusion.

Let us first present a very simple derivation of the drift-diffusion relations, which is very similar to the standard derivation of the Einstein's relations for diffusion in space. The Fokker-Planck equation (V.54) should give the same stationary solution as the original master equation. In the previous section we showed that the attractor of the master equation for the unitary dynamics is the uniform distribution. This means that the locally-uniform distribution should be also a fixed point of the Fokker-Planck equation. But  $\rho_n = \text{const}$  implies  $P(E) = C\Omega(E)$ . Substituting this distribution into Eq. (V.54) we find

$$0 = -\partial_E[A(E)\Omega(E)] + \frac{1}{2}\partial_{EE}^2[B(E)\Omega(E)] \Rightarrow A(E)\Omega(E) + \frac{1}{2}\partial_E[B(E)\Omega(E)] = \text{const.} \quad (\text{V.55})$$

It is clear that the constant term must be zero because if we go to the energies where there are no states  $\Omega(E) \rightarrow 0$ , e.g. approach the ground state energy, we do not expect  $A(E)$  and  $B(E)$  to exponentially blow up. Therefore we see that the following relation should hold

$$A(E) = \frac{\beta}{2}B(E) + \frac{1}{2}\partial_E B(E) \quad (\text{V.56})$$

In large systems, where the energy is extensive the second term is clearly suppressed and therefore we get

$$A(E) \approx \frac{\beta}{2}B(E) \quad (\text{V.57})$$

This result actually states that the unitarity of the evolution and ergodicity put very strong constraint on energy drift and diffusion and that for any quasi-static process energy drift (heating rate) is uniquely related to the energy diffusion. This result also represents the differential form of the second law of thermodynamics in the Thompson form. Because  $B$  is non-negative by definition it guarantees that the average work for a small cyclic process is non-negative provided that the temperature is positive. In the derivation of this relation we made some implicit assumptions. In particular, we assumed that even if  $\rho_{nn}$  is constant locally in energy then the corresponding Fokker-Planck equation should be stationary. This is only the case if the work has a narrow distribution, i.e. we do not allow rare processes which significantly change the energy of the system. Next we will give a more formal derivation of this relation using the fluctuation theorems and see more rigorous conditions for the validity of Eq. (V.56).

Now let us give a more formal microscopic derivation of this result using Eq. (V.46). Again for simplicity we assume that we are dealing with the cyclic process so that  $\Delta F = 0$ . Also to simplify

the derivation we will assume that the process is symmetric in time so that  $R(E, W) = \tilde{R}(E, W)$ . This assumption can be relaxed. Expanding slow functions of work up to the second order in  $W$  we find

$$R(E_m, W) \exp \left[ -\beta W - \frac{1}{2} \frac{\partial \beta}{\partial E} W^2 \right] \approx R(E_m, -W) + W \partial_E R(E_m, -W) + \frac{W^2}{2} \partial_{EE} R(E_m, -W) \quad (\text{V.58})$$

Integrating both parts of this equation over the work  $W$  and again using that  $\langle W \rangle \propto \delta t$  we find

$$\left\langle \exp \left[ -\beta W - \frac{1}{2} \frac{\partial \beta}{\partial E} W^2 \right] \right\rangle \approx 1 - \partial_E \langle W \rangle + \frac{1}{2} \partial_{EE} \langle W^2 \rangle_c \quad (\text{V.59})$$

Now let us take the logarithm of this equation neglecting all the terms proportional to  $\delta t^2$  like  $\langle W \rangle^2$  and  $(\partial_E \langle W \rangle)^2$  and denoting as before  $A(E) = \langle W \rangle$  and  $B(E) = \langle W^2 \rangle_c$ . Then we find

$$-\beta A + \frac{\beta^2}{2} B - \frac{1}{2} \frac{\partial \beta}{\partial E} B \approx -\partial_E A + \frac{1}{2} \partial_{EE} B \quad (\text{V.60})$$

It is easy to check that we recover the relation V.56. But now we know the requirements for this relation to hold. The first requirement that the work is indeed small in a sense that expansion of the entropy into the Taylor series is justified

$$\left| \frac{\partial \beta}{\partial E} \langle W \rangle^2 \right| \ll \langle W \rangle \Leftrightarrow A\tau \ll TC_V, \quad (\text{V.61})$$

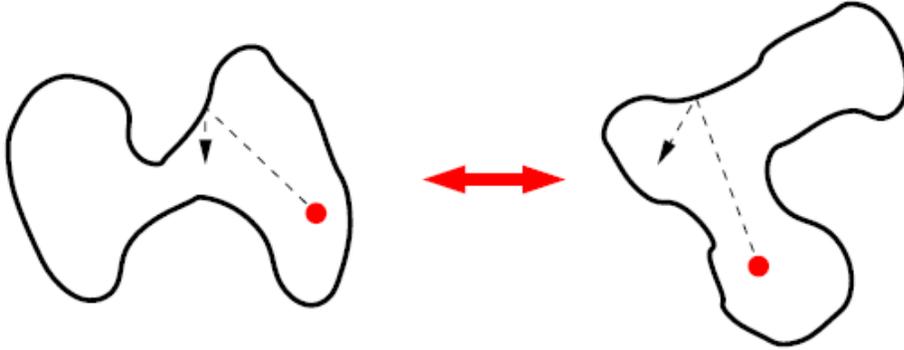
where  $\tau$  is the relaxation time in the system, which defines the minimum value of  $\delta t$  in our quasi-static approach. In other words the energy added to the system during the relaxation time should be small compared to  $TC_V$ . For continuous processes where  $A \propto dt$  this requirement is always satisfied. But we can also consider discrete processes and still be OK. Note that the specific heat  $C_V = T^2 \partial_T E$  is extensive so the ‘‘small’’ work condition can be satisfied for global processes where the energy change is extensive. The second more subtle condition is that the third cumulant in the expansion of the LHS of Eq. (V.59) must be small, which brings are to the requirement that

$$\beta^2 \langle W^3 \rangle_c \ll \beta \langle W \rangle \Leftrightarrow \langle W^3 \rangle_c \ll T^2 \langle W \rangle. \quad (\text{V.62})$$

This requirement physically means that not only we have a small average work, but also this work is done by small increments. For example for a spin one half particle flipping one spin with a small probability guarantees a small work, but the third cumulant of work is not small unless the temperature is large compared to the level splitting. So typically the last requirement implies that we work in a suitable high-temperature limit.

### 3. Application: heating of a particle in a fluctuating chaotic 2D cavity

Let us apply the formalism above to a very simple problem of a classical particle moving in a chaotic cavity with fluctuating boundaries (C. Jarzynski, 1993). The setup is presented in Fig. V.C.3 The assumption that the cavity is chaotic implies that there are no correlations



between consequent collisions. Alternatively we can assume that we move the boundary inducing an energy change then wait until the system relaxes to the stationary (diagonal) distribution and then continue. We also assume for simplicity that we preserve the volume (area) of the cavity so that the density of states does not change in time and we should not worry about adiabatic terms.

First we compute the energy drift and diffusion rates microscopically. Denote the velocity of the particle as  $\vec{v}$  and velocity of the wall as  $\vec{V}/2$ . Because we deal with volume preserving perturbations  $\vec{V}/2$  averaged either over time or over the area of the cavity is zero. Then as we know from elementary mechanics as a result of the collision with the wall the component of the velocity of the particle changes according to

$$\vec{v} \rightarrow \vec{v} - \vec{V} \quad (\text{V.63})$$

This means that the energy change of the particle per collision is

$$m \frac{(\vec{v} - \vec{V})^2}{2} - m \frac{v^2}{2} = m\vec{v}\vec{V} + \frac{m\vec{V}^2}{2} = \pm m v_{\perp} V + \frac{mV^2}{2}, \quad (\text{V.64})$$

where  $v_{\perp}$  is the velocity component orthogonal to the wall and parallel to  $\vec{V}$  with the convention that the plus sign implies the wall and the particle move towards each other and the minus sign implies that the particle and the wall move in the same direction. The probability of collision (per unit area) is proportional to the relative velocity of the particle towards the wall. For the collisions where the velocity of the particle increases the latter is

$$p_{>} = \frac{c}{2}(v_{\perp} + V/2)\delta t, \quad (\text{V.65})$$

where  $c$  is the proportionality constant (for many particles it is proportional to the particle's density) and we inserted a factor of one half for convenience. On the other hand for collisions, where the velocity of particles decreases the probability of collision is

$$p_{<} = \frac{c}{2}(v_{\perp} - V/2)\delta t. \quad (\text{V.66})$$

We will be interested in slow velocity regime of the wall  $V \ll \langle \vec{v} \rangle$ , where the process can be thought of as diffusive, so we will ignore rare situations where  $v_{\perp} < V$ . The average heating rate (energy drift) is thus

$$A = \frac{mV^2}{2}\overline{(p_{>} + p_{<})} + mV\overline{(v_{\perp}p_{>} - v_{\perp}p_{<})}, \quad (\text{V.67})$$

where the overline implies averaging over  $v_{\perp}$ . Using explicit expressions for  $p_{>}$  and  $p_{<}$  we find that both terms give identical contributions and thus

$$A(E) = mV^2\langle v_{\perp} \rangle = mV^2\frac{1}{2\pi}\int_0^{\pi} d\phi \sin(\phi)\sqrt{\frac{2E}{m}}c\delta t = \frac{1}{\pi}\sqrt{2mEV^2}c\delta t. \quad (\text{V.68})$$

To compute the fluctuations of energy change we note that

$$\delta E^2 = \left( m\frac{(\vec{v} + \vec{V})^2}{2} - m\frac{v^2}{2} \right)^2 = m^2v_{\perp}^2V^2 \pm mV^3v_{\perp} + \frac{m^2V^4}{4} \quad (\text{V.69})$$

Since by assumption  $v_{\perp} \gg V$  we can ignore the last two terms in the equation and find that

$$B(E) \approx m^2V^2\overline{v_{\perp}^2(p_{>} + p_{<})} = m^2V^2\left(\frac{2E}{m}\right)^{3/2}\frac{1}{2\pi}c\delta t\int_0^{\pi} d\phi \sin^3(\phi) = \frac{1}{\pi}\sqrt{2E^3}mc\delta t\frac{4}{3} \quad (\text{V.70})$$

So we found the following expressions between the drift and the diffusion coefficients:

$$A(E) = C\sqrt{E}, \quad B(E) = \frac{4}{3}CE^{3/2} \quad (\text{V.71})$$

Now let us check if these satisfy the Einstein relation (V.56). Recall that  $\beta$  entering this relation is simply derivative of the logarithm of the density of states. Since we are dealing with a single particle, this will be a single particle density of states, which is constant in two dimensions  $\Omega(E) = \text{const}$ . Therefore by definition  $\beta(E) = \partial_E \log(\Omega(E)) = 0$ . Thus the Einstein relation reads

$$2A(E) = \partial_E B(E) \quad (\text{V.72})$$

It is obvious that the coefficients  $A(E)$  and  $B(E)$  satisfy these relations. So in fact there was no need of doing these relatively elaborate calculations, it was sufficient to note that  $A(E)$  must be proportional to  $\sqrt{E}$ , which is obvious because the average number of collisions is proportional to the magnitude of  $v_{\perp}$ . Then the Einstein relation immediately fixes the energy dependence of  $B(E)$ .

With the relation V.71 in hand we can rewrite the Fokker-Planck equation describing the heating process as

$$\partial_t P(E, t) = -C \partial_E (\sqrt{E} P(E, t)) + \frac{2}{3} C \partial_{EE} (E^{3/2} P(E, t)) \quad (\text{V.73})$$

Upon careful look we see that if we scale  $t$  as  $\sqrt{E}$  then the equation above becomes dimensionless. We can always fix the constant  $C$  at arbitrary number by redefining the time units. It is convenient to choose  $C = 6$ .

$$P(E, t) = \frac{1}{2\sqrt{Et}} f(\sqrt{E}/t) \equiv \frac{1}{2\sqrt{Et}} f(\xi) \quad (\text{V.74})$$

This form of  $P$  is dictated by the normalization condition

$$1 = \int_0^\infty P(E, t) dE = \int_0^\infty d(\sqrt{E}/t) f(\sqrt{E}/t) = \int_0^\infty d\xi f(\xi). \quad (\text{V.75})$$

Substituting this ansatz into the Fokker-Planck equation above we find

$$-\frac{1}{2\sqrt{Et}^2} f - \frac{1}{2t^3} f' = -\frac{3}{2\sqrt{Et}^2} f' + \frac{2}{\sqrt{Et}^2} f' - \frac{1}{2\sqrt{Et}^2} f' + \frac{1}{2t^3} f'' \quad (\text{V.76})$$

or equivalently

$$\xi f'' + \xi f' + f = 0 \quad (\text{V.77})$$

It is easy to check that this equation is solved by

$$f(\xi) = \xi \exp[-\xi]. \quad (\text{V.78})$$

So we see that the energy distribution asymptotically acquires the universal form

$$P(E, t) = \frac{1}{2t^2} \exp\left[-\frac{\sqrt{E}}{t}\right]. \quad (\text{V.79})$$

This is clearly not the Gibbs distribution, but it shares some of its properties. In particular, it decays with energy faster than any power law so that all the energy moments are well defined. This distribution is definitely wider than the Gibbs distribution so it can be interesting to compare the widths of the two. Computing the first and second moments of the energy we find

$$\langle E \rangle = \int_0^\infty dE E P(E, t) = t^2 \int_0^\infty d\xi \xi^3 \exp[-\xi] = 6t^2, \quad \langle E^2 \rangle = t^4 \int_0^\infty d\xi \xi^5 \exp[-\xi] = 120t^4. \quad (\text{V.80})$$

Therefore

$$\delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2} = \sqrt{84} t^2 = \sqrt{\frac{7}{3}} \langle E \rangle \approx 1.53 \sqrt{E} \quad (\text{V.81})$$

On the other hand for the Gibbs ensemble we have

$$\delta E = \langle E \rangle, \quad (\text{V.82})$$

which follows from  $\delta E = T^2 C_V$ ,  $C_V = 1$  and  $T = \langle E \rangle$ . So we see that the distribution we are getting is approximately a factor 1.5 wider than the Gibbs distribution. If we now assume that we are dealing with a non-interacting gas of many-particles (such that time scales for heating are faster than time scales for re-equilibration of the gas) then the total energy distribution will become Gaussian due to the central limit theorem but the width will remain a factor of 1.5 bigger than the equilibrium Gibbs width. Since we generated a non-equilibrium distribution, it should also have lower entropy than the equivalent Gibbs one. For one particle in two-dimensions (with the constant density of states)

$$\begin{aligned} S(t) &= - \int_0^\infty dE P(E) \log(P(E)) = \log(2t^2) + \int_0^\infty d\xi \xi^2 \exp[-\xi] = \log(2e^2 t^2) \\ &= \log\left(\frac{2e^2}{6} \langle E \rangle\right) \approx 1 + \log[0.906 \langle E \rangle]. \end{aligned} \quad (\text{V.83})$$

While for the exponential Gibbs distribution the entropy is

$$S_{eq} = - \int_0^\infty dE \frac{E}{\langle E \rangle} e^{-E/\langle E \rangle} \log\left(\frac{1}{\langle E \rangle} e^{-E/\langle E \rangle}\right) = 1 + \log[\langle E \rangle] \quad (\text{V.84})$$

So we see that the non-equilibrium heating results in the entropy smaller by  $-\log[0.906] \approx 0.1$  than in the equilibrium case. For many particles this gives an extensive entropy gain equal to  $0.1N$ . This entropy gain can be used, e.g. to build more efficient heat engines and even to beat the fundamental Carnot bound in some cases. Indeed this fundamental bounds are related to the requirement that the entropy increase in the work body of the engine results in minimal losses of energy to the bath, which is  $T\Delta S$ . Smaller entropy increase results in lower bound for energy losses and thus can be used, at least in principle, to construct more efficient non-ergodic engines.

It is interesting that the same setup describes the energy distribution in a Lorentz gas (L. D'Alessio and P. Krapivsky, 2011). This gas is defined as a system of noninteracting light particles colliding with a dense gas of heavy particles moving with some average velocity  $V$ . If the ratio of the masses is very large than there is no effect of the collision on heavy particles so the latter serve precisely the role of moving boundaries. So the resulting kinetic equation for light particles is exactly equivalent to the Fokker-Planck equation we discussed above. Let us point that the ensemble of heavy particles can be viewed as an infinite temperature heat bath. Indeed the average energy of heavy particles  $M\langle V^2 \rangle/2$ , which defines temperature, diverges in the limit  $M \rightarrow \infty$  at

fixed  $\langle V^2 \rangle$ . Thus we see from this simple example that external quasi-static driving of an isolated system is equivalent to the coupling to the infinite temperature bath. In the next section we will see that this statement is actually very general.

#### 4. Exercises

1. Consider a setup of Sec. V.C.3 but in  $d$ -dimensions. Repeat the microscopic derivation of the drift and diffusion coefficients  $A(E)$  and  $B(E)$  in the slow limit for the wall and make sure that they satisfy the Einstein equation with the appropriate density of states. Show that in the large  $d$  limit ( $d \gg 1$ ) the term  $\partial_E B/2$  in the Einstein relation becomes negligible. Using a similar scaling ansatz solve the Fokker-Planck equation and show that at large dimensions  $d \gg 1$  it looks Gaussian but still with non-equilibrium width. *Dimensionality here plays the role of the phase space dimensions so large dimensionality is similar to having many particles.* Find the entropy of the resulting distribution (remember to take into account the correct density of states) and compare it with the equilibrium entropy at the same mean energy.

#### D. Doubly stochastic evolution in open systems. Drift-diffusion and Onsager relations.

So far we focused our attention to isolated systems subject to time-dependent external perturbations. Next we move to open systems. To describe those we do not need to develop a new framework. We will represent an open system as a system  $A$  coupled to another system  $B$  (see Fig. V.D). If the system  $B$  is much bigger than the system  $A$  then it is usually thought of as a heat

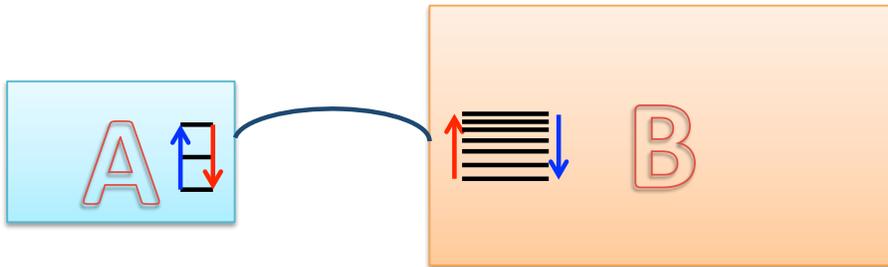


FIG. 23 Schematic representation of an open system as a system  $A$  weakly coupled to another system  $B$ .

bath. For our purposes this assumption is too restrictive, e.g. systems  $A$  and  $B$  can be comparable. But we will assume that the system  $B$  is ergodic in a sense that it satisfies the assumptions of ETH. One can extend our considerations to the situations where the system  $A$  is coupled to more than

one system, e.g. two heat reservoirs at different temperatures or the system  $A$  is externally driven in addition to the coupling to  $B$ . The analysis of such situations will be very similar but will be beyond the scope of these notes. The Hamiltonian describing the total system can be schematically written as

$$H = H_A + H_B + H_{AB}, \quad (\text{V.85})$$

where  $H_A$  is the Hamiltonian, which includes only degrees of freedom of the system  $A$ , likewise  $H_B$  includes only the degrees of freedom of the system  $B$ , and  $H_{AB}$  describes the coupling between then two systems. Initially systems  $A$  and  $B$  are not in equilibrium with each other. We will assume that the process of equilibration is quasi-static in the same way as depicted in Fig. 22, where the coupling  $H_{AB}$  is turned on for a short time then turned off. In between the systems  $A$  and  $B$  equilibrate within themselves, i.e. relax to the diagonal ensemble, and then the process is repeated. Of course in reality this turning on and turning off is not needed and one can use instead a continuous derivation. The only requirement we need is that the relaxation time within the systems  $A$  and  $B$  is much faster than the characteristic time scale of relaxation between the systems  $A$  and  $B$ . As we discussed the relaxation to the diagonal ensemble is a simple dephasing and thus it does not rely on ergodicity. So the system  $A$  can be very simple like a single degree of freedom.

#### 1. Microscopic detailed balance for open systems.

Dynamics as a whole is unitary thus we can use the machinery developed in the previous section. Quasi-static assumption means that at each moment of time the density matrix is approximately diagonal in the basis of decoupled Hamiltonian  $H_A + H_B$ . We will also assume for simplicity that the Hamiltonian obeys the time-reversal symmetry. From these assumptions we can conclude that the microscopic transition rates

$$p_{m \rightarrow n, m' \rightarrow n'} = p_{n \rightarrow m, n' \rightarrow m'}, \quad (\text{V.86})$$

where  $m$  and  $n$  denote the eigenstates of  $H_A$  and  $m'$  and  $n'$  denote the eigenstates of  $H_B$ . There is no tilde in this relation because of the time-reversal symmetry. Because the system is not externally driven the total energy in the system is conserved implying that the rates  $p_{m \rightarrow n, m' \rightarrow n'}$  are non zero only if  $E_n^A - E_m^A = E_{m'}^B - E_{n'}^B = W$ . Because we are interested in properties of the system  $A$  we need to define the transition rates within the system  $A$ , i.e. sum over all final states in the system

$B$ . Then we find

$$p_{m \rightarrow n}^A = \sum_{n'} p_{m \rightarrow n, m' \rightarrow n'} \delta(E_{n'}^B - E_{m'}^B + W) = \bar{p}_{m \rightarrow n, m' \rightarrow n'} \Omega_B(E_B - W), \quad (\text{V.87})$$

where  $\bar{p}_{m \rightarrow n, m' \rightarrow n'}$  is the typical transition matrix element and we used ETH assumptions about the system  $B$  stating that all eigenstates of  $B$  are very similar to each other;  $E_B \equiv E_{m'}^B$ . Similarly we find that

$$p_{n \rightarrow m}^A = \bar{p}_{m \rightarrow n, m' \rightarrow n'} \Omega_B(E_B) \quad (\text{V.88})$$

From the expressions above we see that the probabilities of the transition within the system  $A$  are no longer symmetric. Instead they satisfy the new detailed balance relations

$$\frac{p_{m \rightarrow n}^A}{p_{n \rightarrow m}^A} = \frac{\Omega_B(E_B - W)}{\Omega_B(E_B)}, \quad W = E_n - E_m \quad (\text{V.89})$$

If the energy difference  $W$  is small compared to  $TC_V^B$ , which is always the case if the system  $B$  is big then we can expand the density of states in the expression above and find the standard, usually assumed, detailed balance relation

$$\frac{p_{m \rightarrow n}^A}{p_{n \rightarrow m}^A} = \exp[-\beta_B W]. \quad (\text{V.90})$$

It is interesting that in this derivation we did not use any other assumptions than that the process is quasi-static and that the system  $B$  is ergodic i.e. that it satisfies the ETH.

This detailed balance relation for open systems clearly breaks double-stochasticity of the transition rates. Indeed while

$$\sum_n p_{m \rightarrow n}^A = \sum_{n, n'} p_{m \rightarrow n, m' \rightarrow n'} = 1 \quad (\text{V.91})$$

by the probability conservation

$$\sum_m p_{m \rightarrow n}^A = \sum_{m, n'} p_{m \rightarrow n, m' \rightarrow n'} \neq 1. \quad (\text{V.92})$$

Another interesting point we can make is that in the limit  $\beta_B \rightarrow \infty$  we recover doubly stochastic relations for the transition rates in the system  $A$  obtained before for the unitary evolution. So we come to an important conclusion that for quasi-static processes driving with an external field is similar (and in many cases is equivalent) to the coupling to the infinite temperature reservoir. In other words coupling to an infinite temperature system effectively leads to a unitary dynamics, which can be described by some (possibly random) external force acting on the system. It is easy

to check that the detailed balance V.90 leads to the Gibbs distribution to be an attractor of the dynamics. Indeed writing the master equation

$$\rho_n(t + \delta t) = \sum_m p_{m \rightarrow n} \rho_m(t) = \sum_m p_{n \rightarrow m} e^{-\beta_B(E_n^A - E_m^A)} \rho_m(t) \quad (\text{V.93})$$

and requiring that  $\rho_n(t + \delta t) = \rho_m(t)$  leads to the stationary solution:

$$\rho_n = \frac{1}{Z} e^{-\beta E_n^A}. \quad (\text{V.94})$$

Using the Jensen's inequality and using the relative entropy between the current and the Gibbs distribution as a distance between the two distributions (like in the previous section) one can show that this stationary distribution is indeed an attractor for the dynamics (see exercises).

## 2. Fluctuation theorems and Einstein relations for open systems. Onsager relations.

We will now repeat the same program as we did for isolated systems using new detailed balance relations (V.90). Now we assume that the system  $A$  is also ergodic, i.e. also satisfies the ETH. Then microscopic transition rates are not accessible. Instead as before we consider rates for energy change. In this case energy formally changes not due to work but due to heat but as we know already there is no difference, because from the point of view of thermodynamics work is equivalent to the heat coming from the infinite temperature heat bath. So to avoid switching notations we will still use the letter  $W$  to denote the energy change in the system  $A$ . Because of the assumed ergodicity of the system  $A$  the ratio of rates for energy change  $W$  and the reverse energy change are related by the ratio of the initial density of states in the system  $A$  so we have

$$R_E(W) e^{-(\beta_A - \beta_B)W} \approx R_{E+W}(-W). \quad (\text{V.95})$$

Here we linearized the entropy of the system  $A$  assuming that  $W$  is small. Integrating this equation over  $W$  and ignoring sub-extensive terms proportional to derivatives with respect to the energy we find an analogue of the Jarzynski relation for open systems

$$\langle e^{-(\beta_A - \beta_B)W} \rangle = 1 \quad (\text{V.96})$$

In principle interaction between systems  $A$  and  $B$  can also result in changing some macroscopic parameter affecting  $A$ , e.g. as the system  $A$  heats up its magnetization also changes. Then instead of one in the RHS of this relation one should use  $\exp[-\beta_A \Delta F]$ , where  $\Delta F$  is the free energy

difference and  $\beta_A$  is the initial temperature in the system  $A$ . Expanding Eq. (V.95) in powers of  $W$  we find Einstein relations for drift and diffusion coefficients:

$$2A(E_A) \approx (\beta_A - \beta_B)B(E_A) + \partial_{E_A}B(E_A) \equiv \Delta\beta B(E_A) + \partial_{E_A}B(E_A). \quad (\text{V.97})$$

If the temperatures  $\beta_A$  and  $\beta_B$  are close to each other and the systems  $A$  and  $B$  are separated in space by distance  $\Delta x$  so that

$$\beta_A - \beta_B \approx \nabla\beta \Delta x$$

then the relation above reduces to the standard Einstein relation between energy drift and diffusion with  $A/(\nabla\beta\Delta x)$  playing the role of heat (thermal) conductivity.

Let us now consider a slightly more complicated setup where we have two (or in general more) conserved quantities. For example the energy and the magnetization or the energy and the number of particles. The setup will be the same as before: we have two coupled systems  $A$  and  $B$ , which weakly interact and can exchange energy and the second conserved quantity (for concreteness we assume this is the particle number)  $N$ . We will assume that the energies  $E_A$  and  $E_B$  as well as number of particles  $N_A$  and  $N_B$  are extensive and that we can ignore sub-extensive corrections like  $\partial_{E_A}B$ . The microstates of the systems  $A$  and  $B$  are now characterized by the values  $E_A, N_A$  and  $E_B, N_B$ . Using the same arguments as before we find that the ratio of the transition rates where the energy  $W$  and the number of particles  $N$  flows from  $B$  to  $A$  is equal to the ratio of the final densities of states:

$$\begin{aligned} R(W, N) &\equiv R(E_A, N_A, E_B, N_B \rightarrow E_A + W, N_A + N, E_B - W, N_B - N) \\ &= R(-W, -N) \frac{\Omega_A(E_A + W, N_A + N)\Omega_B(E_B - W, N_B - N)}{\Omega_A(E_A, N_A)\Omega_B(E_B, N_B)} \approx R(-W, -N) \exp[\Delta\beta W + \Delta\lambda N], \end{aligned} \quad (\text{V.98})$$

where  $\Delta\beta = \beta_A - \beta_B$ ,  $\Delta\lambda = \lambda_A - \lambda_B$  and  $\lambda_A = \partial S_A / \partial N_A = -\beta_A \mu_A$ , where  $\mu_A$  is the chemical potential (which is defined as the generalized force with respect to the number of particles). Integrating this relation over  $W$  and  $N$  we find that

$$\langle \exp[-\Delta\beta W - \Delta\lambda N] \rangle = 1. \quad (\text{V.99})$$

There is another independent relation which can be obtained by integrating

$$R(W, N) \exp[-\Delta\beta W] = R(-W, -N) \exp[-\Delta\lambda N], \quad (\text{V.100})$$

which is

$$\langle \exp[-\Delta\beta W] \rangle = \langle \exp[-\Delta\lambda N] \rangle \quad (\text{V.101})$$

Expanding both relations to the second order in cumulants we find

$$-\Delta\beta\langle W \rangle - \Delta\lambda\langle N \rangle + \frac{\Delta\beta^2}{2}\langle W^2 \rangle_c + \frac{\Delta\lambda^2}{2}\langle N^2 \rangle_c + \Delta\beta\Delta\lambda\langle WN \rangle_c = 0 \quad (\text{V.102})$$

$$-\Delta\beta\langle W \rangle + \Delta\lambda\langle N \rangle + \frac{\Delta\beta^2}{2}\langle W^2 \rangle_c - \frac{\Delta\lambda^2}{2}\langle N^2 \rangle_c = 0 \quad (\text{V.103})$$

Adding and subtracting these relations from each other we can rewrite them in the following matrix form (P. Gaspard and D. Andrieux, 2011).

$$\begin{pmatrix} \langle W \rangle \\ \langle N \rangle \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \langle W^2 \rangle_c & \langle WN \rangle_c \\ \langle WN \rangle_c & \langle N^2 \rangle_c \end{pmatrix} \begin{pmatrix} \Delta\beta \\ \Delta\lambda \end{pmatrix} \quad (\text{V.104})$$

These equations are nothing but the celebrated Onsager relations. The left hand side represents the energy and particle relaxation rates (recall that  $W$  and  $N$  as well as all the cumulants are proportional to  $\delta t$ ). The right hand side represents the symmetric fluctuation matrix multiplied by the differences in conjugates to the energy and the number of particles ( $\beta$  and  $\lambda$ ). Note that these relations are non-perturbative in these differences the only real requirements are that the third cumulants of  $W$  and  $N$  are small. In many situations this requirement though is equivalent to the small differences  $\Delta\beta$  and  $\Delta\lambda$ . These Onsager relations predict the symmetry of kinetic coefficients strongly constraining the relaxation process. They also allow one to constrain fluctuations and cross-correlations in the two currents.

### 3. Exercises

1. Using the Jensen's inequality and the Kullback-Libler divergence as a distance between the two distributions prove that the Gibbs distribution is an attractor of the dynamics of the master equation with the transition rates satisfying the detailed balance V.90.
2. Consider two coupled black-bodies at different temperatures separated by a two-dimensional membrane in the  $xy$ -plane transparent to the radiation. The Hamiltonian of the system can be written as

$$H = H_A + H_B + H_{AB}, \quad (\text{V.105})$$

where

$$H_A = \sum_{\vec{k}, \alpha} \hbar c |\vec{k}| a_{\vec{k}, \alpha}^\dagger a_{\vec{k}, \alpha}, \quad H_B = \sum_{\vec{k}, \alpha} \hbar c |\vec{k}| b_{\vec{k}, \alpha}^\dagger b_{\vec{k}, \alpha}, \quad (\text{V.106})$$

are the Hamiltonians representing photons in the two systems  $A$  and  $B$ . Here  $\alpha = 1, 2$  is the polarization index,  $\vec{k}$  is the three-dimensional wave vector and  $a^\dagger, a$  and  $b^\dagger, b$  are the photon creation and annihilation operators in the cavities  $A$  and  $B$  respectively. Consider free boundary conditions (meaning that there are no reflected photons from the membrane). The interaction between systems  $A$  and  $B$  can be described by the following conversion operator:

$$H_{AB} = \hbar c \sum_{\alpha} \int \int dx dy (a_{\alpha}^\dagger(x, y, 0) b_{\alpha}(x, y, 0) + h.c.) \quad (\text{V.107})$$

This operator simply relabels  $A$  photons to the  $B$  photon once it crosses the membrane. Using the Fermi Golden rule (or otherwise) calculate the transition rate for the process of transferring photons from the system  $A$  to  $B$  and back, i.e. the rate per unit time at which photons with momentum  $k$  cross the membrane in both directions. Show that the transition rate from  $A$  to  $B$  is given by

$$p(n_k^{(a)}, n_{k'}^{(b)} \rightarrow n_k^{(a)} - 1, n_{k'}^{(b)} + 1) = \frac{2\pi}{\hbar} \frac{\hbar^2 c^2}{L^2} n_k^{(a)} (1 + n_{k'}^{(b)}) \delta(\hbar c k - \hbar c k'), \quad (\text{V.108})$$

where  $L^2$  is the area of the membrane. Using that each such transition results in energy transfer  $\hbar c k$  from  $A$  to  $B$  and  $-\hbar c k$  for the opposite transition  $p(n_k^{(a)}, n_{k'}^{(b)} \rightarrow n_k^{(a)} + 1, n_{k'}^{(b)} - 1)$  find the average energy transfer rate per unit time and its fluctuations  $A$  and  $B$ . You might express your results as integrals. Check whether the relation

$$2A = \Delta\beta B \quad (\text{V.109})$$

holds for this system and in which regime. Explain your results.

## VI. RELAXATION IN INTEGRABLE AND NEARLY INTEGRABLE SYSTEMS. PRETHERMALIZATION. KINETIC EQUATIONS.

Until now we focused our main attention to ergodic systems satisfying ETH. But we might wonder what happens if the systems are not-ergodic, for example if the systems are integrable. Truly integrable systems are very rare in nature so this question might sound like an academic. However, the reality is much more subtle. Very often we deal with systems, which are nearly

integrable. For example, phonons or photons in a media to the first approximation behave as non-interacting particles and interactions between them or between them and other degrees of freedom are typically very small, especially in the long wave length limit. The same is true about any other situations where we can define particles or quasi-particles: ideal gases, Fermi liquids, superconductors, spin wave excitations and others. In these situations systems are integrable to the first approximation. These systems are quite simple in a sense that they can be described by a gas of weakly interacting bosonic or fermionic excitations. There are more subtle examples of non-linear nearly integrable systems (quantum or classical) with solitonic-like excitations, which are stable complex non-linear objects. And finally there is another class of non-ergodic systems, typically disordered, where particles are localized in space and the relaxational dynamics is glassy, i.e. exponentially slow. We discussed an example of such non-ergodic system, when we considered many-body localization. A natural question to ask how these systems relax (if they relax at all) and what happens with dynamics in these systems if we weakly break integrability. Both topics are currently a subject of an active research, but a few things are already understood.

#### **A. Relaxation in integrable systems. The Generalized Gibbs Ensemble (GGE).**

Let us recall first what happens in equilibrium systems, where we have more than one conserved quantity. It is in fact very common when we deal with two conserved quantities: the energy and the number of particles. It is also quite common that we deal with systems with conserved magnetization, center of mass momentum, angular momentum, volume and a few more. Such systems are generically still ergodic because the number of conservation laws is still small compared to the total number of degrees of freedom but the additional conserved quantities provide additional constraints. It is very important that we always deal with additive conserved quantities. This follows from the basic assumption of the statistical mechanics about the statistical independence of subsystems. The statistical independence implies that the density matrix in equilibrium approximately factorizes into the density matrix of the subsystems. This implies that the logarithm of density matrix can be only a function of the additive conserved quantities. Precisely for this reason it is the energy, not the energy squared, which enters the Gibbs distribution. In 1957 Jaynes formulated a general maximal entropy principle for systems with arbitrary number of conserved quantities. His motivation was coming from the information theory. Namely he postulated that the equilibrium statistical ensemble should maximize the von Neumann's (Shannon) entropy subject

to all constraints (integrals of motion), i.e.

$$\rho_{nm}^{GGE} = \frac{1}{Z} \exp \left[ - \sum_{\alpha} \lambda_{\alpha} I_{\alpha}^{(n)} \right] \delta_{nm}, \quad (\text{VI.1})$$

where  $I_{\alpha}^{(n)}$  are the eigenvalues of the conserved integrals of motion (because they all commute with the Hamiltonian and each other they can be diagonalized simultaneously). It is very important that these integrals of motion are either local in space or can be represented as sums of operators, which are local in space. Indeed only then the exponential form of the density matrix can be justified and the different parts of the system are statistically independent.

While this general Generalized Gibbs Ensemble (GGE) form was proposed more than fifty years ago, there were practically no implications of this conjecture to statistical physics for a very long time. The main reason for this was that integrable systems are usually fine tuned and give only approximate description to real systems. Any infinitesimal generic interaction or the coupling to an environment immediately breaks the integrability and destroys all the integrals of motion except the energy and perhaps few more like the magnetization, or the number of particles. However, recently there have been several experimental advances, which forced us to revisit these issues. First there were realized isolated quantum, mostly one-dimensional, systems, which like the FPU problem do not thermalize on experimental time scales. These systems include cold atoms and ions (T. Kinoshita et. al. 2006), driven exciton-polariton systems (J. Kasprzak et. al. 2006), nuclear spins in various insulators and semiconductors (L. Childress et. al. 2006). In parallel advances in ultra-fast optics allowed experimentalists to access dynamics in ordinary materials at ultra-short time scales. During so short times weakly interacting systems behave approximately as non-interacting and first relax to a non-thermal state, which then slowly relaxes to the true equilibrium. Such two stage relaxation process was termed as prethermalization (J. Berges et. al. 2004).

Let us start from a very simple example of a classical particle in a regular cavity (see Fig. 24) From the figure it is clear that unless we fine tune the trajectory so that it precisely hits the corner the particle will eventually uniformly fill the coordinate space so if we let the particle bounce many times we will loose any information about its position. At the same time the absolute value of the momenta or kinetic energies along the  $x$  and  $y$  directions will be conserved. So in the long time limit the probability distribution for this particle will relax to

$$P(x, y, p_x, p_y, t) \rightarrow_{t \rightarrow \infty} \delta(|p_x| - |p_x^0|) \delta(|p_y| - |p_y^0|) \sim \delta(p_x^2/2m - E_x^0) \delta(p_y^2/2m - E_y^0), \quad (\text{VI.2})$$

where  $p_x^0$  and  $p_y^0$  are the initial values of the momenta along the  $x$  and  $y$  directions ( $E_{x,y}^0 =$

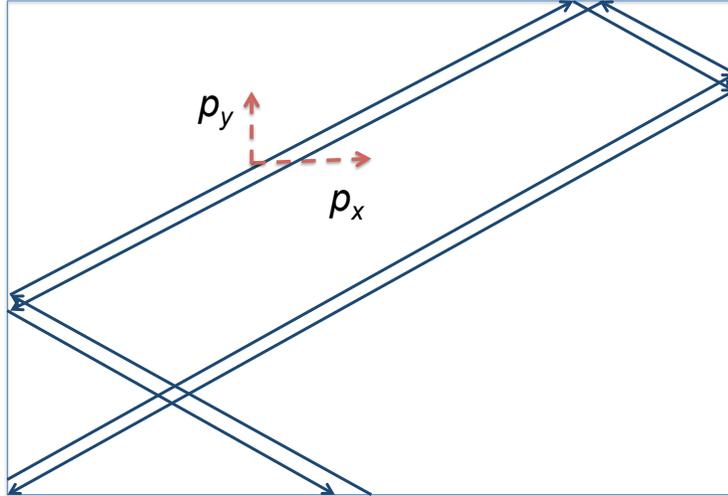


FIG. 24 Example of a motion of a classical particle in an integrable, rectangular, cavity

$(p_{x,y}^0)^2/2m$ ) and the long time limit is understood as before. This example illustrates the main idea of the relaxation in integrable systems to the constraint equilibrium. Because we are dealing with a single particle even in a chaotic regime instead of the relaxation to the Gibbs ensemble we expect the relaxation to the microcanonical ensemble. Similarly in the integrable case the distribution (VI.2) can be viewed as the Generalized Microcanonical Ensemble. The expression (VI.2) is valid if we start from a particle with fixed momenta. However, if we start from an ensemble of particles the relaxation becomes more subtle. In particular, the correlations  $\langle |p_x||p_y| \rangle$  are also preserved in time. Thus if the system is prepared in a correlated state, say  $p_x^0 = p_y^0$  these correlations will be also preserved in time. Thus for the relaxation into a generalized Gibbs (or other) ensemble it is necessary to make sure that the integrals of motion are uncorrelated. Typically this issue becomes unimportant if we are dealing with local integrals of motion or their sums. Then the correlations between these integrals decay in space and thus they become effectively statistically independent.

These ideas were extended to multi-particle systems (M. Rigol et. al. 2007) who postulated that any generic integrable system will relax to the GGE ensemble suggested by Jaynes (VI.1), where the Lagrange multipliers are determined by the initial conditions

$$\text{Tr}[\rho_0 I_\alpha] = \langle I_\alpha \rangle_{GGE} \equiv \text{Tr}[\rho^{GGE} I_\alpha] \quad (\text{VI.3})$$

There is no general proof of this conjecture, but there are rigorous proofs for specific models. These proofs are quite involved so instead we will discuss a relatively simple but yet nontrivial example of a system of one dimensional hard core bosons (equivalent to the one dimensional XY chain in a transverse field) and show the comparison of the anticipated results with numerical simulations.

Our discussion will closely follow the work by M. Rigol et al. (Phys. Rev. Lett. **98**, 050405 (2007)).

1. One-dimensional hard-core bosons and the Jordan-Wigner transformation.

Most known integrable systems in dimensions higher than one are non-interacting. E.g. free quasi-particles in metals or free phonons in solids or liquids. In one dimension there are many non-trivial integrable models with nontrivial properties. We will consider one of the simplest integrable interacting models representing a one dimensional gas of hard core bosons. They can be described by the following lattice Hamiltonian

$$H = -J \sum_j (b_j^\dagger b_{j+1} + h.c.) - \mu \sum_j b_j^\dagger b_j, \quad (\text{VI.4})$$

where  $b_j^\dagger$  and  $b_j$  are the creation and annihilation operators of Hard-core bosons,  $J$  is the hopping and  $\mu$  is the chemical potential, which in equilibrium sets the number of bosons. They commute as long as the sites  $i$  and  $j$  are different from each other:

$$[b_i, b_j] = [b_i^\dagger, b_j] = [b_i^\dagger, b_j^\dagger] = 0 \quad \text{if } i \neq j \quad (\text{VI.5})$$

and they anti-commute on the same site

$$b_i^\dagger b_i + b_i b_i^\dagger = 1, \quad b_i^2 = 0, \quad (b_i^\dagger)^2 = 0 \quad (\text{VI.6})$$

It is easy to check that these anticommutation relations are equivalent to the constraint that no more than one particle can be on a given site. As we discussed earlier in two and more dimensions this hard-core constraint is equivalent to the interactions between the particles leading to the ergodic Hamiltonian. However, in one dimension this is not the case and one can map this problem to the free fermions. Because of this mapping the hard core Boson gas is a relatively simple integrable system, but still its dynamics is very nontrivial. Before proceeding to the mapping to free fermions let us show that hard-core bosons (in any dimension) are equivalent to spin one half degrees of freedom. To see this we use the following identification

$$b_i = \sigma_i^-, \quad b_i^\dagger = \sigma_i^+, \quad b_i^\dagger b_i = \frac{\sigma_i^z + 1}{2}, \quad b_i b_i^\dagger = \frac{1 - \sigma_i^z}{2} \quad (\text{VI.7})$$

or equivalently

$$\sigma_i^x = b_i + b_i^\dagger, \quad \sigma_i^y = i(b_i - b_i^\dagger), \quad \sigma_i^z = 2b_i^\dagger b_i - 1 \quad (\text{VI.8})$$

It is clear that by construction different Pauli matrices commute on different sites as they should and that they satisfy conventional commutation relations on the same site. E.g.

$$\sigma_i^x \sigma_i^y = i(b_i^\dagger b_i - b_i b_i^\dagger) = i(2b_i^\dagger b_i - 1) = i\sigma_i^z. \quad (\text{VI.9})$$

Substituting this representation of the Bosons into the Hamiltonian (VI.4) we find (up to unimportant additive constants)

$$\begin{aligned} H &= -J \sum_j \left[ (\sigma_j^x + i\sigma_j^y)(\sigma_{j+1}^x - i\sigma_{j+1}^y) + h.c. \right] - \frac{\mu}{2} \sum_j \sigma_j^z \\ &= -2J \sum_j (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) - \frac{\mu}{2} \sum_j \sigma_j^z. \end{aligned} \quad (\text{VI.10})$$

This Hamiltonian is known as an isotropic XY model. There is a simple generalization of this Hamiltonian to the anisotropic XY-model, which preserves the integrability

$$H_{XY} = -J \frac{1+\gamma}{2} \sum_j \sigma_j^x \sigma_{j+1}^x - J \frac{1-\gamma}{2} \sum_j \sigma_j^y \sigma_{j+1}^y - h \sum_j \sigma_j^z \quad (\text{VI.11})$$

It is easy to check that the anisotropic term leads to the superconducting type terms  $b_j^\dagger b_{j+1}^\dagger + h.c.$  in the language of the original hard-core bosons. For the anisotropy  $\gamma = 1$  this model is known in literature as the quantum Ising model in the transverse field. It was first introduced and extensively discussed by Schultz and Mattis and Lieb in 1964 (Rev. Mod. Phys. **36**, 856 (1964)).

Now let us discuss the mapping of this model to free fermions using the Jordan-Wigner transformation. This mapping will allow us to understand the structure of the spectrum, eigenstates and the integrals of motion in this system. In parallel the Jordan-Wigner transformation is very instructive because it shows how one can represent anti-commuting fermionic operators through ordinary numbers and  $2 \times 2$  Pauli matrices. The anti-commutation relation of the hard-core bosons on the same site suggest that the fermionic representation should be very similar to bosonic, i.e. on each site we should have

$$f_i \sim \sigma_i^-, \quad f_i^\dagger \sim \sigma_i^+. \quad (\text{VI.12})$$

However, this representation satisfies bosonic, not fermionic commutation relations on each site. So we need to correct this representation. The way to convert the commutation to the anticommutation relations is to effectively introduce the  $\pi$  phase shift on each site whenever we add or remove the boson from the site on the left of site  $j$ . Indeed when we compute the commutator of e.g.  $b_i^\dagger$  and  $b_j$  with say  $i < j$  the term  $b_i^\dagger b_j$  creates an extra particle on the left of the site  $j$ . If we simultaneously change the sign of  $b_i$  then the bosonic commutation relations will automatically

become fermionic. Technically this is achieved via inserting the string of  $\sigma_z$  operators so the correct fermionic representation is

$$f_i = \prod_{j<i} \sigma_z^j \sigma_i^-, \quad f_i^\dagger = \prod_{j<i} \sigma_z^j \sigma_i^+. \quad (\text{VI.13})$$

Let us check that this representation indeed leads to the correct anticommutation relations between fermions. We will do this only for the neighboring sites (see the homework for a more general proof).

First let us compute using that  $(\sigma_z^i)^2 = 1$

$$f_i f_{i+1} + f_{i+1} f_i = \sigma_i^- \sigma_i^z \sigma_{i+1}^z + \sigma_i^z \sigma_i^- \sigma_{i+1}^- = 0, \quad (\text{VI.14})$$

where we used that  $\sigma^- \sigma^z + \sigma^z \sigma^- = 0$ . Similarly  $f_i^\dagger f_{i+1}^\dagger + f_{i+1}^\dagger f_i^\dagger = 0$ . And finally

$$f_i^\dagger f_{i+1} + f_{i+1} f_i^\dagger = \sigma_i^+ \sigma_i^z \sigma_{i+1}^z + \sigma_i^z \sigma_i^+ \sigma_{i+1}^- = 0. \quad (\text{VI.15})$$

The inverse transformation reads

$$\sigma_i^x = \prod_{j<i} (2f_j^\dagger f_j - 1)(f_i + f_i^\dagger), \quad \sigma_i^y = i \prod_{j<i} (2f_j^\dagger f_j - 1)(f_i - f_i^\dagger), \quad \sigma_i^z = 2f_i^\dagger f_i - 1. \quad (\text{VI.16})$$

Using this fermionic representation the Hamiltonian (VI.11) becomes

$$\begin{aligned} H_{XY} &= -J \frac{1+\gamma}{2} \sum_j (f_j + f_j^\dagger)(2f_j^\dagger f_j - 1)(f_{j+1} + f_{j+1}^\dagger) \\ &\quad + J \frac{1-\gamma}{2} \sum_j (f_j - f_j^\dagger)(2f_j^\dagger f_j - 1)(f_{j+1} + f_{j+1}^\dagger) - 2h \sum_j f_j^\dagger f_j \\ &= -J \sum_j (f_j f_{j+1}^\dagger + f_{j+1}^\dagger f_j) - J\gamma \sum_j (f_j f_{j+1} + f_{j+1}^\dagger f_j^\dagger) - 2h \sum_j f_j^\dagger f_j. \end{aligned} \quad (\text{VI.17})$$

Thus the XY - spin chain is equivalent to a one-dimensional BCS superconductor of spinless fermions (so called p-wave superconductor). For the isotropic model  $\gamma = 0$  corresponding to the original hard-core bosons the anomalous term vanishes and the model becomes equivalent to the one-dimensional free electron gas. This Hamiltonian can be always diagonalized via the Bogoliubov transformation (see exercises) so that one can find its energy spectrum and eigenstates as a function of the external parameters  $J, \gamma, h$

It is clear that the Hamiltonian (VI.17) has as many local conserved quantities as the number of degrees of freedom. In particular, occupation numbers of Bogoliubov quasiparticles for each momentum mode are conserved. For the isotropic model  $\gamma = 0$ , which we consider hereafter, the Bogoliubov quasi-particles are simply  $f$  - fermions. There is one subtlety with locality of momentum states because in principle they are defined as the Fourier transform over the whole

system. However, this is not a real issue because we can always construct a localized in space wave packet using the linear combination of the momentum modes. Also the occupation operators can be written in the following form

$$n_k = f_k^\dagger f_k = \frac{1}{L} \sum_{ij} f_i^\dagger f_{i+j} e^{-2\pi ijk}, \quad (\text{VI.18})$$

where  $k$  is quantized in units of  $2\pi/L$ . Because the correlation functions between  $f_i^\dagger$  and  $f_{i+j}$  always decay in space the momentum occupation number effectively represents the sum of local operators and in this sense it is local. From this fermionic operators one can construct local bosonic integrals of motion. The first integral would be simply the total number of particles:

$$I_1 = \sum_k f_k^\dagger f_k = \sum_j f_j^\dagger f_j = \sum_j b_j^\dagger b_j. \quad (\text{VI.19})$$

The next integral will contain the energy

$$\begin{aligned} I_2 &= 2 \sum_k (1 - \cos(k)) f_k^\dagger f_k = \sum_j (2f_j^\dagger f_j - f_j^\dagger f_{j+1} - f_{j+1}^\dagger f_j) \\ &= \sum_j \left[ 2b_j^\dagger b_j - b_j^\dagger (2b_j^\dagger b_j - 1)b_{j+1} - (2b_j^\dagger b_j - 1)b_j b_{j+1}^\dagger \right] = \sum_j (2b_j^\dagger b_j + b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j), \end{aligned} \quad (\text{VI.20})$$

which is clearly a linear combination of the energy and number of particles. The first nontrivial integral of motion will be

$$\begin{aligned} I_3 &= 2 \sum_k (1 - \cos(k))^2 f_k^\dagger f_k = \sum_k (3 - 4\cos(k) + \cos(2k)) f_k^\dagger f_k = -I_1 + 2I_2 + \sum_j f_j^\dagger f_{j+2} + f_{j+2}^\dagger f_j \\ &= -I_1 + 2I_2 + \sum_j \left[ b_j^\dagger (2b_j^\dagger b_j - 1)(2b_{j+1}^\dagger b_{j+1} - 1)b_{j+2} + (2b_j^\dagger b_j - 1)(2b_{j+1}^\dagger b_{j+1} - 1)b_{j+2}^\dagger b_j \right] \\ &= -I_1 + 2I_2 - \sum_j \left[ b_j^\dagger (2b_{j+1}^\dagger b_{j+1} - 1)b_{j+2} + b_{j+2}^\dagger (2b_{j+1}^\dagger b_{j+1} - 1)b_j \right]. \end{aligned} \quad (\text{VI.21})$$

Using explicit calculation (see exercises) one can check that  $I_3$  commutes with the Hamiltonian. In a similar fashion one can construct other integrals of motion, which will be less and less local, i.e. will have larger and larger support in terms of the bosonic operators  $b_i$  and  $b_i^\dagger$ .

Having established the structure of the integrals of motion we can now conjecture that if the system is prepared in some non-equilibrium state it will relax to the generalized Gibbs ensemble

$$\rho_{GGE} = \frac{1}{Z} \exp \left[ - \sum_n \lambda_n I_n \right] = \frac{1}{Z} \exp \left[ - \sum_k \tilde{\lambda}_k n_k \right]. \quad (\text{VI.22})$$

It is clear that if the sum is restricted to the finite number of integrals of motion then the density matrix approximately factorizes into a product of density matrices of different subsystems. Indeed

up to the boundary terms, which involve integrals of motion inter-collating between the subsystems it is just a product of local density matrices. As we mentioned earlier the Lagrange multipliers can be found from the initial conditions fixing the integrals of motion. In Fig. VI.A.1 we show the results of numerical simulations (M. Rigol et. al. (2007)) of the expansion of the hard core Bose gas from a smaller to a larger box (see the caption for details). The two plots show the relaxation

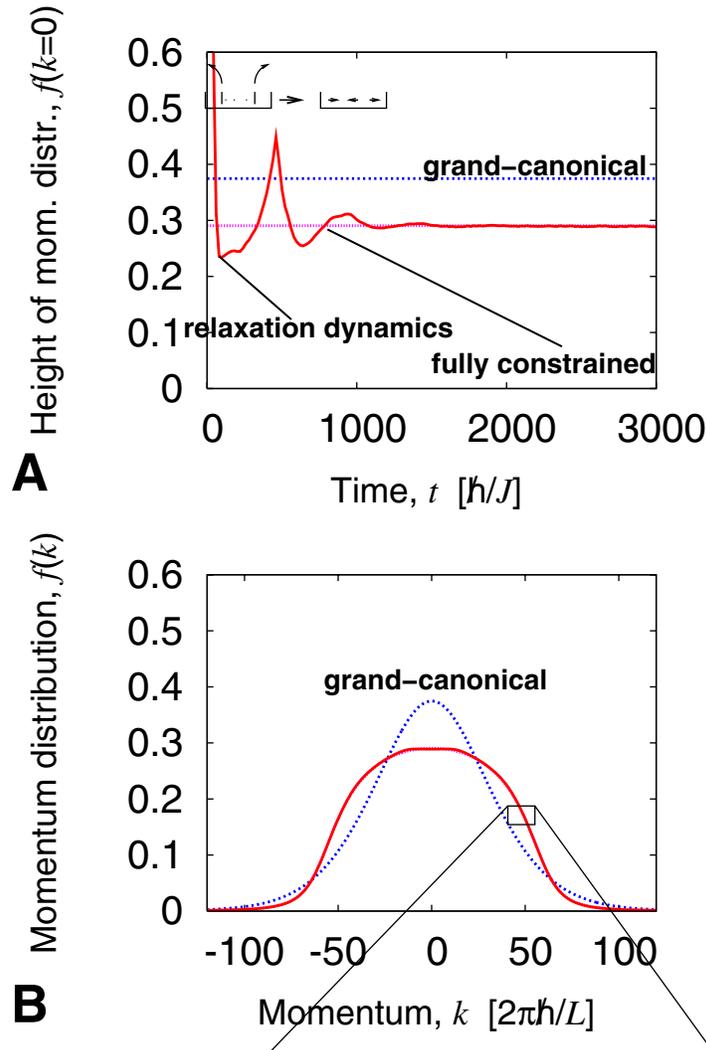


FIG. 25 Results of numerical simulations of the expansion of the hard core Bose gas of  $N = 30$  particles from a box of the width  $L = 150$  to a larger box of the size  $L = 600$ . The top panel shows the time evolution of the zero momentum boson occupation number. The bottom plot shows the whole momentum distribution after the relaxation. The results show that the relaxed system is practically indistinguishable from the GGE. The plots are taken from Ref. M. Rigol, V. Dunjko, V. Yurovsky, and M. Olshanii, Phys. Rev. Lett. **98**, 050405 (2007).

of the zero momentum component of the Bose gas (top) and the full momentum distribution after the relaxation (bottom). The relaxed system is practically indistinguishable from the GGE,

however there are significant deviations from the predictions of the equilibrium grand canonical Gibbs ensemble.

The issue of importance of locality of the integrals of motion was recently analyzed by M. Fagotti and F. Essler for a quench in the transverse field Ising model, described by the Hamiltonian (VI.17) with  $\gamma = 1$  and  $J = 1$ . The integrals in this model have a very similar structure to those in the hard-core bosons. Namely one can always organize them in such a way that  $I_n$  is a sum of products involving up to  $n$  adjacent spin operators. What they rigorously showed is that after a quench the reduced density matrix of a subsystem, which is defined as

$$\rho_A = \sum_{n \in B} \langle n | \rho | n \rangle, \quad (\text{VI.23})$$

where  $A$  is the subsystem of size  $L'$ ,  $B$  is the rest of the system of size  $L - L'$  and  $|n\rangle$  is a complete basis of the system  $B$ , approaches the GGE reduced density matrix in the limit  $L \rightarrow \infty$  and arbitrary fixed  $L'$ . In other words they showed that the subsystem exactly relaxes to the GGE and all observables, both equal time and non-equal time, are exactly described by the GGE in the long time limit. Moreover they showed that only the integrals of motion with  $n < L'$ , i.e. the integrals which can fit into the subsystem, are important. Fig. 26 demonstrates how the norm-distance between the time averaged and GGE density matrix changes with the number of integrals of motion included into GGE. It is clear that once  $n$  becomes bigger than the subsystem size the distance rapidly goes to zero implying that the integrals of motion with  $n > L'$  are not important. The Generalized Gibbs Ensemble provides a nice theoretical framework for understanding the relaxation in integrable systems. However it is still quite ambiguous from the experimental point of view. The main reason for this ambiguity is the large (extensive) number of the conserved quantities, which one needs to fix in order to specify the relaxed state. This number grows linearly with the system size, which is much less than the exponentially growing size of the Hilbert space. Yet this situation is not satisfactory from the point of view of experiments. Most of these integrals are complicated correlation functions, which are hard to measure. One also can not use them as fitting parameters because of their extensive number. So much more work is still needed to understand whether there is a general structure of achievable GGEs and whether they can be described by a non-extensive number of fitting parameters.

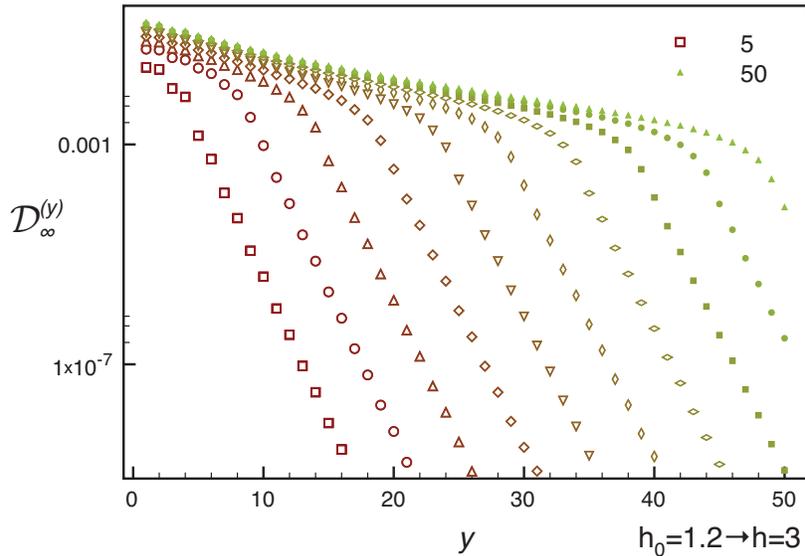


FIG. 26 Norm-distance between the long time limit of the reduced density matrix of a subsystem of size  $L'$  of an infinite transverse field Ising chain after a quench and the reduced density matrix of the GGE ensemble as a function of the number of integrals included into GGE. Different curves correspond to different systems sizes. It is clear that only the integrals with  $n \lesssim L'$  strongly affect this distance. The integrals with  $n > L'$ , i.e. the integrals, which “do not fit” into the subsystem are not important. The plot is taken from Ref. M. Fagotti and F. Essler, Phys. Rev. B, **87**, 245107 (2013)

## 2. Exercises.

1. Prove that the Jordan-Wigner transformation leads to the correct fermionic anti-commutation relations.
2. Rewrite the Hamiltonian (VI.17) in the momentum space. Diagonalize it using the Bogoliubov transformation:  $f_k = u_k \alpha_k + v_k \alpha_{-k}^\dagger$ . Choose coefficients  $u_k$  and  $v_k$  such that the Hamiltonian reads  $H_{XY} = \sum_k \epsilon_k \alpha_k^\dagger \alpha_k$ . What is the spectrum of this Hamiltonian?
3. Check that the integral of motion (VI.21) indeed commutes with the Hamiltonian.

## B. Relaxation in weakly nonintegrable systems. Prethermalization. Quantum kinetic equations.

Let us now assume that the system is nearly integrable, i.e. its Hamiltonian can be written as

$$H = H_0 + H_{\text{int}}, \quad (\text{VI.24})$$

where  $H_0$  is an integrable Hamiltonian and  $H_{int}$  breaks the integrability. This setup is very familiar to us when we consider e.g. weakly interacting quasi-particles, where  $H_0$  is a noninteracting (integrable) Hamiltonian, which can be written as  $H_0 = \sum_k \epsilon_k c_k^\dagger c_k$  and  $H_{int}$  represents interactions between these quasi-particles. In dimensions higher than two this is a standard setup since all integrable theories are non-interacting. In one dimension the structure of  $H_0$  can be more complicated as we discussed above. Note that splitting of the Hamiltonian between  $H_0$  and  $H_{int}$  is not unique in general. In equilibrium there is a well defined procedure of finding  $H_0$  using the renormalization group formalism, which tells us about the structure of low energy excitations. For example, in metals the low energy Hamiltonian can represent a Fermi liquid with dressed quasi-particles, a super-conductor, where elementary excitations are the Bogoliubov quasi-particles or gas of polarons, where fermions are dressed by lattice vibrations. There is no known procedure how to find the best general  $H_0$  away from equilibrium it amounts into optimal splitting of the interaction terms into the integrable part (which can be absorbed into  $H_0$ ) and the remaining part. But if the perturbation  $H_{int}$  is very small then this issue is not really important. Let us point that the same setup can be used to describe a system of weakly coupled grains of some kind. The GGE ensemble will correspond to each grain having its own temperature (the Lagrange multiplier to an approximately conserved local energy). The interaction  $H_{int}$  in this case will represent weak coupling between grains. If the relaxation time with each grain is fast then the setup is precisely the same as we consider here.

If  $H_{int}$  is small then at short times after say a sudden quench the system “does not know” that it is non-integrable and the effect of  $H_{int}$  on dynamics is small. So one can anticipate that the system relaxes to the corresponding GGE ensemble. At longer times  $H_{int}$  can lead to significant effects (small perturbation acting for a long time can lead to a large effect), for example it can force the system to relax to the true thermal equilibrium. This relaxation can be thought of as a slowly evolving GGE, thus the dynamics can be written in terms of the slow evolution of the approximately conserved quantities. Such two stage relaxation scenario was termed as prethermalization in the context of Cosmology (Berges, 2004). This scenario suggests that weakly non-integrable systems have a two stage relaxation process, where first they reach some non-thermal distribution where they spend a significant amount of time and then they ultimately relax to the true thermal state. The two stage relaxation process was found in a series of recent analytical and numerical works (see e.g. M. Moeckel, S. Kehrein, Phys. Rev. Lett. 100, 175702 (2008); M. Eckstein, M. Kollar, P. Werner, Phys. Rev. B 81, 115131 (2010)).

Separation of time scales of relaxation to the GGE (governed by  $H_0$ ) and to the true equilibrium

governed by  $H_{\text{int}}$  can serve as the basis of deriving the kinetic equations (M. Stark and M. Kollar, 2013). Namely, let us try to solve the von Neumann's equation for the density matrix perturbatively

$$i\partial_t\rho = -[\rho, H] = -[\rho, H_0] - [\rho, H_{\text{int}}] \quad (\text{VI.25})$$

with the initial condition that at  $t = 0$  the density matrix is described by some GGE. It is convenient to go to the interaction picture:

$$\rho_I(t) = e^{-iH_0t}\rho e^{iH_0t}, \quad H_{\text{int}}(t) = e^{iH_0t}H_{\text{int}}e^{-iH_0t}.$$

Clearly this transformation does not affect the initial density matrix  $\rho_I(0) = \rho(0)$  because all the integrals of motion appearing in the GGE commute with  $H_0$ . Then the equation of motion for the density matrix becomes

$$i\partial_t\rho_I = -[\rho_I, H_{\text{int}}(t)]. \quad (\text{VI.26})$$

Next we will solve this equation using the time dependent perturbation theory and use it for finding the kinetic equations for the conserved quantities  $I_k$ . Because in the interaction picture  $I_k(t)$  are time independent

$$I_k(t) = e^{iH_0t}I_k e^{-iH_0t} = I_k \quad (\text{VI.27})$$

the equations of motion for their expectation value are

$$d_t\langle I_k \rangle = d_t(\text{Tr}[I_k\rho_I(t)]) = \text{Tr}[I_k d_t\rho_I(t)]. \quad (\text{VI.28})$$

In the leading order of the perturbation theory

$$d_t\rho_I^{(1)} \approx i[\rho_0, H_{\text{int}}(t)]. \quad (\text{VI.29})$$

Substituting this into the equation above we find

$$d_t\langle I_k \rangle \approx i\text{Tr}[I_k(\rho_0 H_{\text{int}}(t) - H_{\text{int}}(t)\rho_0)] = i\langle [H_{\text{int}}(t), I_k] \rangle_0 = 0, \quad (\text{VI.30})$$

where we used the fact that for any operator  $O$  the expectation value of its commutator with  $I_k$  with respect to any GGE ensemble is zero:

$$\langle [O, I_k] \rangle_0 = \sum_n \rho_0^{(n)} \left( \langle n|O|n \rangle I_k^{(n)} - I_k^{(n)} \langle n|O|n \rangle \right) = 0.$$

Thus we need to go to the next order in perturbation theory

$$d_t\langle I_k \rangle \approx i\text{Tr} \left( I_k [\rho_I^{(1)}(t), H_{\text{int}}(t)] \right), \quad (\text{VI.31})$$

where

$$\rho_I^{(1)}(t) = i \int_0^t dt' [\rho_0, H_{\text{int}}(t')] = i \int_0^t d\tau [\rho_0, H_{\text{int}}(t - \tau)] \quad (\text{VI.32})$$

Combining these two expressions we find

$$d_t \langle I_k \rangle \approx - \int_0^t dt' \langle [[I_k, H_{\text{int}}(t - t')], H_{\text{int}}(t)] \rangle_0 \quad (\text{VI.33})$$

Now we can use that within the GGE ensemble (which is translationally invariant in time) correlation functions depend only on time differences and use the time scale separation to send the integration limit to infinity. The latter is indeed justified if the correlation functions of  $H_{\text{int}}$  computed within the GGE ensemble decay much faster than the time scales required for changing the expectation values of the integrals of motion, which in turn define the GGE. This time scale separation is indeed justified if  $H_{\text{int}}$  is small. So finally we get our desired quantum kinetic equations for the integrals of motion

$$d_t \langle I_k \rangle \approx - \int_0^\infty dt \langle [[I_k, H_{\text{int}}(0)], H_{\text{int}}(t)] \rangle_0. \quad (\text{VI.34})$$

These are the nonlinear differential equations because the expectation value of the commutator appearing in the RHS can be a complicated function of the integrals of motions. Nevertheless this equation is much simpler than the original von Neumann's equation because it deals with a system of  $N$  nonlinear differential equations rather than with the exponentially large differential equation for the density matrix.

It is instructive to rewrite the kinetic equations using the Lehman's representation using the basis of  $H_0$ . We will use that

$$\int_0^\infty dt e^{i(\epsilon_n - \epsilon_m)t} = \pi \delta(\epsilon_n - \epsilon_m) + P \frac{i}{\epsilon_n - \epsilon_m}, \quad (\text{VI.35})$$

where  $P$  stands for the principal value. Assuming for simplicity that the system does not break time reversal symmetry we see that the principal value term vanishes from the kinetic equations because it is imaginary. Therefore we find

$$d_t \langle I_k \rangle = 2\pi \sum_{nm} (\rho_{nn}^{GGE} - \rho_{mm}^{GGE}) \langle n | I_k | n \rangle |\langle n | H_{\text{int}} | m \rangle|^2 \delta(\epsilon_n^0 - \epsilon_m^0). \quad (\text{VI.36})$$

In this form it becomes clear that a thermal distribution where  $\rho_{nn}$  is only a function of energy is a stationary solution of these kinetic equations, i.e.  $d_t \langle I_k \rangle = 0$  for any  $I_k$ . Also if we use the energy  $H_0$  as a conserved quantity it is clear that  $d_t \langle H_0 \rangle = 0$  for any  $GGE$  distribution. Both properties are of course expected from general the kinetic theory.

### C. Applications of kinetic equations to weakly interacting particles.

Let us now apply the kinetic equation VI.33 to a common setup dealing with a gas of weakly interacting particles, bosons or fermions (M. Stark, M. Kollar, 2013). For simplicity we assume they are spinless. Also to shorten notations we will use the scalar notation for the momentum, keeping in mind that this is a vector index. Then the Hamiltonian reads

$$H_0 = \sum_k \epsilon_k c_k^\dagger c_k \quad (\text{VI.37})$$

For the integrability breaking term we will take usual (normal ordered) density-density interactions

$$H_{\text{int}} = \sum_{ij} V(i, j) c_i^\dagger c_j^\dagger c_j c_i = \sum_{k_1, k_2, k_3, k_4} c_{k_1}^\dagger c_{k_2}^\dagger V_{k_1, k_2, k_3, k_4} c_{k_3} c_{k_4} \quad (\text{VI.38})$$

For translationally invariant interactions  $V_{k_1, k_2, k_3, k_4}$  is nonzero only when  $k_1 + k_2 = k_3 + k_4$  and it depends only on the transferred momentum  $q = k_1 - k_3$ . But since our formalism applies even if the translational invariance is broken we will keep the interaction matrix element in the most general form. The obvious integrals of motion are the momentum occupation numbers  $\hat{n}_k = c_k^\dagger c_k$ .

Let us first compute the commutator

$$[\hat{n}_{k'}, H_{\text{int}}] = 2 \sum_{k_2, k_3, k_4} [c_{k'}^\dagger c_{k_2}^\dagger V_{k', k_2, k_3, k_4} c_{k_3} c_{k_4} - c_{k_2}^\dagger c_{k_3}^\dagger V_{k_2, k_3, k', k_4} c_{k'} c_{k_4}], \quad (\text{VI.39})$$

where we used the invariance of the interaction matrix element with respect to permutation of  $k_1$  with  $k_2$  and  $k_3$  with  $k_4$ . Next we use that in the interaction representation

$$H_{\text{int}}(t) = \sum_{q_1, q_2, q_3, q_4} e^{iE_{q_1, q_2, q_3, q_4} t} c_{q_1}^\dagger c_{q_2}^\dagger V_{q_1, q_2, q_3, q_4} c_{q_3} c_{q_4}, \quad (\text{VI.40})$$

where  $E_{q_1, q_2, q_3, q_4} = \epsilon_{q_1} + \epsilon_{q_2} - \epsilon_{q_3} - \epsilon_{q_4}$ . We can now evaluate the time integral entering Eq. (VI.34) using

$$\int_0^\infty e^{iE_{q_1, q_2, q_3, q_4} t} dt = \pi \delta(E_{q_1, q_2, q_3, q_4}) + iP \frac{1}{E_{q_1, q_2, q_3, q_4}}, \quad (\text{VI.41})$$

where  $P$  stands for the principal value. And finally let us note that any expectation value of within the generalized Gibbs ensemble of non-interacting particles can be evaluated using the Wick theorem. One can check that only contractions between  $k$  and  $q$  indices give nonzero contribution to the commutator. Because  $d_t n_k$  is real and all contractions are real the principal value part drops from the integral and we find

$$\dot{n}_{k'} \approx 16\pi \sum_{k_2, k_3, k_4} (\tilde{n}_{k'} \tilde{n}_{k_2} n_{k_3} n_{k_4} - n_{k'} n_{k_2} \tilde{n}_{k_3} \tilde{n}_{k_4}) |V_{k', k_2, k_3, k_4}|^2 \delta(E_{k', k_1, k_2, k_3}), \quad (\text{VI.42})$$

where  $\tilde{n}_k = 1 \pm n_k$  with the plus sign referring to bosons and the minus sign referring to fermions. The factor of 16 comes from the factor of two in the commutator (VI.39) another factor of two from two equivalent contributions coming from Eq. (VI.39) and another factor of four coming from Wick's contractions between  $k$  and  $q$  indexes. Classical kinetic equations are obtained by taking the limit  $n_k \ll 1$  and effectively replacing  $\tilde{n}_k$  by unity. Solving these kinetic equations can be tedious but certainly feasible at least numerically for very large systems. Let us check that the thermal distribution is a fixed point of these kinetic equations. E.g. for fermions the equilibrium distribution reads

$$n_k = \frac{1}{1 + \exp[\beta(\epsilon_k - \mu)]} \quad (\text{VI.43})$$

then

$$\begin{aligned} (\tilde{n}_{k'} \tilde{n}_{k_2} n_{k_3} n_{k_4} - n_{k'} n_{k_2} \tilde{n}_{k_3} \tilde{n}_{k_4}) &= (1 - n_{k'} - n_{k_2}) n_{k_3} n_{k_4} - n_{k'} n_{k_2} (1 - n_{k_3} - n_{k_4}) \\ &= [\exp[\beta(\epsilon_{k'} + \epsilon_{k_2} - 2\mu)] - \exp[\beta(\epsilon_{k_3} + \epsilon_{k_4} - 2\mu)]] n_{k'} n_{k_2} n_{k_3} n_{k_4} = 0, \end{aligned} \quad (\text{VI.44})$$

where the last equality relies on the total energy conservation. With more efforts one can show that the equilibrium fixed distribution is the attractor of the kinetic equations.

## VII. PERIODICALLY DRIVEN SYSTEMS.

### A. Floquet theory and the Magnus expansion.

Our previous analysis of dynamical processes in various systems was relying on quasi-static approximation, i.e. the system relaxes or partially relaxes to a steady state (or an approximate steady state) and then slowly evolves in time. Very often, however, we are dealing with an opposite limit when the system is driven at scales fast or comparable to internal relaxation time. In these situations clearly the quasi-static assumptions do not hold. In general behavior of driven systems is not understood. There is, however, an important exception where both experimental and theoretical progress was made, namely periodically driven systems. We already discussed examples of periodic motion using the Kicked rotor, the Fermi Ulam problem and the Kapitza pendulum as primary examples. What we observed that there are both chaotic regions and the islands of stability. If the driving frequency becomes very high the chaotic regions shrink. There is an intuitive reason for this. At high frequencies the system effectively feels the time average potential. In the quantum language the real transition with energy absorption are suppressed because typically the matrix

elements connecting low and high energy states are very small. So effectively one can have only virtual transitions, which lead to the renormalization of the Hamiltonian.

A powerful tool for understanding periodically driven systems is the Floquet theory, which is analogue of the Bloch theory for particles in periodic potential like a crystal lattice. As before we will use the language of quantum mechanics to define the Floquet theory and then we will discuss the classical limit. Consider a Schrödinger equation with some time dependent Hamiltonian.

$$i\hbar\partial_t|\psi\rangle = H(t)|\psi\rangle, \quad (\text{VII.1})$$

where  $H(t+T) = H(t)$ . Its solution can be written as a time ordered exponent

$$|\psi(t)\rangle = T_t \exp\left[-\frac{i}{\hbar} \int_0^t dt' H(t')\right] |\psi_0\rangle, \quad (\text{VII.2})$$

where time ordering simply means that the later times appear on the left, i.e.

$$\begin{aligned} U(t,0) &\equiv T_t \exp\left[-\frac{i}{\hbar} \int_0^t dt' H(t')\right] \\ &= \lim_{N \rightarrow \infty} \exp\left[-\frac{i}{\hbar} H(t_N)\Delta t\right] \exp\left[-\frac{i}{\hbar} H(t_{N-1})\Delta t\right] \dots \exp\left[-\frac{i}{\hbar} H(t_1)\Delta t\right] \exp\left[-\frac{i}{\hbar} H(0)\Delta t\right] |\psi_0\rangle, \end{aligned} \quad (\text{VII.3})$$

where  $t_j = t_j/N$  and  $\Delta t = t/N$ . Note if we are interested in times, which are multiples of the period  $T$  then the evolution operator repeats itself, i.e.  $U(n,T) = U(T)^n$ . The evolution operator  $U(T)$  is a unitary matrix and thus it can be always diagonalized. Because of the unitarity its eigenvalues  $\mu_j$  must satisfy  $\mu_j^* = \mu_j^{-1}$ , i.e.  $\mu_j = \exp[i\lambda_j]$  with some real  $\lambda_j$ . Thus in the diagonal form the evolution operator over one period reads.

$$U(T,0) \equiv U(T) = \text{diag}\left[e^{i\lambda_1}, e^{i\lambda_2}, \dots, e^{i\lambda_M}\right], \quad (\text{VII.4})$$

where  $M$  is the Hilbert space size. Formally the numbers  $\lambda_j$  are defined modulo  $2\pi$ . In this sense  $\lambda_j$  play a role similar to the Bloch momenta. But as we know very often it is convenient to work in the extended Brillouin zone and define  $\lambda_j$  in the whole real axis. Next let us formally define the Floquet Hamiltonian in this diagonal basis as

$$H_F = \text{diag}\left[\frac{\lambda_1\hbar}{T}, \frac{\lambda_2\hbar}{T}, \dots, \frac{\lambda_M\hbar}{T}\right]. \quad (\text{VII.5})$$

By construction the eigenvalues of the Floquet Hamiltonian (Floquet energies) have the right units of energy:

$$\epsilon_j^F = \frac{\lambda_j\hbar}{T}. \quad (\text{VII.6})$$

Then clearly

$$U(T) = \exp \left[ -\frac{i}{\hbar} H_F T \right]. \quad (\text{VII.7})$$

Clearly this relation is independent of the choice of basis. The full evolution operator at arbitrary point of time can be always decomposed as an evolution to the closest nearest multiple of the period and the remainder, i.e. if  $t = nT + \delta t$ , where  $0 \leq \delta t \leq T$  then

$$U(t, 0) = U(\delta t, 0)U(T)^n. \quad (\text{VII.8})$$

Thus an arbitrary solution of the Schrödinger equation reads

$$|\psi(t)\rangle U(\delta t, 0)U(T)^n |\psi_0\rangle \quad (\text{VII.9})$$

This solution can be always expanded in the basis of  $U(T)$  (or equivalently in the basis of the Floquet Hamiltonian)  $|u_j\rangle$ :  $|\psi_0\rangle = \sum_j \alpha_j |u_j\rangle$

$$|\psi(t)\rangle = \sum_j U(\delta t, 0) \exp \left[ \frac{i}{\hbar} \delta t \epsilon_j^F \right] \exp \left[ -\frac{i}{\hbar} \epsilon_j^F t \right] \alpha_j |u_j\rangle = \sum_j \exp \left[ -\frac{i}{\hbar} \epsilon_j^F t \right] \alpha_j |u_j(\delta t)\rangle, \quad (\text{VII.10})$$

where

$$|u_j(\delta t)\rangle = \exp \left[ -\frac{i}{\hbar} \epsilon_j^F t \right] U(\delta t, 0) |u_j\rangle. \quad (\text{VII.11})$$

By construction  $|u_j(\delta t)\rangle$  is a periodic function of  $\delta t$ , i.e.  $|u_j(T)\rangle = |u_j(0)\rangle$ . Eq. (VII.10) is the basis of the Floquet theorem stating that any solution of the evolution operator for a periodically driven system can be written as a superposition of the periodic in time function multiplied by the phase factors  $\exp \left[ -\frac{i}{\hbar} \epsilon_j^F t \right]$ . This statement is very similar to the Bloch theorem discussing the structure of eigenstates of the Hamiltonian in a periodic potential.

If we are not interested in fine structure of the wave function, i.e. its precise behavior between the periods, then the Floquet Hamiltonian gives the complete description of the time evolution of the system. In this sense the dynamics of the system is described by the quench process, where the Hamiltonian jumps to the Floquet Hamiltonian. In the same way we expect that in the long time limit the system will relax the stationary ensemble with respect to  $H_F$ . Thus if the Floquet Hamiltonian is ergodic we can expect that the system will relax to the Floquet thermal state. Then we can extend the whole machinery of statistical mechanics and thermodynamics to the Floquet systems. However, in this reasoning we are hiding an important question under the rug. Namely we have to establish first that the Floquet Hamiltonian is a physical Hamiltonian, i.e. that it is local and non-singular. As we will see below this is not always the case.

Finding the Floquet Hamiltonian is formally equivalent to finding the logarithm of the evolution operator over the period

$$H_F = \frac{i\hbar}{T} \log \left[ T_t \exp \left( -\frac{i}{\hbar} \int_0^T H(t) dt \right) \right]. \quad (\text{VII.12})$$

In general there is no solution for this problem if the Hamiltonian is interacting. Indeed this problem is clearly similar to finding the Free energy as the logarithm of the partition function:

$$F = -T \log [\text{Tr} \exp(-\beta H)]. \quad (\text{VII.13})$$

As we know well this problem can not be solved. Instead one has to rely on various approximation schemes, in particular, on the perturbative high-temperature expansion. We will try to follow the same route for finding the Floquet Hamiltonian from Eq. (VII.12) using the short period expansion instead of the high temperature expansion (in mathematics this is known to be the Magnus expansion). Expanding an exponential under the logarithm in Eq. (VII.12) we find

$$H_F = \frac{i\hbar}{T} \log \left[ 1 - \frac{i}{\hbar} \int_0^T H(t) dt - \frac{1}{\hbar^2} \int_0^T dt_1 \int_0^{t_1} dt_2 H(t_1) H(t_2) + \frac{i}{\hbar^3} \int_0^T dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 H(t_1) H(t_2) H(t_3) + \dots \right] \quad (\text{VII.14})$$

The expansion of the exponent inside the logarithm is clearly time ordered. Next let us expand the logarithm in powers of the period. In the leading order we clearly find

$$H_F^{(1)} = \frac{1}{T} \int_0^T H(t) dt \quad (\text{VII.15})$$

Thus we find a very intuitive result that in the high frequency limit the Floquet Hamiltonian is just the time averaged Hamiltonian. In the next order we find

$$\begin{aligned} H_F^{(2)} &= -\frac{i}{\hbar T} \int_0^T dt_1 \int_0^{t_1} dt_2 H(t_1) H(t_2) - \frac{i\hbar}{2T} \frac{i^2}{\hbar^2} \int_0^T dt_1 \int_0^{t_1} dt_2 H(t_1) H(t_2) \\ &= -\frac{1}{2\hbar T} \int_0^T dt_1 \int_0^{t_1} dt_2 [H(t_1), H(t_2)] \end{aligned} \quad (\text{VII.16})$$

Let us now also show explicitly the third order term without derivation

$$H_F^{(3)} = -\frac{1}{6T\hbar^2} \int_0^T dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([H(t_1), [H(t_2), H(t_3)]] + [H(t_3), [H(t_2), H(t_1)]]) \quad (\text{VII.17})$$

From these expressions we can see the structure of the terms appearing in the Magnus expansion. First we observe this is a short period expansion as expected. Each term carries an extra power of the period (the inverse frequency). Next we observe that for the local Hamiltonians each term in the

Magnus expansion is also local. This follows from the fact that parts of the Hamiltonian separated in space commute with each other and do not contribute to the commutator. This situation is again very similar to the high temperature expansion in thermodynamics, where the expression for the free energy is written in terms of the cumulants of the interaction, which are local. From this observation we see that the convergence of the Magnus expansion is determined by the single particle energy scales. Indeed one can define the Floquet Hamiltonian density  $H_F/V$ , which is volume independent in each order of the Magnus expansion. Therefore only non-extensive energy scale define the convergence. In particular, we can expect convergence of the Magnus expansion if we deal with bounded Hamiltonians like spin chains or Hubbard type models. In systems with unbounded Hamiltonians this expansion can be asymptotic. Let us also point that with each order of Magnus expansion the Hamiltonian becomes less and less local. The easiest way to see this is to consider a spin chain with nearest neighbor interactions. Then generically the commutator of the two such terms will produce a term with three nearest neighbor interactions, e.g.

$$[\sigma_{1x}\sigma_{2x}, \sigma_{2y}\sigma_{3y}] = 2i\sigma_{1x}\sigma_{2z}\sigma_{3y}.$$

If we consider a double commutator of such terms we will generate four spin interactions and so on. If the series does not converge we generically end up with a highly nonlocal (infinite range) Hamiltonian. This will happen if the driving period is not small. On the other hand for low frequency drive we anticipate that the periodicity is not important and the process is effectively quasi-static. So from our previous analysis we expect an infinite heating of the system. Thus we can anticipate that infinite heating is equivalent to the divergent Magnus expansion. The Magnus expansion is well defined classically. Indeed in the limit  $\hbar \rightarrow 0$  we have  $[\dots] \rightarrow -i\hbar\{\dots\}$  and the expression for the Floquet Hamiltonian becomes  $\hbar$ -independent in each order of the expansion. E.g. for the first order term we find

$$H_{F,cl}^{(3)} = \frac{1}{6T} \int_0^T dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 (\{H(t_1), \{H(t_2), H(t_3)\}\} + \{H(t_3), \{H(t_2), H(t_1)\}\}). \quad (\text{VII.18})$$

Like in statistical mechanics quantum language allows for a very simple derivation of this classical result. Other derivations available in literature are much more elaborate. And finally let us note that generically the Floquet Ham

Let us look closer into the setup where the time-dependent Hamiltonian can be written in the form

$$H(t) = H_0 + \lambda(t)V, \quad (\text{VII.19})$$

where  $\lambda(t)$  is some periodic function. Then the second term in the Magnus expansion reads

$$H_F^{(2)} = \frac{1}{2\hbar T} [H_0, V] \int_0^T dt_1 \int_0^{t_1} dt_2 (\lambda(t_1) - \lambda(t_2)) = \frac{1}{2\hbar T} [H_0, V] \int_0^T dt [t\lambda(t) - (T-t)\lambda(T-t)]. \quad (\text{VII.20})$$

For symmetric functions  $\lambda(t) = \lambda(T-t)$ , e.g.  $\lambda(t) = \lambda_0 \cos(2\pi t/T)$ , this integral is clearly zero so there is no second order contribution. For asymmetric functions this integral can be always made zero by an appropriate choice of period, i.e. by an appropriate choice of the interval  $[t_0, t_0 + T]$  defining the Floquet Hamiltonian. This choice is clearly equivalent to the gauge choice since initial evolution of the wave function to  $t_0$  can be thought of as the gauge transformation. The third order of the Magnus expansion has two different contributions:

$$H_F^{(3)} = -\frac{1}{6T\hbar^2} [H, [H, V]] \int_0^T dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 (\lambda(t_3) + \lambda(t_1) - 2\lambda(t_2)) \\ - \frac{1}{6T\hbar^2} [V, [H, V]] \int_0^T dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 (2\lambda(t_3)\lambda(t_1) - \lambda(t_1)\lambda(t_2) - \lambda(t_3)\lambda(t_2)). \quad (\text{VII.21})$$

The integrals in this expression can be evaluated for any periodic function  $\lambda(t)$ . To be specific let us choose  $\lambda(t) = \cos(2\pi t/T)$ . Then the first integral is equal to  $12\pi T^3/(2\pi)^3$  and the second one is  $-3\pi T^3/(2\pi)^3$  so we find

$$H_F^{(3)} = \frac{T^2}{16\pi^2\hbar^2} [V, [H, V]] - \frac{T^2}{4\pi^2\hbar^2} [H, [H, V]]. \quad (\text{VII.22})$$

In the short period limit the  $H_F^{(3)}$  is a small correction to the time average Hamiltonian. So one can naively think that in the regime of convergence (or asymptotic convergence) of the Magnus expansion higher order terms are only small perturbation to the time average Hamiltonian. Thus their effects are generally small (but can be still interesting if e.g. time averaged Hamiltonian is non-ergodic and the first subleading correction breaks integrability). However, the situation is much more interesting. One can get nontrivial high-frequency limit if one scales the amplitude of the perturbation with frequency,  $V \sim 1/T$ . Then clearly the first term in Eq. ( ) has a well defined high frequency limit, while the second term vanishes. If  $V$  is noninteracting, e.g. it represents coupling to an external field, then multiple commutators containing only one  $H$ , which can be complicated and interacting, and arbitrarily many  $V$  terms remain local. Thus the Floquet Hamiltonian also remains local. Another possibility to get a nontrivial Floquet Hamiltonian in the limit  $T \rightarrow 0$  and  $V \sim 1/T$  is to have the Magnus expansion truncated. This happens e.g. if  $H = \sum_j \frac{p_j^2}{2m} + U(x_j)$  and  $V = V(x_j)$ , i.e. if the Hamiltonian is a sum of the quadratic in the momentum kinetic energy and arbitrary momentum independent potential and the driving term is a function of the coordinates only. Then the commutator  $[V, [H, V]]$  becomes a function of the coordinates only and all higher

order commutators of the type  $[V, [V, [H, V]]]$  vanish. Both situations were realized in experiments and we will discuss them in the next section.

## 1. Exercises

1. Prove Eq. (VII.17)

## B. Applications to the Kapitza pendulum and a lattice system in an oscillating potential.

Let us illustrate two applications of the Magnus expansion. The first one will be the Kapitza pendulum, which we discussed earlier in the context of chaos. The other will be a system of interacting particles (bosons or fermions) in a tight-binding potential (Hubbard model) with applied high frequency field. Both problems found practical implications and both illustrate how one can get non-trivial Hamiltonians and associated phases using time-dependent potentials. First let us start from the Kapitza pendulum (see Fig. 4) for the setup. Let us first find the Lagrangian of this system

$$L = T - U = \frac{m\dot{x}^2}{2} + \frac{m\dot{y}^2}{2} - mgy \quad (\text{VII.23})$$

using that  $x = l \sin(\theta)$ ,  $y = a \cos(\omega t) - l \cos(\theta)$ . Then up to unimportant constants

$$L = \frac{ml^2}{2} \dot{\theta}^2 - ml\omega \sin(\omega t) \sin(\theta) \dot{\theta} + mgl \cos(\theta). \quad (\text{VII.24})$$

The equations of motion for this system read

$$\begin{aligned} 0 &= \frac{d}{dt} \frac{\partial L}{\partial \dot{\theta}} - \frac{\partial L}{\partial \theta} = ml^2 \ddot{\theta} - ml\omega^2 \cos(\omega t) \sin(\theta) - ml\omega \sin(\omega t) \cos(\theta) \dot{\theta} \\ &\quad + ml\omega \sin(\omega t) \cos(\theta) \dot{\theta} + mgl \sin(\theta) = ml^2 \ddot{\theta} - ml\omega^2 \cos(\omega t) \sin(\theta) + mgl \sin(\theta) \end{aligned} \quad (\text{VII.25})$$

These equations represent a pendulum in a time-dependent external potential

$$V(t) = -mgl \cos(\theta) \left( 1 - \frac{a\omega^2}{g} \cos(\omega t) \right). \quad (\text{VII.26})$$

The Hamiltonian then can be written as

$$H + V = \frac{p_\theta^2}{2ml^2} - mgl \cos(\theta) + mal\omega^2 \cos(\omega t) \cos(\theta) \quad (\text{VII.27})$$

The periodic potential has the amplitude scaling as a frequency in the limit  $\omega \rightarrow \infty$  if we keep the product  $a\omega$  constant. Thus asymptotically at the high frequency limit we can use only the first term in Eq. (VII.A):

$$H_F^{(3)} \approx \frac{1}{4\omega^2 \hbar^2} m^2 a^2 l^2 \omega^4 \frac{1}{2ml^2} [\cos(\theta), [p^2, \cos(\theta)]] = \frac{ma^2\omega^2}{4} \sin^2(\theta) \quad (\text{VII.28})$$

So in the limit  $\omega \gg \omega_0 = \sqrt{g/l}$  the Kapitza pendulum can be approximately described by the stationary effective Hamiltonian

$$H_F \approx \frac{p^2}{2ml^2} - mgl \cos(\theta) + \frac{ma^2\omega^2}{4} \sin^2(\theta). \quad (\text{VII.29})$$

This Hamiltonian explains emergence of the second metastable equilibrium at  $\theta = \pi$  when

$$\frac{a\omega}{l\omega_0} > \sqrt{2}$$

and explains why the equilibrium at  $\theta = 0$  is further stabilized by the driving. As we discussed earlier because the kinetic energy is quadratic in the momentum, there are no other corrections to the Floquet Hamiltonian in the high frequency limit (if we keep the product  $a\omega$  constant).

The second example we consider deals with a lattice system of particles described by the Hubbard model in a time-dependent periodic field. For simplicity we will assume this is a one-dimensional system, but this is not important in the analysis. Then

$$H + V = -J \sum_j (a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) + \sum_{ij} u_{ij} n_i n_j + \Delta j \cos(\omega t) n_j \quad (\text{VII.30})$$

Here  $n_j = a_j^\dagger a_j$  is the particle density,  $J$  represents the hopping matrix element and  $\Delta$  is the amplitude of the external field (e.g. electric field), which periodically oscillates in time. This Hamiltonian realizes another situation, where we expect to see a nontrivial high-frequency limit if we send  $\omega \rightarrow \infty$  simultaneously scaling the electric field  $\Delta$  with  $\omega$ . This problem can also be solved using the Magnus expansion. But it turns out there is a simpler route, where one first can make a gauge transformation in the Hamiltonian, and then apply the Magnus expansion. Recall that the Heisenberg equations of motion for the creation and annihilation operators are

$$i\dot{a}_j = [a_j, H] = -J(a_{j+1} + a_{j-1}) + 2 \sum_i u_{ij} n_i a_j + \Delta j \cos(\omega t) a_j \quad (\text{VII.31})$$

Let us do the following transformation

$$a_j = \tilde{a}_j e^{-ij(\Delta/\omega) \sin(\omega t)} \quad (\text{VII.32})$$

Then the new equations of motion for  $\tilde{a}_j$  read:

$$i\dot{\tilde{a}}_j = -J \left( \tilde{a}_{j+1} e^{-i\Delta/\omega \sin(\omega t)} + \tilde{a}_{j-1} e^{i\Delta/\omega \sin(\omega t)} \right) + 2 \sum_i n_i \tilde{a}_j. \quad (\text{VII.33})$$

I.e. we effectively moved the time dependence from the effective potential to the hopping (such trick was first suggested by Pirls). So in terms of new fields the Hamiltonian reads

$$H = -J \sum_j \left( \tilde{a}_j^\dagger \tilde{a}_{j+1} e^{-i\Delta/\omega \cos(\omega t)} + \tilde{a}_{j+1}^\dagger \tilde{a}_j e^{i\Delta/\omega \cos(\omega t)} \right) + \sum_{ij} u_{ij} n_i n_j \quad (\text{VII.34})$$

This is a time dependent Hamiltonian, however, it can not be represented in the form  $H + V(t)$  but rather  $H + V(t) + V^\dagger(t)$ . This introduces additional terms in the Magnus expansion, in particular, non-vanishing  $H_F^{(2)}$ . But the general structure of the expansion remains the same. Note that in principle all observables should be also re-expressed through  $\tilde{a}_j$  and  $\tilde{a}_j^\dagger$ . But at times, which are multiple of the driving period clearly  $\tilde{a}_j = a_j$  so we do not need to worry about this subtlety if we are interested in the stroboscopic description of the system and thus can drop the tilde sign. Because the amplitude in the hopping term is bounded at any value of  $\Delta$  and  $\omega$  we can take an infinite frequency limit and obtain an effective Floquet Hamiltonian

$$H_F \approx -JJ_0(\Delta/\omega) \sum_j (a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) + \sum_{ij} u_{ij} n_i n_j, \quad (\text{VII.35})$$

where  $J_0$  is the Bessel function. This simple time-average is in fact an infinite resummation of the original Magnus expansion (see exercises). Note that if we take the limit  $\omega \rightarrow \infty$  at fixed  $\Delta$  we will reproduce the time-average of the original Hamiltonian (VII.30) as expected. But if we keep the ratio  $\Delta/\omega$  fixed we can get a highly nontrivial Hamiltonian with e.g. vanishing or negative hopping strength. We can thus create Hamiltonians with interesting properties, which are impossible to achieve in equilibrium

### 1. Exercises

1. Show that in the high frequency limit the leading terms in the Magnus expansion for the Hamiltonian (VII.30) one can reproduce Eq. (VII.35). One can match the Taylor series of the Bessel function with the Magnus expansion term by term.

## VIII. ACKNOWLEDGMENTS

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## IX. FINAL PRESENTATIONS

### A. Schedule

- Tuesday, Dec. 3.  
9:15-9:50 Adam Iazzi  
9:50-10:25 Michael Chernicoff  
10:25-11:00 Tom Iadecola
  
- Thursday Dec. 5  
9:15-9:50 Chester Curme  
9:50-10:25 Marin Bukov  
10:25-11:00 Shainen Davidson
  
- Friday Dec. 6  
9:15-9:50 Nick Lubbers  
9:50-10:25 Gabriel Birzu  
10:25-11:00 Uttam Bhatt  
  
11:00-11:30 Coffee  
  
11:30-12:05 Bernardo Zubillaga  
12:05-12:40 Rashi Verma  
  
12:40-1:30 Lunch  
  
1:30-2:05 Cancan Zhang  
2:05-2:40 Mahsa Mokhtarzadeh  
2:40-3:15 Ching-Hao Wang
  
- Tuesday, Dec. 10  
9:15-9:50 Rajita Menon  
9:50-10:25 Na Xu  
10:25-11:00 Xin Yuan

## B. Theoretical

1. Thermalization and prethermalization after interaction quench in the Hubbard model. M. Moeckel, S. Kehrein, Phys. Rev. Lett. 100, 175702 (2008); M. Eckstein, M. Kollar, P. Werner, Phys. Rev. B 81, 115131 (2010). [Na Xu, Dec. 10](#)
2. C. Shannon, A mathematical theory of communication, <http://www3.alcatel-lucent.com/bstj/vol127-1948/articles/bstj27-3-379.pdf>, [Rajita Menon, Dec.10](#)
3. Statistics of work in interaction quenches and its relation to the Loschmidt echo. A. Silva, Phys. Rev. Lett. 101, 120603 (2008) [Rashi Verma, Dec. 6](#)
4. Chirikov criterion for ergodicity in the classical FPU model: F.M. Izrailev and B.V. Chirikov, Statistical properties of a nonlinear string, Sov. Phys. Dokl., 11, 30 (1966): <http://lptsv4.ups-tlse.fr/chirikov/refs/chi1966e.pdf> [Cancan Zhang, Dec. 6](#)
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6. S. Fishman, D.R. Grempel and R.E. Prange, Phys. Rev. Lett. 49, 509 (1982).
7. Relaxation to the generalized Gibbs ensemble in an integrable model after a quench (quite mathematical). Maurizio Fagotti, Fabian H.L. Essler, Phys. Rev. B 87, 245107 (2013)
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9. Steady state fluctuations in driven-dissipative systems. G. Bunin and Y. Kafri, [arXiv:1202.5053v1.pdf](#) (2012) [Nick Lubbers Dec. 6](#)
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11. Quantum chaos and effective thermalization using Husimi representation (similar to the Weyl-Wigner rep.). A. Altland, F. Haake, Phys. Rev. Lett. 108, 073601 (2012), New J. Phys 14, 73011 (2012) [Shainen Davidson](#)

12. Local conservation laws in many-body localized states. M. Serbyn, Z. Papi, D. A. Abanin, Phys. Rev. Lett. 111, 127201 (2013); D. A. Huse and V. Oganesyan, arXiv:1305.4915 (2013) **Adam Iaizzi. Dec. 3**
13. Different phase space representations in Quantum Optics (Glauber P, Positive P, Q (Husimi). Walls and Milburn, Quantum Optics, Chapter 4; Gardiner and Zoller, Quantum Noise, Chapter 4; M. J. Steel et al, Phys. Rev. A 58, 4824 (1998)
14. Emergent irreversibility and entanglement spectrum statistics, Claudio Chamon, Alioscia Hamma, Eduardo R. Mucciolo, arXiv:1310.2702 **Bernardo Zubillaga. Dec. 6**

### C. Experimental

15. Information to energy conversion and Maxwell demon (experiment + theory). S. Toyabe et. al., Nature Physics 6, 988992 (2010) **Gabriel Birzu Dec. 6**; Information Thermodynamics: Maxwell's Demon in Nonequilibrium Dynamics, T. Sagawa, M. Ueda **Uttam Bhatt. Dec. 6**
16. Observation of Floquet topological insulators (experiment + theory). Y. H. Wang, H. Steinberg, P. Jarillo-Herrero, N. Gedik <http://arxiv.org/abs/1310.7563>; Benjamin M. Fregoso, Y.H. Wang, N. Gedik, Victor Galitski <http://arxiv.org/abs/1305.4145>. **Tom Iadecola, Dec. 3**
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18. W. Hu et. al. Enhancement of superconductivity in periodically driven YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.5</sub>: arXiv:1308.3204 (2013); arXiv:1205.4661 (2012) **Mahsa Mokhtarzadeh, Dec. 6**.
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21. Experimental test of Hatano Sasa's nonequilibrium steady-state equality, E. H. Trepagnier et. al., PNAS 101, 15038 (2004) **Ching-Hao Wang, Dec. 6**