Lecture Notes for Modern Theoretical Condensed Matter

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Contents

1 Introduction

There are many rich frameworks used to describe various exotic regimes like the quantum hall regime, crystalline solids, topologically ordered phases of matter, and the phase transitions between them. But all of this progress has been built on two pillars of equilibrium statistical mechanics:

1. Thermalization

2. Phase structure

We assume, when studying phase transitions in the general sense, that the system is in thermal contact with some kind of bath/reservoir, and the system exchanges heat, particles, etc. with this bath, and eventually it reaches equilibrium at late times. This state is characterized by a few variables like temperature, chemical potential, etc. depending on the conservation laws in this

system. Then the properties are developed by analysis of observables or order parameters:

$$\rho_{eq}(T, \mu, ...) \tag{1}$$

$$\langle O \rangle = Tr[\rho_{eq}O] \tag{2}$$

The definition of a phase only makes sense in the thermodynamic limit, where we only care about the asymptotics of millions and millions of particles at late times. The central problem in statistical mechanics is how to keep track of all of this data. This is where equilibrium statistical mechanics comes in: a standard assumption of equilibrium statistical mechanics is the ergodic hypothesis, which states that, in time, all of phase space is explored, so we can replace all of these detailed equations of motion with macroscopic averages. These macrostates are characterized by a couple parameters like temperature, chemical potential... to find the equilibrium state, or, if we're at zero temperature, the ground state, and then characterize phases and phase transitions by evaluating correlation functions, order parameters, etc.

One question is what can we say about the dynamics of *isolated* many-body quantum systems, where there is no bath. How does such a system reach equilibrium? Usually we think about some sort of irreversible change from a tiny fraction of phase space, and, after a long time, having no way to know what that tiny fraction was. However, under unitary time evolution, we know where the initial state was. Thus the first question is what thermal equilibrium even means in this context.

Remark 1. *This is actually deeply connected to the black hole information paradox. According to Hawking's calculation for an evaporating black hole, the Hawking radiation should only be characterized by a small number of paramters such as the temperature or mass of the black hole, but a quantum black hole evolving unitarily doesn't forget any information.*

1.1 Thermalization & Localization

Here we will consider highly excited, strongly interacting many-body systems. A standard assumption of statistical mechanics is that this system goes to thermal equilibrium at late times. This makes sense, but must this always be true? What does "thermal equilibrium" mean in this context, and how is it reached? How does classical hydrodynamics emerge from unitary quantum dynamics? Anderson, in 1958, gave the first example of a system which could be many-body "localized" and fail to go to thermal equilibrium. (*Absence of Diffusion in Certain Random Lattices*) The question he raised in 1958 is: Can an isolated, strongly interacting many-body system act as its own "bath" and bring its subsystems to thermal equilibrium? The two *generic* (not fine-tuned in any way) answers are

1. Yes: the system is thermalizing

2. No: the system is many-body localized. E.g. integrable models. These have extensively many conservation laws, so any thermalization must obey these conservation laws, so they don't generically thermalize to a Gibbs ensemble where temperature is a parameter; instead they thermalize to generalized Gibbs ensembles.

There are some systems that are sort of intermediate to the above two possibilities. E.g. many-body scars, ie. systems where the vast majority of initial states do approach thermal equilibrium, but there are states that don't.

If you have thermalizing on one hand and localization on the other hand, what is the whole chaos between the two? As of now, our current understanding is that there are only two *generic* possibilities, i.e. if we have one intermediate system and perturb it in parameter space, it goes to one or the other.

In thinking about these new systems, we think about different classes of models. We have

1. Time-independent Hamiltonians: $U(t) = e^{-iHt}$

2. Floquet systems: $H(t + T) = H(t), U(nT) = [U(T)]^T$

3. Unitary circuits (e.g. from quantum information theory)

Remark 2. *The Google experiment claiming quantum supremacy really just implemented a random unitary circuit and characterized the behavior of that circuit.*

A natural question is whether systems with more structure, e.g. have many-body eigenstates, is there more structure implied?

The **Eigenstate Thermalization Hypothesis** (ETH) states that if all "reasonable" initial states reach thermal equilibrium, then eigenstates of H must be thermal:

$$H \left| n \right\rangle = E_n n \tag{3}$$

$$Tr_B \left| n \right\rangle \left\langle n \right| = Tr_B \frac{e^{-\beta_n H}}{Z} \tag{4}$$

Eigenstates are time-independent, so how would an eigenstate reach thermal equilibrium in time? ETH says that they must already be thermal. This means that, in systems that are thermalizing and obey ETH, every single eigenstate is thermal and forms a microcanonical ensemble.

The only "generic" (that we're aware of) exception to thermalization is localization. This occurs in systems that are not translationally invariant. An actual experiment verifying this was done in a system of cold atoms (Choi et. al. Science (2016), Screiber et. al (2015)). A localized system

retains local memory of its initial conditions forever i.e. is observable. Globally, unitary dynamics preserves all information, but locally we preserve local information.

So, when is ETH obeyed? Yes: (strong version) for all eigenstates at finite temperature. (weak version) for most eigenstates at finite temperature. This weak version occurs in many body quantum scars. For examples, the AKLT chain. No: In many body localized systems, integrable systems (generalized Gibbs ensemble). For some observable O at some temperature $\frac{1}{\beta}$,

$$\langle O \rangle_\beta = \frac{1}{Z} Tr[e^{-\beta H} O] \tag{5}$$

if $\tau = \infty, \beta = 0$, and

$$\langle O \rangle_{\beta=0} = \frac{Tr[O]}{Z} \tag{6}$$

The observable could be energy density. Most eigenstates entropically will live near this energy density. Each state has a global energy (with T some global temperature) and energy density E/V. For ρ for the whole system, we have

$$Tr_B[\rho] = \rho_A(t) \xrightarrow{t, Vol_B \to \infty} Tr_B[\rho_{thermal}(t)] \tag{7}$$

so if we have a thermal density matrix ρ at the temperature set by the energy density of the state we're considering (which, for an eigenstate, is just the energy density), the reduced density energy matrix of the subregion at late times approaches the reduced density matrix appropriate to a thermal density matrix.

1.2 Entanglement Dynamics

In systems that reach thermal equilibrium, the states approach a **volume law** which states that the rest of the region B can act as a bath for all spins in A. Then the Von Neumann entanglement entropy for region A agrees with the thermodynamic entropy at the temperature that's appropriate to the eigenstate/initial state that we're considering, so the entanglement entropy scales with the volume. On the other hand, one of the best diagnostics of locallization (because transport doesn't really work) is in the dynamics of entanglement in the eigenstates of an MBL system. In MBL systems, states have an **area law** for entanglement: only the spins right near the edge in A are entangled to the spins in B, and B is not able to act like a bath and bring all states in A to thermal equilibrium. So in MBL systems, entanglement entropy scales with the perimeter of the subregion, so the difference between thermalization and localization is really examining the entanglement

properties of the system.

2 Thermalization & the Eigenstate Thermalization Hypothesis

In strongly interacting, highly excited systems, we have the natural question: Do these systems reach thermal equilibrium under their *own* internal unitary dynamics? As above, thermalizing systems answer yes, MBL systems, integrable systems, etc. answer no. For both cases, how and why to the dynamics establish equilibrium or not? Furthermore, how does unitary dynamics lead to apparently irreversible changes? The types of systems we'll consider are

1. Time-independent Hamiltonians $H(t) = H$, where energy is conserved, and we consider eigenstates of H

2. Floquet systems $H(t+T) = H(t)$. This means, in the way that momentum is not conserved in Bloch settings, energy is not conserved, although quasi-energy (energy mod ω) is conserved.

3. Random $H(t)$ with no symmetries.

For the first item, we have $U(t) = \tau e^{-i \int_0^{t'} dt' H(t')}$, which, since $H(t) = H$, we have the energy eigenstates form a complete basis, so

$$|\psi_0\rangle = \sum_\alpha c_\alpha |\alpha\rangle \tag{8}$$

$$|\psi(t)\rangle = \sum_\alpha c_\alpha e^{-iE_\alpha t} |\alpha\rangle \tag{9}$$

All of the complexity is hidden in E_α and $|\alpha\rangle$. In traditional statmech, we have a system S within an environment E, with $|S| << |E|$. Then we specify the laws of conservation: we want to talk about the total energy or the total particle number, etc. These conservation laws define the appropriate equilibrium states as the maximum entropy states consistent all these different conservation laws. Usually the way this works is we take variables conjugate to the energy density or the particle number, assume the environment is at some fixed temperature or chemical potential, and the system and the environment are exchanging energy, particles, etc. and the system is going to reach thermal equilibrium at late times as a result of this change. Thus we want

$$\rho_S(t) \to \rho_{eq}^S(T, \mu, ...) \tag{10}$$

where ρ_{eq}^S is the maximum entropy state consistent with all of the conservation laws in this system.

Implicitly in this system we take advantage of classical chaos. A classically chaotic system ergodically explores all of phase space, so we can replace very detailed descriptions of all of these particles with macroscopic descriptions. What is the analogue in the many-body setting? We are still exploring how to correctly describe quantum chaos, and what the notion of ergodicity means in this many-body setting. What we do know how to define is the concept of thermalization.

Definition 1. *In a closed quantum system, **thermalization** is the property that the system successfully acts as a bath for its subsystems and brings them to equilibrium at late times and for large sizes.*

Definition 2. *A **subsystem** is a subset of the degrees of freedom of the whole system. For a subsystem A of system B (A's complement, as a bath), we require (imprecisely) $||A|| << ||B||$, $\mathcal{H}_A = \{|a\rangle_A\}$, $\mathcal{H}_B = \{|b\rangle_B\}$, $\mathcal{H}_{total} = \mathcal{H}_A \otimes \mathcal{H}_B$ spanned by $\{|a\rangle_A \otimes |b\rangle_B\}$ with hamiltonian $H = H_A + H_B + H_{AB}$.*

We assume that there are some local degrees of freedom, e.g. spins on some site. The subsystem is some low-order constructions in terms of these local operators. The observables are also going to be low-order constructions in terms of local observables.

$$\sum_{i \in A} O_i \tag{11}$$

for O_i local operators. These are a vanishing subset of all the operators defined on our Hilbert space.

Definition 3. ***States*** *can be pure or mixed. A state is given by its density matrix ρ. This corresponds to the probability density in state space. We know $Tr[\rho] = 1$, and $\rho = \sum_n p_n |n\rangle |n\rangle$. In general $Tr[\rho]^2 \leq 1$, with equality if and only if it is a pure state. The time evolution of this state is, again, given by the Schrödinger equation.*

So now we have a state defined in AB given by ρ_{AB}. If we want to define the state on the subsystem we take the reduced-density matrix $Tr_B[\rho_{AB}]$.

Definition 4. *What we mean by **thermal equilibrium** is*

$$\lim_{t, B \to \infty} \rho_A(t) = Tr_B(\rho_{AB}) \to Tr_B[\rho_{eq}] \tag{12}$$

The appropriate equilibrium state ρ_{eq} (which is not unique) respects all conservation laws in our system.

Remark 3. *There are classes known as integrable systems that have infinitely many local conserved quantities, taking the form*

$$N_q = \sum_i c_{q,i} O_{q,i} \tag{13}$$

$$q = \{0, 1, ...\} \tag{14}$$

where the sum is over every site i.

Now we need to specify conserved quantities. We know energy density E/V is conjugate to temperature, number density is conjugate to chemical potential, and we need these quantities to be well-defined in the thermodynamic limit. We have the expectations $\langle E \rangle \propto V, \langle \Delta E \rangle \propto V^2, \alpha < 1$. Only when we have

$$\lim_{V \to \infty} \frac{\langle \Delta E \rangle}{\langle E \rangle} \to 0 \tag{15}$$

do we have a well-defined energy density. Only then can we have a well-defined temperature for our system as a whole. So if we have initial states which are macroscopic superpositions of states that have very different (extensively different, to be precise) expectation values for energy or number, then the energy is so uncertain that we don't know what energy we're supposed to be thermalizing to, so we can't define an appropriate equilibrium ensemble because we don't know what the right temperature should be.

Definition 5. *If we start with an out-of-equilibrium initial state $|\psi_0\rangle$, which could be a product state, and we time-evolve it under a Hamiltonian, we see what the dynamics look like. We prepared $|\psi_0\rangle$ by preparing the ground state of some Hamiltonian and then, immediately after time $t = 0$ **quench** to a different Hamiltonian, which means we vary the experimental parameters as fast as we can to time evolve our initial state under a different Hamiltonian. In practice people start with product states. All such initial states behave well, i.e. have sub-extensive uncertainties in all conserved quantities.*

Suppose we have a state ρ which is a candidate thermal state. ρ can be mixed or pure. From ρ we get $\rho_A = Tr_B(\rho)$. We say ρ is thermal if $\rho_A \to \rho_A^{eq}$. In the ETH, we consider eigenstates as

our candidate states. These are pure states, but the eigenstate can individually be thermal if, in this limit, if (for $|n\rangle$ the nth energy eigenstate)

$$Tr_B(|n\rangle \langle n|) \to \rho_A^{eq} \tag{16}$$

(One candidate for ρ^{eq} is $\frac{1}{Z} \sum_n e^{-\beta E_n} |n\rangle \langle n|$)

Remark 4. *For a system with no eigenstates, it is considered thermalized if we reach the maximum entropy state. E.g. for Floquet systems or $H(t)$ with no conservation laws, $\rho_A^{eq} \propto 1_A$. The Gibbs ensemble at infinite temperature also approaches the identity.*

If we have a thermal state, all local information is set by the conserved quantities, and has forgotten everything about the initial condition, i.e. if $\rho_0 \to \rho_{eq}$, all local information at late times is only set by the macroscopic conserved quantities, and all other information about the initial state is hidden in non-observable operators.

The ETH has two versions. The strong version states that every MB eigenstate at finite $t > 0$ is a thermal state (the weak version states most). Suppose $|\psi_0\rangle$ is a non-equilibrium initial pure state. Then $\langle E \rangle = \langle \psi_0| H |\psi_0\rangle, \langle \Delta E \rangle = \sqrt{\langle \psi_0| H^2 |\psi_0\rangle - \langle H \rangle^2}$. If $|\psi_0\rangle$ is a well-defined state, then $\frac{\Delta E}{E} \to 0$ as $V \to \infty$. Then $|\psi_0\rangle$ has a well-defined energy density. We can use the energy-entropy curve to define temperature via $\frac{dS}{dE} = \frac{1}{T}$. If we wait over time, $|\psi_0\rangle \xrightarrow{t} Tr_B[|\psi_0(t)\rangle \langle \psi_0(t)|] = Tr_B[\rho_0(t)] = Tr_B[\frac{e^{-\beta H}}{Z}]$. Notice that the state determines the temperature, because the system is isolated. For an energy eigenstate,

$$H |\alpha\rangle = E_\alpha |\alpha\rangle \tag{17}$$

$$|\psi_0\rangle = \sum_\alpha c_\alpha |\alpha\rangle \tag{18}$$

$$|\psi(t)\rangle = \sum_\alpha c_\alpha e^{-iE_\alpha t} |\alpha\rangle \tag{19}$$

$$\langle \psi(t)| O |\psi(t)\rangle = \sum_{\alpha,\beta} c_\beta^* c_\alpha e^{-i(E_\alpha - E_\beta)\tau} \langle \beta| O |\alpha\rangle \tag{20}$$

$$= \sum_\alpha |c_\alpha|^2 O_{\alpha\alpha} + \sum_{\alpha \neq \beta} c_\beta^* c_\alpha e^{-i(E_\alpha - e_\beta)\tau} O_{\beta\alpha} \tag{21}$$

so we have all of these random phases $e^{-i(E_\alpha - e_\beta)\tau} O$. In these hamiltonians, we assume there are no degeneracies. Degeneracies usually come from symmetries, but we consider that we are working in one block of the hamiltonian, i.e. all symmetries have already been accounted for. If we have

$$E_{\beta_1} + ... + E_{\beta_n} = E_{\alpha_1} + ... + E_{\alpha_n} \tag{22}$$

Then we know that $|\beta_1...\beta_n\rangle$ is some permutation of $|\alpha_1...\alpha_n\rangle$ so there are no symmetries in the problem.

$||\mathcal{H}_{AB}|| \propto \exp(V)$, e.g. 2^L for spin-$\frac{1}{2}$ in a 1-dimensional chain. The energies are extensive, so if we take the full spectrum from E_0 to E_{2^L-1}, we know since E_0, E_{2^L-1} scale with V, then $E_{2^L-1} - E_0 \propto V$. We have jammed in 2^L energy levels in this extensive spacing. Thus we have

$$\frac{E_0}{E_{2^L-1} - E_n} = \frac{\alpha V}{2^V} \propto e^{-V} \tag{23}$$

so we have exponentially decaying energy differences as the system grows. In the limit as $t \to \exp(V)$, we have that all of the differences become some random numbers and the $e^{-i(E_\alpha - e_\beta)\tau}$ term goes to zero, so we are left with the diagonal term $\sum_\alpha |c_\alpha|^2 O_{\alpha\alpha}$.

So thermal equilibrium is the diagonal piece $\sum_\alpha |c_\alpha|^2 O_{\alpha\alpha} \to O_{eq} = Tr[O\rho_{Gibbs}(t)]$. If this expression has to hold for absolutely every initial state, then we know that $O_{\alpha\alpha}$ must be thermal. This is the ETH. Srednicki's statement in particular is

$$\langle a| O |\beta\rangle = O(E)\delta_{\alpha\beta} + e^{-\frac{S(E)}{2}} f(E,\omega)R_{\alpha\beta} \tag{24}$$

where O is a smooth function of $E := E_\alpha + E_\beta 2$ $((E) = \langle O \rangle_{Th} + \mathcal{O}(V^{-1}), \langle O \rangle_{Th} = \frac{1}{Z}Tr[e^{-\beta H}O])$, and $\delta_{\alpha\beta}$ is the diagonal part, $f(E,\omega)$ is a smooth function of E and ω (usually decaying for large ω), and $R_{\alpha\beta}$ is a random number of mean 0 and standard deviation 1. This tells us that off-diagonal matrix elements are exponentially small.

3   Quantum Statistical Mechanics

The Transverse Field Ising Model (TFIM) is the system with Hamiltonian

$$H = -J \sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x \tag{25}$$

The ground state of H is ferromagnetically ordered when $J > h$, is a paramagnet for $h > J$, and the system undergoes a phase transition when $h = J$. For a system of L spins, let

$$\sigma_i^\alpha = 1 \otimes ... \otimes 1 \otimes \sigma^\alpha \otimes 1 \otimes ... \otimes 1, \alpha \in \{x, y, z\} \tag{26}$$

3.1 Block-diagonalization

The TFIM has a symmetry with the operator $P = \prod_i \sigma_i^z$, which flips all spins in the z basis. It is easy enough to create P and H using scipy's sparse matrix methods. Since P flips all spins, $P^2 = 1$, so P's eigenvalues are ± 1. Thus we can transform H into a block-diagonal matrix, corresponding to the +1 and -1 sectors. By finding the eigenvectors and eigenvalues of these matrices, we can greatly speed up the solving of the Hamiltonian: (the following code is in python using numpy and scipy sparse matrix methods)

```python
def diagonalize_with_P_v1(H, P, L):
    '''assuming P is diagonal, i.e. using
       P = gen_op_prod(sz_list)'''
    diagP = P.diagonal()
    posP_inds = np.where(diagP==1)[0]
    posP_sector = np.ix_(posP_inds, posP_inds)
    negP_inds = np.where(diagP==-1)[0]
    negP_sector = np.ix_(negP_inds, negP_inds)
    Hfull = H.toarray()
    H_negP = Hfull[negP_sector]
    H_posP = Hfull[posP_sector]
    evals_negP = linalg.eigh(H_negP, eigvals_only=True)
    evals_posP = linalg.eigh(H_posP, eigvals_only=True)
    return [evals_negP, evals_posP]
```

Here is an alternative method for block-diagonalizing H: (using argsort)

```python
def permute_in_place(M, p):
    '''reorder rows and columns of matrix M
       according to permutation vector p'''
    N = M.shape[0]
    for i in range(N):
        M[:,i] = M[p,i]
    for i in range(N):
        M[i,:] = M[i,p]


def plot_matrix_structure(H):
    plt.imshow(np.where(np.abs(H)>1e-5,1,0),cmap='Greys')
    plt.xlabel(r'index $i$')
```

```python
    plt.ylabel(r'index $j$')
    plt.title(r'$H_{ij}$')
    plt.show()


def diagonalize_with_P_v2(H, P, L, print_Hfull = False):
    '''assuming P is diagonal, i.e. using
       P = gen_op_prod(sz_list)'''

    def get_block_inds(conserved_op_eigs):
        _, inds = np.unique(conserved_op_eigs, return_index = True)
        return inds


    diagP = P.diagonal()
    perm = np.argsort(diagP)
    Hfull = H.toarray()
    permute_in_place(Hfull, perm)

    if print_Hfull:
        plot_matrix_structure(Hfull)

    _, block_inds = np.unique(diagP, return_index = True)
    block_inds = np.append(block_inds, [Hfull.shape[0]])

    evals = []
    for i in range(len(block_inds)-1):
        evals = np.append(evals, np.linalg.eigvalsh(Hfull[block_inds[i]:block_inds[i+1], 

    evals = np.sort(evals)


    return evals
```
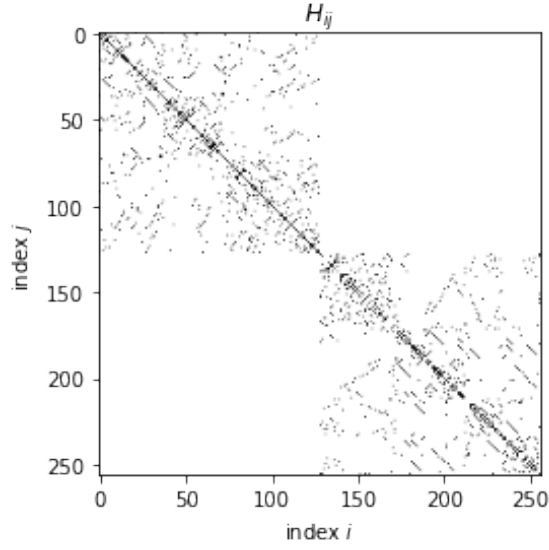
After this block-diagonalization, we get the following matrix representation of H with $L = 8$:

H_{ij}

Thus we've partially split the Hamiltonian into two blocks of size $2^{L-1} \times 2^{L-1}$.

In general, to diagonalize H using parity symmetry, we need the eigenvectors of P. In the x-basis, they are of the form $|\pm_1, \pm_2, ..., \pm_L\rangle$. This is done in the following code:

```python
def gen_parity_eigenstate(n, L):
    '''generates the n'th parity eigenstate
    by taking binary representation of n and
    translating 0 -> |+> and 1 -> |-> '''
    b = np.binary_repr(n, width=L)
    state = [1,1] if b[0]=='1' else [1,-1]
    for j in range(1,L):
        if b[j]=='1':
            state = sparse.kron(state,[1,1],'csc')
        else:
            state = sparse.kron(state,[1,-1],'csc')
    state = state/ 2**(L/2) # properly normalize
    return state


def diagonalize_with_P_v3(H, P, L, print_Hfull = False):
    '''assuming P is in x-basis, i.e. using
    P = gen_op_prod(sx_list) '''

    even_projector = np.zeros((2**(L-1),2**L))
    odd_projector = np.zeros((2**(L-1),2**L))
```

```python
        even_counter, odd_counter = 0, 0

    for n in range(2**L):
        state = gen_parity_eigenstate(n, L)

        if state[0,0]==state[0,2**L-1]:
            even_projector[even_counter, :] = state.toarray()
            even_counter += 1
        else:
            odd_projector[odd_counter, :] = state.toarray()
            odd_counter += 1

    if print_Hfull:
        U = np.zeros((2**L,2**L))
        U[:2**(L-1), :] = even_projector
        U[2**(L-1):, :] = odd_projector
        H_transformed = U@H@U.T
        plot_matrix_structure(H_transformed)

    # Get the parity sectors of the Hamiltonian with the projectors
    H_even = even_projector@H@even_projector.T
    H_odd = odd_projector@H@odd_projector.T
    evals_even = linalg.eigh(H_even, eigvals_only=True)
    evals_odd = linalg.eigh(H_odd, eigvals_only=True)
    return np.sort(np.concatenate((evals_even, evals_odd)))
```
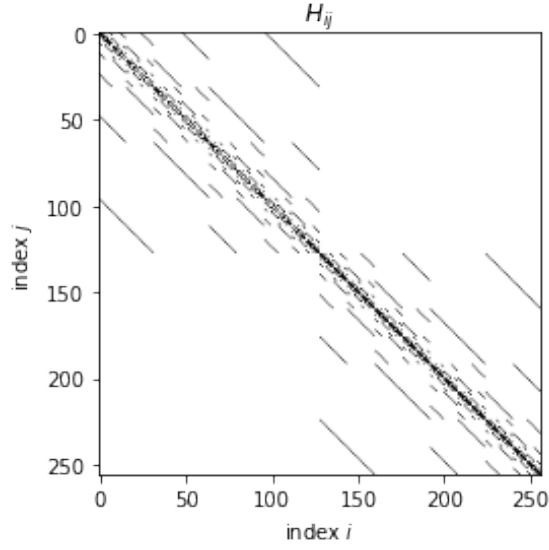
Resulting in the following matrix:

H_{ij}

3.2   Open boundary conditions, parity and reflection

For open systems, we have spatial reflection symmetry, with reflection operator $R : i \to L - i$. For periodic systems, we have R, but we also have spatial translation invariance, with translation operator $T : i \to i + 1$.

Remark 5. *Notice that $[H, R] = [H, T] = 0, [R, T] \neq 0$.*

For open boundary conditions, we can simultaneously diagonalize H using R and P. $R^2 = 1$, so the eigenvalues of R are ± 1. This simultaneous diagonalization should gives blocks of size $2^L/4$.

Let $|\Psi_P\rangle$ be the eigenstates of P, i.e. states of the form $|\pm_1, \pm_2, ..., \pm_L\rangle$. Then

$$|\Psi_{RP}\rangle := \frac{|\Psi_P\rangle \pm R |\Psi_P\rangle}{\sqrt{2}} \tag{27}$$

are eigenstates of both P and R. We implement this with the following code:

```
def bin2int(b):
    L = len(b)
    n = 0
    for i in range(L):
        if b[i] == '1':
            n += 2**(L - i - 1)
    return n


def lex_order(b1, b2):
    '''order bit strings based on the value of their
```

```python
            integers in base 10. Smallest first.'''
    n1, n2 = bin2int(b1), bin2int(b2)
    if n1 == n2:
        return 0
    elif n1 > n2:
        return 1
    else:
        return -1


def gen_reflection_op(L):
    N = 2**L
    row, col = np.arange(N), np.zeros(N)
    data = np.ones(N)
    for i in range(N):
        col[i] = bin2int(np.binary_repr(i,width=L)[::-1])
    R = sparse.csr_matrix((data, (row, col)), shape=(N, N))
    return R


def ispalindrome(b):
    return (bin2int(b) == bin2int(b[::-1]))


def get_bitstring_parity(b):
    return 1 if b.count('0')%2 == 0 else -1


def diagonalize_with_PR(H, P, R, L, print_Hfull = False):
    P_even_R_even_states = []
    P_even_R_odd_states = []
    P_odd_R_even_states = []
    P_odd_R_odd_states = []

    for i in range(2**L):
        b = np.binary_repr(i,width=L)

        if ispalindrome(b):
            state = gen_parity_eigenstate(i, L)
```

```python
    peig = get_bitstring_parity(b)
    if peig > 0:
      P_even_R_even_states.append(state.toarray()[0])
    else:
      P_odd_R_even_states.append(state.toarray()[0])


  if lex_order(b, b[::-1]) <= 0:
    continue


  state = gen_parity_eigenstate(i, L)
  reflected_state = gen_parity_eigenstate(bin2int(b[::-1]), L)


  R_even_state = (state + reflected_state)/np.sqrt(2)
  R_odd_state = (state - reflected_state)/np.sqrt(2)


  peig = (R_even_state*P*R_even_state.H).toarray()[0,0]
  if peig > 0:
    P_even_R_even_states.append(R_even_state.toarray()[0])
    P_even_R_odd_states.append(R_odd_state.toarray()[0])
  else:
    P_odd_R_even_states.append(R_even_state.toarray()[0])
    P_odd_R_odd_states.append(R_odd_state.toarray()[0])


if print_Hfull:
  U_PR = sparse.csr_matrix(np.array(P_even_R_even_states+P_even_R_odd_states+P_odd_
  H_PR = U_PR * H * U_PR.H
  plot_matrix_structure(H_PR.toarray())


ee_projector = sparse.csr_matrix( np.array(P_even_R_even_states))
eo_projector = sparse.csr_matrix( np.array(P_even_R_odd_states))
oe_projector = sparse.csr_matrix( np.array(P_odd_R_even_states))
oo_projector = sparse.csr_matrix( np.array(P_odd_R_odd_states))


H_ee = ee_projector@H@ee_projector.H
H_eo = eo_projector@H@eo_projector.H
```

```python
    H_oe = oe_projector@H@oe_projector.H
    H_oo = oo_projector@H@oo_projector.H


    evals_ee = linalg.eigh(H_ee.toarray(), eigvals_only=True)
    evals_eo = linalg.eigh(H_eo.toarray(), eigvals_only=True)
    evals_oe = linalg.eigh(H_oe.toarray(), eigvals_only=True)
    evals_oo = linalg.eigh(H_oo.toarray(), eigvals_only=True)
    return np.sort(np.concatenate((evals_ee, evals_eo, evals_oe, evals_oo)))
```

This results in the diagonalization
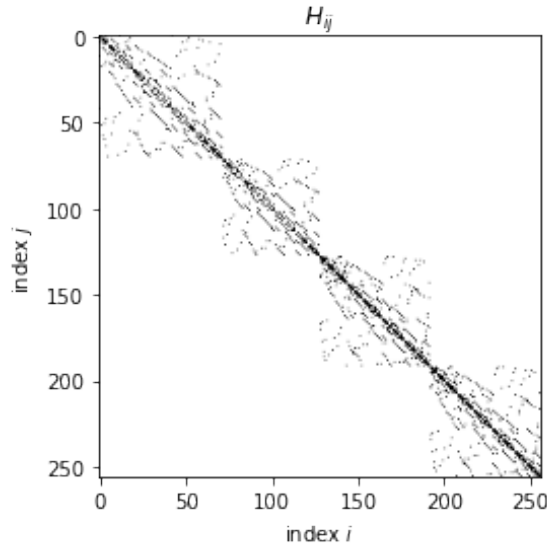
3.3   Periodic boundary conditions, parity and translation

For periodic boundary conditions, we can use P and T. T splits the Hilbert space roughly into L blocks of length $2^L/L$. This is a much greater advantage than the factor of 2 from spatial reflection. P further splits each of these blocks into 2, giving a total of $2L$ blocks with size $\sim 2^L/(2L)$.

```python
def translate_bitstring(b, d):
    '''translates the bitstring b by d positions '''
    b1 = b[0 : d]
    b2 = b[d :]
    return b2 + b1


def get_cycle_length(b):
    '''computes the number of translations
       allowed before bitstring b comes back
```

```python
        to itself'''
    n = bin2int(b)
    L = len(b)
    for i in range(1,L):
        if n == bin2int(translate_bitstring(b, i)):
            return i
    return L


def get_T_representatives(L):
    '''get one representative from each set
      of basis states that are equivalent
      up to action of the translation op T'''
    reps = []
    for n in range(2**L):
        flag = False
        b = np.binary_repr(n, width=L)
        for d in range(1, L):
            if translate_bitstring(b, d) in reps:
                flag = True
        if not flag:
            reps.append(b)
    return reps


def get_PT_eigenstate(rep, k ,L, cycle):
    state = gen_parity_eigenstate(bin2int(rep), L)
    for i in range(1, cycle):
        state += np.exp(2 * np.pi * 1j * k * i/L) * \
        gen_parity_eigenstate(bin2int(translate_bitstring(rep, i)), L)
    state = state/np.sqrt(cycle)
    return state


def diagonalize_with_PT(H, P, L, print_Hfull = False):
    tol = 0.1/L
    P_even_states = []
    P_odd_states = []
```

```python
reps = get_T_representatives(L)
cycle_lengths = {r:get_cycle_length(r) for r in reps}
n_up = {r:r.count('1') for r in reps}

countkp = 0
countkm = 0

indsplus = []
indsminus = []

for k in range(L):
  indsplus.append(countkp)
  indsminus.append(countkm)

  for r in reps:
    tmp = k*cycle_lengths[r]/L
    if np.abs(np.round(tmp) - tmp) < tol:
      state = get_PT_eigenstate(r, k, L, cycle_lengths[r])
      peig = np.real( (state*P*state.H).toarray()[0,0])
      if peig > 0:
        P_even_states.append(state.toarray()[0])
        countkp = countkp+1
      else:
        P_odd_states.append(state.toarray()[0])
        countkm = countkm+1
indsplus.append(countkp)
indsminus.append(countkm)

U_PT = sparse.csr_matrix(np.array(P_even_states+P_odd_states))
H_PT = U_PT * H * U_PT.H
Hfull = H_PT.toarray()

if print_Hfull:
  plot_matrix_structure(Hfull)
```

```
block_inds = np.append(np.array(indsplus), np.array(indsminus[1:])+indsplus[-1])

evals = []
for i in range(len(block_inds)-1):
    evals = np.append(evals, np.linalg.eigvalsh(Hfull[block_inds[i]:block_inds[i+1], 

evals = np.sort(evals)
return evals
```
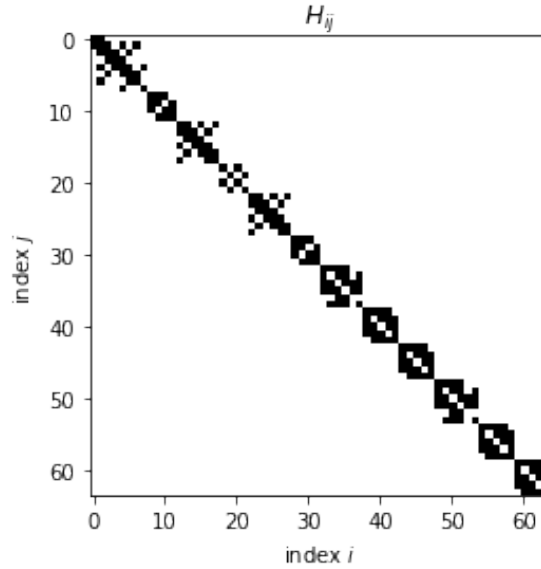
This results in the diagonalization

While R and T do not commute, in the $k = 0$ and $k = \pm\pi$ sectors, reflection symmetry/anti-symmetry can still be utilized. This does not provide a large speed-up in general as compared to the gains seen by T.

4 Quantum chaos

We've seen that it is already pretty hard to extend what thermalization means from the classical to quantum context. It is similarly difficult to do this with chaos.

In classical chaos we usually use the description of a **Lyapunov exponent**

$$\lambda_L \sim \frac{dq(t)}{dq_0} \tag{28}$$

but having a Lyapunov exponent in the quantum case is harder because there's already a phase ambiguity, and the Schrödinger equation is linear; evolving using unitary time evolution doesn't change the amplitude. In quantum chaos we use "**OTOCs**," or **Out-of-Time-Ordered Correlators**; and these are useful quantities for probing chaos in systems like black holes or a system with many degrees of freedom (large n systems). But for spin systems or very quantum systems we consider here it is difficult to make this work; they fail to give exponential dependence when considering strongly quantum spin-$\frac{1}{2}$ systems.

We also have to consider the quantum analogue of **ergodicity**, or the exploration of phase space. Traditionally this is described using canonical coordinates (q, p), which are conjugate coordinates, and again it is hard to translate this to the quantum context because we can't even define position and momentum at the same time due to Heisenberg uncertainty.

The point is that, although we have some tools to describe these, like OTOCs and Random Matrix Theory (RMT), we need a whole new framework. We also can use the Riemann Zeta function; the eigenvalues of a random matrix are related to the zeros of the Riemann Zeta function via *Montgomery's Conjecture*. The relationship with RMT and quantum chaos is difficult via **Gutzwiller's Trace Formula**, which links the spectrum of random matrices in terms of the density of states with something classical which is a sum over periodic orbits:

$$\rho(E) \sim \sum_{\rho_0} A_{p_0} e^{iS\rho_0/\hbar} \tag{29}$$

There is a distinction between few-particle quantum chaos with a semiclassical analogue; we need to think about few particle quantum chaos in the semiclassical limit vs many-body quantum chaos for systems that are far from any kind of semiclassical limit (e.g. strongly spin-$\frac{1}{2}$ systems). There this notion of periodic orbits becomes far less well-defined because there isn't any natural classical analogue. Lyapunov exponents have to do with small perturbations in phase space leading to exponential differences in trajectories.

In classical chaos, we have a $2n$-dimensional phase space

$$\mathcal{R} = (q_1, ..., q_n, p_1, ..., p_n) \tag{30}$$

evolving via Hamilton's equations

$$\frac{dq}{dt} = -\frac{\partial H}{\partial p} \tag{31}$$

$$\frac{dp}{dt} = \frac{\partial H}{\partial q} \tag{32}$$

Already in this system we assume that energy is conserved, and anything additionally conserved constrains our motion in phase space even more, which is why if we say in an integrable system, in the classical context we are constrained to the **invariant torus**. Classically, 2-body motion is pretty easy to do, but adding a third body classically makes the problem very difficult to solve.

4.1   Random Matrix Theory

This was started in the 1950's by Wigner, trying to write down Hamiltonians for interactions within nuclei. We wrote a Hamiltonian as an $N \times N$ randome matrix

$$
H \to \begin{pmatrix} x_{11} & ... & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{N1} & ... & x_{NN} \end{pmatrix} \tag{33}
$$

where the entries were from a Gaussian distribution. The mean doesn't usually matter, but the variance is important.

Definition 6. *Entries taken from a Gaussian distribution independent from one another is denoted **i.i.d.** (This doesn't mean they are taken from a Gaussian but they are independently identically taken from this Gaussian distribution)*

Remark 6. *The universal properties of the spectra of a nuclei looks remarkably well like that of a random matrix. A random matrix has become one of the best known diagnostics of quantum chaos. When you have a system which is chaotic, ergodic, or whatever, the spectra of these systems end up sharing many universal properties with these random matrices.*

The whole problem with RMT is starting from a matrix such as the one above and computing the characteristic equation i.e. finding the eigenvalues $\lambda_1, ..., \lambda_n$. We start with some probability distribution on our entries, $p(x_{11}, ..., x_{NN})$. It they're all random we have N^2, if symmetric then $\frac{N(N+1)}{2}$. Then we want to find a probability distribution on the eigenvalues $p(\lambda_1, ..., \lambda_n)$ but most of the time on the spacings $p(s_1, ..., s_{n-1}), s_i = \lambda_{i+1} - \lambda_i$.

Example 1. *For a random real and symmetric 2×2 matrix, we have*

$$H = \begin{pmatrix} x_1 & x_2 \\ x_2 & \\ x_3 & \end{pmatrix} ; x_1, x_3 \in N(0,1), x_2 \in H(0, \frac{1}{2}) \tag{34}$$

$$p(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} \tag{35}$$

$$-\lambda^2 + Tr[H]\lambda + \det(H) = 0 \tag{36}$$

$$\lambda_{1,2} = \frac{1}{2}\Gamma(x_1 - x_3)^2 \pm \sqrt{f(x_1, x_2, x_3)} \tag{37}$$

$$S =_2 -\lambda_1 = \sqrt{(x_1 - x_3)^2 + 4x_2^2} \tag{38}$$

$$p(s) = \int dx_1 \int dx_2 \int dx_3 p(x_1)p(x_2)p(x_3) \int (s - \sqrt{(x_1 - x_3)^2 + 4x_2^2}) \tag{39}$$

$$\tag{40}$$

We then get the level spacings as

$$p(s) \propto s^\beta e^{-s^2} \tag{41}$$

*where $\beta = 1$ for real entries and $\beta = 2$ for complex entries. This is known as **Wigner's Surmise**.*

The ensemble that we draw our entries from depends on the symmetries of the Hamiltonian. If we have a real Hamiltonian, it is described by the **Gaussian Orthogonal Ensemble** (GOE), rather than the **Gaussian Unitary Ensemble** (GUE). The diagonals always have to be real to make the matrix Hermitian. We also have a symplectic ensemble (GSE), in which $\beta = 4$.

Remark 7. *In the GOE ensemble we can diagonalize our Hamiltonian via an orthogonal matrix, and this means that the entries are real, which means we have a system which have time-reversal symmetry because energy is conserved. Thus if we have a system with time-reversal symmetry we're going to want to draw our matrices from the GOE, while if we have a Hamiltonian that breaks time-reversal symmetry we'll want to model it with the GUE. One representative of time-reversal symmetry is complex conjugation.*

In one particle quantum chaos we can see the use of RMT. For something with a classical analogue, e.g. a billiard ball in an ellipsis-shaped area, the system is chaotic: it bounces all around the ellipsis. In the quantum case, we have $\hat{H} = \frac{\hat{p}^2}{2m} + V$ in the geometry in the problem and

look at these quantum energy levels and look at the distribution of level spacings, we get that, for quantum systems that have a classical analogue to a classically chaotic system, we end up getting BFS statistics. One the other hand, for quantum systems for which the classical limit is integrable, we end up with Poisson level statistics. This is known as the quantum chaos conjecture.

Now we are getting to many-body quantum chaos, where we consider systems like strong spin-$\frac{1}{2}$ systems, and there is no semi-classical analogue. There is no classical analogue to a spin-$\frac{1}{2}$ ising chain or XXZ chain. For thermalizing systems, their spectra look like results from RMT. For integrable systems or MBL, there are many symmetries in our problem, our level statistics end up looking Poisson.

In large N, $p(s)$ for RMT and Hamiltonians match very well. For the density of states $p(E)$, the rnadom matrix gives a semicircle, while near the edges, for most physical Hamiltonians, $p(E)$ looks much more like a Gaussian.

Definition 7. *We have been considering $\lambda_{i+1} - \lambda_i$. There is another diagonstic called the **Spectral Form Factor** that probes the correlations between all distances of spectrum as a function of time $K(t)$. If we go to early times we find large distances and if we look at later times we look at very nearby energies.*

Taking the staircase function $N(E) := \sum_n O(E - E_n)$ and going to the density of states $\rho(E) = \frac{dN}{dE} = \sum_n \delta(E - E_n)$, and then we go from the density of states to a two-point function $R(E) = \langle \rho(E_0 + \frac{E}{2})\rho(E_0 - \frac{E}{2})\rangle_{E_0}$ (in a small-energy window), and then going from the two-point function we get the spectral form factor by taking the Fourier transform of the two-point function:

$$N(E) \to \rho(E) \to R(E) \to K(t) \qquad (42)$$

$$\sum_n O(E - E_n) \to \sum_n \delta(E - E_n) \to \langle \rho(E_0 + \frac{E}{2})\rho(E_0 - \frac{E}{2})\rangle_{E_0} \xrightarrow{F.T.} \int e^{iEt} R(E)dE \qquad (43)$$

$$= \frac{1}{N} \sum_{n,m} e^{it(E_n - E_m)} \qquad (44)$$

with some normalization. $K(t)$ decreases in time until we reach the **Thouless time**, where level repulsion starts kicking in, and then $K(t)$ increases with time. This manifests itself in what is known as a "ramp" in $K(t)$. For large time, since the exponent is negative, we essentially get random phases that add to zero, so we reach a plateau in $K(t)$ starting at the **Heisenberg time**, which is around the dimension of the Hilbert space. The height of this plateau depends on how we normalize the spectral form factor $(\frac{1}{N})$ and if we have degeneracies, because if we have degeneracies we don't need $n = m$ for $E_n = E_m$; therefore if we have degeneracies the plateau is essentially higher. The benefits of studying $K(t)$ are:

1. It is not sensitive to being in the correct symmetry sector (not proven but checked numerically for many systems)

2. We can calculate $K(t)$ without having to know our full spectrum: $K(t) \sim \sum_{p_0} A_{p_0} e^{i \frac{S_{p_0}}{\hbar}}$ in the semi-classical limit.