

Quantum Matter & Information

— Spring 2018 —

These notes are an evolving an incomplete endeavor. I thank Vitor R. Vieira for his attentive reading, many suggestions and comments. Errors and mistakes herein are of my entire responsibility. Comments and corrections are welcome, please email them to ribeiro.pedro@gmail.com.

Pedro Ribeiro

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1 Introduction

1.1 Whats and Whys

What? These set of lectures is an attempt to give a (partial and incomplete) view on some topics covering areas such as Quantum Information and Computation, Condensed Matter, Quantum Thermodynamics, Quantum Optics, and more. Some of these topics and links between these areas are relatively new (such as entanglement-based classifications of matter) and some have been known for a long time (such as the relation between Shanon and thermodynamic entropies). The overall idea is to navigate among them with an information theoretical perspective

Why? There are many reasons (besides building a quantum computer), mainly they are of two kinds:

- (i) the manipulation of information requires a physical support, so it is important to understand the restrictions and opportunities physical implementations impose.
- (ii) the framework and concepts developed within information theory might help to shed light to other areas of physics. In some cases it has already been proven useful to understand certain phases of matter with a substantial degree of success.

We will try to address both of these viewpoints as we go.

Who? The lectures are directed to students interested in theoretical physics including Condensed Matter and Quantum Information, but also from other areas. The course is part of the graduate physics program and is aimed at students with diverse backgrounds. It assumes a previous background on Quantum Mechanics, including second quantization, and some basics of Solid State Physics, such as band theory and tight-binding models. Otherwise, the lectures try to be self-contained.

How? We will try to address a list of subjects that (roughly) includes:

1. Introduction

What's and whys

1. On the nature of Quantum Systems

locality | physical states

2. Quantum Information Theory

quantifying information | entanglement measures | distance measures

3. Characterizing Matter

response and correlation functions | phases | phase transitions | symmetry |
Landau theory in a nutshell | models

4. Entanglement in many-body systems

area laws | phase transitions | topological phases of matter

5. Simulating quantum systems

canonical simulation methods, matrix product states and generalizations

6. Closed quantum systems

dynamics | thermalization

7. Open Quantum Systems

super-operators | master equations | relaxation and decoherence | transport |
decoherence-free subspaces

8. Quantum thermodynamics

work and information | work distribution | Jarzynski equalities | counting statistics

9. Other possible topics:

Realizations of qubits (SC qubits, Adiabatic QC) | Quantum Computation (algorithms, error correcting codes) | Quantum Communication (noisy channels)

When?

	Fev.	Mar.	Apr.	May
# classes	4	6 (5?)	8 (7)	8 (7)
Topics	1,2,3	3,4,5	5,6,7	8,9

1.2 Objectives

New methods and techniques developed in the context of quantum information and computation have been introduced in Condensed Matter Physics during the last 10 to 15 years. As they often allow for a fresh approach and shine a new light on long-standing problems the topic is of growing importance. On the other hand, Condensed Matter Physics naturally provides quantum information and even quantum computation the physical devices for their implementation. The purpose of this course is to provide the students with an integrated knowledge of both areas.

1.3 References

- [N&C] [Quantum Computation and Quantum Information](#), M. A. Nielsen , I. L. Chuang
- [AFOV] [Rev Mod. Phys. 80 517 \(2008\)](#) by L. Amico, R. Fazio, A. Osterloh and V. Vedral
- [ZCW] [Quantum Information meets Quantum Matter](#), B. Zeng et al.
- [McG] [Quantum information is physical](#), Lecture notes by J. McGreevy
- [Laf] [Quantum entanglement in condensed matter systems](#), N. Laflorencie
- [Pre] [Quantum Computation](#), Lecture Notes by John Preskill

This is a growing list... More references are given along the text.

1.4 Course Logistics

1.4.1 Contacts

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1.4.2 Lectures Schedule

Tuesday 11:00 - 13:00 - Room: 2-8.11
 Thursday 11:00 - 13:00 - Room: 2-8.11

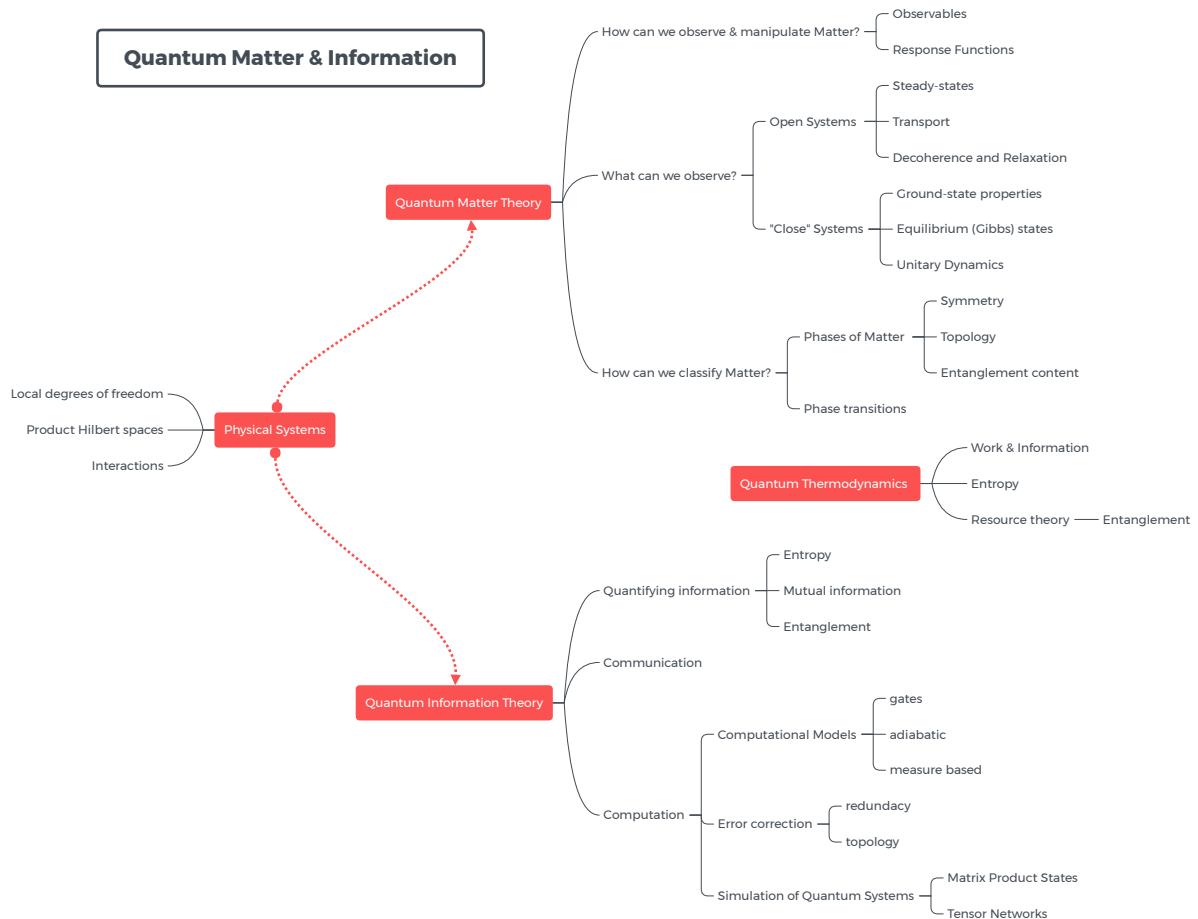
1.4.3 Office hours

- 11:00-12:00 Wednesday - Office 3- 8.14

1.4.4 Evaluation

- (i) 3 exercise series - 30%
- (ii) Project: 4-page document (journal article format) + Oral presentation.

1.5 A bird's eye view on the path



2 On the nature of Quantum Systems

2.1 Locality

Physical systems (at least most of the ones we will be considering in this course) are constituted of a collection of local degrees of freedom coupled to each other. A state of the constituent local system can be written using a basis for the local Hilbert space \mathcal{H}_r : $|\psi(r)\rangle = \sum_{n=1}^{d_r} c_n |\phi_n(r)\rangle$, with dimension d_r . Note that $d_r = 2$ for a qubit, with $|\phi_1\rangle = |\uparrow\rangle$ and $|\phi_2\rangle = |\downarrow\rangle$. A basis for the total Hilbert space can be obtained by a tensor product of local basis states

$$|\phi_{n_1}(r_1), \phi_{n_2}(r_2), \dots\rangle = |\phi_{n_1}(r_1)\rangle \otimes |\phi_{n_2}(r_2)\rangle \otimes \dots \quad (1)$$

and thus the total Hilbert space $\mathcal{H} = \otimes_r \mathcal{H}_r$, has dimension $d_{\mathcal{H}} = \prod_r d_{\mathcal{H}_r}$ ¹. A state of the total system can be written as

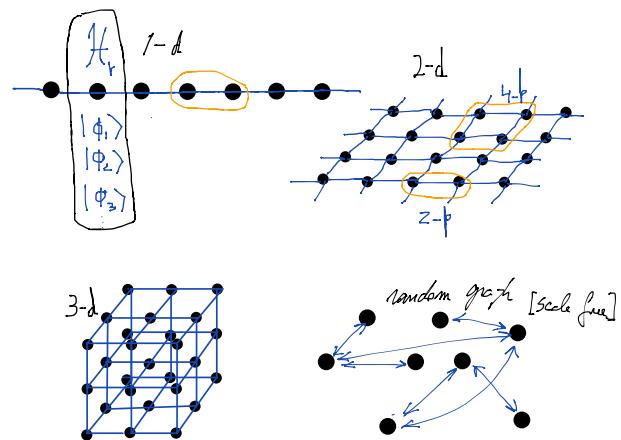
$$|\Psi\rangle = \sum_{n_1 n_2 \dots} c_{n_1 n_2 \dots} |\phi_{n_1}(r_1), \phi_{n_2}(r_2), \phi_{n_3}(r_3), \dots\rangle. \quad (2)$$

This means that there is a sense on asking how two degrees of freedom are correlated, or how one of them is correlated with the rest of the system (more in the following).

Due to the nature of the physical forces it is also plausible to assume that the interactions between degrees of freedom are pair-wise or limited to a few-body term, i.e. an operator can be written as $O = \sum_r O_r + \sum_{rr'} O_r O_{r'} + \sum_{rr'r''} O_r O_{r'} O_{r''} + \dots$, where O_r , $O_{r'}$ and $O_{r''}$ only on degrees of freedom at site r , r' and r'' , with $+\dots$ being finite number of terms. Operators that act non-trivially in k sites are called k -local².

In most physically systems there is also a notion of locality, i.e. of proximity between degrees of freedom. Two local degrees of freedom can only interact if they are sufficiently close. This happens since interacting potentials have a finite characteristic length³. Fully connected models, or random graphs may also be considered but often care must be taken in interpreting the results and defining the interactions for sometimes even simple thermodynamic properties are not well defined. Most physical systems have well defined spacial (and temporal) structure and a notion of distance (i.e. a metric) between sites (or positions) in which the degrees of freedom live.

Due to the local nature of degrees of freedom and to the fact that interactions are restricted to few terms, the Hamiltonian and (local) observables can be written as $O = \sum_r O_r$ where O_r is bounded to a few (say k) lattice sites. This fact alone has consequences, for example:



¹This is the case for the degrees of freedom we are going to study in this course, however for some effective degrees of freedom like “anyons” the structure of the local Hilbert space is not that of a simple product space. See, for example <https://arxiv.org/abs/0902.3275>.

²see for example [ZCZW] chapter 4.

³For example the Coulomb potential is not of this kind however there are two ways of rendering it local: (1) if we consider the electromagnetic field as a dynamic degree of freedom the theory is local, (2) screening of the electromagnetic fields, in metals or superconductors, that renders the interaction local. Which one is a good approximation depends on the physical problem.

- It is meaningful to ask how correlations decay. In fact we can even classify systems according to the nature of that decay.
- We can ask how fast a localized perturbation can spread. There are results called Lieb-Robinson bounds⁴ regarding the spread of information that can be derived based on these assumptions. The question of how fast the information of a perturbation can spread is definitely something for which quantum information tools can help.

2.2 The Vastness of the Hilbert space

The above characterization of the Hilbert space of a many-body system has an essential problem: the number of variables we need to encode a state grows exponentially with the number of degrees of freedom. This means diagonalizing the Hamiltonian of a few qubits becomes very fast an impossible task (the current record using the symmetries is around 30 two-level systems). This is clearly not enough since we want to be able to say something about properties of systems with much more degrees of freedom, that being electrons in a crystal (say in a mole of atoms 10^{23}) or qubits in an useful (to be created) quantum memory (say a megabyte $2^{20} \simeq 10^6$ bytes).

As long as thermodynamic properties are concerned there are a lot of details that we clearly will not care about. Computing specific heat, compressibility, conductivity... should not require the knowledge of all the wave function. Many-body theory developed within the context of Condensed Matter systems provides a useful set of tools to compute such quantities. However, things might be different if you are concerned with other properties, in particular if we want to follow the time evolution of a system, its full counting statistics⁵ or work distribution⁶.

In this context information theory has given important contributions. For example, it was shown that ground states and Gibbs (i.e. thermal) states are substantially simpler than a generic state, in particular their entanglement follows a so-called area law⁷ (some of these results we will cover in the course). Some of these states can be described in a much more compact way then Eq.(2). Matrix Product States⁸ (that I hope we will be able to cover briefly) are a clever way of encoding the wave-function in a few degrees of freedom.

It has also been intensively investigated the way generic states, evolving under generic local Hamiltonians, thermalize, i.e. observables after a long time only depend on generic conserved quantities like energy and number of particles and are relatively indifferent to the nature of the initial state otherwise (I hope we will be able to cover this topic briefly). Some results⁹ (that I hope to discuss later) also indicate that physically meaningful states only explore a corner of the Hilbert space in reasonable (non-exponential) time scales.

2.3 Physical states

Traditionally, Condensed Matter Physics deals with equilibrium states, that being ground states (that are pure states) or finite temperature states (described by density matrices).

That is because most systems interact, at least weakly with their environment, and, when left on their own, relax to an equilibrium condition, with a temperature (and other thermodynamic potentials) fixed by their surroundings.

⁴See for example: <https://arxiv.org/pdf/1004.2086.pdf> or <https://arxiv.org/abs/1008.5137>.

⁵Find ref!!

⁶Find ref!!

⁷Quantum entanglement in condensed matter systems, N. Laflorencie

⁸See for example Orus, Annals of Physics 349 117-158, (2014)

⁹Poulin, et al., Phys. Rev. Lett. 106, 170501 (2011)

Under rather general conditions (maybe we will have time to dig into them) the density matrix of the equilibrium state has a Gibbs form

$$\rho = \frac{1}{Z} e^{-\beta H} \quad (3)$$

with $Z = \text{tr}(e^{-\beta H})$ and where H is the Hamiltonian of the system and β is the inverse temperature.

There are a set of techniques that were developed to deal with these states, to compute observables and the response function when the system is perturbed slightly away from this equilibrium from. You can learn about these in the course of [Many Body Physics](#) where, among other things, you will see the so called Matsubara formalism that provides an easy prescription to compute finite temperature observables. We will try to avoid using such techniques in this course.

Assuming that H is local (in the sense discussed in the previous section) it turns out that thermal states of the form (3) inhabit a rather special and small corner of the Hilbert space.

An easy way of seeing this, that sometimes appear under the name typicality¹⁰, is to realize that, for most states of the Hilbert space $\langle O_r \rangle \approx \text{tr}(O_r)$ (where \approx can be made precise in the thermodynamic limit) and $\langle O_r O_{r'} \rangle \approx \text{tr}(O_r) \text{tr}(O_{r'})$ (assuming O_r does contain operators of the degrees of freedom of r' and vice-versa). Therefore the correlations $\langle (O_r - \langle O_r \rangle)(O_{r'} - \langle O_{r'} \rangle) \rangle \approx 0$ vanish in most states, whereas for a thermal state at finite temperature we expect $\langle (O_r - \langle O_r \rangle)(O_{r'} - \langle O_{r'} \rangle) \rangle \approx f(|r - r'|)$ with $f(r)$ some decreasing function of r . This means that almost all states in the Hilbert space are like infinite temperature states (since for $\beta \rightarrow 0$: $\text{tr}(\rho O) = \text{tr}(O)$). On the other hand finite temperature states are special in the sense that correlations know about the spatial structure of the system.

Note that this discussion only makes sense for systems with a large number of degrees of freedom. For when the Hilbert space is small, like that of a qubit, we can explore it all!

Another remarkable property of thermal states (that seems somehow to contradict what we just said) is that they are much less entangled (in a sense we will precise later) than most states in the Hilbert space.

Quantum information tools allow us to understand some of the unique properties of “physical” states, i.e. states that we are likely to observe in real systems.

Lecture 2

3 Quantum Information - The basics

3.1 Mixed States

3.1.1 Density Matrix

Let us discuss some properties of density matrices and mixed states that will use throughout the course.

¹⁰See: S. Popescu, A. J. Short, and A. Winter, *Nature Phys.* 2, 754 (2006) and S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghi, *Phys. Rev. Lett.* 96, 050403 (2006)

Mixed states can be obtained by a probabilistic preparation. For example, preparing the state $|\phi_i\rangle$ with probability p_i we obtain the density matrix

$$\rho = \sum_i p_i |\phi_i\rangle \langle \phi_i|.$$

Another way of producing mixed states is by looking to a subsystem of a composite system. For example, assume that the Hilbert space is a direct product of system A and B with base orthonormal base $|\phi_i^A\rangle \otimes |\phi_j^B\rangle$, and the system is in a pure state $|\psi\rangle = \sum_{ij} \psi_{ij} |\phi_i^A\rangle \otimes |\phi_j^B\rangle$. If we look only to A:

$$\langle O_A \rangle = \text{tr}(O_A |\psi\rangle \langle \psi|) = \text{tr}_B(O_A \rho_A)$$

with $\rho_A = \sum_{ii'j} \psi_{ij} \bar{\psi}_{ji} |\phi_i\rangle \langle \phi_{i'}|$. If $\psi_{ij} = \sqrt{p_i} \delta_{ij}$ then ρ_A is diagonal.

Properties of a (physical) density matrix are:

- (1) Hermiticity: $\rho_A^\dagger = \rho_A$
- (2) Positivity: $\langle \varphi | \rho_A | \varphi \rangle \geq 0$
- (3) Unit trace: $\text{tr} \rho_A = 1$

These condition imply that ρ_A can be diagonalized in some orthogonal base $|\tilde{\phi}_i^A\rangle$, in which case: $\rho_A = \sum_a p_i |\tilde{\phi}_i^A\rangle \langle \tilde{\phi}_i^A|$. The density matrix obtained in this way is the same as the one obtained by a probabilistic preparation using an orthogonal set of vectors $|\tilde{\phi}_i^A\rangle$.

Note that, as a consequence $\text{tr} \rho_A^2 \leq 1$ with $\text{tr} \rho_A^2 = 1$ if ρ_A is a pure state.

3.1.2 Schmidt Decomposition

The Smith decomposition is a useful tool we will use in the course. It is a procedure to obtain an orthogonal base of A and B such that $|\psi\rangle = \sum_i \sqrt{p_i} |\tilde{\phi}_i^A\rangle \otimes |\tilde{\phi}_i^B\rangle$. An advantage of this form is that both ρ_A and ρ_B are diagonal in this base. Another advantage is to give us a canonical way to study the entanglement between the two systems. To see how to construct the basis starting from an initial state $|\psi\rangle = \sum_{ij} \psi_{ij} |\phi_i^A\rangle \otimes |\phi_j^B\rangle$ we consider the amplitudes ψ_{ij} as a $m \times n$ matrix and preform a singular value decomposition

$$\psi = \mathbf{U} \mathbf{D} \mathbf{V}^\dagger$$

where \mathbf{U} and \mathbf{V} are unitary (i.e. $\mathbf{U}\mathbf{U}^\dagger = 1$), respectively $m \times m$ and $n \times n$ matrices, and \mathbf{D} is a $m \times n$ diagonal matrix with non-negative entries. Using this decomposition we write

$$\begin{aligned} |\psi\rangle &= \sum_{ijk} U_{ik} D_{kk} V_{kj}^\dagger |\phi_i^A\rangle \otimes |\phi_j^B\rangle \\ &= \sum_i \underbrace{D_{kk}}_{\sqrt{p_k}} \left(\underbrace{\sum_i U_{ik} |\phi_i^A\rangle}_{|\tilde{\phi}_k^A\rangle} \right) \otimes \left(\underbrace{\sum_j V_{kj}^\dagger |\phi_j^B\rangle}_{|\tilde{\phi}_k^B\rangle} \right) \end{aligned}$$

The unitarity of \mathbf{U} and \mathbf{V} ensure that the states $|\tilde{\phi}_k^{A/B}\rangle$ are orthogonal¹¹.

¹¹Prove that!

3.1.3 Purification

The purification of a state is somehow the converse of the Smith decomposition. This is to say that any density matrix of a subsystem A can be obtained from a pure state of a composite system, i.e.

$$\rho_A = \text{Tr}_B [|\psi\rangle\langle\psi|].$$

After our discussion, we know that such state is of the form

$$|\psi\rangle = \sum_i \sqrt{p_i} |\tilde{\phi}_i^A\rangle \otimes |\tilde{\phi}_i^B\rangle$$

However the states $|\tilde{\phi}_j^B\rangle$ are now defined up to an unitary transformation since the only condition is that they form an orthogonal base, the set of states $U|\tilde{\phi}_j^B\rangle$ would give an equally good purification.

3.2 Quantifying information

3.2.1 Shanon Entropy

In its diagonal base $\rho = \sum_i p_i |\tilde{\phi}_i\rangle\langle\tilde{\phi}_i|$ can be interpreted as a classical probability distribution since $\langle A \rangle = \sum_i p_i A_i$ with $A_i = \langle \tilde{\phi}_i | A | \tilde{\phi}_i \rangle$. A useful quantity to quantify the degree of uncertainty of such probability distribution is the Shanon entropy of a random process $X = \{x, p_x\}$

$$H(X) = - \sum_x p_x \ln p_x$$

that has a number of remarkable properties:

1. This quantity represents the amount of information (number of bits if we replace $\ln \rightarrow \log$) needed to encode effectively a message if the letter x occurs with a probability p_x
2. It is maximized by the uniform distribution $q_x = \frac{1}{\Omega}$, with $\Omega = \sum_x 1$. Defining $s(p) = -p \ln p$ we have that $s(\sum_n \lambda_n p_n) \geq \sum_n \lambda_n s(p_n)$ where $\sum_n \lambda_n = 1$. Thus $\frac{1}{\Omega} \sum_x s(p_x) \leq s\left(\frac{1}{\Omega} \sum_x p_x\right)$.
3. It is stable against the addition of other possible outcomes with zero probability $H(p_1, p_2, \dots, p_\Omega) = H(p_1, p_2, \dots, p_\Omega, 0, \dots)$
4. Information is extensive: Let $XY = \{(x, y), p_{x,y}\}$ be a stochastic process. Describe an elements (x, y) as the object x belonging to box y . $Y = \{y, p_y = \sum_{x \in y} p_{x,y}\}$ is the probability for an element to be in box y and $X_y = \{x, p_{x|y} = \frac{p_{x,y}}{\sum_x p_{x,y}}\}$ the probability of a particular element within box y . The entropy of the two descriptions is the same

$$\begin{aligned} H(XY) &= H(Y) + \sum_y p_y H(X_y) \\ &= - \sum_y p_y \ln p_y - \sum_{yx} p_y \frac{p_{x,y}}{p_y} \ln \left(\frac{p_{x,y}}{p_y} \right) \\ &= - \sum_{yx} p_{x,y} \ln (p_{x,y}) \end{aligned}$$

5. Information decreases ignorance: for the random process $XY = \{(x, y), p_{x,y}\}$, $Y = \{y, p_y = \sum_x p_{x,y}\}$ is the probability of outcome y , and $p_{x|y} = \frac{p_{x,y}}{p_y}$ is the probability of x given y . Then the entropy after outcome y is $H(X_y)$ with $X_y = \{x, p_{x|y}\}$. The average entropy over the possible values of y is given by

$$H(X|Y) = \sum_y p_y H(X_y) = -\sum_{xy} p_{x,y} \ln \frac{p_{x,y}}{p_y} = H(XY) - H(Y) < H(XY)$$

this quantity is called the conditional entropy of x given y . This quantity represents the additional amount of information (number of additional bits per letter) needed to specify both x and y once y is known. The amount of information learned on x by knowing y is given by

$$\begin{aligned} I(X;Y) &= H(X) - H(X|Y) \\ &= H(X) + H(Y) - H(XY) \end{aligned}$$

is a symmetric quantity in x and y called mutual information. If $I(X;Y) = 0$, X and Y are completely uncorrelated.

3.2.2 Von Neumann Entropy

The Von Neumann entropy is the quantum generalization of the Shanon entropy for a density matrix $\rho = \sum_x p_x |\tilde{\phi}_x\rangle\langle\tilde{\phi}_x|$:

$$S(\rho) = -\text{tr}\rho \ln \rho = -\sum_x p_x \ln p_x$$

It also has a number of remarkable properties:

1. $S(|\varphi\rangle\langle\varphi|) = 0$
2. $S(U\rho U^{-1}) = S(\rho)$
3. $S(\rho) \leq \log d$, with d the dimensionality of the Hilbert space
4. $S(\sum_n \lambda_n \rho_n) \geq \sum_n \lambda_n S(\rho_n)$ here $\sum_n \lambda_n = 1$ (same as the Shanon Entropy)
5. $S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B)$, called subadditivity - we know more if we also know correlations
6. for pure states $\rho_{AB} = |\varphi\rangle\langle\varphi|$ then $S(\rho_A) = S(\rho_B)$
7. The mutual information $I(A;B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$ is non-negative
8. Triangle inequality $S(\rho_{AB}) \geq |S(\rho_A) - S(\rho_B)|^{12}$. This is to be contrasted with $H(XY) \geq H(X), H(Y)$ that states that the Shanon entropy of a part cannot be greater than that of the hole system: i.e encoding x and y takes more bits than encoding only x . This property holds only in the classical case! For example, it can be simply violated for a pure state $\rho_{AB} = |\varphi\rangle\langle\varphi|$. There is a similar statement for the quantum conditional entropy, defined as

$$S(A|B) = S(\rho_{AB}) - S(\rho_B)$$

This quantity is always positive classically $H(X|Y) > 0$ translating the fact that information decreases ignorance. However this is not true quantum mechanically since it is also trivially violated by a pure state.

¹²Assume $\rho_{ABC} = |\varphi\rangle\langle\varphi|$ and $\rho_{AB} = \text{tr}_C[\rho_{ABC}]$. We have that since ρ_{ABC} is pure $S(\rho_A) = S(\rho_{BC})$ and $S(\rho_C) = S(\rho_{AB})$. Then $S(\rho_A) = S(\rho_{BC}) \leq S(\rho_B) + S(\rho_C) = S(\rho_B) + S(\rho_{AB})$ i.e. $S(\rho_{AB}) \geq S(\rho_A) - S(\rho_B)$ and the same with $A \leftrightarrow B$.

3.3 State distinguishability - Fidelity

In the space of pure states, the similarity between two states $|\psi\rangle$ and $|\varphi\rangle$ can be given by their overlap $|\langle\psi|\varphi\rangle|^2$ also called fidelity. For density matrices it is not so easy to come up with a generalization of this simple notion. A quantity that does the trick is

$$F(\rho, \sigma) = \left(\text{tr} \sqrt{\rho^{\frac{1}{2}} \sigma \rho^{\frac{1}{2}}} \right)^2 = \left\| \sigma^{\frac{1}{2}} \rho^{\frac{1}{2}} \right\|^2.$$

with $\|A\| = \text{tr} \sqrt{A^\dagger A}$ the trace norm.

The fidelity has a number of interesting properties. One is how the fidelity of a state is related with that of its purification. To see that we can write

$$\begin{aligned} |\psi_\rho(U)\rangle &= \sum_i \sqrt{p_i} |\phi_i^A\rangle \otimes U |\phi_i^B\rangle = \sum_i \sqrt{p_i} |\phi_i^A\rangle \otimes U |\phi_i^B\rangle = \left(\rho^{\frac{1}{2}} \otimes U \right) \sum_i |\phi_i^A\rangle \otimes |\phi_i^B\rangle \\ |\psi_\sigma(U')\rangle &= \sum_i \sqrt{p'_i} |\tilde{\phi}_i^A\rangle \otimes U' |\phi_i^B\rangle = \dots = \left(\sigma^{\frac{1}{2}} \otimes U' \right) \sum_i |\tilde{\phi}_i^A\rangle \otimes |\phi_i^B\rangle \end{aligned}$$

and compute the overlap

$$\langle \psi_\sigma(U') | \psi_\rho(U) \rangle = \left(\sum_i \langle \tilde{\phi}_j^A | \otimes \langle \phi_j^B | \right) \left(\sigma^{\frac{1}{2}} \rho^{\frac{1}{2}} \otimes U'^\dagger U \right) \left(\sum_i |\phi_i^A\rangle \otimes |\phi_i^B\rangle \right)$$

We now use the fact that the state $\sum_i |\phi_i^A\rangle \otimes |\phi_i^B\rangle$ is invariant under $V_A \otimes V_B^{\dagger T}$ with V_A and V_B unitary transformations $V_A = \sum_{ij} V_{ij} |\phi_j^A\rangle \langle \phi_j^A|$ and $V_B = \sum_{ij} V_{ij} |\phi_j^B\rangle \langle \phi_j^B|$, i.e. $V_A \otimes V_B^{\dagger T} (\sum_i |\phi_i^A\rangle \otimes |\phi_i^B\rangle) = \sum_{ijk} V_{ji} V_{ki}^{\dagger T} |\phi_j^A\rangle \otimes |\phi_k^B\rangle = \sum_i |\phi_i^A\rangle \otimes |\phi_i^B\rangle$. So we have

$$\begin{aligned} \langle \psi_\sigma(U') | \psi_\rho(U) \rangle &= \left(\sum_i \langle \tilde{\phi}_j^A | \otimes \langle \phi_j^B | \right) \left(\sigma^{\frac{1}{2}} \rho^{\frac{1}{2}} (U'^\dagger U)^{T\dagger} \otimes 1 \right) \left(\sum_i |\phi_i^A\rangle \otimes |\phi_i^B\rangle \right) \\ &= \text{tr} \left[\sigma^{\frac{1}{2}} \rho^{\frac{1}{2}} (U'^\dagger U)^{T\dagger} V \right] = \text{tr} \left[\tilde{U} \sqrt{\rho^{\frac{1}{2}} \sigma \rho^{\frac{1}{2}}} (U'^\dagger U)^{T\dagger} V \right] \end{aligned}$$

using $|\phi_i^A\rangle = V |\tilde{\phi}_i^A\rangle$ the polar decomposition $A = \tilde{U} \sqrt{A^\dagger A}$ with \tilde{U} a unitary matrix. In the basis where $\sigma^{\frac{1}{2}} \rho^{\frac{1}{2}} = \sum_a |a\rangle \lambda_a \langle a|$ is diagonal it finally writes

$$\langle \psi_\sigma(U') | \psi_\rho(U) \rangle = \sum_a \lambda_a \langle a | (U'^\dagger U)^{T\dagger} V \tilde{U} | a \rangle$$

since the λ_a 's are non-negative the inner product is maximal for $(U'^\dagger U)^{T\dagger} V \tilde{U} = 1$. Therefore,

$$F(\rho, \sigma) = \max_{U, U'} |\langle \psi_\sigma(U') | \psi_\rho(U) \rangle|^2$$

In particular

$$F(\rho_{AB}, \sigma_{AB}) \leq F(\rho_A, \sigma_A).$$

The fidelity also allows to define a distance between states, called Bures distance

$$D_B(\rho, \sigma) = 2 \left[1 - \sqrt{F(\rho, \sigma)} \right]$$

We will come back to the fidelity and Bures distance, it will be important to understand what happens near phase transitions...

3.4 Actions on a quantum state

3.4.1 Unitary evolution and Measurements

The most familiar type of actions one can perform to a quantum state is to evolve it under the action of a unitary operator $|\psi\rangle \rightarrow U|\psi\rangle$. We can also measure a quantum state, projecting it into the eigenspace of the measured operator $A = \sum_x a_x |x\rangle\langle x| = \sum_a a E_a$ where $E_a = \sum_x \delta_{a_x=a} |x\rangle\langle x|$ is a projector and $\sum_a E_a = 1$. After the measure we have

$$|\psi\rangle \rightarrow \begin{cases} \frac{E_a |\psi\rangle}{\sqrt{\langle \psi | E_a | \psi \rangle}} \\ \text{classical outcome } a \text{ happening with probability } p_a = \langle \psi | E_a | \psi \rangle \end{cases}$$

For a density matrix we have similarly, for a unitary evolution or a measure:

$$\rho \rightarrow U\rho U^\dagger$$

$$\rho \rightarrow \begin{cases} \frac{E_a \rho E_a}{\text{tr} \rho E_a} \\ \text{classical outcome } a \text{ happening with probability } p_a = \text{tr} \rho E_a \end{cases}$$

If we decide to measure but not yet know the classical outcome then

$$\rho \rightarrow \sum_a p_a \frac{E_a \rho E_a}{\text{tr} \rho E_a} = \sum_a E_a \rho E_a$$

3.4.2 Generalized measurements

Unitary evolution and measurements are however not the most generic thing we can do to a quantum state. For example we could put it in contact with another system and perform a unitary evolution of the full system but agree only to measure the observable $O_B = \sum_i b_i |b_i\rangle\langle b_i|$ with $b_i \neq b_j$ for $i \neq j$, of the auxiliary subsystem. The first step we can write as

$$|\psi\rangle_A \otimes |0\rangle_B \rightarrow |\psi'\rangle_{AB} = U(|\psi\rangle_A \otimes |0\rangle_B) = \sum_i [\langle b_i | U(|\psi\rangle_A \otimes |0\rangle_B)] \otimes |b_i\rangle = \sum_i M_i |\psi\rangle_A \otimes |b_i\rangle$$

where $\langle a | M_i | a' \rangle = (\langle a |_A \otimes \langle b_i |_B) U(|a'\rangle_A \otimes |0\rangle_B)$, and the second

$$\rho'_{AB} \rightarrow \begin{cases} \rho''_{AB} = \frac{M_i |\psi\rangle_A \langle \psi|_A M_i^\dagger}{\langle \psi|_A M_i^\dagger M_i |\psi\rangle_A} \otimes |b_i\rangle\langle b_i| \\ \text{classical outcome probability } b_i \text{ with probability } p_i = \langle \psi|_A M_i^\dagger M_i |\psi\rangle_A \end{cases}$$

Now, disregarding the subsystem B (since we only care about the fact it was measured), we obtain

$$\rho''_A = \sum_i \frac{M_i |\psi\rangle_A \langle \psi|_A M_i^\dagger}{\langle \psi|_A M_i^\dagger M_i |\psi\rangle_A} p_i = \sum_i M_i |\psi\rangle_A \langle \psi|_A M_i^\dagger$$

Since U preserved the norm, $\langle \psi' | \psi' \rangle_{AB} = \sum_i \langle \psi |_A M_i^\dagger M_i |\psi\rangle_A$ for any state $|\psi\rangle_A$ it follows that $\sum_i M_i^\dagger M_i = 1$.

This action can be generalized to density matrices:

$$\rho_A \rightarrow \rho'_A = \sum_i M_i \rho_A M_i^\dagger$$

As a result of this procedure we know the classical outcome b_i with probability $\text{tr} [M_i \rho_A M_i^\dagger]$ was obtained but we are (still) not aware what that value was. This turns out to be the most generic transformation that takes a physical density matrix into another and it is called a positive operator-valued measure (POVM). Unitary evolution and measurements are just particular examples.

However, there is a redundancy in choosing the operators M_i . To see this let us consider the purification of the state ρ'_A assuming $\rho_A = |\psi_A\rangle\langle\psi_A|$, we have

$$\begin{aligned} |\psi'_{AB}\rangle &= \sum_i M_i |\psi_A\rangle \otimes |\phi_i\rangle \\ &= \sum_{ij} M_i |\psi_A\rangle \otimes U_{ij} |\tilde{\phi}_j\rangle \\ &= \sum_i \tilde{M}_i |\psi_A\rangle \otimes |\tilde{\phi}_i\rangle \end{aligned}$$

with $U_{ij} = \langle \tilde{\phi}_j | \phi_i \rangle$ and $\tilde{M}_j = \sum_i M_i U_{ij}$. So,

$$\sum_i M_i |\psi_A\rangle \langle\psi_A| M_i^\dagger = \sum_i \tilde{M}_i |\psi_A\rangle \langle\psi_A| \tilde{M}_i^\dagger$$

for any $|\psi_A\rangle\langle\psi_A|$ and thus

$$\sum_i M_i \rho_A M_i^\dagger = \sum_i \tilde{M}_i \rho_A \tilde{M}_i^\dagger$$

for $\tilde{M}_j = \sum_i M_i U_{ij}$.

Lecture 3

4 Entanglement and Entanglement Measures

Entanglement is a generic name to characterize the fact that a quantum state cannot be written as a direct product of states of its subsystems. In fact, separable states are a set of measure zero. As we will see there is no unique way to quantify the degree of entanglement but rather different measures that try to capture the many ways states can be entangled. Moreover it turns out that it is much more difficult to characterize entanglement in mixed states. We will look at some measures of entanglement with particular emphasis on those we will use in the following [13](#).

4.0.1 Requirements

A good measure of entanglement should satisfy some requirements. For example, it should not increase if nothing is done to increase the “quantum” correlations of the system, i.e. $E(\rho) \geq E(\rho')$ if ρ' is obtained from ρ by Local Operations and Classical Communication (LOCC).

¹³you can find a review in Plenio, M. B., and S. Virmani, 2007, Quantum Inf. Comput. 7, 1. The discussion here follows [\[AFOV\]](#).

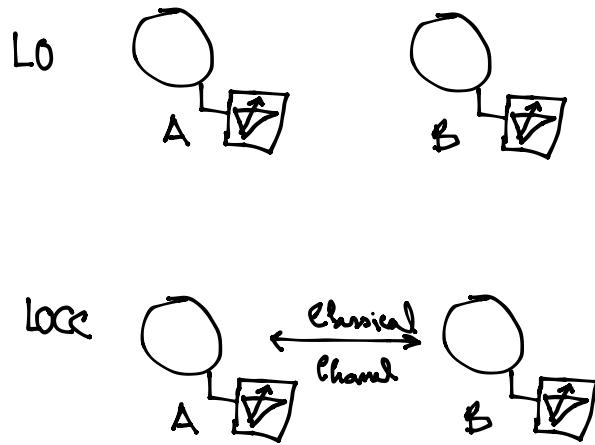
The most general set of local operations one can perform without communication is to do an independent set of POVM's in each system i.e.

$$\rho_{AB} \rightarrow \rho'_{AB} = \sum_{ik} M_i^A \otimes M_k^B \rho_A M_i^{A\dagger} \otimes M_k^{B\dagger}$$

If the observers of system A and B are allowed to communicate classically before or after they perform a POVM, their actions may depend upon the outcomes of previous measuring operations. In general this set of allowed operations is quite complicated and there is no simple explicit characterization of that class of operators. An important class is the set of separable operations:

$$\rho_{AB} \rightarrow \rho'_{AB} = \sum_k M_k^A \otimes M_k^B \rho_A M_k^{A\dagger} \otimes M_k^{B\dagger}$$

with $\sum_k M_k^{A\dagger} M_k^A \otimes M_k^{B\dagger} M_k^B = 1 \otimes 1$. Note that this can not be written as two independent POVM's as before.



Armed with this new concept of LOCC let us now write a wish-list for the properties of entanglement measures¹⁴:

1. Separable states contain no entanglement: $E(\rho_A \otimes \rho_B) = 0$
2. All non-separable states are entangled: if ρ cannot be put of the form $\rho_A \otimes \rho_B$ for some ρ_A and ρ_B , then $E(\rho) > 0$
3. The entanglement does not increase under LOCC transformations: $E(\rho) \geq E(\rho')$ if ρ' is obtained from ρ by LOCC
4. Entanglement does not change under Local Unitary operations: $E(U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger) = E(\rho)$
5. There are maximally entangled states

4.0.2 Entanglement Cost

A possible way of defining an entanglement measure is to take an entangled reference state and ask what is the cost of transforming it into the state we want to measure. But the cost in what? What is the resource? One possible resource is the number of copies of the system!

Take the reference state $|\Phi^+\rangle = 1/\sqrt{2}(|01\rangle + |10\rangle)$ with density matrix $P_+ = |\Phi^+\rangle\langle\Phi^+|$. How many $|\Phi^+\rangle$ do I need to produce n copies of the state $|\psi_{AB}\rangle$, if I can only do LOOC?

Let's see some examples:

- State $|\psi_{AB}\rangle = |00\rangle_A \otimes |00\rangle_B$. I need 0 copies of $|\Phi^+\rangle$! I just tell A and B to prepare two qubits in the state 0.

¹⁴Plenio, M. B., and S. Virmani, 2007, Quantum Inf. Comput. 7, 1.

- State $|\psi_{AB}\rangle = \frac{1}{\sqrt{2}} [|00\rangle_A \otimes |00\rangle_B + |11\rangle_A \otimes |11\rangle_B]$. (1) I give one copy of the state $|\Phi^+\rangle$ to A and B. (2) I ask B to perform a σ_x on his/her qubit

$$1 \otimes \sigma_x |\Phi^+\rangle = 1/\sqrt{2} (|00\rangle + |11\rangle)$$

(3) I tell both to add a local qubit in the state 0

$$[1 \otimes \sigma_x |\Phi^+\rangle] \otimes [|0\rangle_{A_2} \otimes |0\rangle_{B_2}] = 1/\sqrt{2} (|00\rangle_A \otimes |00\rangle_B + |10\rangle_A \otimes |10\rangle_B)$$

(4) Finally, I ask A and B to do a control not on their qubits

$$[\text{CNOT} \otimes \text{CNOT}] [1 \otimes \sigma_x |\Phi^+\rangle] \otimes [|0\rangle_{A_2} \otimes |0\rangle_{B_2}] = 1/\sqrt{2} (|00\rangle \otimes |00\rangle + |11\rangle \otimes |11\rangle)$$

So, I need one copy of the state $|\Phi^+\rangle$!

- State $|\psi_{AB}\rangle = \frac{1}{2} [|00\rangle_A \otimes |00\rangle_B + |10\rangle_A \otimes |10\rangle_B + |01\rangle_A \otimes |01\rangle_B + |11\rangle_A \otimes |11\rangle_B]$. (1) I give two copies of $|\Phi^+\rangle$ to A and B

$$\begin{aligned} |\Phi^+\rangle \otimes |\Phi^+\rangle &= \frac{1}{2} (|0\rangle_{A1} \otimes |1\rangle_{B1} + |1\rangle_{A1} \otimes |0\rangle_{B1}) \otimes (|0\rangle_{A2} \otimes |1\rangle_{B2} + |1\rangle_{A2} \otimes |0\rangle_{B2}) \\ &= \frac{1}{2} (|00\rangle_A \otimes |11\rangle_B + |01\rangle_A \otimes |10\rangle_B + |10\rangle_A \otimes |01\rangle_B + |11\rangle_A \otimes |00\rangle_B) \end{aligned}$$

(2) I ask B to perform a $\sigma_x^{B1} \otimes \sigma_x^{B2}$ operation

$$\begin{aligned} [1^{A1} \otimes 1^{A2}] \otimes [\sigma_x^{B1} \otimes \sigma_x^{B2}] |\Phi^+\rangle \otimes |\Phi^+\rangle &= \\ \frac{1}{2} (|00\rangle_A \otimes |00\rangle_B + |01\rangle_A \otimes |01\rangle_B + |10\rangle_A \otimes |01\rangle_B + |11\rangle_A \otimes |11\rangle_B) & \end{aligned}$$

So I need two copies of $|\Phi^+\rangle$!

More generally the entanglement cost quantifies the rate m/n at which it is possible to convert $P_+^{\otimes m}$ into $\rho^{\otimes n}$ with a LOCC operation $\Lambda(P_+^{\otimes m}) \simeq \rho^{\otimes n}$. More precisely

$$\underset{\text{cost}}{(\langle \Phi^+ | \Phi^+ \rangle)^{\otimes m}} \xrightarrow{\text{Locc}} \rho^{\otimes n}$$

$$E_C(\rho) = \inf \left\{ r : \lim_{n \rightarrow \infty} \inf_{\Lambda} \{ F[\rho^{\otimes n}, \Lambda(P_+^{\otimes rn})] \} = 1 \right\}$$

Although computing $E_C(\rho)$ is difficult it still gives a way to think about entanglement in a precise sense.

$$\rho^{\otimes n} \xrightarrow{\text{Locc}} (\langle \Phi^+ | \Phi^+ \rangle)^{\otimes m}$$

4.0.3 Entanglement Distillation

This measurement is the converse of the previous one and asks: how many states of P_+ can I prepare with n copies of ρ

$$E_D(\rho) = \inf \left\{ r : \lim_{n \rightarrow \infty} \inf_{\Lambda} \{ F[P_+^{\otimes rn}, \Lambda(\rho^{\otimes n})] \} = 1 \right\}$$

Given these two entanglement measures it is natural to ask whether $E_C = E_D$. This means that the transformations become reversible “entanglementwise” in the asymptotic limit.

This happens for pure state transformations: ¹⁵

$$E_C(|\psi\rangle\langle\psi|) = E_D(|\psi\rangle\langle\psi|) = E(|\psi\rangle\langle\psi|)$$

where E is called the entropy of entanglement

$$E(|\psi\rangle\langle\psi|) = S(\text{tr}_A |\psi\rangle\langle\psi|) = S(\text{tr}_B |\psi\rangle\langle\psi|)$$

¹⁵C. H. Bennett, H. Bernstein, S. Popescu and B. Schumacher, Phys. Rev. A 53, 2046 (1996)

4.0.4 Entanglement of Formation and Concurrence

Inspired by the case of pure states one can define another measure of entanglement

$$E_F(\rho) = \inf \left\{ \sum_i p_i E(|\psi_i\rangle\langle\psi_i|) : \rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \right\}$$

taken over all the possible ways one can write ρ in terms of pure states.

For the case of two qubits there is an explicit expression for the entanglement of formation

$$E_F(\rho) = - \sum_{\sigma=\pm 1} \frac{\sqrt{1 + \sigma C^2(\rho)}}{2} \ln \frac{\sqrt{1 + \sigma C^2(\rho)}}{2}$$

where $C(\rho)$ is another measure of entanglement called concurrence given by

$$C(\rho) = \max \{ \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0 \}$$

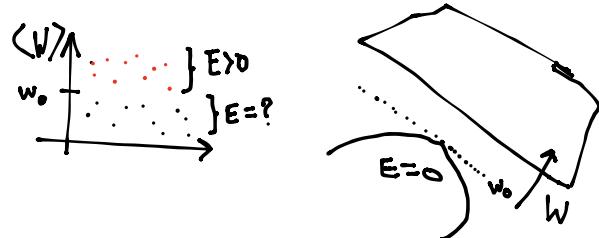
where $\lambda_1^2 \geq \dots \geq \lambda_4^2$ are the eigenvalues of the matrix $R(\rho) = \sqrt{\rho} (\sigma^y \otimes \sigma^y) \rho^* (\sigma^y \otimes \sigma^y) \sqrt{\rho}$.

Having an explicit entanglement measure for mixed states, even if only for two qubits, is extremely useful - in a system of many qubits one can ask what is the entanglement between two of them pairwise.

4.0.5 Entanglement Witnesses, partial transpose and positive maps

It is not just the quantification of entanglement which is difficult. Even, to tell in general whether a state of n parties is separable or not is still an open problem. Some observables may nevertheless help in particular cases. An entanglement witness W is a Hermitian operator able to detect entanglement. The idea is similar to that of the Bell inequalities: if the expectation value of W exceeds certain bounds the state is entangled:

$$\text{tr}(\rho W) > w_0 \Rightarrow \rho \text{ is not separable.}$$



However the converse is not true. An example is $W = [|\Phi^+\rangle\langle\Phi^+| - \frac{1}{2}]$, for $\text{tr}[\rho W] > 0$, ρ is not separable¹⁶, however for $\rho = |\Phi^-\rangle\langle\Phi^-|$ we have $W = -1/2 < 0$ and this state is maximally entangled.

The geometrical idea behind this is simple: since the set of separable states is convex there always exist some observable that can discriminate points that do not belong to the set.

Entanglement witnesses are a special case of a more general concept - positive maps. We already give examples of the so called completely positive maps POVMs:

$$\rho_A \rightarrow \rho'_A = \Phi(\rho_A) = \sum_i M_i \rho_A M_i^\dagger$$

¹⁶Prove this!

These maps take a physical density matrix (i.e. non-negative, Hermitian with unit trace) to another physical matrix. They are called completely positive because their action can be extended to a larger space and the result is always a physical density matrix:

$$\rho_{AB} \rightarrow \rho'_{AB} = (\Phi \otimes 1)(\rho_{AB}) = \sum_i (M_i \otimes 1) \rho_{AB} (M_i^\dagger \otimes 1)$$

Actually POVMs are the most generic linear transformations with such a property and we could have obtained the same form by axiomatizing ¹⁷ this property. However there are maps that are positive but not completely positive. An example is the transposition $\rho \rightarrow \Phi(\rho) = \rho^T$. ρ^T is a honest density matrix since transposition does not change eigenvalues but the extension to a larger space ($\Phi \otimes 1$) called the partial trace

$$\rho_{AB} \rightarrow (\Phi \otimes 1)(\rho_{AB}) = \rho'_{AB}$$

with

$$\begin{aligned} \rho_{AB} &= \sum_{ii'jj'} |a_i\rangle \otimes |b_i\rangle [\rho_{AB}]_{ij;i'j'} \langle a_{i'}| \otimes \langle b_{j'}| \\ \rho'_{AB} &= \sum_{ii'jj'} |a_i\rangle \otimes |b_i\rangle [\rho_{AB}]_{i'j;ij'} \langle a_{i'}| \otimes \langle b_{j'}| \end{aligned}$$

might not be an honest density matrix. Let us look at the example of a maximal entangled state of two qubits $|\Phi^+\rangle = 1/\sqrt{2}(|10\rangle + |01\rangle)$:

$$\begin{array}{c} \rho = \frac{1}{2} \times \begin{array}{|cc|} \hline 00 & 01 & 10 & 11 \\ \hline 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ \hline \end{array} \rightarrow \rho' = \rho^{TA} = \frac{1}{2} \times \begin{array}{|cc|} \hline 00 & 01 & 10 & 11 \\ \hline 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ \hline \end{array} \\ \lambda \in \{1, 0, 0, 0\} \qquad \qquad \qquad \lambda' \in \left\{ -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right\} \end{array}$$

Partial transpose is an example of a positive but not completely positive map. These maps are important for entanglement theory since it can be proven that a state ρ_{AB} is entangled if and only if a positive (but not completely positive) map exists such that $(\Phi \otimes 1)(\rho_{AB}) \not\succeq 0$. The example above is particularly simple because for two qubits a positive map can be written as $\Phi = CP_1 + CP_2 T_B$, i.e. the non-complete positive part is entirely due to the partial transposition. In the general case of many qubits or tensor products of states with larger local Hilbert space the partial trace is an entanglement witness.

An associated measure of entanglement is the negativity $N(\rho_{AB}) = \sum_i -\lambda'_i \Theta(-\lambda'_i)$, where Θ is the Heaviside theta function.

4.0.6 Other measures of entanglement

Other measures also relay on the comparison to a reference state for example:

Relative entropy of entanglement:

$$E(\rho) = \inf_{\sigma \in \mathcal{D}} S(\sigma|\rho) = \inf_{\sigma \in \mathcal{D}} \text{tr}[\sigma(\ln \sigma - \ln \rho)]$$

where \mathcal{D} is the manifold of separable states that can be written as $\sigma = \sum_i p_i \sigma_i^A \otimes \sigma_i^B$. The difficulty in computing this measure is to find the disentangled state closest to ρ , which is still an open problem, even for two qubits! Although it can be done numerically there are only a few classes of states for which exact results are known.

¹⁷see chapter 8.2.4 of [N&C]

4.0.7 Comments on entanglement measures

There is much more to say about entanglement but we will stop here in this course. A few more comments though:

- There are subtleties in defining entanglement for indistinguishable particles that we will avoid by considering entanglement between sites on a lattice.
- For 3 qubits or more there are several kinds of entanglement, that quantify the true n -party non-separability, $(n - 1)$ -party non-separability, and so on...
- To quantify this many kinds of entanglement one can use entanglement invariants which are a complete set of numbers that describe the orbits of the group $U_1 \otimes U_2 \otimes \dots$. However these quantities grow exponentially with the Hilbert space size and are only known explicitly for a very small number of cases.

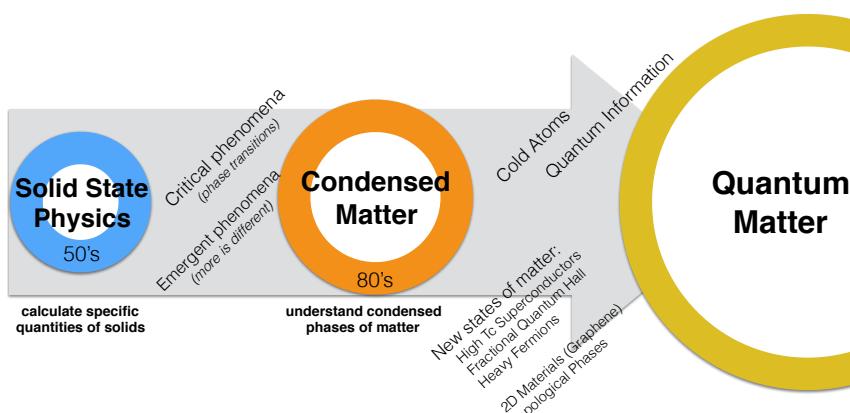
Lecture 4

5 Quantum Matter - The basics

5.1 Matter and Condensed Matter

Wikipedia on Condensed matter physics:

- “deals with the physical properties of condensed phases of matter, where particles adhere to each other”;
- “seeks to understand the behavior of these phases by using physical laws. In particular, they include the laws of quantum mechanics, electromagnetism and statistical mechanics.”



What we today refer to as condensed matter has been an evolving concept, starting from the 50's with the characterization of specific properties of solids (crystallography, metallurgy, elasticity, magnetism), to the 80's where the emphasis passed to the qualitative understanding of phases of matter and their emerging excitations. More recently, advances in quantum optics and in the field of cold atoms permitted to study systems with many particles, with a degree of control that was unprecedented and with a set of new techniques that are quite different from the traditional

solid-state ones. Therefore nowadays, when referring to condensed matter we typically mean phenomena way more vast than just the study of “rocks”.

For the purposes of this course I will call Quantum Matter the study of phenomena at low enough energy scales such that quantum effects have to be taken into account and where the interactions between particles are exclusively mediated by electromagnetic forces. At these energy scales, outer shell electrons, ions and photons can be considered as “fundamental particles”. Even if it seems restrictive (after all we have 3 more forces and many more particles to play with) the collective behavior of these fundamental constituents is extremely rich and has never stopped to provide new physics.

5.2 What is observed?

Traditional experimental condensed matter techniques can be categorized as¹⁸:

- experiments probing thermodynamic coefficients (specific heat, static susceptibilities (magnetic, charge,...) with no information on spatial structures nor dynamical features);
- transport experiments (for example, Scanning tunneling microscopy (STM), current spectroscopy, point contacts, Hall currents);
- spectroscopy (Angle-resolved photoemission spectroscopy (ARPES), Nuclear magnetic resonance spectroscopy (NMR)).

These last two, transport and spectroscopic measurements, may be used to obtain detailed information on the spatio-temporal structure of the excitations of a system. In cold atomic systems one may access other properties, often much more local, such as the position or the state of an atom.

Almost all of these properties can be understood by studying how the particular system in question reacts to an external electromagnetic stimulus that is in general much weaker than the internal correlations of the system.

5.2.1 Linear response theory

The theoretical framework that deals with the response of an equilibrium system to an external small perturbation is called linear response theory: for a system initially in thermal equilibrium with Hamiltonian H_0 , the change in the expectation value of observable A due to a perturbation to the system's Hamiltonian of the form $H = H_0 + V$ with $V = \int dr' b(t', r') B(r')$ is given by

$$\langle A(t, r) \rangle = \langle A(t, r) \rangle_0 + \int dt' \int dr' \chi_{AB}^R(t, r; t', r') b(t', r') + O(b^2),$$

where the subscript 0 means that the expectation value and the time evolution are computed with respect to the unperturbed Hamiltonian. The operator A is written in the Heisenberg representation $A(t, r) = U(t_0, t) A(r) U(t, t_0)$ with $U(t, t') = T e^{-i \int_{t'}^t d\tau H(\tau)}$ and $U(t_0, t) = U(t, t_0)^\dagger$ for some initial time t_0 such that $b(t, r) = 0$ for $t < t_0$.

We can derive an explicit expression for the quantity $\chi_{AB}^R(t, r; t', r')$ called the (retarded) susceptibility of A to B . Writing $U(t, t')$ in powers of the perturbation field b we obtain $U(t, t') =$

¹⁸Condensed Matter Field Theory, A. Altland and B. Simons

$U_0(t, t') \left[1 - i \int_0^t dt' \int dr' U_0(t', \tau) b(\tau, r') B(r) U_0(\tau, t') \right] + O(b^2)$.¹⁹ Taking $t_0 \rightarrow -\infty$ and using the development of U we obtain²⁰

$$\chi_{AB}^R(t, r; t', r') = -i\Theta(t - t') \langle [A(t, r), B(t', r')] \rangle_0. \quad (4)$$

This formula is very important because it relates correlation functions, that can be computed, with observables that can be measured experimentally.

Typically the unperturbed system in question is invariant under translations in space and time (i.e. its Hamiltonian is time independent), in that case $\chi_{AB}^R(t, r; t', r') = \chi_{AB}^R(t - t', r - r')$ and we consider instead the Fourier transformed quantities

$$\chi_{AB}^R(\omega, q) = \int dt \int dr e^{i(\omega t - qr)} \chi_{AB}^R(t, r).$$

The Θ -function in front of Eq.(4) ensure that the response cannot precede the perturbation. As a consequence of this causal structure of the retarded susceptibility, there is a relation between the real and imaginary parts of $\chi_{AB}^R(\omega, q)$. Writing $\chi_{AB}^R(\omega, q) = \chi'_{AB}(\omega, q) + i\chi''_{AB}(\omega, q)$ these so-called Kramers-Kronig relations are given by²¹

$$\begin{aligned} \chi''_{AB}(\omega, q) &= -\frac{1}{\pi} \int d\nu \frac{\chi'_{AB}(\nu, q)}{\omega - \nu} \\ \chi'_{AB}(\omega, q) &= \frac{1}{\pi} \int d\nu \frac{\chi''_{AB}(\nu, q)}{\omega - \nu} \end{aligned}$$

Although response functions that allow to directly measure χ_{AB}^R are the most common, for some cases it is possible to measure $A(t, r)B(t', r')$ and $B(t', r')A(t, r)$ independently (i.e. not only the commutator $[A(t, r), B(t', r')]$). At equilibrium these two quantities

$$\begin{aligned} \chi_{AB}^>(t, r; t', r') &= -i \langle A(t, r) B(t', r') \rangle_0 \\ \chi_{AB}^<(t, r; t', r') &= -i \langle B(t', r') A(t, r) \rangle_0 \end{aligned}$$

are not independent and obey the so-called fluctuation dissipation relations²²

$$\chi_{AB}^<(\omega, q) = -e^{-\beta\omega} \chi_{AB}^>(\omega, q),$$

or, equivalently,

$$\frac{\chi_{AB}^>(\omega, q) - \chi_{AB}^<(\omega, q)}{\chi_{AB}^>(\omega, q) + \chi_{AB}^<(\omega, q)} = \coth\left(\frac{\beta}{2}\omega\right).$$

This finished a crash course on linear response theory. A notion to bear in mind is that by computing correlations and response functions such as the ones referred above we can predict the outcomes of an experiment.

5.3 Emergent degrees of freedom

The fact that the basic building blocks of the theory are limited to electrons, ions and photons does not mean that the model systems we will consider in the following are only limited to these degrees of freedom. In fact, often the useful degrees of freedom to consider at sufficiently low energies are collective modes which might be completely different from the excitations of the initial microscopic theory²³.

¹⁹Prove this!

²⁰Also prove this relation.

²¹Prove the Kramers-Kronig relations relations.

²²Prove the fluctuation dissipation relations.

²³If this ideas are new to you, read [More Is Different](#), P. W. Anderson.

5.3.1 The relation between the Anderson and Kondo models

Here I'm going to give a simple example of how emergent degrees of freedom may appear in which an electron system becomes effectively as a spin degree of freedom. Consider the following Hamiltonian

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_k \left(V_k d_\sigma^\dagger c_{k\sigma} + V_k^* c_{k\sigma}^\dagger d_\sigma \right) + E_1$$

of a system of itinerant electrons with dispersion relation ϵ_k that can hop to a localized site, d where the electron-electron interaction is strong, and V_k is the hybridization integral in momentum space which for a local coupling is given by $V_k = 1/\sqrt{\mathcal{V}}$ with $\mathcal{V} = \sum_k 1$. This is called the **Single impurity Anderson model (SIAM)**.

If U and $-\varepsilon_d$ are both large and positive the states that minimize the energy of the local level are those having a single electron either with spin up or down. $|\uparrow\rangle$ and $|\downarrow\rangle$ have degenerate energies and the contact with the itinerant electrons will lift this degeneracy in a non-trivial way. We want to express the Hamiltonian in the subspace of degenerate states in the first non-trivial order of perturbation in t . There are several ways of doing this that go under the name of Schrieffer-Wolff transformations, the easiest is just to use degenerate perturbation theory²⁴:

- Let $P_0 = (1 - n_{d\uparrow})(1 - n_{d\downarrow})$, $P_1 = (1 - n_{d\uparrow})(n_{d\downarrow}) + n_{d\uparrow}(1 - n_{d\downarrow})$ and $P_2 = n_{d\uparrow}n_{d\downarrow}$ be the projectors into the subspace with $n = 0, 1, 2$ localized electrons, the eigenstate condition can be written as

$$\begin{pmatrix} H_{00} & H_{01} & H_{02} \\ H_{10} & H_{11} & H_{12} \\ H_{20} & H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} |\psi_0\rangle \\ |\psi_1\rangle \\ |\psi_2\rangle \end{pmatrix} = E \begin{pmatrix} |\psi_0\rangle \\ |\psi_1\rangle \\ |\psi_2\rangle \end{pmatrix}$$

where $|\psi_n\rangle = P_n |\psi\rangle$ and $H_{nn'} = P_n H P_{n'}$. Note that the off-diagonal elements come from the hybridization term. Since this changes the number of electrons by one $H_{20} = H_{02}$. For the other terms we have

$$\begin{aligned} H_{10} &= \sum_{k\sigma} V_k d_\sigma^\dagger (1 - n_{d,-\sigma}) c_{k\sigma} \\ H_{12} &= \sum_{k\sigma} V_k^* c_{k\sigma}^\dagger d_\sigma n_{d,-\sigma} \end{aligned}$$

and $H_{01} = H_{10}^\dagger$, $H_{21} = H_{12}^\dagger$. Thus we have

$$\begin{pmatrix} (H_{00} - E) |\psi_0\rangle + H_{01} |\psi_1\rangle \\ H_{10} |\psi_0\rangle + (H_{11} - E) |\psi_1\rangle + H_{12} |\psi_2\rangle \\ H_{21} |\psi_1\rangle + (H_{22} - E) |\psi_2\rangle \end{pmatrix} = 0$$

Since we are interested in the amplitude $|\psi_1\rangle$ we eliminate $|\psi_0\rangle$ and $|\psi_2\rangle$ for the eigenvalue equation

$$\left[H_{10} (E - H_{00})^{-1} H_{01} + H_{11} + H_{12} (E - H_{22})^{-1} H_{21} \right] |\psi_1\rangle = E |\psi_1\rangle$$

Let us now evaluate

$$H_{12} (E - H_{22})^{-1} H_{21} = \sum_{kk'\sigma\sigma'} V_k^* V_{k'} c_{k\sigma}^\dagger d_\sigma (E - H_{22})^{-1} d_{\sigma'}^\dagger c_{k'\sigma'}$$

²⁴This argument is taken from [The Kondo Problem to Heavy Fermions](#), A.Hewson

At leading order in V we have $|\psi_1\rangle = |\uparrow\rangle \otimes |\text{FS}\rangle + |\delta\psi_\uparrow\rangle + O(V^2)$ or $|\psi_1\rangle = |\downarrow\rangle \otimes |\text{FS}\rangle + |\delta\psi_\downarrow\rangle + O(V^2)$ where we chose E_1 such that $\left(\sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_\sigma \epsilon_d n_{d\sigma}\right) |\uparrow, \downarrow\rangle \otimes |\text{FS}\rangle = 0$ is the full Fermi sea. Therefore, to leading order in V we can write

$$\begin{aligned} H_{12}(E - H_{22})^{-1} H_{21} |\psi_1\rangle &\simeq \sum_{kk'\sigma\sigma'} V_k^* V_{k'} c_{k\sigma}^\dagger d_\sigma (E + \epsilon_{k'} - U - \epsilon_d)^{-1} n_{d,-\sigma'} d_{\sigma'}^\dagger c_{k'\sigma'} |\psi_1\rangle \\ &\simeq \sum_{kk'\sigma\sigma'} -\frac{V_k^* V_{k'}}{U + \epsilon_d} c_{k\sigma}^\dagger d_\sigma n_{d,-\sigma'} d_{\sigma'}^\dagger c_{k'\sigma'} |\psi_1\rangle \end{aligned}$$

where we consider the regime $\epsilon_F, E \ll U + \epsilon_d$ where $\epsilon_F \simeq \epsilon_{k'}$ is the Fermi energy. These terms can also be written as²⁵

$$H_{12}(E - H_{22})^{-1} H_{21} |\psi_1\rangle = \sum_{kk'} \frac{V_k^* V_{k'}}{U + \epsilon_d} \left[\sum_{ss'} \left(c_{ks}^\dagger \boldsymbol{\sigma}_{ss'} c_{ks'}^\dagger \right) \cdot \mathbf{s}_d + \frac{1}{2} \sum_s c_{ks}^\dagger c_{k's}^\dagger \right] |\psi_1\rangle$$

where $\mathbf{S}_d = \frac{1}{2} \sum_{uu'} d_u^\dagger \boldsymbol{\sigma}_{uu'} d_{u'}^\dagger$ respects the $su(2)$ commutation relations. In the same way

$$H_{10}(E - H_{00})^{-1} H_{01} |\psi_1\rangle = \sum_{kk'} \frac{V_k^* V_{k'}}{-\epsilon_d} \left[\sum_{ss'} \left(c_{ks}^\dagger \boldsymbol{\sigma}_{ss'} c_{ks'}^\dagger \right) \cdot \mathbf{S}_d + \frac{1}{2} \sum_s c_{ks}^\dagger c_{k's}^\dagger \right] |\psi_1\rangle$$

Therefore, in the subspace of one electron occupying the d level we have

$$\begin{aligned} H_{\text{eff}} &= \left[H_{10}(E - H_{00})^{-1} H_{01} + H_{11} + H_{12}(E - H_{22})^{-1} H_{21} \right] \\ &\simeq \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{kk's} V_k^* V_{k'} \left(\frac{1}{U + \epsilon_d} + \frac{1}{-\epsilon_d} \right) c_{ks}^\dagger c_{k's}^\dagger + \sum_{kk'} V_k^* V_{k'} \left(\frac{1}{U + \epsilon_d} + \frac{1}{-\epsilon_d} \right) \sum_{ss'} \left(c_{ks}^\dagger \boldsymbol{\sigma}_{ss'} c_{ks'}^\dagger \right) \cdot \mathbf{S}_d \end{aligned}$$

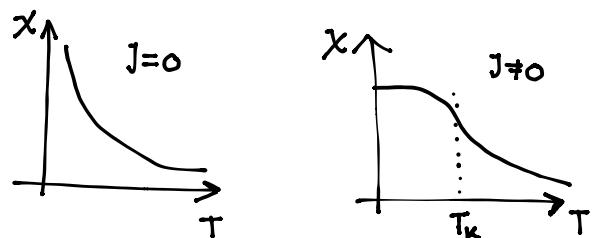
which for a local hybridization can be written as

$$H_{\text{eff}} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + U_0 \underbrace{\sum_s c_{0s}^\dagger c_{0s}^\dagger}_{\text{Potential Scattering}} + J \underbrace{\sum_{ss'} \left(c_{0s}^\dagger \boldsymbol{\sigma}_{ss'} c_{0s'}^\dagger \right) \cdot \mathbf{S}_d}_{\text{Kondo term}}$$

with $J = \left(\frac{1}{U + \epsilon_d} + \frac{1}{-\epsilon_d} \right)$, $U_0 = \left(\frac{1}{U + \epsilon_d} + \frac{1}{-\epsilon_d} \right)$. This is the **Kondo model** and it has had an important role in the understanding of non-perturbative effects and asymptotic freedom in the context of Condensed Matter.

First calculations, using perturbative methods in J , showed that logarithmic divergencies render the perturbative results invalid below some temperature scale, dubbed the Kondo temperature T_K .

Later P. Anderson came up with perturbative renormalization group method - so called Poor Man's Scaling - that showed that when temperature is decreased the effective coupling between the spin and itinerant electrons diverges. Finally, the Kondo problem was solved by K. Wilson that used his ideas of renormalization to devise a numerical renormalization group method that showed that the susceptibility of the impurity saturates as temperature goes to zero.

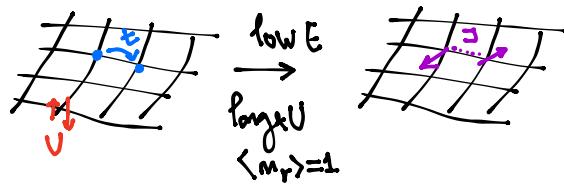


What we just proved was that the Anderson model in some regime behaves like the Kondo model, i.e. an electron degree of freedom, that has 4 possible states, can sometimes be reduced to a spin degree of freedom, that has only two states. This reduction arises because we want to study the systems at relatively low energies. If we study the high energy states this reduction is not possible.

This example is relatively easy and straightforward.
²⁵Prove that!

Other examples of this kind are the reduction of the Hubbard Model defined as

$$H = t \sum_{\langle rr' \rangle \sigma} c_{r\sigma}^\dagger c_{r'\sigma} + U \sum_r n_{r\uparrow} n_{r\downarrow},$$



where the sum over $\langle rr' \rangle$ runs over all nearest neighbors of the lattice, at half-filling $\langle n_\uparrow + n_\downarrow \rangle = 1$ and large U , to the Heisenberg model

$$H = J \sum_{\langle rr' \rangle} \mathbf{S}_r \cdot \mathbf{S}_{r'}$$

with $J \simeq t^2/U$. Other examples are much less evident, for example the low energy degrees of freedom of Fractional Quantum Hall states are particles with non-abelian statistics. The concept of emergent degrees of freedom thus tells you that **the microscopic degrees of freedom you start with may not be the ones that are helpful to understand the physics all low energy scales.**

The Kondo and the SIAM are examples of impurity models where a **zero dimensional** system interacts with a bunch of other degrees of freedom we will call bath or environment. The Kondo model is an example of a system where decoherence is very important if you prepare any state of the spin (qubit) after a time of the order of the inverse of T_K .

The Hubbard and Heisenberg models can be defined in a d -dimensional lattice and are used to model materials where correlations are important. In one dimension there are exact results for both models but for 2 and higher dimensions one has to rely on approximations. The Hubbard model in two dimensions is considered to be particularly interesting and rich, as some people think that it might explain some of the physics of the high-temperature superconductors and other strong correlated materials that are made out of quasi-2d layers. The Heisenberg model gives rise to very interesting physics, specially for frustrated lattices (such as a triangular lattice).

Lecture 5

5.4 More on models

I do not want to give you here an extensive review of all the models used in Condensed Matter, cold atoms or any other setup. The idea of this chapter is to introduce and motivate some models that we will see in some form or another in the reminder of the course or just models that are so common that you will probably encounter them at some point. Along the way I'll be doing some comments about their properties and the systems they are used to describe.

5.4.1 Bosons

Bosonic models are perhaps the most ubiquitous, appearing in the description of systems of photons, phonons, atoms and many low energy effective descriptions. In the context of Condensed Matter they are first encountered to describe phonons, i.e. vibrational models of a lattice. For example, in 1-dimension we have

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 \sum_{\langle ij \rangle} (x_i - x_j)^2$$

where m is the mass of the atom and $k = \omega^2 m$ is the force constant. Using $a_i = \sqrt{\frac{m\omega}{2}} (x_i + \frac{i}{m\omega} p_i)$ this can be transformed to

$$H = \sum_i \omega \left(a_i^\dagger a_i + \frac{1}{2} \right) + \sum_{\langle ij \rangle} (a_i^\dagger + a_i) (a_j^\dagger + a_j).$$

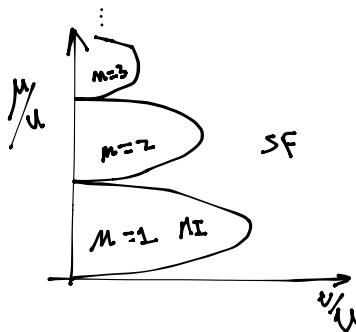
This is an example of a quadratic model that can be solved exactly. Once diagonalized (we will see how to do this) the dispersion relation of the eigen-modes is $\omega_k = 2\omega |\sin(\frac{k}{2})|$.

Cold atoms systems are usually described by a continuum model of an **interacting Bose gas**²⁶:

$$H = \int d^d r \left[\psi^\dagger(r) \left(-\frac{1}{2m} \nabla^2 + V(r) - \mu \right) \psi(r) \right] + \int d^d r d^d r' \psi^\dagger(r) \psi(r) U(r - r') \psi^\dagger(r') \psi(r')$$

where $V(r)$ is an external potential and U in the interaction term. In some cases a contact approximation: $U(r - r') = g\delta(r - r')$, is assumed. The model has been used to explain the phenomena of superfluidity. Note that this Hamiltonian has a global $U(1)$ symmetry, i.e. it is invariant by the transformation $\psi^\dagger(r) \rightarrow e^{i\phi} \psi^\dagger(r)$. In a superfluid phase, this symmetry is spontaneously broken (more on symmetries and broken phases later...).

The phenomenology of an interacting Bose gas is remarkable. For example, by imposing a $V(r)$ periodic potential induced by a laser field a periodic lattice can be constructed. If the lattice potential is sufficiently strong, a tight binding approximation, similar of that used for electrons, can be employed and the model reduces to the **Bose-Hubbard model**



$$H = -t \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i (n_i - 1) - \mu \sum_i n_i$$

parametrized by the hopping amplitude t of the bosons in the lattice, the on-site interaction U (which can be attractive or repulsive), and the chemical potential μ , which sets the total number of particles. Depending on its parameters a Bose-Hubbard system might be in a Mott insulating phase for $t/U \ll 1$, or in a superfluid state for $t/U \gg 1$.

Photons trapped in cavities in the context of Cavity Quantum Electrodynamics setups can also be described by bosonic Hamiltonians. Typically this modes couple to atoms that are considered as few level systems. We will look at some of these models later.

5.4.2 Fermions

We already mentioned several fermionic models such as the Single Impurity Anderson model and the Hubbard model. However, the simplest and most used fermionic models are quadratic ones of the type

$$H = \sum_{ij} c_i^\dagger h_{ij} c_j$$

where \mathbf{h} is an $N \times N$ Hermitian matrix. For Hamiltonians where fermions (i.e. electrons with spin) live on a number of sites \mathbf{r} , we have $i = (\mathbf{r}, \sigma)$. But i can index other kinds of quantum

²⁶see Jens O. Andersen, Rev. Mod. Phys. 76, 599 (2004)

numbers such as the kind of atom in a multi-band model. Typically we have $h_{ij} = 0$ if i and j refer to sites that are far apart. Tight binding Hamiltonians are also of this form with $h_{\mathbf{r}\sigma;\mathbf{r}'\sigma'} = -t\delta_{\sigma\sigma'}\delta_{|\mathbf{r}-\mathbf{r}'|,1}$. As in the bosonic case, these models can be obtained as an effective low energy theory starting from a continuum description of a fermionic field and assuming the sites correspond to potential wells where one fermions pass most of its time, only tunneling from time to time to other wells.

The Bardeen-Cooper-Schrieffer (BCS) theory was the first microscopic theory that explained superconductivity. After the electron-phonon interaction had been identified as the source of attractive interaction between the electrons there was the need to obtain some mean-field description of the superconducting phase. However, quadratic Hamiltonians of the kind we have just seen before seem not to do the job. A key observation of Bardeen, Cooper and Schrieffer was to consider also anomalous terms $c_i^\dagger c_j^\dagger$ and $c_j c_i$. Therefore, more generically, we can write a quadratic Hamiltonian as

$$H = \frac{1}{2} C^\dagger \mathbf{H} C$$

with $C = \{c_1, \dots, c_N, c_1^\dagger, \dots, c_N^\dagger\}$ and

$$\mathbf{H} = \begin{pmatrix} \mathbf{h} & \Delta \\ \Delta^\dagger & -\mathbf{h}^T \end{pmatrix}$$

and where $\mathbf{h}^\dagger = \mathbf{h}$ and $\Delta^T = -\Delta$ are $N \times N$ matrices. These kind of Hamiltonians arise as mean-field descriptions of interacting ones and will be important for us in the following. Classifying ground-states of these Hamiltonians will lead us to the notion of a topological phase.

Beyond non-interacting system there are several well studied models of interacting Fermions. You already saw the Kondo and the (fermionic) Hubbard model but there are many generalizations.

5.4.3 Spins and Spin Chains

We already saw how spin degrees of freedom emerge for electronic ones. Spin models are very important to understand magnetic properties of solids. Here, we already mentioned the Heisenberg model where spins sit on a lattice and interact via an exchange coupling $\propto \mathbf{S}_r \cdot \mathbf{S}_{r'}$. There are many generalization of this model by adding anisotropy terms $\propto S_r^\alpha S_{r'}^\alpha$ or magnetic fields $\propto \mathbf{h}_r \cdot \mathbf{S}_r$. Here, I want to mention an important family of models in one dimension - the so called spin chain models. The most general is the *XYZ* model

$$H = \sum_r J_x S_r^x \cdot S_{r+1}^x + J_y S_r^y \cdot S_{r+1}^y + J_z S_r^z \cdot S_{r+1}^z + h_z S_r^z.$$

A solution of this model (at least for $h_z = 0$) is known by a method called Bethe ansatz, but it is quite involved and extracting physical properties from it is not easy. For $J_x = J_y$ and $J_z = \Delta$ this is called the XXZ model also solvable by Bethe ansatz. A model we are going to study in some detail is the spin-1/2 XY model, when $J_z = 0$. This model can be transformed by a clever trick to a quadratic model of fermions that can then be solved by the methods in the next section. This model will be our drosophila both to study phase transitions and topological phases.

Another kind of spin models can be used to understand the physics of two-level atoms in an optical trap. The two states of the atoms can be labeled $|\uparrow\rangle$ and $|\downarrow\rangle$. In a cavity the cloud is quite confined by an optical trap and the atoms interact strongly with each other in a way that every atom can be assumed to interact in the same way with every other atom. Moreover an

effective field can be applied to the atoms to favor one of the states. The resulting Hamiltonian can be written as

$$H = \sum_{\alpha i, j} J_\alpha S_i^\alpha S_j^\alpha + h \sum_i S_i^z$$

where J_α characterizes the anisotropy of the interaction, and h is the synthetic magnetic field. Moreover defining the total spin operators $S_T^\alpha = \sum_j S_j^\alpha$ we can write

$$H = \sum_\alpha J_\alpha S_T^\alpha S_T^\alpha + h S_T^z + c$$

where c is a constant. This model is called the Lipkin Meshkov Glick (LMG) model and has applications in condensed matter and cold atomic systems. It is also a toy model to study phase transitions.

5.4.4 Models with multiple species of degrees of freedom

Many models consider interactions of degrees of freedom between different species. We have already mentioned the Kondo model that features one spin 1/2 interacting with electrons. Another classical example in Condensed Matter is the **Holstein model**

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \omega \sum_i a_i^\dagger a_i + \lambda \sum_i c_{i\sigma}^\dagger c_{i\sigma} (a_i^\dagger + a_i)$$

which is the simplest model that captures the effect of interaction between electrons and lattice phonons. The interaction with the phonons eventually leads to an attractive effective interaction between the electrons that gives rise to a superconducting phase at low energies.

The **Rabi model** is one of the simplest models describing a photonic modes that interacts with one atom and is a setup routinely realized in cavity QED experiments. The atom is considered as a two level system

$$H = \omega a^\dagger a + g \sigma_x (a + a^\dagger) + \Delta \sigma_z$$

This model admits an exact solution²⁷. However, a simpler version - called the **Jaynes-Cummings model** - valid for the resonance condition $2\Delta \simeq \omega$ and for weak coupling $g \ll \omega$ is widely used:

$$H = \omega a^\dagger a + g (\sigma^+ a + \sigma^- a^\dagger) + \Delta \sigma_z.$$

We will do some exercises about this model.

5.5 ... and how to solve (some of) them

5.5.1 Canonical Transformations

There are a number of physically relevant systems which may be modeled by quadratic (or bilinear) Hamiltonians. Examples include: superconductors, superfluids and ferromagnets and antiferromagnets in the spin-wave approximation and many more. To be able to compute physical observables the first step is to diagonalize these Hamiltonians by what are known as Bogoliubov transformations, which mix creation and annihilation operators, but preserving the commutation relations. Before making a more general approach to these quadratic models we will workout two simple examples²⁸.

²⁷D. Braak. Phys. Rev. Lett. 107, 100401 (2011)

²⁸The examples were taken from John Chalker, Quantum Theory of Condensed Matter, Lecture notes

Example I - Fermions Let us consider the Hamiltonian

$$H = \epsilon (c_1^\dagger c_1 + c_2^\dagger c_2) + \lambda (c_1^\dagger c_2^\dagger + c_2 c_1)$$

which arises in the context of the BSC theory superconductivity, we can also write it as

$$\begin{aligned} H &= \frac{1}{2} \begin{pmatrix} c_1 \\ c_2 \\ c_1^\dagger \\ c_2^\dagger \end{pmatrix}^\dagger \begin{pmatrix} \epsilon & & \lambda & \\ & \epsilon & -\lambda & \\ & -\lambda & -\epsilon & \\ \lambda & & & -\epsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_1^\dagger \\ c_2^\dagger \end{pmatrix} + \epsilon \\ &= \frac{1}{2} \begin{pmatrix} c_1 \\ c_2^\dagger \\ c_2 \\ c_1^\dagger \end{pmatrix}^\dagger \begin{pmatrix} \epsilon & \lambda & & \\ \lambda & -\epsilon & & \\ & & \epsilon & -\lambda \\ & & -\lambda & -\epsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2^\dagger \\ c_2 \\ c_1^\dagger \end{pmatrix} + \epsilon \end{aligned}$$

where in the second equality I just reshuffle the indices to emphasize the block diagonal structure. In order to diagonalize it further we consider the transformation

$$\begin{aligned} c_1^\dagger &= u d_1^\dagger + v d_2 \\ c_2^\dagger &= u d_2^\dagger - v d_1 \end{aligned}$$

This transformation is only useful only if the fermionic anticommutation relations are obeyed by both c 's and d 's. From this condition and $\{c_1, c_2\} = 0$ we have

$$\{c_1^\dagger, c_1\} = u^2 \{d_1^\dagger, d_1\} + v^2 \{d_2^\dagger, d_2\}$$

which implies $u^2 + v^2 = 1$ and suggests the parametrization $u = \cos \theta$, $v = \sin \theta$. Since

$$\begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} = R \begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix}$$

with $R = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}$, we can diagonalize the Hamiltonian's upper block by choosing R such that

$$R^\dagger \begin{pmatrix} \epsilon & \lambda \\ \lambda & -\epsilon \end{pmatrix} R = \begin{pmatrix} \tilde{\epsilon} & 0 \\ 0 & -\tilde{\epsilon} \end{pmatrix}$$

where $\tilde{\epsilon} = \sqrt{\epsilon^2 + \lambda^2}$ and $\tan 2\theta = -\lambda/\epsilon$. The transformation in the lower block is also determined. Joining both results we obtain

$$H = \tilde{\epsilon} (d_1^\dagger d_1 + d_2^\dagger d_2^\dagger) - \tilde{\epsilon} + \epsilon$$

Example II - Bosons Bogoliubov transformations for a bosonic systems are similar to those of fermions but different in some important details. Consider now an Hamiltonian of the same form as before, but where the particles are bosonic:

$$H = \epsilon (c_1^\dagger c_1 + c_2^\dagger c_2) + \lambda (c_1^\dagger c_2^\dagger + c_2 c_1)$$

This kind of Hamiltonians arises in the context of superfluidity and spin wave theory. We now use a transformation of the form

$$\begin{aligned} c_1^\dagger &= u d_1^\dagger + v d_2 \\ c_2^\dagger &= u d_2^\dagger + v d_1 \end{aligned}$$

which, as far as commutation relations are concerned, gives

$$[c_1^\dagger, c_1] = u^2 [d_1^\dagger, d_1] - v^2 [d_2^\dagger, d_2]$$

implying that $u^2 - v^2 = 1$ and suggests the parametrization $u = \cosh \theta$, $v = \sinh \theta$. Writing the Hamiltonian in matrix form

$$\begin{aligned} H &= \frac{1}{2} \begin{pmatrix} c_1 \\ c_2 \\ c_1^\dagger \\ c_2^\dagger \end{pmatrix}^\dagger \begin{pmatrix} \epsilon & & \lambda \\ & \epsilon & \lambda \\ & \lambda & \epsilon \\ \lambda & & \epsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_1^\dagger \\ c_2^\dagger \end{pmatrix} - \epsilon \\ &= \frac{1}{2} \begin{pmatrix} c_1 \\ c_2^\dagger \\ c_2 \\ c_1^\dagger \end{pmatrix}^\dagger \begin{pmatrix} \epsilon & \lambda & & \\ \lambda & \epsilon & & \\ & & \epsilon & \lambda \\ & & \lambda & \epsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2^\dagger \\ c_2 \\ c_1^\dagger \end{pmatrix} - \epsilon \end{aligned}$$

and going over the same steps as before, we obtain

$$H = \tilde{\epsilon} (d_1^\dagger d_1 + d_2^\dagger d_2^\dagger) + \tilde{\epsilon} - \epsilon$$

with $\tilde{\epsilon} = \sqrt{\epsilon^2 - \lambda^2}$ and $\tanh 2\theta = -\lambda/\epsilon$.

In this case the transformation requires $\epsilon > \lambda$, otherwise the initial problem is not well defined since the Hamiltonian represents a system at an unstable equilibrium point.

Lecture 6

Quadratic Hamiltonians Quadratic bosonic and fermionic models can be diagonalized by canonical transformations also called Bogoliubov or Bogoliubov-Valatin transformations. A Bogoliubov transformation is an isomorphism between of the canonical commutation or anti-commutation algebra. A quadratic generic Hamiltonian of N bosonic or fermionic modes can be written as

$$H = \frac{1}{2} A^\dagger \mathbf{H} A$$

with the Nambu vector $A = \{a_1, \dots, a_N, a_1^\dagger, \dots, a_N^\dagger\}$ and

$$\mathbf{H} = \begin{pmatrix} \mathbf{h} & \boldsymbol{\Delta} \\ \boldsymbol{\Delta}^\dagger & \xi \mathbf{h}^T \end{pmatrix}$$

where $\xi = 1$ for bosons and $\xi = -1$ for fermions. $\mathbf{h} = \mathbf{h}^\dagger$ and $\boldsymbol{\Delta} = -\boldsymbol{\Delta}^T$ are complex-valued $N \times N$ matrices. Note that, $\mathbf{S}A = A^{\dagger T}$, with $\mathbf{S} = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$, which implies that the Hamiltonian is particle-hole symmetric²⁹ i.e. $\hat{\mathbf{H}} = \xi \mathbf{H}$ with $\hat{\mathbf{H}} = \mathbf{S} \mathbf{H}^T \mathbf{S}$.

Invariant condition The computation or anti-commutation relations $a_i a_j^\dagger - \xi a_j^\dagger a_i = \delta_{i,j}$ can be summarized in the form

$$AA^\dagger - \xi (A^{\dagger T} A^T)^T = \mathbf{J}$$

²⁹Prove this.

where

$$AA^\dagger = \left(\begin{array}{cc|c} a_1 a_1^\dagger & a_1 a_2^\dagger & \\ a_2 a_1^\dagger & \ddots & \\ \hline & & a_1^\dagger a_1 & a_1^\dagger a_2 \\ & & a_2^\dagger a_1 & \ddots \\ & & a_2^\dagger a_2 & \ddots \end{array} \right); \quad [A^T A^{\dagger T}]^T = \left(\begin{array}{cc|c} a_1^\dagger a_1 & a_2^\dagger a_1 & \\ a_1^\dagger a_2 & \ddots & \\ \hline & & a_1 a_1^\dagger & a_2 a_1^\dagger \\ & & a_1 a_2^\dagger & \ddots \\ & & a_2 a_2^\dagger & \ddots \end{array} \right)$$

and $\mathbf{J} = \begin{pmatrix} \mathbf{1} & \\ & -\xi \mathbf{1} \end{pmatrix}$. Therefore a linear transformation $A \rightarrow A' = \mathbf{R}A$ that transforms bosonic (fermionic) degrees of freedom into bosonic (fermionic) degrees of freedom has to respect the same commutation relations

$$A' A'^\dagger - \xi (A'^{\dagger T} A'^T)^T = \mathbf{J}$$

which implies \mathbf{R} leaves the matrix \mathbf{J} invariant

$$\mathbf{R} \mathbf{J} \mathbf{R}^\dagger = \mathbf{J},$$

while the particle-hole symmetry implies

$$\mathbf{R}^\dagger = \mathbf{S} \mathbf{R}^T \mathbf{S}.$$

$q-p$ representation For fermions, \mathbf{R} is an unitary transformation while for bosons the group of transformation that respect the commutation relations is called the symplectic group. A way of justifying these denominations is to look at the representation

$$X = \frac{1}{\sqrt{2}} \begin{pmatrix} a + a^\dagger \\ i(a^\dagger - a) \end{pmatrix} = \mathbf{V}A$$

with $\mathbf{V} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1} & \mathbf{1} \\ -i\mathbf{1} & i\mathbf{1} \end{pmatrix}$. For bosons this is a generalized $q-p$ (position-momentum) representation while for fermions this is called the Majorana representation. Since $X^\dagger = X^T$ the commutation relations can be written as

$$XX^T - \xi (XX^T)^T = \tilde{\mathbf{J}}$$

where

$$\tilde{\mathbf{J}} = \mathbf{V} \mathbf{J} \mathbf{V}^\dagger = \begin{cases} i \begin{pmatrix} & \mathbf{1} \\ -1 & \end{pmatrix} & \text{bosons} \\ \begin{pmatrix} \mathbf{1} \\ & \mathbf{1} \end{pmatrix} & \text{fermions} \end{cases}$$

and a canonical transformation $X \rightarrow X' = \tilde{\mathbf{R}}X$ respects

$$\begin{aligned} \tilde{\mathbf{R}}^\dagger &= \tilde{\mathbf{R}}^T \\ \tilde{\mathbf{R}} \tilde{\mathbf{J}} \tilde{\mathbf{R}}^T &= \tilde{\mathbf{J}} \end{aligned}$$

For bosons this corresponds to the linear transformations that leave invariant the symplectic quadratic form $\Omega = \begin{pmatrix} & \mathbf{1} \\ -1 & \end{pmatrix}$ of conjugated classical variables. This group of transformations is called Real Symplectic Group $Sp(N, \mathbb{R})$. For fermions the set of transformations obeying $\tilde{\mathbf{R}} \tilde{\mathbf{R}}^T = \mathbf{1}$ form the Orthogonal group $O(2N)$, which is also a real group.

Equations of motion Now that we discovered the properties of the transformations that we allow for bosons and fermions let us consider the evolution of A under H . The Heisenberg equations of motion are given by³⁰

$$\partial_t A(t) = i[H, A(t)] = -i\mathbf{J}\mathbf{H}A(t).$$

We can now define $A' = \mathbf{R}A$ to diagonalize the matrix $\mathbf{K} = \mathbf{J}\mathbf{H}$

$$\partial_t A'(t) = -i\mathbf{R}\mathbf{K}\mathbf{R}^{-1}A'(t) = -i\mathbf{K}'A'(t)$$

From the Hermiticity of the Hamiltonian we have

$$\mathbf{K}^\dagger = \mathbf{H}\mathbf{J} = \mathbf{J}\mathbf{K}\mathbf{J}$$

and thus for each left eigenvector of \mathbf{K} with energy ϵ

$$\mathbf{K}|v\rangle = \epsilon|v\rangle$$

corresponds to a right eigenvector

$$\langle v|\mathbf{J}\mathbf{K} = \epsilon\langle v|\mathbf{J}$$

From the particle-hole symmetry we have $\hat{\mathbf{K}} = \mathbf{S}\mathbf{K}^T\mathbf{S} = \mathbf{S}\mathbf{H}^T\mathbf{J}\mathbf{S} = -\xi\mathbf{S}\mathbf{H}^T\mathbf{S}\mathbf{J} = -\mathbf{K}$ and thus for each $|v\rangle$ we can associate another eigenvector $|\hat{v}\rangle = \mathbf{S}\cdot\mathbf{J}\langle v|^T$ with negative energy

$$\mathbf{K}|\hat{v}\rangle = -\mathbf{S}\mathbf{K}^T\mathbf{S}\mathbf{S}\cdot\mathbf{J}\langle v|^T = -\mathbf{S}(\langle v|\mathbf{J}\mathbf{K})^T = -\epsilon|\hat{v}\rangle$$

Thus we can write

$$\mathbf{K} = \sum_{\epsilon_i > 0} \epsilon_i [|v_i\rangle\langle v_i| J - |\hat{v}_i\rangle\langle \hat{v}_i| J]$$

and the diagonalized form of the operator \mathbf{K} is given as

$$\mathbf{K}' = \mathbf{R}\mathbf{K}\mathbf{R}^{-1} = \begin{pmatrix} \epsilon_1 & & & \\ & \epsilon_2 & & \\ & & \ddots & \\ \hline & & & -\epsilon_1 \\ & & & & -\epsilon_2 \\ & & & & & \ddots \end{pmatrix}$$

Thus, we can finally write the Hamiltonian in diagonal form

$$\begin{aligned} H &= \frac{1}{2}A^\dagger\mathbf{H}A = \frac{1}{2}A'^\dagger\mathbf{J}\mathbf{R}\mathbf{K}\mathbf{R}^{-1}A' \\ &= \frac{1}{2}A'^\dagger\mathbf{J}\mathbf{K}'A' = \sum_i \epsilon_i \left(a_i'^\dagger a_i' + \frac{\xi}{2} \right) \end{aligned}$$

Implementing a canonical transformation numerically To diagonalize numerically the Hamiltonian things can get a bit tricky because the list of eigenvalues of \mathbf{K} will generically not be given in the right order and the list of eigenvectors might not have the correct normalization. In order to ensure that we end up with the right matrix \mathbf{R} we have to manipulate the numerical results in an appropriate way. Let us assume that we obtain a list of eigenvalues $\mathbf{D} = \text{diag}(d_1, \dots, d_{2N})$ and eigenvectors given by the matrix $\mathbf{U} = (v_1, \dots, v_{2N})$ such that $\mathbf{K} = \mathbf{U}\mathbf{D}\mathbf{U}^{-1}$. We have seen that

³⁰Prove this.

the eigenvalues come in pairs. Therefore the first task is to order the eigenvalues and eigenvectors such that

$$\begin{aligned}\mathbf{D}' &= \text{diag}(d_{i_1}, d_{i_2} \dots d_{i_N}, d_{i_{N+1}}, d_{i_{N+2}} \dots d_{i_{2N}}) \\ \mathbf{U}' &= (v_{i_1}, v_{i_2} \dots v_{i_N}, v_{i_{N+1}}, v_{i_{N+2}} \dots v_{i_{2N}})\end{aligned}$$

such that $d_{i_j} = -d_{i_{j+N}} > 0$. However, in general the matrix \mathbf{U}' does not fulfill the conditions

$$\begin{aligned}\mathbf{U}' \mathbf{J} \mathbf{U}'^\dagger &= \mathbf{J} \\ \mathbf{U}'^\dagger &= \mathbf{S} \mathbf{U}'^T \mathbf{S}\end{aligned}$$

required for the transformation to obey the commutation relations and the particle-hole symmetry. Note that a matrix

$$\mathbf{R} = \mathbf{U}' \cdot \Theta$$

with $\Theta = \text{diag}(\theta_1, \dots, \theta_N, \theta'_1, \dots, \theta'_N)$ a diagonal matrix, also diagonalizes $\mathbf{K} = \mathbf{R} \mathbf{D}' \mathbf{R}^{-1}$ since Θ and D commute. We will now choose such that \mathbf{R} obeys the conditions

$$\begin{aligned}\mathbf{R} \mathbf{J} \mathbf{R}^\dagger &= \mathbf{J} \\ \mathbf{R}^\dagger &= \mathbf{S} \mathbf{R}^T \mathbf{S}\end{aligned}$$

Solving in order to Θ this yields

$$\begin{aligned}\Theta^{\dagger-1} \mathbf{J} \Theta &= \mathbf{U}'^\dagger \mathbf{J} \mathbf{U}' \\ \mathbf{S} \Theta^{T-1} \mathbf{S} \mathbf{J} \Theta^{-1} &= \mathbf{S} \mathbf{U}^T \mathbf{S} \cdot \mathbf{J} \mathbf{U}'\end{aligned}$$

since two sides of the equations are diagonal matrices we can write

$$\begin{aligned}\text{diag} \left[(\theta_1 \bar{\theta}_1)^{-1}, \dots, (\theta_N \bar{\theta}_N)^{-1}, -\xi (\theta'_1 \bar{\theta}'_1)^{-1}, \dots, -\xi (\theta'_N \bar{\theta}'_N)^{-1} \right] &= \text{diag} (u_1, \dots, u_N, u'_1, \dots, u'_N) \\ \text{diag} \left[(\theta_1 \bar{\theta}'_1)^{-1}, \dots, (\theta_N \bar{\theta}'_N)^{-1}, -\xi (\theta_1 \bar{\theta}'_1)^{-1}, \dots, -\xi (\theta_N \bar{\theta}'_N)^{-1} \right] &= \text{diag} (w_1, \dots, w_N, w'_1, \dots, w'_N)\end{aligned}$$

A possible choice is to take $\theta_i = u_i^{-\frac{1}{2}}$ to be real and $\theta'_i = (\theta_i \bar{w}_1)^{-1}$. The matrices \mathbf{R} defined in this way thus respect the commutation relations and the particle-hole symmetry.

Implementing a canonical transformation with a unitary operator The many-body operator that implements the transformation \mathbf{R} is actually the exponential of a quadratic operator $e^{-i\Omega} = e^{-i\frac{1}{2}A^\dagger \Omega A}$ where the matrix Ω respects the same symmetry condition as the Hamiltonian. To see this we can explicitly compute ³¹

$$e^{i\frac{1}{2}A^\dagger \Omega A} A e^{-i\frac{1}{2}A^\dagger \Omega A} = e^{-i\mathbf{J}\Omega} A$$

and thus $e^{i\mathbf{J}\Omega} \mathbf{J} e^{-i\Omega\mathbf{J}} = \mathbf{J}$ as requested by a canonical transformation.

The magic of quadratic Hamiltonians Once in a diagonalized form we can easily compute all quantities of a quadratic Hamiltonian in terms of its single particle Hamiltonian matrix \mathbf{H} . This means that we can compute quantities of a Hilbert space that has dimension 2^N in the case of fermions and D^N (where D is a suitable truncation of the Hilbert space of one boson) in the case of bosons by using only a $N \times N$ matrix! This fact renders quadratic Hamiltonians manageable

³¹Prove the following.

even for a very large number of degrees of freedom. For example, the partition function of the Hamiltonian H_0 is given by ³²

$$Z = \text{tr} \left(e^{-\beta H_0} \right) = \left\{ \det \left[\left(e^{\beta \mathbf{J} \mathbf{H}_0} - \xi \mathbf{1} \right) \mathbf{J} \right] \right\}^{-\frac{\xi}{2}}$$

and the single-particle correlation matrix, defined by $\chi_0 = \langle AA^\dagger \rangle_0$, can be computed as ³³

$$\chi_0 = \text{tr} \left(\frac{e^{-\beta H_0}}{Z} AA^\dagger \right) = [\mathbf{1} + \xi n_\xi(\mathbf{J} \mathbf{H}_0)] \mathbf{J}$$

where

$$n_\xi(z) = \frac{1}{e^{\beta z} - \xi}$$

is the Bose-Einstein (for $\xi = 1$) or Fermi Dirac (for $\xi = -1$) distribution. Finally, for a unitary evolution with a quadratic Hamiltonian $\chi(t) = \langle A(t) A^\dagger(t) \rangle$ is given by ³⁴

$$\chi(t) = e^{-i\mathbf{J} \mathbf{H} t} \chi_0 e^{i\mathbf{J} \mathbf{H} t}$$

With this matrix we can compute the mean values of any observable $O = \frac{1}{2} A^\dagger \mathbf{O} A$ and we obtain ³⁵

$$\langle O(t) \rangle = \frac{1}{2} \text{tr} \left[\rho_0 \left(A^\dagger(t) \mathbf{O} A(t) \right) \right] = \frac{1}{2} \xi \text{tr} [\mathbf{O} \chi(t)]$$

Entropy of quadratic density matrices As for observables, the entanglement entropy of a density matrix $\rho = \frac{e^{-\beta H}}{Z}$ is particularly simple in terms of the single particle correlation matrix ³⁶

$$S = -\text{tr} [\rho \ln \rho] = \xi \text{Tr} [\mathbf{J} \chi \ln \chi]$$

This is extremely helpful to compute the entanglement entropy of ground states of quadratic Hamiltonians. The key is to realize that starting with a density matrix

$$\rho_{AB} = \frac{e^{-\beta H_{AB}}}{Z_{AB}}$$

with $H_{AB} = \frac{1}{2} A^\dagger \mathbf{H}_{ABA} A$, after partial trace over subsystem B , the resulting density matrix remains quadratic:

$$\rho_A = \text{tr}_B \left[\frac{e^{-\beta H_{AB}}}{Z_{AB}} \right] = \frac{e^{-\beta \tilde{H}_A}}{Z_A}$$

with $\tilde{H}_A = \frac{1}{2} \sum_{ij \in A} A_i^\dagger \tilde{\mathbf{H}}_{i,j}^A A_j$ and $Z_A = \text{tr} e^{-\beta \tilde{H}_A}$. Moreover, we can explicitly obtain \tilde{H}_A since any mean value computed for an operator only living in subsystem A has to coincide when computed with ρ_{AB} with ρ_A

$$\chi_{ij}^A = [\chi]_{i,j \in A} = \text{tr} \left[A_i A_j^\dagger \frac{e^{-\beta H_{AB}}}{Z_{AB}} \right] = \text{tr} \left[A_i A_j^\dagger \frac{e^{-\beta \tilde{H}_A}}{Z_A} \right]$$

and thus, we can obtain $\chi_A = [\mathbf{1} + \xi n_\xi(\mathbf{J} \tilde{H}_A)] \mathbf{J}$. Therefore, computing the entropy of subsystem A amounts simply to evaluate

$$S_A = -\text{tr} [\rho_A \ln \rho_A] = \xi \text{Tr} [\mathbf{J} \chi_A \ln \chi_A].$$

³²Prove this!

³³Prove this!

³⁴Prove this!

³⁵Prove this!

³⁶Prove this!

5.5.2 The XY model and the Jordan Wigner Mapping

The XY Chain We are now going to see all the machinery of quadratic Hamiltonians working in an example that starts actually with spins. Let us consider the following Hamiltonian of a spin-1/2 chain of length L , which we will assume to have periodic boundary conditions,

$$H = -J \sum_{m=0}^{L-1} \frac{1}{2} [(1 + \gamma) \sigma_m^x \sigma_{m+1}^x + (1 - \gamma) \sigma_m^y \sigma_{m+1}^y] + h \sum_m \sigma_m^z$$

This model is called the *XY* model in a transverse field h , where γ regulates the anisotropy of the interaction along the x and y directions. In the following we are going to work in units such that $J = 1$.

Besides translational symmetry, there is another symmetry that leaves this Hamiltonian invariant:

$$\begin{aligned} \sigma_r^x &\rightarrow -\sigma_r^x \\ \sigma_r^y &\rightarrow -\sigma_r^y \\ \sigma_r^z &\rightarrow \sigma_r^z \end{aligned}$$

This corresponds to a π rotation along the z axis that can be implemented by the operator $U = \otimes_r e^{i\pi\sigma_r^z}$. This extra symmetry group of the Hamiltonian is $\{1, U\}$ and is isomorphic to \mathbb{Z}_2 . So we say that the model has a \mathbb{Z}_2 symmetry.

Ground-state and Symmetry Broken Phase Let us now consider some particularly simple points. Take, for example, the Ising case $h = 0, \gamma = 1$, where the system is fully diagonal in the x basis. Here the ground-state is doubly degenerate within a subspace generated by $\otimes_{i=0}^{L-1} |\rightarrow_x\rangle$ and $\otimes_{i=0}^{L-1} |\leftarrow_x\rangle$, where $|\rightarrow_x\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$ and $|\leftarrow_x\rangle = (|\uparrow\rangle - |\downarrow\rangle)/\sqrt{2}$ are the fully polarized states along the x -axes.

States in this subspace are quite special because $\langle \sigma_r^x \sigma_{r'}^x \rangle = 1$ no matter what is the distance between points r and r' . This is what is called a system with long-range order because degrees of freedom that are far apart are still correlated although on average $\langle \sigma_r^x \rangle = 0$.

Applying a small magnetic field along the x direction, i.e. $h_x \sum_r \sigma_r^x$, breaks this degeneracy and one of the two ground-states will win, yielding $\langle \sigma_r^x \rangle = \pm 1$. This effect is called spontaneous symmetry breaking. What is spontaneous about it is that any infinitesimal perturbation chooses one of the two states. In a real system one of the two is actually realized since there are always small perturbations that select one of them.

For points in phase space close to $h = 0, \gamma = 1$, we still expect to have a similar behavior $\lim_{|r-r'| \rightarrow \infty} \langle \sigma_r^x \sigma_{r'}^x \rangle = \phi^2$. This statement is equivalent to say that $\lim_{h_x \rightarrow \pm 0} \langle \sigma_r^x \rangle = \pm \phi$. For $h = 0$ we have $\phi = 1$ but quantum fluctuations, at small but non vanishing h , reduce the value of ϕ .

For excitations around the ground state it is also useful to consider the Ising limit ($h = 0, \gamma = 1$). Excitations correspond to domain walls where the local orientation changes

$$\dots |\rightarrow_x\rangle |\rightarrow_x\rangle |\leftarrow_x\rangle |\leftarrow_x\rangle \dots$$

which have an energy cost of 1 (in units of J).

Let us look now to the other particularly simple case $h/J \rightarrow +\infty$. The ground state is given by $\otimes_r |\downarrow\rangle$. In this phase $\langle \sigma_r^z \sigma_{r'}^z \rangle = 1$ but this is not very exciting since $\langle \sigma_r^z \rangle = -1$ and this

value is stable to any perturbation since the ground-state is unique. Excitations around the fully polarized state cost $2h$ and correspond to flipping one spin up. Moreover $\langle \sigma_r^x \sigma_{r'}^x \rangle = 0$. Again, this should be stable around the $h/J \rightarrow +\infty$ point. For large but finite h , we expect $\langle \sigma_r^z \rangle > -1$ due to the quantum fluctuations. Working in perturbation theory in small J/h , we can obtain that

$$\langle \sigma_r^x \sigma_{r'}^x \rangle \propto e^{-|r-r'|/\xi}$$

where ξ is called the correlation length. A similar argument can be done for $h \rightarrow -\infty$.

These are two special points in parameter space and their vicinities correspond to qualitatively different ground-states. After the thermodynamic limit is taken, it is impossible to pass from one case to the other smoothly. Thus, we expect that, at some point in the space of parameters - called critical point - there is a sudden change in the ground-state properties. Precisely at this point we will see that correlations become neither infinite-range nor exponentially decaying but instead power-law in the separation $|r - r'|$. This point also corresponds to non-analyticities of thermodynamic quantities, such as the spin susceptibility.

For generic systems, besides obtaining exact solutions for some special points and doing perturbation theory around them, one has to generically rely on approximations and numerical method. However the XY model admits an exact solution that is sufficiently simple and instructive for us to look into it.

Jordan-Wigner transformation We will solve this model by a clever mapping to fermions known as the Jordan-Wigner transformation. This transformation explores the fact that the Hilbert space of fermions on a lattice and of spins-1/2 has the same dimensionality. However commutation relations of spins and fermions are different and it is in general difficult to write a useful mapping from the spin operators to creation and annihilation operators of fermions. In one dimension this mapping is particularly simple. To see how it works let us recall that

$$\begin{aligned} \{\sigma_m^-, \sigma_m^+\} &= 1 & \{c_m, c_m^\dagger\} &= 1 \\ (\sigma_m^+)^2 &= (\sigma_m^-)^2 = 0 & (c_m^\dagger)^2 &= (c_m)^2 = 0 \\ [\sigma_m^-, \sigma_n^+] &= 0 & \{c_m, c_n^\dagger\} &= 1 \quad n \neq m \end{aligned}$$

So the only difference is that the last relation differs due to the anti-commutation relations of fermions. However, defining

$$\begin{aligned} c_m &= e^{i\pi \sum_{j=0}^{m-1} \sigma_j^+ \sigma_j^-} \sigma_m^- \\ c_m^\dagger &= e^{i\pi \sum_{j=0}^{m-1} \sigma_j^+ \sigma_j^-} \sigma_m^+ \end{aligned}$$

reproduces the correct commutation relations with

$$\frac{1}{2} \sigma_z + 1 = \sigma_m^+ \sigma_m^- = c_m^\dagger c_m$$

Conversely we have

$$\begin{aligned} \sigma_m^- &= e^{i\pi \sum_{j=0}^{m-1} c_j^\dagger c_j} c_m \\ \sigma_m^+ &= e^{i\pi \sum_{j=0}^{m-1} c_j^\dagger c_j} c_m^\dagger \end{aligned}$$

The operator $S(m-1, 0) = e^{i\pi \sum_{j=0}^{m-1} c_j^\dagger c_j}$ is sometimes called the string operator.

Therefore

$$\sum_m \sigma_m^z = \sum_m (2c_m^\dagger c_m - 1)$$

For $m \leq L-2$ we have that

$$\begin{aligned} \sigma_m^+ \sigma_{m+1}^- &= e^{i\pi \sum_{j=0}^{m-1} c_j^\dagger c_j} c_m^\dagger e^{i\pi \sum_{j=0}^m c_j^\dagger c_j} c_{m+1} \\ &= c_m^\dagger e^{i\pi c_m^\dagger c_m} c_{m+1} \\ &= c_m^\dagger c_{m+1} \end{aligned}$$

since $c_m^\dagger e^{i\pi c_m^\dagger c_m} |n_m = 1\rangle = 0$ and $c_m^\dagger e^{i\pi c_m^\dagger c_m} |n_m = 0\rangle = 0$, in a similar way

$$\begin{aligned} \sigma_m^+ \sigma_{m+1}^+ &= c_m^\dagger c_{m+1}^\dagger \\ \sigma_m^- \sigma_{m+1}^+ &= -c_m c_{m+1}^\dagger \end{aligned}$$

If $m = L-1$ things get a bit more complicated due to the periodic boundary conditions

$$\begin{aligned} \sigma_{L-1}^+ \sigma_0^- &= e^{i\pi \sum_{j=0}^{L-2} c_j^\dagger c_j} c_{L-1}^\dagger c_0 \\ &= \left(e^{i\pi \sum_{j=0}^{L-1} c_j^\dagger c_j} \right) \left(e^{i\pi c_{L-1}^\dagger c_{L-1}} \right) c_{L-1}^\dagger c_0 \\ &= -(-1)^M c_{L-1}^\dagger c_0 \\ \sigma_{L-1}^+ \sigma_0^+ &= -(-1)^M c_{L-1}^\dagger c_0^\dagger \\ \sigma_{L-1}^- \sigma_0^+ &= (-1)^M c_{L-1} c_0^\dagger \end{aligned}$$

where

$$(-1)^{\sum_{j=0}^{L-1} c_j^\dagger c_j} = (-1)^{\sum_{j=0}^{L-1} (\frac{1}{2}\sigma_j^z + 1)} = (-1)^M$$

is a constant of motion because all bilinear operators of fermions conserve the parity of the number of states.

Hamiltonian in momentum space Putting this all together we can write the Hamiltonian as

$$H = -J \sum_{m=0}^{L-1} \left[(c_m^\dagger c_{m+1} + c_{m+1}^\dagger c_m) + \gamma (c_m^\dagger c_{m+1}^\dagger + c_{m+1} c_m) \right] + h \sum_m (2c_m^\dagger c_m - 1)$$

where we defined that $c_L^\dagger = (-1)^M c_0^\dagger$ to account for the term $(-1)^M$ coming from the $m = L-1$ term.

Since the system is translational invariant we want to write the Hamiltonian in a momentum space representation. For that we write

$$c_m = \frac{1}{\sqrt{L}} \sum_{m=0}^{L-1} e^{iqm} \tilde{c}_q$$

In order to ensure that $c_L = c_0 (-1)^M$ we have to set $q = \frac{2\pi}{L} n$ for M even and $q = \frac{\pi+2\pi n}{L}$ for M odd. Note that in general if we have $c_L = e^{i\phi} c_0$ the momentum quantization reads $e^{iqL} = e^{i\phi}$ and thus $q = \frac{2\pi n + \phi}{L}$. Substituting this in the Hamiltonian and using the identity $\frac{1}{\sqrt{L}} \sum_{m=0}^{L-1} e^{i(q-q')m} = \delta_{q,q'}$ we obtain

$$H = \sum_{q=0}^{L-1} \left[iJ\gamma \sin(q) c_{-q}^\dagger c_q^\dagger + 2(h - J \cos q) c_q^\dagger c_q - iJ\gamma \sin(q) c_q c_{-q} \right] - hL$$

The Hamiltonian is now in a form that can be easily diagonalizable by a suitable Bogoliubov transformation. In fact this transformation is the same as in our simple example for the fermions with $c_q = c_1$, $c_{-q} = -ic_2$, $\epsilon = 2(h - \cos q)$ and $\lambda = 2\gamma \sin(q)$. Note that I absorbed the phase $-i$ in the definition of c_2 . Using the results of the previous section we have (up to an unimportant constant)

$$H = \sum_q \varepsilon_q \left(d_q^\dagger d_q - \frac{1}{2} \right)$$

with

$$\varepsilon_q = 2J \sqrt{\left(\frac{h}{J} - \cos q \right)^2 + \gamma^2 (\sin q)^2}.$$

Phase diagram Let us now analyze the band structure of the model to learn more about the phase diagram of the model. For a generic point in the phase space $\gamma - h$ the dispersion relation is gapped, i.e. there is no wave-vector k for which $\varepsilon_q = 0$. This means that all excitations on top of the ground states $|0\rangle_d$, defined as the vacuum of d 's, $d_q |0\rangle_d = 0$, cost a finite amount of energy. This has important implications. For example, take the ground-state correlation function of two arbitrary operators made from fermionic creation and annihilation in position space, that can be schematically decomposed as

$$\langle A_r B_{r'} \rangle = \int dq_1 \dots dq_n e^{iq_1 r} \dots \langle d_{q_1}^\dagger d_{q_2} \dots \rangle \langle \phi_{c,q_1} | \phi_{d,q_2} \rangle \dots$$

where the number of d 's appearing in $\langle \dots \rangle$ is finite. If $\tan \frac{\theta}{2}$ of the Bogoliubov transformation, and the occupation function $n_F(\varepsilon_q) = \Theta(-\varepsilon_q)$ are analytic functions for all q , the Fourier transform on the left-hand side will yield a function that decays exponentially with $|r - r'|$. This is a direct consequence of the fact that the FT of a analytic function decays exponentially. Since these conditions are meet for a generic point, we expect exponentially decaying correlations almost everywhere.

However, when $\varepsilon_q = 0$ for some q , this changes. At that point $n_F(\varepsilon_q)$ becomes non-analytic, generically, the decay of correlations is a power-law. This arises for $|h| = 1$ and for $\gamma = 0$ and corresponds to three lines in phase space $\gamma - h$ where the nature of the ground-state changes - these correspond to the phase transitions lines of both the initial XY model and the fermionic model we obtained by JW transformation. Points that can be linked to each-other without crossing these lines are said to be in the same phase because they share the same qualitative properties. Moreover, we can see that the energy cost of excitations at the Ising point and for $h \rightarrow \infty$ does correspond to ε_q in this limits.

Subtleties of the JW transformation We saw that by analyzing the case spin Hamiltonian in the Ising case that there were two degenerate ground-states. However in terms of the electrons the ground state is unique and is simply given by the vacuum of d 's, i.e.

$$d_q |\Psi_0\rangle = 0$$

The key here is to remember that there was a quantum number $P = (-1)^{\sum_{j=0}^{L-1} c_j^\dagger c_j}$ that we had to fix and thus we have to look at the two sectors $P = \pm 1$. Thus, we have two ground-states $|\Psi_0^{P=\pm 1}\rangle$. We obtain other eigenstates from these two by

$$|\{q_1, \dots, q_n\}\rangle_{P=\pm 1} = d_{q_1}^\dagger \dots d_{q_n}^\dagger |\Psi_0^{P=\pm 1}\rangle$$

However, we now have twice the states than the ones in the initial Hilbert space! The solution is again to remember that $P |\{q_1, \dots, q_n\}\rangle_{P=\pm 1} = \pm |\{q_1, \dots, q_n\}\rangle_{P=\pm 1}$. This only happens to half the states in each sector, to see this suppose that $P |\Psi_0^{P=1}\rangle = |\Psi_0^{P=1}\rangle$, then $Pd_{q_1}^\dagger |\Psi_0^{P=1}\rangle = -d_{q_1}^\dagger |\Psi_0^{P=1}\rangle$ has a different parity because the d 's are linear combinations of c 's and c^\dagger 's and thus is not a physical state of the spin system.

Regarding the ground-state manyfold, inside the symmetry broken (or ordered) phases we have $P |\Psi_0^{P=1}\rangle = |\Psi_0^{P=1}\rangle$ and $P |\Psi_0^{P=-1}\rangle = -|\Psi_0^{P=-1}\rangle$, so the ground-states of both sectors are physical and have the same energy in the limit $L \rightarrow \infty$. For the disordered phases one of the ground-states is not physical. Since there is a finite gap to excitations, the less energetic state of that sector already has to pay an energetic price when compared with the ground-state of the other sector.

Another subtlety of the JW transformation is the mapping between correlation functions. In the beginning we convince ourselves that the spin system has long range order. However, we just argued that the electronic state has either exponentially decaying correlation functions or, at most, power law vanishing ones. Here we have to remember that

$$\sigma_m^+ \sigma_{m'}^- = \begin{cases} e^{i\pi \sum_{j=m'+1}^{m-1} c_j^\dagger c_j} c_m^\dagger c_{m'} & m > m' \\ e^{i\pi \sum_{j=m+1}^{m'-1} c_j^\dagger c_j} c_m^\dagger c_{m'} & m < m' \end{cases}$$

and similarly for the other correlation functions. Therefore in terms of the fermions the limit $|r - r'| \rightarrow \infty$ does not yield an expression with a finite number of c 's and c^\dagger 's. This operator can be exactly computed in the asymptotic limit $|r - r'| \rightarrow \infty$ ³⁷, although we are not going to do it here.

Finite temperature What we discussed up no now where properties of ground-state. We could also study the system at finite temperature. Here the free energy $f = -\frac{1}{\beta L} \ln \text{tr} [e^{-\beta H}]$ per volume is given by

$$f = -\frac{1}{2} \frac{1}{\beta} \int \frac{dq}{2\pi} \ln (2 \cosh \beta \varepsilon_q)$$

which has no non-analyticity for β finite. We therefore conclude that the phase transition only occurs at zero temperature. In particular the correlation functions, even in the broken symmetry phase decay exponentially with a correlation length that diverges at $T = 0$.

Classical and quantum phase transitions We can also study the properties of correlation functions that are time dependent

$$\begin{aligned} C_{\alpha\beta}(r, t) &= \langle \sigma_r^\alpha(t) \sigma_0^\beta(0) \rangle \\ &= \text{tr} \left[\sigma_r^\alpha(t) \sigma_0^\beta(0) \frac{e^{-\beta H}}{Z} \right] \end{aligned}$$

where $O(t) = e^{iHt} O e^{-iHt}$. Response functions to a time and space dependent field can also be computed from the equilibrium Hamiltonian. For example the response to a time dependent magnetic field is given by the susceptibility

$$\chi_{\alpha\beta}(r, t) = -i \langle T [\sigma_r^\alpha(t), \sigma_0^\beta(0)] \rangle$$

³⁷See: E. Lieb, T. Schultz and D. Mattis, Annals of Physics 16, 407 (1961)

where T is the time order operator.

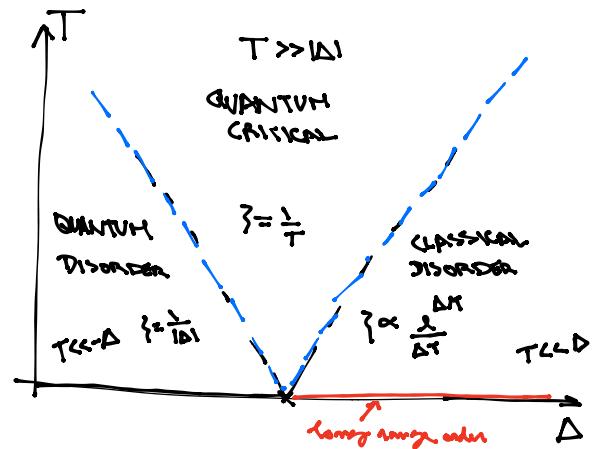
At criticality not only the spacial correlation functions but also time correlations decay algebraically. As in classical systems, away from a critical point, correlation functions typically have an exponential decay.

The physical consequence of an algebraic decay in the time domain has long memory to perturbations and long re-equilibration times. This effect is sometimes called critical slowing down.

Order parameter and susceptibility The order parameter of the transverse field Ising model is the magnetization along σ_x , this is the quantity that has a broken symmetry in the ordered phase. However, in order to obtain a finite magnetization one has to impose a field h_x along the x direction and perform the limit $\langle \sigma_x \rangle_{\pm} = \lim_{h_x \rightarrow 0^{\pm}} \lim_{L \rightarrow \infty} \langle \sigma_x \rangle_{h_x}$. Unfortunately in the presence of a finite h_x field the system is no longer solvable, exponents can be obtained by other methods but the computations are more involved and we will not study them here.

Another quantity of interest is $\chi_{xx}(r, t)$ given by the linear response to time dependent and spacial dependent field. This quantity can be computed taking into account the string operators. Again we will not compute it explicitly but just list the results for $\gamma = 1$ ³⁸.

Equal time correlations:



$$C_{xx}(r, 0) \propto e^{-|r|/\xi}$$

$$\xi \propto \begin{cases} \frac{1}{\sqrt{\Delta T}} e^{\Delta/T} & \Delta \gg T \\ \frac{1}{T} & |\Delta| \ll T \\ \frac{1}{|\Delta|} & -\Delta \gg T \end{cases}$$

with $\Delta = 2J(1 - h/J)$.

Equal space correlations:

$$C_{xx}(0, t) \propto e^{-|t|/\tau_\varphi}$$

$$\tau_\varphi \propto \begin{cases} \frac{1}{\Delta T} e^{\Delta/T} & \Delta \gg T \\ \frac{1}{T} & |\Delta| \ll T \\ \frac{1}{T} e^{|\Delta|/T} & -\Delta \gg T \end{cases}$$

where τ_φ is the phase coherence time (memory).

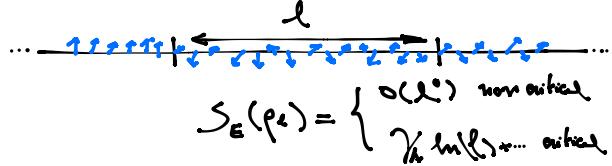
Entanglement entropy Another important feature about the XY chain is that the entanglement entropy of a subsystem A consisting on a set of sites of the chain is equal to the entanglement entropy of the fermionic model³⁹.

³⁸A discussion on this is given in [Quantum Phase transitions](#), Sachdev

³⁹This non-trivial and was shown for the first time in [Entanglement in Quantum Critical Phenomena](#). G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev. Phys. Rev. Lett. 90, 227902 (2003)

A natural question to ask regarding the entanglement entropy is: suppose you are in the ground-state of the system, say for an infinite chain, how much a segment of length ℓ of this chain is entangled with the rest? We will go back to this question much more in detail later when we talk about area laws. For now I will just state the results. Inside a phase of the XY model the entanglement entropy saturates

$$\lim_{\ell \rightarrow \infty} S_E(\rho_\ell) = O(\ell^0)$$



At the phase transition lines, however,

$$\lim_{\ell \rightarrow \infty} S_E(\rho_\ell) = \gamma_A \log \ell + \gamma_0$$

where $\gamma_A = 1/3$ is a universal quantity that does not depend on the details of the system and γ_0 is a constant that does. The fact that the entanglement entropy diverges at phase transition points as a function of system size is a trend that we will study further as a way to detect phase transition points.

5.5.3 Mean-field and beyond - The LMG model

Thermal phase transition in the LMG model Mean field theories provide approximations to interacting models by studying simpler ones whose parameters are obtained self-consistently. For some systems the mean-field solution is exact in some controlled limit. However, in most cases, it is only an educated (or physically motivated) guess whose validity has to be confirmed by other means.

Here, we are going to study a spin model for which the mean-field solution is asymptotically exact in the thermodynamic limit:

$$H = -\frac{J}{N} \sum_{i,j} S_i^x S_j^x + h \sum_i S_i^z$$

where the summations are over the N spins-1/2. This is a version of LMG model that we introduced before. The mean-field approximation consists considering that the term

$$S_i^x S_j^x = S_i^x \langle S_j^x \rangle + \langle S_i^x \rangle S_j^x - \langle S_i^x \rangle \langle S_j^x \rangle + (S_i^x - \langle S_i^x \rangle) (S_j^x - \langle S_j^x \rangle)$$

can be well approximated by

$$S_i^x S_j^x \simeq S_i^x \langle S_j^x \rangle + \langle S_i^x \rangle S_j^x - \langle S_i^x \rangle \langle S_j^x \rangle$$

by neglecting the fluctuations $(S_i^x - \langle S_i^x \rangle) (S_j^x - \langle S_j^x \rangle)$. This means that

$$H_{\text{MF}} \simeq -2J\phi \sum_i S_i^x + JN\phi^2 + h \sum_i S_i^z$$

with $\phi = \frac{1}{N} \langle S_j^x \rangle$. The Hamiltonian now is simple to handle and many quantities can be computed exactly.

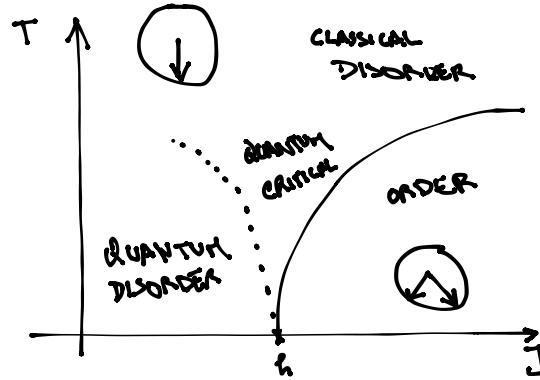
Solving the mean-field equations⁴⁰ one finds

$$\tanh\left(\frac{1}{2}\beta\sqrt{h^2 + 4J^2\phi^2}\right) = \frac{1}{J}\sqrt{h^2 + 4J^2\phi^2}$$

in addition $\phi = 0$ is always a solution.
⁴⁰The details of the calculation will be worked-out in the exercise series.

The phase diagram thus consists of two phases with $\phi = 0$ and $\phi \neq 0$. In the case where more than one solution exists, one can determine the one with less energy by looking at the mean-field free energy per spin, defined as $f_{\text{MF}} = -\frac{1}{\beta N} \ln \text{tr} (e^{-\beta H_{\text{MF}}})$.

As for the XY model the phase with $\phi \neq 0$ breaks the \mathbb{Z}_2 symmetry of the initial Hamiltonian and thus the ground-state is twice degenerate in the thermodynamic limit. Here, the ordered phase exists for a finite temperature region.



Quantum Phase Transition - Symmetric sector

A drawback of this approximation is that the entanglement between the degrees of freedom is lost. There are several ways of going beyond this approximation to correct this. In the following, we will look only at zero temperature - i.e. to the ground-state - in which case we can consider only the symmetric spin sector, for which $S^2 = s(s+1)$ with $s = 2N$. In this sector the Hamiltonian writes

$$H = -\frac{J}{N} (S^x)^2 + h S^z + c$$

where $S^\alpha = \sum_i S_i^\alpha$ is the total spin and c is an unimportant constant. The Hilbert space of the system is spanned by the $2s+1$ states $|s, -m\rangle, \dots, |s, m\rangle$.

To proceed, we are going to use the same philosophy as for the spin chain and transform the spin Hamiltonian in something we know how to solve: in this case in a bosonic Hamiltonian. For that we use the so-called Holstein-Primakoff transformation

$$S^z = -s + a^\dagger a \quad (5)$$

$$S^+ = a \sqrt{2s - a^\dagger a} \quad (6)$$

$$S^- = \sqrt{2s - a^\dagger a} a^\dagger \quad (7)$$

where a and a^\dagger are bosonic creation and annihilation operators. Note that the bosonic expressions respect the $su(2)$ commutation relations.

The idea is then to assume that $2s \gg a^\dagger a$, and expand the Hamiltonian in powers of $2s$. The first non-trivial order term yields a quadratic Hamiltonian of the form

$$H = \left(h - \frac{J}{2} \right) a^\dagger a - \frac{J}{4} (a^\dagger a^\dagger + a a) + c'$$

and thus, it can be solved exactly. To obtain results at higher orders one can then use perturbation theory in $1/(2s)$.

Note that, at leading order we have

$$\langle \mathbf{S} \rangle = \left\{ 0, 0, -s + a^\dagger a \right\} + O(s^{-1/2})$$

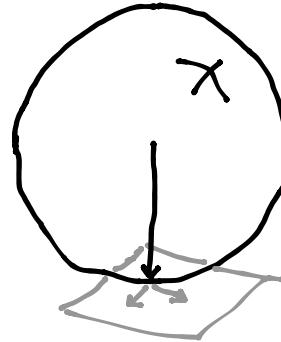
and thus the higher order corrections correspond to small fluctuations around this value.

This is only possible if the ground-state is well approximated by the fully polarized state pointing to the south pole. In the following we will assume $h > 0$, and we get

$$\mathbf{K}' = \mathbf{J} \mathbf{H}' = \begin{pmatrix} \sqrt{h} \sqrt{h-J} & 0 \\ 0 & -\sqrt{h} \sqrt{h-J} \end{pmatrix}$$

with $\mathbf{K} = \mathbf{R} \mathbf{K}' \mathbf{R}^{-1}$. From here we can see that something drastic happens when $h = J$. That can also be seen by computing the deviations to the magnetization

$$a^\dagger a = \frac{1}{4} \left(\frac{1}{\sqrt{1-J/h}} + \sqrt{1-J/h} \right) - \frac{1}{2}$$

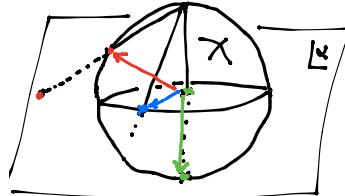


that diverge at $J = h$. For $h < J$ the bosonic energies become negative and this bosonic quadratic model can no longer be used. This point corresponds to the zero temperature point of the phase transition we have seen before.

The key to understand the symmetry broken phase is to consider the generalized HP transformation by adding a shift $a \rightarrow a + \sqrt{2s} \frac{\alpha}{\sqrt{1+\bar{\alpha}\alpha}}$, with $\alpha \in \mathbb{C}$, to the bosonic operators. Developing the HP relations to leading order in s after the shift one obtains

$$\langle \mathbf{S} \rangle = s \left\{ \frac{\alpha + \bar{\alpha}}{1 + \bar{\alpha}\alpha}, i \frac{\alpha - \bar{\alpha}}{1 + \bar{\alpha}\alpha}, 1 - \frac{2}{1 + \bar{\alpha}\alpha} \right\} + O(\sqrt{s})$$

which is simply the stereographic projection from the complex plain to the sphere.



Therefore, developing the HP expressions around a finite value of α corresponds to studying fluctuations around a different fully polarized state. To know which fully polarized state better approximates the ground-state we can just minimize the leading order term H_0 in the Hamiltonian

$$H = 2s H_0(\alpha) + \sqrt{2s} H_1(\alpha) + H_2(\alpha) + O\left(\frac{1}{\sqrt{2s}}\right),$$

where $H_i(\alpha)$ has a number i of creation or annihilation operators.

For $h > J$, $\alpha = 0$ is the minimum of H_0 , however this changes for $h < J$, where two degenerate minima appear. Choosing α corresponding to one of these degenerate minima makes $H_1(\alpha)$ to vanish. Corrections to the magnetization can be obtained as before by diagonalizing $H_2(\alpha)$.

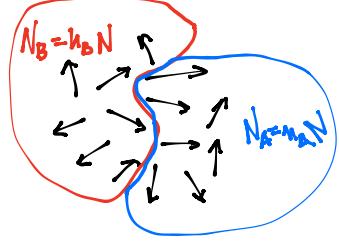
Entanglement Entropy Let us now analyze the entanglement entropy of the ground-state. However there is a problem with the description we just used in terms of a single spin since there is no sub-system we can trace over.

A solution to this problem consists on considering two sets containing $N_A = 2s_A$ and $N_B = 2s_B$ spins.⁴¹

⁴¹This was done in Entanglement Entropy beyond the Free Case, T. Barthel, S. Dusuel, J. Vidal. PRL 97, 220402 (2006)

Note however that the Hilbert space of the composite system is larger than the initial space. The identification between the Hilbert spaces has to be done with the states of highest total spin. Thus we have that $s_A + s_B = s$ and $S_A^\alpha + S_B^\alpha = S^\alpha$. The Hamiltonian writes

$$H = -\frac{J}{N} (S_A^x + S_B^x)^2 + h (S_A^z + S_B^z) + c$$



We can now introduce two H-P transformations

$$S_A^z = -s_A + a^\dagger a; \quad S_B^z = -s_B + b^\dagger b; \quad (8)$$

$$S_A^+ = a\sqrt{2s_A - a^\dagger a}; \quad S_B^+ = b\sqrt{2s_B - b^\dagger b}; \quad (9)$$

$$S_A^- = \sqrt{2s - a^\dagger a} a^\dagger; \quad S_B^- = \sqrt{2s - b^\dagger b} b^\dagger; \quad (10)$$

As before one can apply a shift to both bosonic operators to access the symmetry broken phase. Here we will only look at the entropy within the disordered phase. Therefore we develop, as before, the Hamiltonian in powers of $s_A = sn_A$ and $s_B = s(1 - n_A)$ and obtain

$$H = \frac{1}{2} A^\dagger \mathbf{H} A - h \left(1 + \frac{1}{4s} \right) + c$$

where

$$\begin{aligned} A &= \{a, b, a^\dagger, b^\dagger\} \\ \mathbf{H} &= \begin{pmatrix} \mathbf{h} & \Delta \\ \Delta^\dagger & \mathbf{h}^T \end{pmatrix} \\ \mathbf{h} &= \begin{pmatrix} -h - \frac{J}{2n_A} & -\frac{J}{2\sqrt{n_A(1-n_A)}} \\ -\frac{J}{2\sqrt{n_A(1-n_A)}} & -h - \frac{J}{2(1-n_A)} \end{pmatrix} \\ \Delta &= \begin{pmatrix} -\frac{J}{2n_A} & -\frac{J}{2\sqrt{n_A(1-n_A)}} \\ -\frac{J}{2\sqrt{n_A(1-n_A)}} & -\frac{J}{2(1-n_A)} \end{pmatrix} \end{aligned}$$

Diagonalizing the Hamiltonian we obtain

$$H = \sqrt{h(h-J)} \left(\tilde{a}^\dagger \tilde{a} - \frac{1}{2} \right) + h \left(\tilde{b}^\dagger \tilde{b} - \frac{1}{2} \right) + h(1+s) + c$$

and

$$\chi_A = n_A \begin{pmatrix} 1 + \frac{2\sqrt{1-\frac{J}{h}} - \frac{J}{h}}{4\sqrt{1-\frac{J}{h}}} & \frac{\frac{J}{h}}{4\sqrt{1-\frac{J}{h}}} \\ \frac{\frac{J}{h}}{4\sqrt{1-\frac{J}{h}}} & \frac{2\sqrt{1-\frac{J}{h}} - \frac{J}{h}}{4\sqrt{1-\frac{J}{h}}} \end{pmatrix}$$

The eigenvalues of $\mathbf{J}\chi_A$ are ν and $1 - \nu$ where

$$\nu = \frac{1}{2} \left(1 - \sqrt{1 + \frac{2(1 - \frac{J}{h}) + (\frac{J}{h} - 2)\sqrt{1 - \frac{J}{h}}(n_A - 1)n_A}{1 - \frac{J}{h}}} \right)$$

which yields an entanglement entropy

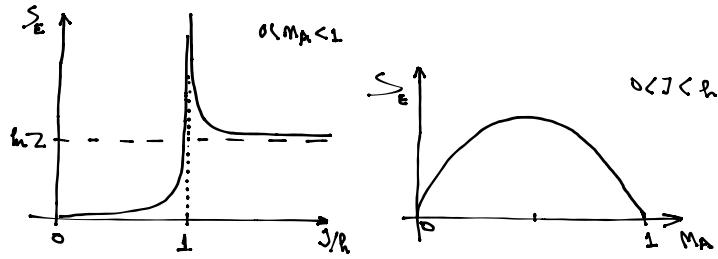
$$S = \text{Tr} [\mathbf{J}\chi \ln(\chi)] = \nu \ln(-\nu) + (1 - \nu) \ln(1 - \nu)$$

that diverges at the transition. For a finite system the entanglement entropy diverges logarithmically in s at the phase transition point.

Symmetric Sector vs All sectors

One last remark about the LMG model. If we look at the finite temperature behavior restricted to the symmetric sector we are going to conclude that there is no transition at finite temperature. This is not in contradiction with our mean-field calculation because there we used all spin sectors.

The symmetric sector is only a good approximation here because we considered the ground-state, i.e. the zero-temperature, case. The finite temperature transition makes all the spin sectors intervene.



5.5.4 Reference to exact methods and numerical approaches

We have seen two methods to solve interacting models. In both cases they consist on reducing the problem to a bosonic or fermionic Hamiltonian that can then be treated analytically.

Exact results Quadratic models are by far the most used due to their simplicity and ability to capture some important phases of matter.

Besides quadratic bosons or fermions, there are a number of systems for which exact solutions can be obtained. These are known as integrable models and they share some of the integrability features of classical systems.

In one spacial dimension the wave function of integral models can be obtained by a method called Bethe ansatz. In its most elementary form, this method consist on writing the wave function when the particles (or excitations) are far apart and then matching the different amplitudes by gluing the different sectors of the wave function. The same method has been re-phrased in a completely algebraic fashion that permits to apply it to other systems, including some fully connected models.

Numerical techniques Exact diagonalization: is the most straightforward technique to use and allows access to ground-state, thermal and dynamic properties but is limited to small size systems. Dynamic and thermal properties require to obtain all the spectrum and eigenstates which is quite costly. Ground-state and low energy properties that can be obtained computed a limited fraction of the spectrum are less costly.

Matrix product states (MPS): is a powerful numerical technique for one dimensional systems. It is a variational technique that allows to encode a quantum state efficiently. It is very efficient for ground-states of local gapped Hamiltonians but can also be applied in the gapless case. It is also used to obtain dynamics but is limited to small times.

Tensor networks: These are generalizations of MPS to higher dimensions. Even if they are efficient in describing ground states of some local gapped Hamiltonians, until now it is not clear how efficient these methods are for generic cases. There are many examples where they fail.

Quantum Monte Carlo: It is a quite ubiquitous method and has many variants. Its basic form is based on Trotter slicing the partition function and performing a sum over the possible histories of the system. Its efficiency has to be verified on a case-by-case basis. Fermionic and spin systems may suffer from the so-called sign-problem that inhibits the convergence of the algorithm. It is

commonly used to obtain thermal properties and to extrapolate to zero temperature to get the properties of the ground state. It has also been used to compute dynamics but it is limited to rather short times.

5.6 Comments on Phase transitions

This is not a course of phase transitions, however, since we talked so much of them during the course I decided to include a small discussion about these remarkable phenomena.

5.6.1 Spontaneous symmetry breaking

In the approach presented so far we observed that, at a phase transition point and along coexistence lines, the order parameter becomes multivalued. In practice, the physical translation of this statement is that the system “spontaneously” chooses a particular value for the order parameter. By doing so the system becomes ordered and the physical observables explicitly break the symmetry of the Hamiltonian.

Up to now we regarded such process as a limiting procedure of a vanishing conjugated field ($h^x \rightarrow 0^\pm$, for the transverse field Ising model). An equivalent way of interpreting this phenomena is the imposition of a restriction to the set of configurations of the non-symmetry broken Hamiltonian (i.e. at $h = 0$). The restriction on the number of micro-states results from the particular kinetic processes that render increasingly unlikely (in fact impossible at the thermodynamic limit) the passage from an ordered phase to another. To do so the system would have to pass by configurations with vanishing probability. This is indeed needed to understand why the system chooses a particular ordered state among all the ones related by symmetry: the chosen states depends on the history of the dynamics in configuration space.

5.6.2 The role of symmetry and dimensionality

For the XY model the symmetry group is \mathbb{Z}_2 . Spontaneous symmetry breaking implies here that the system chooses a subset of configurations yielding to a positive or negative magnetization. However, spontaneous symmetry breaking is even more remarkable when the symmetry group is a continuous one such as for example in the Heisenberg model where the symmetry group is $O(3)$, the group rotation in $d = 3$. Intuitively it seems easily for the system to pass from an ordered state to another avoiding states of very low probability.

The thermodynamic limit does provide a route for the establishment of ordered states even in this case. Nonetheless, the fact that it is easy for thermal fluctuations to destroy order in this case translated to the lack of order of the Heisenberg model in $d \leq 2$. The fact that ordered phases become more stable with increasing dimensionality can be traced to the fact that the number of neighbors that surround a given degree of freedom also increases. As d increases interactions become dominant and can overcome quantum or thermal fluctuations. For sufficiently large d a mean-field like description, that typically overestimates the order phase, provides a good description of the transition.

5.6.3 Scaling

Away from phase transitions intensive physical quantities are smoothly varying and are independent of size. They can therefore be listed and cataloged which would be senseless otherwise.

However this changes drastically close to critical points where critical quantities can vary abruptly and even diverge when a parameter is changed by a small amount. One should therefore find another way of classifying such systems. This classification is based on some universal properties that all phase transitions that share some common features have such as critical exponents.

All the considerations and the importance we give to critical exponents are motivated by the fact that the same critical exponents arise in very different models. There is a universality hypothesis that underlines our understanding of critical phenomena: All phase transitions problems can be divided into a small number of different classes depending upon the dimensionality of the system and the symmetry of the ordered phase. Within each class, all phase transitions have identical behavior in the critical region, only the names of the variables change.

Related to the idea of universality is the concept of scaling. Universality implies that the microscopic details of the system are unimportant near the critical point. Universal quantities like critical exponents (and scaling functions) cannot depend on the details of the system and microscopic scales.

Consider a physical quantity near the phase transition, it is in principle a function of ω, q, ξ, h and other “irrelevant” parameters, such as the lattice constant, etc, we denote as p . According to the scaling hypothesis this observable becomes an homogeneous function near the critical point

$$O(\omega, q, \xi, h, p) \simeq O(\omega, q, \xi, h) = \xi^{x_O} f_O(\xi^z \omega, q \xi, h \xi^{x_h})$$

where the exponents x_O and x_h are unknown as well as the function f_O , called a scaling function.

5.6.4 Critical exponents

Let $t = g - g_c$ be distance to the transition and h the field conjugated to the order parameter, a summary of critical exponents is:

Physical quantity	$t > 0$	$t < 0$
specific heat	$c_v \propto A_{cv} t ^{-\alpha}$	$c_v \propto A'_{cv} t ^{-\alpha'}$
order parameter ($h = 0$)	$\eta = 0$	$ \eta \propto t ^\beta$
order parameter ($t = 0$)		$ \eta \propto h ^{\frac{1}{\delta}}$
susceptibility	$\chi \propto A_\chi t ^{-\gamma}$	$\chi \propto A'_\chi t ^{-\gamma'}$
correlation length	$\xi \propto A_\xi t ^{-\nu}$	$\xi \propto A'_\xi t ^{-\nu}$
correlation time	$\tau \propto \xi^z \propto A_\tau t ^{-\nu z}$	$\tau \propto \xi^z \propto A'_\tau t ^{-\nu z}$
spacial correlations	$G(r) = A_G r^{-d+2-\eta}$	$G(r) = A'_G r^{-d+2-\eta'}$

The primed quantities refer the behavior for $t < 0$. Critical exponents are universal and will be shown to be equal in each side of the transition. Even if the amplitudes are not universal quantities their ratio A'/A is.

Lecture 6

6 Entanglement in Many Body Systems

In this section we will discuss the entanglement content, as measured by the entanglement entropy, of ground-states of local Hamiltonians.

As stressed before, ground states of local Hamiltonians are very different from generic states taken randomly from the Hilbert space. A striking manifestation of this is the entanglement entropy of a subregion. For a large class of systems the ground state entanglement entropy of a subregion A grows as the area of the subregion. For systems with gapless excitations there are eventually some logarithmic corrections that violate the area law. We have already encountered this for the case of the XY spin chain.

In the following we will try to summarize a set of results regarding area laws and their violation and provide the main arguments. Materials in this section were mainly taken from the following sources:

Entanglement in many-body systems. Luigi Amico, Rosario Fazio, Andreas Osterloh, and Vlatko Vedral Rev. Mod. Phys. 80, 517 (2008)

Colloquium: Area laws for the entanglement entropy. J. Eisert, M. Cramer, and M. B. Plenio Rev. Mod. Phys. 82, 277 (2010);

Quantum Entanglement in condensed matter. [Grégoire Misguich, \(2015\)](#)

6.1 Area law

6.1.1 Ground-state

The concept of an area law for the entropy was first encountered in quantum field theory partly driven by the suggested connection to black hole entropy in the 80's and early 90's.

In the early 2000's there was a revival of interest in the problem within the context of quantum many-body systems due to the appearance of new techniques and perspectives from quantum information theory. Part of the motivation came from trying to understand the efficiency of numerical methods such as DMFT and tensor networks.

Before starting let us agree on some nomenclature: (a) By non-critical systems I will mean those having a finite energy gap between the ground-state manifold, consisting of a finite number of states that does not grow with the system size, and the rest of the excited states. (b) By the correlation length I mean a quantity ξ such that the mean value of any two observables, A_r and $B_{r'}$ that have a finite support around r and r' respectively, behaves as $\lim_{|r-r'| \rightarrow \infty} \langle A_r B_{r'} \rangle \simeq e^{-|r-r'|/\xi}$.

An intuitive argument for the area law is the following:

- assume that all connected correlation functions decay exponentially and take a subsystem A with a subsystem size much larger than the correlation length
- correlations of degrees of freedom inside A and inside the complement of A , i.e. \bar{A} , do not contribute to S_A
- the only contributions come from the correlations between A and \bar{A} that take place along the boundary of A
- the size of the region where the correlations are important is $L^{d-1} \times \xi$ therefore we expect $S_A \simeq L^{d-1} \xi$
- assuming that the size of the local Hilbert space is D (for example $D = 2$, for a qubit) expect $S_A < \ln D L^{d-1} \xi$.

Figure

6.1.2 Finite temperature

For finite temperature the system is in a mixed state and the entanglement entropy is no longer a good measure of the entanglement between degrees of freedom.

However area laws can still be obtained for the mutual information⁴². Recall that $I(A|B) = S(\rho_A) + S(\rho_B) - S(\rho_A \otimes \rho_B)$ with $S(\rho) = -\text{tr}\rho \ln \rho$.

The mutual information measures all correlations between system A and B , not necessarily quantum. Indeed there is an important bound on the mutual information

$$I(A|B) \geq \frac{\langle O_A O_B \rangle - \langle O_A \rangle \langle O_B \rangle}{2 \|O_A\|^2 \|O_B\|^2}$$

which we will prove in the exercise sessions.

Note that for zero temperature we recover that $I(A|B) = 2S_A$. At finite temperature the only way of getting an area law is that the volume contributions cancel.

The way to prove the area law at finite temperature is quite simple and instructive⁴³ :

- Consider the Free energy $F(\rho) = \text{tr}(H\rho) - \frac{1}{\beta}S(\rho)$.
 - This quantity is minimized by the Gibbs state $\rho = \frac{e^{-\beta H}}{Z}$. Therefore $F(\rho_A \otimes \rho_B) \geq F(\rho_{AB})$.
 - We can thus write
- $$\begin{aligned} \text{tr}[(H_A + H_{\bar{A}} + H_{\partial A})(\rho_A \otimes \rho_{\bar{A}})] - \frac{1}{\beta}[S(\rho_A) + S(\rho_{\bar{A}})] &\geq \text{tr}[(H_A + H_{\bar{A}} + H_{\partial A})(\rho_{A\bar{A}})] - \frac{1}{\beta}S(\rho_{A\bar{A}}) \\ \text{tr}[H_{\partial A}(\rho_A \otimes \rho_{\bar{A}} - \rho_{A\bar{A}})] &\geq \frac{1}{\beta}I(A|\bar{A}) \end{aligned}$$

i.e.

$$\frac{1}{\beta}I(A|\bar{A}) \leq \text{tr}[H_{\partial A}(\rho_A \otimes \rho_{\bar{A}} - \rho_{A\bar{A}})] \simeq \Omega(\partial A)$$

Thus, for finite temperature the existence of an area law is a very general result!

For zero temperature things are more complicated....

6.1.3 Finite temperature

6.2 Area law

6.2.1 One dimension

Most results on area laws are for one dimensional systems because there is a large number of techniques that are specially suited to tackle these problems and because they seem to be substantially simpler than their higher dimension counterparts.

In one dimensional systems the area law is particularly simple since the border is of order $O(L)$.

We will look at the behavior of free bosons (Harmonic chains), free fermions (and the XY model) and discuss some general results for interacting systems.

⁴²Area Laws in Quantum Systems: Mutual Information and Correlations. Michael M. Wolf, Frank Verstraete, Matthew B. Hastings, and J. Ignacio Cirac Phys. Rev. Lett. 100, 070502 (2008)

⁴³Area Laws in Quantum Systems: Mutual Information and Correlations. Michael M. Wolf, Frank Verstraete, Matthew B. Hastings, and J. Ignacio Cirac Phys. Rev. Lett. 100, 070502 (2008)

Harmonic chains The first set of results on entanglement entropy was obtain for a Klein-Gordon field that is the continuous version of an harmonic chain.

One of the important early results in one dimension⁴⁴

6.3 Violations of the area law

6.4 Entanglement near phase transitions

⁴⁴M. B. Hastings, *J. Stat. Mech.* 2007, P08024 (2007).

7 Geometry of Hilbert Spaces

7.1 Bures Metric

7.2 Gauge Invariance

7.3 Parallel Transport

7.4 Berry Phase

7.5 Uhlman Phase

8 Topological Phases

8.1 Kitaev Chain

8.2 Haldane Model

8.3 Topological Superconductors

8.4 Kitaev's Toric Code

9 Simulation of Many Body Systems

10 Dynamics of Closed Quantum Systems

11 Open Quantum Systems