Entanglement and Black Holes

A Thesis

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BS-MS Dual Degree Programme

by

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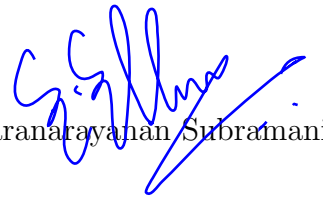
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Certificate

This is to certify that this dissertation entitled "Entanglement and Black Holes" towards the partial fulfilment of the BS-MS dual degree programme at the Indian Institute of Science Education and Research, Pune represents study/work carried out by Sugat Kokiloo at Indian Institute of Science Education and Research under the supervision of Shankaranarayanan Subramaniam , Professor of Physics at Indian Institute of Technology Bombay, Department of Physics , during the academic year 2021-2022.



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This thesis is dedicated to my family and friends that supported and helped me through all the tough times.

Declaration

I hereby declare that the matter embodied in the report entitled Entanglement and Black Holes are the results of the work carried out by me at the Department of Physics, Indian Institute of Science Education and Research, Pune, under the supervision of Shankaranarayanan Subramaniam and the same has not been submitted elsewhere for any other degree.



Sugat Kokiloo

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Abstract

Black Holes have an entropy that can be shown to depend on the area of its horizon. In this context, we look at the possibility of entanglement of quantum field modes across the horizon being the source of this entropy and look at the entanglement entropies of various quantum fields. In this thesis, we start by looking at two methods to calculate entanglement entropy for the scalar quantum field theory and study their various properties. The first method relies majorly on numerical simulations while the second method (covariance matrix approach) gives analytical results. The numerical method can help show the area law dependence of the entropy of a scalar field. Through the covariance matrix approach we see that the entanglement entropy of a scalar field at leading order behaves differently in different regimes of a parameter ζ. It is shown that for Neumann boundary conditions, the entanglement entropy diverges as $\log\log$ in the regime $\zeta \ll 1$ and diverges as $\log$ in the regime $\zeta \gg 1$. Then, we try to generalize the above results for a fermionic field, with the goals of seeing area law dependence, the above crossover in behaviour of entanglement entropy and obtaining Hawking temperature in this theory. Lastly, we also have a look at Black Hole thermodynamics and study the concept of cosmological particle creation, which leads to concepts like the Unruh effect and Hawking Radiation.

"If I have seen further it is by standing on the shoulders of Giants."

-Sir Isaac Newton

0.1 Elements in this thesis

This thesis will occasionally have blue boxes around equations. These are the important equations in the relevant chapter or are the important results in this thesis. An example for this would look like

$$T_H = \frac{1}{8\pi M}. \tag{0.1.1}$$

This thesis also contains many clickable chapters, equation numbers, references and URLs. A legend for identifying them is given as

- All clickable links to chapters like [chapter 1], clickable links to sections/subsections etc like [section 0.1] and clickable links to equations like (0.1.1) have the color blue.
- All clickable links to the citation of academic papers/books like [1] have the color red.
- All clickable links to URLs like `https://www.iiserpune.ac.in` have the color violet.

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Chapter 1

Entanglement and Black Holes: An introduction

"Entanglement is not one but rather the characteristic trait of quantum mechanics."

– Erwin Schrödinger

1.1 A brief history of entanglement

Physics before the 20th century was successfully explained by what is occasionally termed as "classical physics." At the center of it lie Newtonian mechanics, which is rooted in ideas of energy and momentum conservation and concerned itself with the motion of bodies under the effect of "forces". These laws painted a picture of the world as a system of gears working together in a *deterministic* way. The 20th century brought many observations and ideas that fundamentally challenged the then-accepted physical laws. It started when the German Bureau asked Max Planck about ways to make light bulbs more efficient such that they would give the maximum amount of light for the minimum amount of power. This led to Planck looking at the prevalent theory of radiation, which allowed for the light waves to have any arbitrary (and continuous) value of their energy.

As a result, the theoretical spectrum of energy radiated at a temperature kept on disagreeing with the experimental results as the energy radiated at short wavelengths (ultraviolet range and below) was theoretically tending to infinity. At the same time, the experiments pointed towards finite values lesser than the theory. This mismatch led to Plank hypothesizing that light energy came in discrete packets (the quantum of quantum mechanics) instead of the continuous form assumed in classical mechanics and thus eliminating this "Ultraviolet catastrophe". Although Planck himself hated this idea, it led to the birth of Quantum Mechanics, a theory that successfully explained physics at the small scales which the older theory of classical mechanics failed to do.

This description of reality was *probabalistic*, rather than *deterministic*. At the center of this theory was the postulate of a wavefunction, an abstract quantity that encoded all the information that can be known about the system. The connection to the physical world occurs in this theory by the operators that act on the wave function and give values of the corresponding physical quantity as eigenvalues. These operators were not necessarily commuting, which implies that precise knowledge of one variable precluded knowledge of the other. There were many unsettling parts to this theory, discussions upon which led to what was called *"entanglement"*. The primary line of thought that spurred the idea of entanglement concerned itself with the description of physical reality in quantum mechanics. Einstein, Podolsky, and Rosen (henceforth referred to as EPR) in their seminal 1935 paper [1] state that

"*If, without in any way disturbing a system, we can predict with certainty (i.e., with probability equal to unity) the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity.*"

This view renders a quantity in the theory physical only when one can confidently tell its value without disturbing the system. Looking at the problem of the incompatible observables, we can say that when we know the momentum of a particle, its

co-ordinate does not have a physical reality. This definition implied that either

(a) The wavefunction description has to be incomplete (which meant that every element of a physical reality **did not** have a counterpart in the physical theory) or

(b) The two physical quantities corresponding to the incompatible observers do not have simultaneous reality.

To look at this more carefully, EPR proposed a thought experiment.

EPR thought experiment

Let us say there are two systems, system 1 and 2 that start interacting with each other at time $t = 0$ untill $t = T$. After $t = T$ the systems are isolated and do not interact. This composite system is described fully by its wavefunction Ψ. We now look at the physical quantity represented by an operator A, with eigenvalues $a_1, a_2 \cdots$ and corresponding wavefunctions as $u_1(x_1), u_2(x_1), \cdots$. Here x_1 represents the first system's variables and x_2 the second system's variables. We then have

$$\Psi = \sum_n \psi_n(x_2) u_n(x_1).$$

Now upon measurement of A if system 1 is found to have a value of a_k, then from the equation above we interpret it as system 1 being in the state $u_k(x_1)$, and system 2 being in the state $\psi_n(x_2)$. The states u_k that system 1 would take depends on the choice of the operator A. If we had chosen a different operator B with eigenvalues $b_1, b_2 \cdots$ and corresponding wavefunctions as $v_1(x_1), v_2(x_1), \cdots$, the wavefunction would have taken the form

$$\Psi = \sum_s \varphi_s(x_2) v_s(x_1).$$

Now upon measurement of B if system 1 is found to have a value of b_r, we interpret it as system 1 being in the state $v_r(x_1)$ and system 2 being in the state $\varphi_r(x_2)$. Thus EPR concluded that by measuring A or B in system 1, the 2nd system had to be in one of the two possible states. Since the measurement was done *after* the interaction

took place, no real change should have happened in the 2nd system as a consequence of measurement in the 1st system; hence, it was possible to prescribe two different wavefunctions to system 2's reality.

Now, if both ψ_k and φ_r happen to be eigenstates of arbitrary operators P (with eigenvalue p_k) and Q (with eigenvalue q_k) that act on system 2, we would be able to confidently predict without disturbing the 2nd system the value of P or Q by measuring system 1. That is, by measuring A on system 1, we know if system 2 has a value of p_k for the physical observable P, or by measuring B on system 1 we know if system 2 has a value of q_k for the physical observable Q, all without disturbing system 2. By the definition of "physical reality" above, they concluded that P was an element of physical reality when A was measured on system 1 and Q was an element of physical reality when B was measured on system 1.

Hence if we assume that the "wavefunction" is a complete description of physical reality, we can show that two incompatible operators can have simultaneous reality. The above meant that negation of the point (a) leads to the negation of the only other possible choice (b). This led EPR to believe that the quantum mechanical description of reality using wavefunctions is incomplete.

This was the core idea of entanglement that EPR stumbled upon. This paper incited much debate amongst the scientific community and quickly became the centerpiece of any discussion about the interpretation of quantum mechanics. Bohr and Schrödinger (who coined the term "entanglement") both published their rebuttals against Einstein's arguments in 1935 [2, 3, 4]. Bohr insisted that EPR's interpretation of the phrase "without in any way disturbing the system" was ambiguous and that disturbance is inevitable in the measuring process. Schrödinger gave his famous thought experiment with the cat, where the cat was said to be both dead and alive, analogous to how system 2 in the above example had two physical realities. Majority of the scientific community seemed to accept Bohr and Schrödinger's views following

the great success of quantum mechanics as a theory.

Einstein's disagreement with Bohr and Schrödinger came from his view on reality, as the EPR paper states. He believed that nature could not be fundamentally random and refused to believe a probabilistic description of reality. One can see his discomfort with entanglement in the arguments described above, through particular definitions of "physical reality" and quotes like

"Quantum theory yields much, but it hardly brings us close to the Old One's secrets. I, in any case, am convinced he does not play dice with the universe."

Over the next many years, Einstein stood his ground on these views and solidified his view on demanding the theory to be local. He believed that if one were to take a similar composite system that have interacted for some time and take these particles far from each other, then measurements on particle 1 should not be able to immediately affect the state of particle 2. Entangled particles seemed to do just that, and it was this non-local nature he referred to when saying *"spooky action at a distance"*. This non-local nature of quantum mechanics forced him to look for a hidden variable theory [5], which gave the explanations of quantum mechanical phenomena using hypothetical variables that are un-observable which completed this incomplete theory of wavefunctions.

But all qualms were put to the ground in 1964, when John Bell showed that a local theory with hidden variables can never give all the statistical outcomes possible if one compares it to the results and observations of quantum mechanics [6]. This meant that quantum mechanics is fully incompatible with local hidden-variables theory, and the "spooky action at a distance" or "entanglement" is not an artifact of an incomplete description, *but rather the characteristic trait of quantum mechanics.*

As everyone, Einstein's views and intuition rooted from physical experiences mak-

ing it extremely hard to accept such correlations. The fact that quantum mechanics allows for such wavefunctions/states that have such non trivial correlations (while being a local theory) was hard to accept from a classical point of view. It was not that there is some non-locality, but rather that systems could be in a combined state even when they are not "interacting" classically, due to which measurement on one system invariably affects the other one as well.

The topic of quantum mechanics became the bread and butter for physicists looking to explain any phenomena at atomic scales. At the same time (1920-1930s), Paul Dirac's attempts at quantizing the electromagnetic field led to the idea of a "quantum field theory", which was a fully quantum mechanical theory involving matter and electromagnetic fields. Quantum mechanics as it was could not account for relativistic particles. Since photons were relativistic objects, a description of electromagnetism could hence not be given by a an ordinary theory of quantum mechanics. This led to the idea of a quantum field theory, which could account for relativistic particles. Shortly after, almost all forces (leaving gravity) came to be well described by ideas in this theory, leading to a great understanding of how nature might work (or atleast how we can model it). We now ask, what does being entangled mean for these quantum fields?

1.2 What does being entangled mean for fields?

Let us take a bipartite system with individual Hilbert spaces represented by $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively. The bipartite system then has the Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. The states of this bipartite system, which belong to $\mathcal{H}$ look like $|\Psi_1\rangle \otimes |\Psi_2\rangle$. We write an arbitrary state as:

$$|\Psi\rangle = \sum_i c_i |\Psi_{1i}\rangle \otimes |\Psi_{2i}\rangle. \tag{1.2.1}$$

Here i represents the sum index; it runs over the dimension of $\mathcal{H}$. The density matrix for the bipartite system is given by

$$\rho = |\Psi\rangle\langle\Psi| = \sum_{i,j} c_i c_j^* |\Psi_{1i}\rangle\langle\Psi_{1j}| \otimes |\Psi_{2i}\rangle\langle\Psi_{2j}|.$$

Partial trace: If we want to get to know about the probabilities of a state in the system 1 (assuming we do not know anything about the state of the system 2), we perform a partial trace of the system 2 in ρ. Partial tracing is similar to integrating out a variable from a joint probability distribution. This is because ρ encodes probabilities. For example if you consider a state which is in a superposition, the diagonal terms of the density matrix represent the probabilities to find the system in a particular state. The method of partial tracing can be seen as

$$\rho_1 = \mathrm{Tr}_2\rho = \sum_{i,j,k} c_i c_j^* |\Psi_{1i}\rangle\langle\Psi_{1j}| \otimes \langle\Psi_{2k}|\Psi_{2i}\rangle\langle\Psi_{2j}|\Psi_{2k}\rangle = \sum_{i,j} c_i c_j^* |\Psi_{1i}\rangle\langle\Psi_{1j}|$$
$$\otimes \sum_k \langle\Psi_{2j} \underbrace{|\Psi_{2k}\rangle\langle\Psi_{2k}|}_{=\mathbb{I}} \Psi_{2i}\rangle = \sum_{i,j} c_i c_j^* |\Psi_{1i}\rangle\langle\Psi_{1j}| \otimes \langle\Psi_{2j}|\Psi_{2i}\rangle. \quad (1.2.2)$$

Separability: A state $|\Psi\rangle$ of the composite system can be written as $|\Psi_1\rangle \otimes |\Psi_2\rangle$ when $\rho^2 = \rho$ and vice versa. This separability of $|\Psi\rangle$ into $|\Psi_1\rangle$ and $|\Psi_2\rangle$ leads to "pure states". As said before, ρ encodes probabilities. If ρ_1 is independent of the system 2 i.e $\rho_1 \neq f$(variables of system 2), then that means probabilities about measurement of things in system 1 don't have any information about the state of system 2 (or equivalently are not affected by system 2).

Lastly, note that if $|\Psi\rangle$ in (1.2.1) were to be in a pure state, then there would only be one term in the summation, and the constant outside would be equal to 1. This would then also mean the scalar product in (1.2.2) is 1 as it is normalized and we retrieve $\rho_1 = \sum_i c_i c_i^* |\Psi_{1i}\rangle\langle\Psi_{1j}|$ and all the properties of a pure state.

However if $|\Psi\rangle$ cannot be separated as $|\Psi_1\rangle \otimes |\Psi_2\rangle$, it implies that ρ_1 is a function of state of system 2 as in (1.2.2). Measurements involving system 1 using ρ_1 also depend on the state of the system 2 and hence the states are *"entangled"*, and so are the observables for this state (from $\langle O\rangle = \mathrm{Tr}(\rho O)$!). These states also have $\rho^2 \neq \rho$. Entanglement is not a rare feature, it occurs quite often in systems with interactions

and is ubiquitous. Many systems despite starting with a pure state, evolve into an entangled state with the slightest of interactions with the environment.

Correlations: We now state this in a slightly different way. For an entangled state, measurements done on system 1 depend on the state of the system 2. In other words, there can be correlations between outcomes of measurements. For example, consider a particular outcome in the system 1 only happens when system 2 is in a particular state. It is then possible that by measuring system 1, we can confer, or *correlate* what state system 2 has to be in after the measurement. Hence there are nontrivial correlations for entangled states, and we say the **observables or operators are entangled**.

In general, when the states are separable, we can write:

$$\langle\Psi|\mathcal{O}_1\otimes\mathcal{O}_2|\Psi\rangle = (\langle\Psi_1|\otimes\langle\Psi_2|)(\mathcal{O}_1\otimes\mathcal{O}_2)(|\Psi_1\rangle\otimes|\Psi_2\rangle) = \langle\Psi_1|\mathcal{O}_1|\Psi_1\rangle.\langle\Psi_2|\mathcal{O}_2|\Psi_2\rangle.$$

This statement is similar to saying $E[XY] = E[X]E[Y]$, which tells us that the two variables are uncorrelated. Similarly in a pure state, the systems and measurements done upon it are uncorrelated while for entangled states we have the following inequality signalling about some correlation:

$$\langle\Psi|\mathcal{O}_1\otimes\mathcal{O}_2|\Psi\rangle \neq \langle\Psi_1|\mathcal{O}_1|\Psi_1\rangle.\langle\Psi_2|\mathcal{O}_2|\Psi_2\rangle.$$

Moving to a quantum field, we take the two systems as two different regions of space-time where the field exists and ask if the quantum fields (operators) in the two regions are entangled. Therefore, for two points x_1 and x_2, we are looking if the following inequality is true [7]

$$\langle\Psi|\phi(x_1)\otimes\phi(x_2)|\Psi\rangle \neq \langle\Psi_1|\phi(x_1)|\Psi_1\rangle.\langle\Psi_2|\phi(x_2)|\Psi_2\rangle. \tag{1.2.3}$$

If this inequality is true, then the operators $\phi(x_1)$ and $\phi(x_2)$ are entangled, and their values depend on each other. To analyze this, we can look at the inequality in the limit $x_1, x_2 \to x$. The LHS of (1.2.3) can be shown [8] to behave like:

$$\lim_{x_1,x_2\to x}\langle\Psi|\phi(x_1)\otimes\phi(x_2)|\Psi\rangle = \lim_{x_1,x_2\to x}\frac{U(x_1,x_2)}{\sigma(x_1,x_2)} \to \infty.$$

Here U is a smooth function and σ represents the squared geodesic distance. When $x_1, x_2 \to x$, the denominator goes to zero and hence the LHS diverges. For the RHS, we get:

$$\lim_{x_1,x_2\to x} \langle\Psi_1|\phi(x_1)|\Psi_1\rangle.\langle\Psi_2|\phi(x_2)|\Psi_2\rangle = [\langle\Psi_1|\phi(x)|\Psi_1\rangle]^2.$$

The above expression is just the expectation value of the field operator, and it does not necessarily diverge. Therefore in general LHS≠RHS. The calculation done here was only for $x_1, x_2 \to x$, but by plugging the general form of the field operators, it can be shown to be held in general as well. Hence the field operators in different regions are entangled! The observables in one region are hence correlated to observables in another region, as all observables can be constructed from the quantum field.

1.2.1 Entropy of fields: a heuristic argument

Let us look at a free scalar field in ground state. We construct its density matrix and try to find the reduced density matrix after integrating the degrees of freedom inside a sphere. If the radius of this sphere is R, we typically would expect the entropy to scale as R^3.

However, when we have a composite system in a pure state, it can be shown that the reduced density matrix with degrees of freedom inside a region traced out has the same eigenvalues as the reduced density matrix with degrees of freedom outside the region traced out, i.e., ρ_{in} has the same eigenvalues as ρ_{out}. This can be done by looking at the Schmidt decomposition of the state. This means that these two density matrices will give the same Von-Neumann Entropy i.e

$$S = -\sum_n \rho_n \ln \rho_n, \lambda_{out,i} = \lambda_{in,i} \implies S_{out} = S_{in}. \tag{1.2.4}$$

The above entropy is interesting to look at since it is a measure of entanglement. The equality above is puzzling because even if one decides to make this sphere bigger, the entanglement entropy for both regions will still be equal. But as we make this sphere bigger, the volume inside the sphere increases and outside reduces. The fact that entropy corresponding to inner degrees of freedom traced out is still equal to the

entropy corresponding to outer degrees of freedom traced out means that it depends on the boundary of the two regions. It can only depend on a degrees of freedom common to both regions, i.e., the boundary separating the two regions which stays common for both under any scaling of the sphere. Interestingly, this has connections to Black Holes and their entropy, as it also follows an area law. In the following section, we will describe Black Holes and their entropy, and motivate the need to look at entanglement entropy of scalar fields.

1.3 Laws of Black Hole thermodynamics and the area law

General relativity is a well-tested theory of gravity. In the past few decades, it has been established that Black Holes are thermodynamic objects, objects having properties like temperature and entropy [9, 10]. With these advances came a few crucial results, now often called the law of Black Hole thermodynamics. These are completely analogous to the laws of thermodynamics.

- Hawking in 1975 showed that a Black Hole radiates. Moreso, this radiation has a thermal spectrum, which means we can assign a temperature to the Black Hole. A detailed derivation of this temperature is given in [appendix A, see (A.4.10)]. The temperature in SI units is given by

$$T_{BH} = \frac{\hbar c^3}{8\pi G k_b M_{BH}}. \tag{1.3.1}$$

We can then find the entropy associated with this temperature as:

$$T_{\mathrm{BH}} dS_{\mathrm{BH}} = dE_{\mathrm{BH}} = dM_{\mathrm{BH}} c^2.$$

$$\implies \int dS_{\mathrm{BH}} = c^2 \int dM_{\mathrm{BH}} \frac{8\pi G k_b M_{\mathrm{BH}}}{\hbar c^3} = \frac{4\pi G k_b M_{\mathrm{BH}}^2}{\hbar c}$$

$$\boxed{S_{\mathrm{BH}} = \frac{A_{\mathrm{BH}}}{l_p^2} . \frac{k_b}{4}} \tag{1.3.2}$$

Where l_p is the Planck length and A_{BH} is the area of the Black Hole. This area is equal to $4\pi r_c^2$ with r_c being the Schwarzschild radius.

- The first law of Black Hole thermodynamics is a statement of energy conservation, analogous to thermodynamics. It says:

$$dE_{\text{BH}} = \frac{\kappa}{8\pi} dA_{\text{BH}} + \Omega_{\text{BH}}\, dJ_{\text{BH}}. \tag{1.3.3}$$

  Here J_{BH} is the angular momentum, and Ω_{BH} is the angular velocity of the Black Hole. Using (1.3.1) and (1.3.2), we can identify the first term as the TdS term.

- The force applied by an observer to hold a unit mass at the event horizon (this force is referred to as surface gravity κ) is the same everywhere on the horizon for a static Black Hole. This is analogous to the zeroth law of thermodynamics, which defines what temperature means. Here it defines surface gravity (interestingly, the hawking temperature can also be written as $T_H = \kappa/2\pi$).

- Massive objects that fall into the Black Hole end up increasing its mass, and hence its radius and area. This property of the area of a Black Hole is reminiscent of the second law of thermodynamics, which says that the entropy always increases in a thermodynamic process. Extending the analogy, we now get:

$$\frac{dA}{dt} \geq 0. \tag{1.3.4}$$

  This analogy of entropy with area holds in many different situations, for example, in Black Hole mergers. If two Black Holes with areas A_1 and A_2 merge, forming a Black Hole with area A, it can be shown that:

$$A \geq A_1 + A_2. \tag{1.3.5}$$

- The third law of Black Hole thermodynamics states that if we start with a Black Hole with finite surface gravity, it is impossible to reduce its surface gravity to zero by any sequence of operations. This is analogous to the third law of thermodynamics, where absolute zero temperature can never be achieved.

A few questions

We can now ask a few questions based on the laws defined above.

1. A problem arises when we try to look at Black Hole entropy from the perspective of quantum fields. Imagine a star that is collapsing into a Black Hole. We can assume that before the collapse, we know everything about the matter fields in the space-time. Hence we start with a pure state, and the entropy is zero. But at a later time, after the Black Hole is formed, the Black Hole has non-zero entropy, i.e. it is in a mixed state, a thermal state. However, we know that this process of time evolution should be unitary (the time evolution operator in quantum mechanics is unitary); hence we shouldn't be able to time evolve a pure state into a mixed state for an isolated system. This is the *Black Hole information paradox* [11]. Unitary time evolution means that information about the state is always conserved.

2. Why does Black Hole entropy depend on the area? Typically entropy is an extensive quantity and depends on the volume (can be seen from $S = k_b \ln W$, with W being the number of microstates). However the Black Hole entropy depends explicitly on the final area. Moreover, its past history or any initial condition like what star it was made of, etc., does not matter; only the final area matters.

3. We can also ask what are the microstates that contribute to the entropy. What is the source of this entropy? There are many candidates for this question, but it is not clear which one it is.

All of these questions are still largely open questions. There has been a lot of work towards answering some of these questions. One approach involves associating S_{BH}'s microstates to degrees of freedom of a full theory of quantum gravity (for example strings, D-branes etc [12, 13]). Another approach involves associating S_{BH} to entropy of matter quantum fields in a space-times with horizons. This can be done by thinking of **entanglement of quantum field modes inside and outside a region** [14,

15]. Looking at the last section, we can now connect the two possibly linked ideas and look at entanglement entropy as a source of Black Hole entropy. In this thesis, the second approach is taken to produce results like the area law.

The entanglement entropy corresponding to scalar fields can be calculated across a Black Hole horizon on a discretized lattice, and it can be shown to have the behavior [15]

$$S = k_1\left(\frac{A}{a^2}\right) + k_2\left(\frac{A}{a^2}\right)^{\nu}. \tag{1.3.6}$$

Here k_1 and k_2 are constants, ν is a number between 0 and 1 and a is the lattice separation. The leading order result will be derived in later sections through two different methods, through numerical estimation of entropy using harmonic chains and the covariance matrix approach.

Leading term: Clearly, the leading term is similar to the expression for entropy for Black Holes. The a^2 in the denominator also behaves like the Planck length, as it is the smallest area scale in the problem, just like l_p^2 is the smallest area scale in the other problem. Since $S \propto W$, it is as if each lattice cell (or Planck cell for the Black Hole) corresponds to a degree of freedom/micro-state. This similarity is highly remarkable.

Sub-leading terms: The sub-leading terms is corrections to the area law. The crucial point to remember is that the derivation of Black Hole entropy is based on the semi-classical derivation of Hawking temperature. In the limit where quantum effects and gravitational effects are dominant, ($A \approx l_p^2$) we expect the semi-classical analysis to break down or have modifications. Hence if entanglement (a purely quantum phenomena) is indeed the source of Black Hole entropy, then sub-leading terms would give us the corrections one would receive from a theory of quantum gravity.

Finally, we can now ask if there is any logical connection between Black Hole entropy and entanglement entropy or if it is just similarities we have seen in expressions.

Following [15], imagine a collapsing star and a faraway observer who is observing the collapse. Let us assume that they can see everything that is happening, and so they have all the information about the collapsing star and hence $S = 0$. However, as soon as the Black Hole is formed, the faraway observer does not know about matter fields inside the horizon as that part is causally disconnected. The observer has no information about the degrees of freedom that are inside the horizon. This separation gives finite entanglement entropy between two regions in a space-time with horizons. On the other hand, entanglement entropy is also attributed to the presence of the same horizon, a boundary. Hence both of the entropies are associated with the presence of the horizon.

Another way to motivate why to look at entanglement entropies of scalar fields can be shown by considering the Einstein-Hilbert action and looking how it changes under small perturbations to the space-time like $g_{\mu\nu} \to g_{\mu\nu} + h_{\mu\nu}$ [15]. Using this, the linearized action (E-H action with a small perturbation to metric) can be shown to look like the action for a massive scalar field propagating in a background space-time with metric $g_{\mu\nu}$. Moreover, for spherically symmetric space-times, equation of motion for these perturbations looks exactly like equation of motion for a test particle propagating in Black Hole space-time. This means that by calculating the entanglement entropy of scalar fields, we get the entropy of a set of metrics that are perturbations to a background space-time, and hence might help us in understanding the role entanglement plays in the area law behavior of Black Hole entropy. Lastly, we can also show that a scalar field in Black Hole space-time for a fixed Lemaitre time reduces down to scalar field in flat space. This will be shown in full detail in chapter 2 as well.

With these motivations, it is only natural to look at the problem of entanglement entropy of scalar fields and its behavior. The following chapter 2 will discuss one method of calculating entropy of scalar fields, building its way up from simple toy models. This method relies on numerics mostly and does not allow for many analytical results. Given the importance of entanglement entropies of fields, we try to explore

the characteristics of entanglement entropy in scalar fields analytically in chapter 3 with the covariance method approach. This approach analyzes the calculation of entanglement entropy carefully and shows a change in leading order behavior of the entropy in different regimes of the quantity ζ, leading to different information content in these regimes.

Chapter 4 describes the current work in progress towards evaluating entanglement entropy for a fermionic field. It shortly describes the problems faced when one tries to discretize a fermionic field, and how to overcome these problems. Then, a potential method of calculating entanglement entropy for fermionic field is discussed.

Apart from these ideas, another goal during this project was to understand Black Hole thermodynamics and cosmological particle creation in space-times in order to gain a better background for the physics behind concepts like Hawking radiation and Black Hole entropy. Appendix A contains most of the relevant work in detail, where we will look at the topic of time dependent harmonic oscillators, scalar fields in expanding space-time and finally the Unruh and Hawking radiation. This appendix chapter demonstrates particle creation in each of these cases and the role played by the vacuum in these scenarios.

Chapter 2

Entanglement entropy for systems

This section intends to find the entanglement entropy for scalar fields in Minkowski space without and with a horizon. We show that scalar fields under discretization reduce down to a chain of harmonic oscillators. We try to approach this complex problem by looking at a simpler problem before, the simplest case of the harmonic chain: a coupled harmonic oscillator. Then we tackle the case of the harmonic chain and finally scalar fields in spacetimes. Throughout this chapter, we follow the methods used in [16, 15].

2.1 Coupled harmonic oscillator

We start with examining a quantum coupled harmonic oscillator in the ground state and calculating its entanglement entropy. The procedure is to find the ground state wavefunction and then calculate its density matrix. Then, using the eigenvalues of the density matrix, find the Von-Neumann Entanglement entropy.

2.1.1 Finding the ground state and the density matrix

The Hamiltonian of the system is given by:

$$\mathcal{H} = \frac{1}{2m}\Big[p_1^2 + p_2^2 + k_o(x_1^2 + x_2^2) + k_1(x_1 - x_2)^2\Big]. \tag{2.1.1}$$

The goal here is to find the entanglement entropy of this system when one of the oscillators is traced out from the total density matrix. We will start by finding the ground state wavefunction, and from there construct the density matrix, trace out one of the oscillators and finally compute the Von-Neumann entropy. Instead of solving this problem interactions, we go to the normal co-ordinates using experience from classical problems. We hence diagonalize the Hamiltonian by introducing new variables in (2.1.1) as

$$x_\pm = \frac{x_2 \pm x_1}{\sqrt{2}}, p_\pm = \frac{p_2 \pm p_1}{\sqrt{2}}.$$

$$\implies \mathcal{H} = \frac{1}{2m}\Big[p_+^2 + p_-^2 + k_0 x_+^2 + (k_0 + 2k_1)x_-^2\Big]. \tag{2.1.2}$$

Hence, we have two uncoupled oscillators and we can write the ground state of the system as the product of the ground state of the individual oscillators by

$$\Psi_0 = \left(\frac{\sqrt{k_0}}{\pi}\right)^{\frac{1}{4}} \exp\left\{\left[-\frac{\sqrt{k_0}x_+^2}{2}\right]\right\}.\left(\frac{\sqrt{k_0+2k_1}}{\pi}\right)^{\frac{1}{4}} \exp\left\{\left[-\frac{\sqrt{k_0+2k_1}x_-^2}{2}\right]\right\}.$$

Writing $\omega_+ = \sqrt{k_0}$ and $\omega_- = \sqrt{k_0 + 2k_1}$, we get

$$\Psi_0 = \left(\frac{\omega_+\omega_-}{\pi^2}\right)^{\frac{1}{4}} \exp\left\{\left[-\frac{1}{2}\big(\omega_+ x_+^2 + \omega_- x_-^2\big)\right]\right\}. \tag{2.1.3}$$

Now, we can find the density matrix, $\rho = |\Psi_0\rangle\langle\Psi_0|$ and trace out one oscillator, with $x = x_1$

$$\rho_{red} = \mathrm{Tr}_{\mathrm{osc}}\rho.$$

$$\implies \rho_{red}(x_2, x_2') = \sum_{\text{e.s of } x_1} \langle x_1|\Psi_0\rangle\langle\Psi_0|x_1\rangle = \int dx_1 \Psi_0(x_1, x_2)\Psi_0^\dagger(x_1, x_2')$$

$$= \int dx_1 \left(\frac{\omega_+\omega_-}{\pi^2}\right)^{\frac{1}{2}} \exp\left\{\left[-\frac{1}{2}\big(\omega_+ x_+^2 + \omega_- x_-^2 + \omega_+ x_+'^2 + \omega_- x_-'^2\big)\right]\right\}.$$

Expressing $x_\pm$ in terms of x_1, x_2, completing the square and evaluating the gaussian integral we get

$$= \left(\frac{\omega_+\omega_-}{\pi^2}\right)^{\frac{1}{2}} \exp\left\{\left[-\frac{1}{4}(\omega_+\omega_-)(x_2^2 + x_2'^2)\right\}\right] \int dx_1 \exp\left\{\left[-\frac{1}{4}\big(2x_1^2(\omega_+ + \omega_-) + 2x_1(\omega_+\omega_-)(x_2 + x_2')\big)\right\}\right]$$

$$= \left(\frac{\omega_+\omega_-}{\pi^2}\right)^{\frac{1}{2}} \exp\left\{\left[-\frac{1}{4}(\omega_+\omega_-)(x_2^2+x_2'^2)\right\}\right] \exp\left\{\left[\frac{(\omega_+-\omega_-)^2(x_2+x_2')^2)}{8(\omega_++\omega_-)}\right\}\right] \sqrt{\frac{\pi}{\frac{\omega_++\omega_-}{2}}}$$

$$\implies \rho_{red}(x_2, x_2^{'}) = \sqrt{\frac{2\omega_+\omega_-}{(\omega_++\omega_-)\pi}} \exp\left\{\left[-\frac{1}{2}\gamma(x_2^2+x_2'^2)+\beta x_2 x_2^{'}\right]\right\}$$

$$\equiv \sqrt{\frac{\gamma-\beta}{\pi}} \exp\left\{\left[-\frac{1}{2}\gamma(x_2^2+x_2'^2)+\beta x_2 x_2^{'}\right]\right\}, \tag{2.1.4}$$

where $\beta = \frac{(\omega_+-\omega_-)^2}{4(\omega_++\omega_-)}$ and $\gamma-\beta = \frac{2\omega_+\omega_-}{(\omega_++\omega_-)}$.

2.1.2 Density matrix eigenvalues and entanglement entropy

Now we need to diagonalize the operator $\rho_{red}(x_2, x_2^{'})$ so that we can calculate the Von-Neumann entropy. All we need are the eigenvalues, so we look at the eigenvalue equation. Since ρ is an operator, we can think of it as an outer product $|a\rangle\langle b|$. Upon acting on a vector $|c\rangle$, we obtain is a scalar product. This can be viewed as the $\rho_{red}(x_2, x_2^{'})$ acting on a function and integrating one of the indices out. Hence the eigenvalue equation looks like

$$\int dx' \rho_{red}(x_2, x_2^{'}) f_n(x') = p_n f_n(x).$$

The eigenvalues of this operator are given by $p_n = (1-\xi)\xi^n$ and the eigenvectors are $f_n(x) = H_n(\alpha^{\frac{1}{2}}x).\exp\left\{\left(-\frac{\alpha x^2}{2}\right)\right\}$ where $\alpha = \sqrt{\gamma^2-\beta^2}$ and $\xi = \frac{\beta}{\alpha+\gamma}$ and H_n's are the nth order Hermite polynomials.

Given the eigenvalues, we can now find the entropy to be

$$S = -\sum_n p_n \ln p_n = -(1-\xi)\sum_n \xi^n \ln[(1-\xi)\xi^n]$$

$$= -(1-\xi)\left[\sum_n \xi^n \ln(1-\xi) + \sum_n \xi^n \ln \xi^n\right]$$

$$= -(1-\xi)\left[\ln(1-\xi)\frac{1}{1-\xi} + \ln\xi \sum_n n\xi^n\right]. \tag{2.1.5}$$

Where we used the sum for an infinite GP in the first sum above. The second sum can be solved by writing it as a derivative and switching the sum and the derivative

as

$$\ln\xi\sum_n n\xi^n = \xi\ln\xi\sum_n n\xi^{n-1} = \xi\ln\xi\sum_n \frac{d}{d\xi}\xi^n = \xi\ln\xi\frac{d}{d\xi}\sum_n \xi^n = \xi\ln\xi\frac{d}{d\xi}\frac{1}{1-\xi}$$
$$= \xi\ln\xi\frac{1}{(1-\xi)^2}. \quad (2.1.6)$$

On putting this back into (2.1.5), we get

$$\boxed{S(\xi) = -\ln(1-\xi) - \frac{\xi}{1-\xi}\ln\xi.} \quad (2.1.7)$$

Hence we have now fully calculated entanglement entropy for the coupled harmonic oscillator in terms of the known parameters.

2.2 Harmonic chain

Now that we have solved for the entropy for coupled oscillator, we use that experience to similarly solve for the harmonic chain system. The procedure remains the same as before, we try to go to the normal mode basis and find the ground state, and then the entropy.

2.2.1 Finding the ground state and the density matrix

The general Hamiltonian can be written as

$$\mathcal{H} = \frac{1}{2m}\Big[\sum_i p_i^2 + \sum_{i,j=1}^{N} x_i K_{ij} x_j\Big]. \quad (2.2.1)$$

K is the coupling matrix, and it contains all the information about the interactions and the boundary conditions. Note that there is no requirement that $i > j$, hence the interaction terms are divided into the off-diagonal terms, implying that K is a symmetric matrix. We try to match the results from the last subsection. For $N = 2$ and from (2.1.1) we get

$$K = \begin{bmatrix} k_0 + k_1 & -k_1 \\ -k_1 & k_0 + k_1 \end{bmatrix}.$$

Hence $\sum_{i,j=1}^{N} x_i K_{ij} x_j = (k_0+k_1)x_1^2 + (k_0+k_1)x_2^2 - 2k_1 x_1 x_2 = k_o(x_1^2+x_2^2) + k_1(x_1-x_2)^2$. Then the transformation to variables $x_\pm, p_\pm$ diagonalizes this matrix and is just a transformation to its eigenbasis. This can be written in matrix language via a unitary matrix transformation as

$$\mathbf{x}^T.K.\mathbf{x} = \underbrace{\mathbf{x}^T U^T}_{x_\pm^T}.\underbrace{UKU^T}_{K_D}.\underbrace{U\mathbf{x}}_{x_\pm} = \mathbf{x}_\pm^T.K_D.\mathbf{x}_\pm.$$

Where $K_D = \text{Diag}(k_0, k_0+2k_1)$. Each of the diagonal elements then contributes one exponential in the ground state expression. With this formalism, we can easily generalize and write down the ground state wavefunction for the harmonic chain as

$$\Psi_0 = \left(\frac{\prod_j \omega_j}{\pi^N}\right)^{\frac{1}{4}} \prod_i \exp\left[-\frac{x_i'^2\sqrt{(K_D)_{ii}}}{2}\right] = \det\left(K^{\frac{1}{2}}\right).\pi^{-\frac{N}{4}} \exp\left[-\frac{\sum_i x_i'^2\sqrt{(K_D)_{ii}}}{2}\right]$$

$$\implies \Psi_0 = \det\left(K^{\frac{1}{2}}\right).\pi^{-\frac{N}{4}} \exp\left[-\frac{\mathbf{x}_\pm^T.K^{\frac{1}{2}}.\mathbf{x}_\pm}{2}\right]. \tag{2.2.2}$$

Note that repeated indices do not imply a sum here. Since the determinant is unchanged in a unitary transformation, we can replace K_D with K at places. As before, we now know $\rho = |\Psi_0\rangle\langle\Psi_0|$ and we now calculate the reduced density matrix by tracing out n of the N oscillators. Using (2.2.2), we get

$$\rho_{red}(x_{n+1}\cdots x_N, x'_{n+1}\cdots x'_N) = \int \prod_{i=1}^{n} dx_i \Psi_0(x_1,\cdots x_n, x_{n+1},\cdots x_N)\Psi_0^\dagger(x_1,\cdots x_n, x'_{n+1},\cdots x'_N)$$

$$\implies \rho_{red} = \pi^{-\frac{N}{2}}(\det K^{\frac{1}{2}})^2 \int \prod_{i=1}^{n} dx_i \exp\left[-\frac{\mathbf{x}^T.K^{\frac{1}{2}}.\mathbf{x} + \mathbf{x}'^T.K^{\frac{1}{2}}.\mathbf{x}'}{2}\right]. \tag{2.2.3}$$

We can see in (2.2.3) that we still have the matrix products. We now aim to separate these products into sub-matrices to carry out the integration. Since the first n indices are being integrated, we divide the state vector into two parts of length n and $N-n$. We then appropriately also divide the matrix $K_D^{\frac{1}{2}}$ into sub-matrices A($n\times n$), B($n\times$

$N-n$), C($N-n\times n$) and D($N-n\times N-n$) as

$$\begin{pmatrix} x_1 \\ . \\ . \\ x_n \\ . \\ . \\ x_N \end{pmatrix} \rightarrow \begin{pmatrix} X_n \\ X_N \end{pmatrix}, K^{\frac{1}{2}} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} A & B \\ B^T & D \end{bmatrix}.$$

Putting this into the terms inside the exponential of (2.2.3) we get

$$\mathbf{x}^T.K^{\frac{1}{2}}.\mathbf{x}+\mathbf{x}'^T.K^{\frac{1}{2}}.\mathbf{x}' = \begin{pmatrix} X_n & X_{N-n} \end{pmatrix} \begin{bmatrix} A & B \\ B^T & D \end{bmatrix} \begin{pmatrix} X_n \\ X_{N-n} \end{pmatrix} + \begin{pmatrix} X_n & X'_{N-n} \end{pmatrix} \begin{bmatrix} A & B \\ B^T & D \end{bmatrix} \begin{pmatrix} X_n \\ X'_{N-n} \end{pmatrix}$$

$$= X_nAX_n + X_nBX_{N-n} + X_{N-n}B^TX_n + X_{N-n}CX_{N-n} + X_nAX_n + X_nBX'_{N-n} + X'_{N-n}B^TX_n + X'_{N-n}CX'_{N-n}. \quad (2.2.4)$$

The terms containing only $N-n$ are not integrated in expression of ρ_{red} . Substituting (2.2.4) into (2.2.3) and simplifying, we get:

$$\rho_{red} = \pi^{-\frac{N}{2}}(\det K^{\frac{1}{2}})^2 \exp\left[-\frac{X_{N-n}CX_{N-n} + X'_{N-n}CX'_{N-n}}{2}\right] \int \prod_{i=1}^{n} dx_i \exp\left[-X_nAX_{N-n} - (X_{N-n}B^T + X'_{N-n}B^T)X'_n\right]$$

This is the standard gaussian integral for matrices. Performing the integral and simplifying, we get:

$$\rho_{red} = \pi^{-\frac{N}{2}}(\det K^{\frac{1}{2}})^2 \sqrt{\frac{(2\pi)^n}{\det A}} \exp\left[-\frac{X_{N-n}\big(C-\frac{1}{2}B^TA^{-1}B\big)X_{N-n}}{2} \right.$$
$$\left. \frac{+X'_{N-n}(C-\frac{1}{2}B^TA^{-1}B\big)X'_{N-n} - 2X_n\big(\frac{1}{2}B^TA^{-1}B\big)X'_n}{2}\right].$$

Calling $\gamma = C-\frac{1}{2}B^TA^{-1}B$ and $\beta = \frac{1}{2}B^TA^{-1}B$, we get

$$\rho_{red} = \pi^{-\frac{N}{2}}(\det K^{\frac{1}{2}})^2 \sqrt{\frac{(2\pi)^n}{\det A}} \exp\left[-\frac{X_{N-n}.\gamma.X_{N-n} + X'_{N-n}.\gamma.X'_{N-n} - 2X_n.\beta.X'_n}{2}\right]. \quad (2.2.5)$$

Hence we have found the reduced density matrix for the harmonic chain.

2.2.2 Density matrix eigenvalues and entanglement entropy

Now as before, we have the task to find eigenvalues of ρ_{red}. We would like to reduce this complicated problem to a problem we already know, i.e (2.1.4). To do this, we need to convert the matrix equation above into individual copies of (2.1.4). This corresponds to diagonalizing the matrices γ and β in the exponential. We do this by first tackling γ, by choosing an orthogonal matrix V such that $\gamma_D = V\gamma V^T$ and choose another basis y such that $X_{N-n} = V^T\gamma_D^{-\frac{1}{2}}Y_{N-n}$. Inserting that in (2.2.5), we get

$$\rho_{red} = \pi^{-\frac{N}{2}}(\det K^{\frac{1}{2}})^2\sqrt{\frac{(2\pi)^n}{\det A}}\exp\left[-\frac{Y_{N-n}.Y_{N-n}+Y'_{N-n}.Y'_{N-n}}{2}+Y_{N-n}.\underbrace{\gamma_D^{-\frac{1}{2}}V\beta V^T\gamma_D^{-\frac{1}{2}}}_{\beta'}.Y'_{N-n}\right].$$

Now we can do another transformation that diagonalizes β' and leaves the inner products $Y_{N-n}.Y_{N-n}$ and $Y'_{N-n}.Y'_{N-n}$ unchanged. Let $Y_{N-n} = Wz_{N-n}$, where W is a unitary transformation matrix that diagonalizes β', i.e $\beta'_{D'} = W\beta' W^T$. Hence $\beta'_D = \text{Diag}(\beta'_{n+1}, \beta'_{n+2}, \cdots \beta'_N)$ where β'_i are the eigenvalues of β'. Finally, since the matrices are now diagonal, we can write

$$= \pi^{-\frac{N}{2}}(\det K^{\frac{1}{2}})^2\sqrt{\frac{(2\pi)^n}{\det A}}\exp\left[-\frac{1}{2}\sum_{i=n+1}^{N}(z_i^2+z'^2_i+\beta'_i z_i z'_i)\right]$$

$$\implies \rho_{red}(z,z') = \pi^{-\frac{N}{2}}(\det K^{\frac{1}{2}})^2\sqrt{\frac{(2\pi)^n}{\det A}}\prod_{i=n+1}^{N}\exp\left[-\frac{1}{2}(z_i^2+z'^2_i+\beta'_i z_i z'_i)\right]. \tag{2.2.6}$$

These are just $N-n$ copies of (2.1.4) with $\gamma \leftrightarrow 1$ and $\beta \leftrightarrow \beta'_i$. Hence the total operator can be diagonalized in a similar way with the eigenvalue being the product of all eigenvalues of the $N-n$ copies. The total entropy is hence given with the help

of (2.1.7) by

$$S = \sum_{i=n+1}^{N} S(\xi_i), \qquad \text{Where } S(\xi_i) = -\ln(1-\xi_i) - \frac{\xi_i}{1-\xi_i}\ln\xi_i \text{ and } \xi_i = \frac{\beta_i'}{1-(1-\beta_i'^2)}. \tag{2.2.7}$$

Hence the entropy for a harmonic chain can be calculated numerically by doing the above summation.

2.3 Free scalar field in 3+1 dimensions

Finally, we have the case of a free scalar field. We try to compute its entropy by connecting it to the results we have found above. To do so, we start with writing the Hamiltonian for the field in spherical harmonic basis, where then the connection to (2.2.1) is more apparent.

2.3.1 Hamiltonian in spherical harmonic basis

We begin by writing the Hamiltonian

$$\mathcal{H} = \frac{1}{2}\int d^3x \Big[m^2\phi^2 + |\nabla\phi|^2 + \pi^2\Big]. \tag{2.3.1}$$

We now write this Hamiltonian in real spherical harmonic basis, i.e $Z_l^m(x,\phi)$. We have the transformation equations as:

$$\phi(\mathbf{x}) = \sum_{lm} \frac{\varphi_{lm}(r)}{r} Z_l^m(x,\varphi) \qquad \pi(\mathbf{x}) = \sum_{lm} \frac{\pi_{lm}(r)}{r} Z_l^m(x,\varphi). \tag{2.3.2}$$

Using (2.3.2) in (2.3.1) and expressing volume in spherical coordinates we can simplify $\mathcal{H}$. Lets look at this term by term. Noting that $\int d\Omega Z_l^m Z_{l'}^{m'} = \delta_{ll'}\delta_{mm'}$. For the φ^2 term, we get

$$\int d\Omega \sum_{lm}\sum_{l'm'} \frac{\varphi_{lm}(r)}{r} Z_l^m(x,\varphi) \frac{\varphi_{l'm'}(r)}{r} Z_{l'}^{m'}(x,\varphi) \overset{\text{compl}}{=} \sum_{lm} \frac{\varphi_{lm}^2}{r^2}. \tag{2.3.3}$$

Similarly for the π^2 term we get

$$\int d\Omega \sum_{lm}\sum_{l'm'} \frac{\pi_{lm}(r)}{r} Z_l^m(x,\varphi) \frac{\pi_{l'm'}(r)}{r} Z_{l'}^{m'}(x,\varphi) \overset{\text{compl}}{=} \sum_{lm} \frac{\pi_{lm}^2}{r^2}. \tag{2.3.4}$$

For the gradient term, we use the expansion for gradient in spherical polar co-ordinates and then evaluate the squared terms as

$$\int d\Omega \left| \sum_{lm} \left[\frac{\partial}{\partial r}\left(\frac{\varphi_{lm}}{r}\right) Z_l^m + \frac{\varphi_{lm}}{r^2} \frac{\partial Z_l^m}{\partial x} \vec{e_x} + \frac{\varphi_{lm}}{r^2 \sin x} \frac{\partial Z_l^m}{\partial \varphi} \vec{e_\varphi} \right] \right|^2.$$

Expanding the square and noting that all $2ab$ terms vanish because of the dot products, we get:

$$\int d\Omega \sum_{ll'mm'} \left[\frac{\partial}{\partial r}\left(\frac{\varphi_{lm}}{r}\right) \frac{\partial}{\partial r}\left(\frac{\varphi_{l'm'}}{r}\right) Z_l^m Z_{l'}^{m'} + \frac{\varphi_{lm}\varphi_{l'm'}}{r^4} \frac{\partial Z_l^m}{\partial x} \frac{\partial Z_{l'}^{m'}}{\partial x} + \frac{\varphi_{lm}\varphi_{l'm'}}{r^4 \sin^2 x} \frac{\partial Z_l^m}{\partial \phi} \frac{\partial Z_{l'}^{m'}}{\partial \phi} \right]. \tag{2.3.5}$$

Since the φ_{lm} is a function of r only, it can be taken out of the integral, and the first term is evaluated using the completeness as:

$$\sum_{ll'mm'} \frac{\partial}{\partial r}\left(\frac{\varphi_{lm}}{r}\right) \frac{\partial}{\partial r}\left(\frac{\varphi_{l'm'}}{r}\right) \int d\Omega Z_l^m Z_{l'}^{m'} = \sum_{lm} \left[\frac{\partial}{\partial r}\left(\frac{\varphi_{lm}}{r}\right) \right]^2. \tag{2.3.6}$$

Similarly calculating the other terms, we finally get:

$$\mathcal{H} = \frac{1}{2} \int r^2\, dr \sum_{lm} \left[\left(\frac{\partial}{\partial r}\left(\frac{\varphi_{lm}}{r}\right) \right)^2 + \frac{l(l+1)}{r^4} \varphi_{lm}^2 + m^2 \frac{\varphi_{lm}^2}{r^2} + \frac{\pi_{lm}^2}{r^2} \right]$$

$$\implies \mathcal{H} = \frac{1}{2} \sum_{lm} \int dr \left[r^2 \left\{ \frac{\partial}{\partial r}\left(\frac{\varphi_{lm}}{r}\right) \right\}^2 + \left(\frac{l(l+1)}{r^2} + m^2 \right) \varphi_{lm}^2 + \pi_{lm}^2 \right]. \tag{2.3.7}$$

2.3.2 Discretization and connection with harmonic chain result

To connect to the results obtained in (1.3.6), we need to have a discrete theory. We discretize the theory by working in a lattice of spacing a, where now $r = j.a \implies \int dr \to a \sum_i$. Since we do not sum overall space but rather over a spherical box of

radius $L = (N+1)a$, we demand the field vanishes at points farther than $L = Na$. This is the relevant boundary condition. For the first term in curly brackets, we can use the midpoint discretization:

$$r^2\left\{\frac{\partial}{\partial r}\left(\frac{\varphi_{lm}(r)}{r}\right)\right\}^2 \to (j+\frac{1}{2})^2\left\{\frac{\frac{\varphi_{lm}(j+1)}{j+1}-\frac{\varphi_{lm}(j)}{j}}{(j+1)-(j)}\right\}^2 = (j+\frac{1}{2})^2\left\{\frac{\varphi_{lm}(j+1)}{j+1}-\frac{\varphi_{lm}(j)}{j}\right\}.$$

The $j+\frac{1}{2}$ can be thought of being chosen as the midpoint between j and $j+1$ to give a better estimate for the area, i.e $f(x)\partial_x g \to f_{j+\frac{1}{2}}\left(\frac{g_{j+1}-g_j}{a}\right)$.

We can now write the Hamiltonian as:

$$\mathcal{H} = \frac{1}{a}\sum_{lm}\frac{1}{2}\sum_{j}\left[(j+\frac{1}{2})^2\left\{\frac{\varphi_{lm}(j+1)}{j+1}-\frac{\varphi_{lm}(j)}{j}\right\}^2+\left(\frac{l(l+1)}{j^2}+a^2m^2\right)\varphi_{lmj}^2+\pi_{lmj}^2\right].$$

$$= \frac{1}{a}\sum_{lm}\tilde{\mathcal{H}}_{lm} \tag{2.3.8}$$

Now we can connect this to (2.2.1). The square terms in the curly bracket and terms in φ^2 bracket contribute to the diagonal elements of K, and the $2ab$ terms will get split into the off-diagonal terms. Each $\tilde{\mathcal{H}}_{lm}$ will contribute a term to the ground state and hence the density matrix. Hence as in the harmonic chain, the total entropy will be the sum of entropies of $\tilde{\mathcal{H}}_{lm}$'s. In particular, since (2.3.8) is independent of m, the m summation just gives out $2l+1$. With that, the total entropy is given by

$$\boxed{S = \sum_{lm} S_{lm}(\xi_i(n,N)) = \sum_{l}(2l+1)S_l(\xi_i(n,N)).} \tag{2.3.9}$$

As in the harmonic chain, n corresponds to the number of oscillators traced out. With this, we can numerically find S for a given size of the system N and n. Since the area of the "sphere" now depends on the number of oscillators we are tracing out, we define the radius of the sphere to be $R = (n+\frac{1}{2})a$. This gives the endpoint of the radius vector to be between the nth integrated out oscillator and the $(n+1)$th oscillator, which is not integrated.

We can now choose different n, corresponding to choosing a bigger sphere (whose entropy we are calculating). The graph is shown below in (Fig. 2.1) and fits beautifully by the line $S = 0.3\frac{R^2}{a^2}$. Note that this result is for $m = 0$.

Note here that the entropy still diverges in the continuum limit $a \to 0$. This straight-line behavior shows that the entanglement entropy of a scalar field follows an area law.

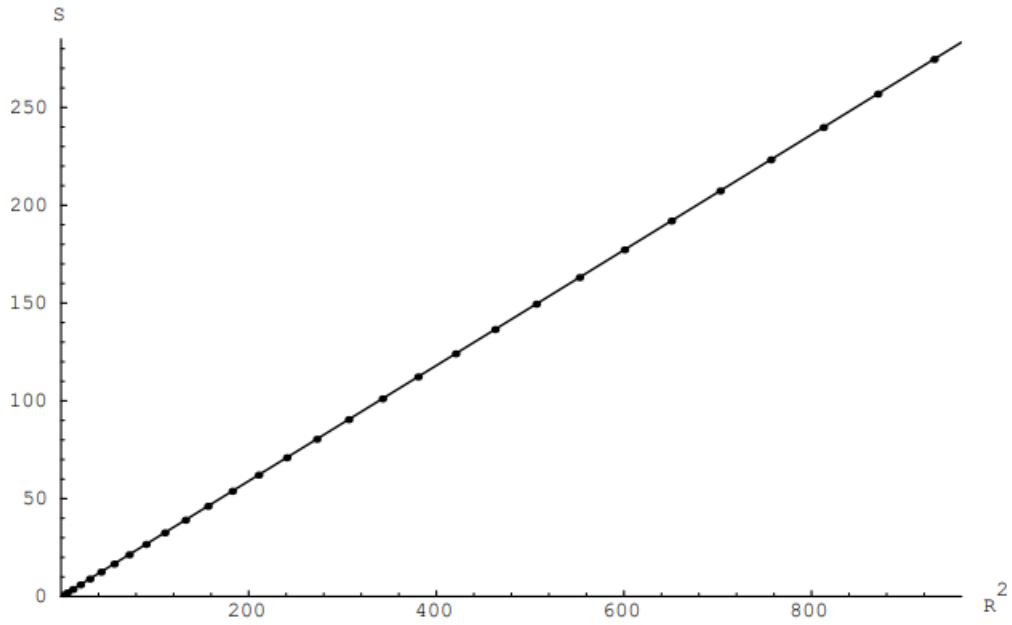


Figure 2.1: Entropy scaling with the variable R. Points here correspond to to a radial lattice discretization with N=60. Reprinted from [16]

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2.4 Massless scalar field in presence of a horizon

With all the examples done in this section, we can now finally move to the problem of finding the entanglement entropy of a scalar field in the presence of a horizon and confirm (1.3.6). We follow [15] for this section. Consider a free massless scalar field propagating in a spherically symmetric Black Hole space-time. We now ask what the Hamiltonian of such a system would be. The plan is to write the action on a spherical harmonic basis and then get the Hamiltonian.

2.4.1 The Hamiltonian

We start with the action for a free massive scalar field in a Black Hole space-time.

$$S = -\frac{1}{2}\int d^4x\sqrt{-g}.g_{\mu\nu}(\partial_\mu\varphi)(\partial_\nu\varphi).$$

The product $d^4x\sqrt{-g}$ is a quantity that is invariant under any co-ordinate changes. Now we need to choose a metric to work in. Black Hole space-times can be described by many metrics like Lemaitre, Kruskal, Painleve-gullstrand, Schwarzschild etc. We will work here in Lemaitre co-ordinates. The line element for this metric looks like

$$ds^2 = -d\tau^2 + \frac{r_c}{r}\,d\rho^2 + r^2(\,dx^2 + \sin^2 x\,d\phi^2). \tag{2.4.1}$$

And

$$\sqrt{-g} = \sqrt{-(-1).(\frac{r_c}{r}).(r^2).(r^2\sin^2 x)} = r^2\sqrt{\frac{r_c}{r}}\sin x.$$

$$S = -\frac{1}{2}\int d^4x.r^2\sqrt{\frac{r_c}{r}}\sin x\left[-(\partial_\tau\varphi)^2 + \frac{r_c}{r}(\partial_\rho\varphi)^2 + r^2(\partial_x\varphi)^2 + r^2\sin^2 x(\partial_\phi\varphi)^2\right].$$

As in the previous section, we change to the spherical harmonic basis and integrate out the angular variables using properties of spherical harmonics. After a little algebra, we get:

$$S = \int d\tau\,d\rho\sum_{lm}\frac{1}{2}\left[r^2\sqrt{\frac{r_c}{r}}(\partial_\tau\varphi_{lm})^2 - r^2\sqrt{\frac{r}{r_c}}(\partial_\rho\varphi_{lm})^2 - \sqrt{\frac{r_c}{r}}l(l+1)\varphi_{lm}^2\right]. \tag{2.4.2}$$

We now try to write down the Hamiltonian for this Lagrangian. Note that

$$\Pi_{lm} = \frac{\partial \mathcal{L}}{\partial(\partial_\tau \varphi_{lm})} = r^2\sqrt{\frac{r_c}{r}}(\partial_\tau \varphi_{lm}).$$

Using this, we finally get the Hamiltonian as

$$\mathcal{H} = \sum_{lm}\left\{\int_\tau^\infty d\rho \frac{1}{2}\left[\frac{1}{r^2}\sqrt{\frac{r}{r_c}}\Pi_{lm}^2 + r^2\sqrt{\frac{r}{r_c}}(\partial_\rho\varphi_{lm})^2 + \sqrt{\frac{r_c}{r}}l(l+1)\varphi_{lm}^2\right]\right\} = \sum_{lm} H_{lm}. \tag{2.4.3}$$

This Hamiltonian is time dependent because of the presence of ρ which is a function of time. Note that the Lemaitre co-ordinate only takes values from $(\tau, \infty]$. Now, for constant angular variables ($d\phi = \ dx = 0$) and a fixed proper time ($\tau = \tau_0$, wlog set $\tau_0 = 0$), we get from (2.4.1)

$$ds^2 = \frac{r_c}{r}\, d\rho^2 = \ dr^2. \tag{2.4.4}$$

The last equality can be obtained by using the relation between Schwazschild and Lemaitre co-ordinates. With that, we can replace $d\rho$ and ∂_ρ in favour of r and ∂_r. We finally write (2.4.3) as

$$\mathcal{H} = \sum_{lm}\left\{\int_0^\infty dr \frac{1}{2}\left[\frac{1}{r^2}\frac{r}{r_c}\Pi_{lm}^2 + r^2(\partial_r\varphi_{lm})^2 + l(l+1)\varphi_{lm}^2\right]\right\}. \tag{2.4.5}$$

We can already see the similarities between (2.4.5) and (2.3.8). To connect them, do a canonical transformation to absorb all factors outside Π. Finally we also divide φ by r^2 to reach the required equation. We hence have the transformation

$$\pi_{lm} = \frac{1}{r}.\sqrt{\frac{r}{r_c}}.\Pi_{lm}, \qquad\qquad \Phi_{lm} = \phi_{lm}.r,$$

$$\implies \mathcal{H} = \sum_{lm}\left\{\int dr \frac{1}{2}\left[\pi_{lm}^2 + r^2\left(\frac{\partial}{\partial r}\left(\frac{\Phi_{lm}}{r}\right)\right)^2 + l(l+1)\frac{\Phi_{lm}^2}{r^2}\right]\right\}. \tag{2.4.6}$$

Hence, this Hamiltonian takes the same form as for a scalar field that we have already solved! Therefore the entropy will have the same form as calculated in the last section. This result is only for one particular time slicing. Again note that in the continuum limit, the entanglement entropy diverges.

This method of calculating entropy used in this chapter usually resorts to doing numerical simulations to sum (2.3.9). This illustrates the general trend of the entanglement entropy well, but we can analytically solve this by using the *covariance method* as well. This analytical solution lets us tune the system in a controlled way. With it, we can also study properties of entanglement entropy that were earlier not known in full detail, for example, the log to log log crossover of the leading order term in entanglement entropy under a change in boundary conditions. Next, the analytical method helps understand this crossover better and explains precisely how the leading order term depends on the system's physical parameters in different boundary conditions.

Hence we will now focus on calculating the entanglement entropy of a scalar field using the covariance matrix method and understand its properties and divergence more carefully in the continuum limit.

Chapter 3

Entanglement entropy of a scalar field: Covariance matrix method

We start with the Hamiltonian for a scalar field in (1+1) dimensions and try to discretize this theory to connect it to (2.2.1). Unlike last chapter, we will not use the spherical harmonic basis. After that, we shall look at the covariance matrix is and how it is connected to the entanglement entropy. Then finally, we can find the covariance matrix for the scalar field and compute the entanglement entropy. The main idea of calculating its entanglement entropy using the covariance matrix in this chapter closely follows [17].

3.1 Discretizing the theory

We start with the Lagrangian of a massive scalar field in 1+1 dimensions

$$L = \int dx\mathcal{L} = \frac{1}{2}\int dx\Big(\partial^\mu\varphi\partial_\mu\varphi - m^2\varphi^2\Big) = \frac{1}{2}\int dx\Big(\dot{\varphi}^2 - (\nabla\varphi)^2 - m^2\varphi^2\Big).$$

We can now get the corresponding Hamiltonian density by a Legendre transformation. First we find the conjugate momentum:

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\varphi}} = \dot{\varphi}, \qquad \mathcal{H} = \pi\dot{\varphi} - \mathcal{L}.$$

The Hamiltonian is given by

$$H = \int dx \mathcal{H} = \frac{1}{2} \int dx \Big(\pi^2 + (\nabla \varphi)^2 + m^2 \varphi^2 \Big). \tag{3.1.1}$$

Now we discretize the space by working on a lattice with lattice spacing a and length $L = (N-1)a$. This means that $x \to x_n = an$, and hence $\int dx \to a \sum_{n=0}^{N-1}$. Moreover, we can write $\pi(x) = \frac{p_n}{a}$, as $\pi(x)$ was the momentum *density*. Finally, for the derivative term, we write $\nabla \varphi \to \frac{\varphi_{n+1} - \varphi_n}{a}$. With all this we write the Hamiltonian in (3.1.1) as:

$$H = \frac{a}{2} \sum_{n=0}^{N-1} \left[\frac{p_n^2}{a^2} + \Big(\frac{\varphi_{n+1} - \varphi_n}{a} \Big)^2 + m^2 \varphi_n^2 \right] = \frac{1}{2a} \sum_{n=0}^{N-1} \left[p_n^2 + \big(\varphi_{n+1} - \varphi_n \big)^2 + \underbrace{a^2 m^2}_{\Lambda} \varphi_n^2 \right] = \frac{\tilde{H}}{a}.$$

$\tilde{H}$ is the rescaled Hamiltonian. We intend to find the entanglement entropy. It can be shown that the rescaled Hamiltonian has the same entanglement entropy as the original Hamiltonian.[18] Keeping that in mind, we work only with the rescaled Hamiltonian.

$$\boxed{\tilde{H} = \frac{1}{2} \sum_{n=0}^{N-1} \left[p_n^2 + \big(\varphi_{n+1} - \varphi_n \big)^2 + \Lambda \varphi_n^2 \right].} \tag{3.1.2}$$

As before, we write it in the standard form of (2.2.1), where Λ and the φ_{n+1}, φ_n terms in the parenthesis will contribute to the diagonal elements of K (coupling matrix). The cross-terms ($2ab$ terms) will contribute to the off-diagonal entries. Note that we still need to choose the boundary condition, which will determine what values like φ_N etc. contribute to K. To understand the workings of the covariance matrix method, we take a detour to understand the fundamental properties of the covariance matrix.

3.2 Covariance matrix

In this section we look at the covariance matrix and how it helps us in the problem of calculating the entanglement entropy.

3.2.1 Whats covariance?

When dealing with a dataset, we can come up with many quantities that help us characterize the dataset's properties. For example, we have a few numbers in a plane. The average of these points would tell us roughly where their "center of mass" would lie. Similarly, we can talk about variance, which indicates how much points deviate from this average. A high variance dataset would look spread out, and a low variance would look clustered. However, consider the situation where a dataset looks like the (Fig. 3.1).

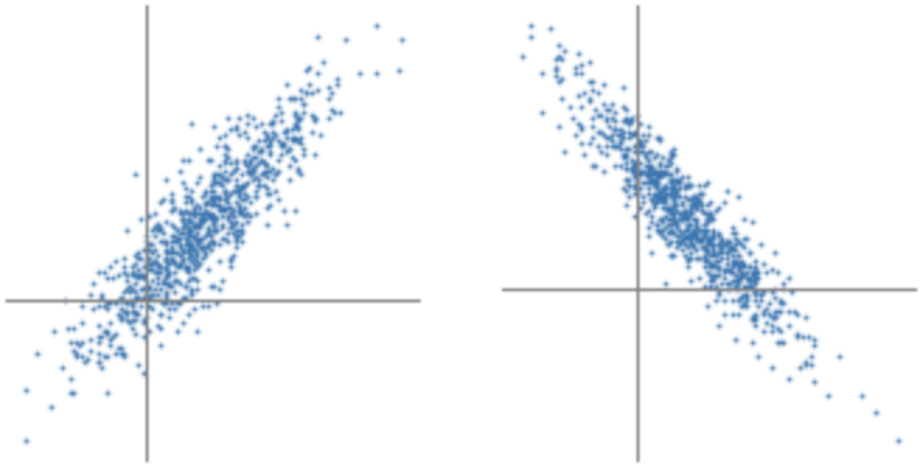


Figure 3.1: Dataset

If we were to calculate how they are spread, we would get the same answer. Nevertheless, they are two different datasets. How can we distinguish them? We look at how they vary with each other and how y changes when x changes. Clearly, in the left image, x increases as y increases, but it is the opposite for the right figure. Hence "covariance" is a valid statistical quantity. Mathematically, we can write it as:

$$Cov(X,Y) = \langle (X - \langle X \rangle)(Y - \langle Y \rangle) \rangle = \langle XY \rangle - \langle X \rangle \langle Y \rangle, \tag{3.2.1}$$

where $\langle X \rangle$ denotes the average value of X, or the expectation of X. Clearly, since we were looking how they "co-vary", we multiply the two increments and deduce from that. For example, consider a 2-D data set. One way to neatly put these statistical

quantities into a matrix form is as:

$$\gamma = \begin{pmatrix} Cov(X,X) & Cov(X,Y) \\ Cov(Y,X) & Cov(Y,Y) \end{pmatrix} = \begin{pmatrix} Var(X) & Cov(X,Y) \\ Cov(Y,X) & Var(Y) \end{pmatrix} = \begin{pmatrix} \sigma_{XX} & \sigma_{XY} \\ \sigma_{YX} & \sigma_{YY} \end{pmatrix}.$$

, where Var represents variance. This is called the *covariance matrix*. We algebraically write it as

$$\gamma_{kl} = \frac{1}{2}\langle X_k X_l + X_l X_k \rangle - \langle X_k \rangle \langle X_l \rangle. \tag{3.2.2}$$

3.2.2 Covariance matrix for a harmonic chain

Lets now try to find the covariance matrix for a harmonic chain. We take the general Hamiltonian to be like (2.2.1), i.e

$$\mathcal{H} = \hat{x}^T K \hat{x} + \hat{p}^T \mathbb{I} \hat{p}. \tag{3.2.3}$$

Here K is the coupling matrix. We now switch to the symplectic notation, where instead of working with x and p, we work with a single vector of dimension $2n$, with n of its components as x_i and n of them as p_i. i.e

$$R = \begin{pmatrix} x_1 \\ . \\ . \\ x_n \\ p_1 \\ . \\ . \\ p_n \end{pmatrix} = \begin{pmatrix} \mathbf{x} \\ \mathbf{p} \end{pmatrix}, \qquad \mathcal{H} = \hat{R}^T \begin{pmatrix} K & 0 \\ 0 & \mathbb{I} \end{pmatrix} \hat{R}. \tag{3.2.4}$$

Following the methods of [19, 20], we now wish to diagonalize $\mathcal{H}$ by a transformation. This procedure is technically the same as in section 2.2, but in symplectic notation. The variables x and p follow canonical commutation relations, i.e $[x_k, p_l] = i\delta_{kl}$. Under a transformation, we want the CCR to stay the same. This means the transformation has to be symplectic. It can be shown that in order to preserve the CCR, the matrices

S have to follow $S^T\Omega S = \Omega$, where $R \to SR$ and Ω has the form

$$\Omega = \begin{pmatrix} 0 & \mathbb{I}_{n\times n} \\ -\mathbb{I}_{n\times n} & 0 \end{pmatrix}, \qquad \text{CCR: } [R_k, R_l] = i\Omega_{kl}.$$

The matrices S then belong to the symplectic group $Sp(2n, \mathbb{R})$. We now choose such a transformation that diagonalizes the Hamiltonian. Since one of the diagonal terms in the Hamiltonian is identity, it makes the job easy. We postulate a symplectic transformation as

$$S = \begin{pmatrix} M & 0 \\ 0 & M \end{pmatrix}.$$

The condition $S^T\Omega S = \Omega$ can be trivially checked. We put the condition that M is an orthogonal matrix ($M^TM = \mathbb{I}$) and that M diagonalizes K ($M^TKM = D$ where D=Diag($d_1 \cdots d_n$), i.e. d_i are eigenvalues of K). Using this in (3.2.4), we get

$$\mathcal{H} = \hat{R'}^T S^T \begin{pmatrix} K & 0 \\ 0 & \mathbb{I} \end{pmatrix} S\hat{R'} = \hat{R'}^T \begin{pmatrix} M^TKM & 0 \\ 0 & M^TM \end{pmatrix} \hat{R'} = \hat{R'}^T \begin{pmatrix} D & 0 \\ 0 & \mathbb{I} \end{pmatrix} \hat{R'}.$$

Hence we have successfully diagonalized the Hamiltonian by going into the R' basis. As seen before, this corresponds to uncoupling of all the oscillators. The Hamiltonian in x and p now has the form

$$\mathcal{H} = \hat{x'}^T D\hat{x'} + \hat{p'}^T\mathbb{I}\hat{p'} = \sum_i d_i^2 x'^2_i + \sum_i p'^2_i = \sum_{i=1}^{n}(d_i^2 x'^2_i + p'^2_i). \tag{3.2.5}$$

We want to write this in terms of creation and annihilation operators. Consider the product $(a+ib)(a-ib)$. Clearly

$$(a+ib)(a-ib) = a^2 - iab + iba + b^2 \implies a^2 + b^2 = (a+ib)(a-ib) + i[a,b]. \tag{3.2.6}$$

For $a = d_i^{\frac{1}{2}} x'_i$ and $b = p'_i$ in (3.2.6), and with some rearranging we get

$$\mathcal{H} = \sum_i \left[\left(d_i^{\frac{1}{2}} x'_i + ip'_i\right)\left(d_i^{\frac{1}{2}} x'_i - ip'_i\right) + i[d_i^{\frac{1}{2}} x'_i, p'_i] \right] = \sum_i \left[\left(d_i^{\frac{1}{2}} x'_i + ip'_i\right)\left(d_i^{\frac{1}{2}} x'_i - ip'_i\right) - d_i^{\frac{1}{2}} \right]$$

$$\implies \sum_i 2d_i^{\frac{1}{2}} \left[\underbrace{\left(\frac{id_i^{\frac{1}{2}} x'_i - p'_i}{\sqrt{2d_i}}\right)}_{a_i^\dagger} \underbrace{\left(\frac{id_i^{\frac{1}{2}} x'_i + p'_i}{\sqrt{2d_i}}\right)}_{a_i} + \frac{1}{2} \right] = \sum_i 2d_i^{\frac{1}{2}} \left[a_i^\dagger a_i + \frac{1}{2} \right]. \tag{3.2.7}$$

Hence we have broken the system into harmonic oscillators. This is no different to what we did before. Diagonalizing the Hamiltonian converts the chain to a set of uncoupled harmonic oscillators. Now we try to find the covariance matrix for the ground state, i.e a gaussian state.

Covariance matrix for a single oscillator

Let us take the example of a single oscillator and find its covariance matrix. The Hamiltonian for a single oscillator is

$$\mathcal{H} = \frac{1}{2}\Big[p^2 + \omega^2 x^2\Big]. \tag{3.2.8}$$

In the symplectic notation, we have

$$\mathcal{H} = R^T \begin{pmatrix} \frac{\omega^2}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} R. \tag{3.2.9}$$

Quantum averages can be calculated with the help of the density matrix by $\langle O\rangle = \mathrm{Tr}(\rho O)$. Using this in (3.2.1), we can get the form of covariance matrix as

$$\gamma_{kl} = \langle (R_k - \langle R_k\rangle)(R_l - \langle R_l\rangle)\rangle = \mathrm{Tr}\big[\rho(R_k - \langle R_k\rangle)(R_l - \langle R_l\rangle)\big],$$

$$= \mathrm{Tr}\big[\rho(R_k - \mathrm{Tr}(\rho R_k))(R_l - \mathrm{Tr}(\rho R_k))\big].$$

Now for the ground state of the oscillator, $\rho = |0\rangle\langle 0|$. The first moments are zero and the covariance matrix expression just becomes $\sigma_{kl} = \mathrm{Tr}\big[\rho \hat{R}_k \hat{R}_l\big]$. Now we can write the $\hat{x}$ and $\hat{p}$ in terms of creation and annihilation operators. As an example we can calculate σ_{XX}:

$$x = \frac{1}{\sqrt{2\omega}}\big(a + a^\dagger\big) \implies \gamma_{XX} = \frac{1}{2\omega}\mathrm{Tr}\Big[|0\rangle\langle 0|\big(a^2 + {a^\dagger}^2 + aa^\dagger + a^\dagger a\big)\Big]$$

$$= \frac{1}{2\omega}\mathrm{Tr}\Big[\langle 0|\big(a^2 + {a^\dagger}^2 + aa^\dagger + a^\dagger a\big)|0\rangle\Big] = \frac{1}{2\omega}.$$

We can calculate other components similarly. The final covariance matrix reads

$$\sigma = \frac{1}{2}\begin{pmatrix} \frac{1}{\omega} & 0 \\ 0 & \omega \end{pmatrix}. \tag{3.2.10}$$

Coming back to harmonic chain

In the new basis R', we have n uncoupled oscillators. In this basis, the covariance matrix γ' would be diagonal as well! Each oscillator will have a covariance matrix like (3.2.10). In the single oscillator problem we had ω^2 as the factor before x^2 and in chain Hamiltonian we had the matrix K. In the diagonal basis each harmonic oscillator will have frequency $\omega^2 = d_i$. Therefore the covariance matrix of a single oscillator would look like

$$\sigma_i = \frac{1}{2}\begin{pmatrix} \frac{1}{\sqrt{d_i}} & 0 \\ 0 & \sqrt{d_i} \end{pmatrix}.$$

Hence the covariance matrix has $\gamma'_{ii} = \frac{1}{2\sqrt{d_i}}$ for $i \leq n$ and $\gamma'_{ii} = \frac{\sqrt{d_i}}{2}$ for $i > n$, and all off diagonal terms zero. Finally, we can switch back to the old basis and get the desired γ by the transformation

$$\gamma = S^T \gamma' S = \begin{pmatrix} M^T & 0 \\ 0 & M^T \end{pmatrix} \gamma' \begin{pmatrix} M & 0 \\ 0 & M \end{pmatrix} = \frac{1}{2}\begin{pmatrix} K^{-\frac{1}{2}} & 0 \\ 0 & K^{\frac{1}{2}} \end{pmatrix}. \tag{3.2.11}$$

3.2.3 Covariance matrix and its link to entanglement entropy

Thermal states

A density matrix that represents Gaussian states is the thermal density matrix. Hence, calculating any quantity in a gaussian state can be done by taking its density matrix as a thermal density matrix. We now derive a few results for the thermal density matrix. [21]

Let us take an m-mode thermal state. The thermal density matrix will be the direct product of all individual density matrices, since they are independent modes. Just as in last section, the covariance matrix is the direct sum of all individual covariance matrices:

$$\rho = \bigotimes_{k=1}^{m} \rho_{th}(n_k), \qquad \gamma_{th} = \bigoplus_{k=1}^{m} \gamma_k,$$

where n_k is the occupation number of the kth mode. This clearly means the covariance matrix is diagonal. We now use virial theorem. Virial theorem states that

$$\text{If } V \propto r^a \implies \langle T \rangle = \frac{a}{2}\langle V \rangle.$$

For $a = 2$, $\langle T\rangle = \langle V\rangle = \frac{E}{2}$. Since total energy is just ($\hbar = 1$): $E = \omega_k(n_k + \frac{1}{2})$, we have

$$\frac{1}{2}\omega_k^2\langle x_k^2\rangle = \frac{1}{2}\omega_k\big(n_k + \frac{1}{2}\big), \qquad \frac{1}{2}\langle {p_k}^2\rangle = \frac{1}{2}\omega_k\big(n_k + \frac{1}{2}\big),$$

$$\langle x_k^2\rangle = \frac{1}{2\omega_k}\big(2n_k + 1\big), \qquad \langle {p_k}^2\rangle = \frac{\omega_k}{2}\big(2n_k + 1\big). \tag{3.2.12}$$

These values in (3.2.12) are the variances, which are exactly the diagonal elements we want. With that we can write the covariance matrix as

$$\gamma_k = \begin{pmatrix} \frac{1}{\omega_k}\big(n_k + \frac{1}{2}\big) & 0 \\ 0 & \omega_k\big(n_k + \frac{1}{2}\big) \end{pmatrix}. \tag{3.2.13}$$

Finally, we can perform a canonical transformation in (3.2.13) $x_k \to x_k\sqrt{\omega_k}$ and $p_k \to \frac{p_k}{\sqrt{\omega_k}}$ (It leaves the CCR unchanged as products remain unchanged!). The covariance matrix has the form

$$\gamma_k = \begin{pmatrix} n_k + \frac{1}{2} & 0 \\ 0 & n_k + \frac{1}{2} \end{pmatrix}. \tag{3.2.14}$$

Hence the eigenvalues are

$$\lambda_k = n_k + \frac{1}{2} \implies n_k = \lambda_k - \frac{1}{2}. \tag{3.2.15}$$

Now with that result, we calculate the total entropy in this thermal state of m modes by

$$S = \sum_{k=1}^{m} S(\rho_{th}(n_k)). \tag{3.2.16}$$

Density matrix for thermal states

We now derive an expression for $\rho_{th}(n_k)$. In the thermal state, the system can be in any of the states $|0\rangle, |1\rangle, \cdots |n\rangle$ with probability of being in that state being proportional to $\exp\{-\beta E_n\} = \exp\{-\beta\omega n\}$. We consider this statistical mixture and hence write down the expression of the density matrix as

$$\rho = \sum_{n=0}^{\infty} \frac{\exp\{-\beta\omega n\}}{Z}|n\rangle\langle n|. \tag{3.2.17}$$

First, we calculate the partition function by simply tracing the operator or summing all probabilities to 1, i.e

$$Z = \sum_{n=0}^{\infty} \exp\{-\beta\omega n\} = \frac{1}{1-\exp\{-\beta\omega\}}. \tag{3.2.18}$$

Where we have summed the infinite geometric progression. Next we want to write this in terms of the average number, so we calculate average number of quanta in the mode by $\langle n\rangle = \mathrm{Tr}(\rho n)$, i.e

$$\langle n\rangle = \sum_{n=0}^{\infty} n\frac{\exp\{-\beta\omega n\}}{Z}. \tag{3.2.19}$$

We use a similar trick we used in (2.1.6) to solve this sum.

$$\langle n\rangle = \sum_{n=0}^{\infty} n\frac{\exp\{-\beta\omega n\}}{Z} = \sum_{n=0}^{\infty} \frac{\partial}{\partial(\beta\omega)}\Big(\frac{-\exp\{-\beta\omega n\}}{Z}\Big) = \frac{-1}{Z}\frac{\partial}{\partial(\beta\omega)}\sum_{n=0}^{\infty} -\exp\{\beta\omega n\}$$

$$= \frac{-1}{Z}\frac{\partial}{\partial(\beta\omega)}\frac{1}{1-\exp\{-\beta\omega\}} = \frac{1}{Z}\frac{\exp\{-\beta\omega\}}{(1-\exp\{-\beta\omega\})^2} = \frac{\exp\{-\beta\omega\}}{1-\exp\{-\beta\omega\}}. \tag{3.2.20}$$

Where in the last equality we used (3.2.18). We now invert this relation to find the exponential in terms of the average as

$$\exp\{-\beta\omega\} = \frac{\langle n\rangle}{1+\langle n\rangle}. \tag{3.2.21}$$

Finally, we put (3.2.18) and (3.2.21) into the expression (3.2.17) to get

$$\rho = \sum_{n=0}^{\infty} \frac{\langle n\rangle^n}{(\langle n\rangle+1)^{n+1}}|n\rangle\langle n|. \tag{3.2.22}$$

Entropy for thermal states

Before we can finally go back to (3.2.16), we need to calculate the entropy for a given thermal state. We do that by computing

$$S(\rho_{th}(\langle n_k\rangle)) = -\sum_{j=0}^{\infty} \frac{\langle n_k\rangle^j}{(1+\langle n_k\rangle)^{j+1}} \ln\left(\frac{\langle n_k\rangle^j}{(1+\langle n_k\rangle)^{j+1}}\right)$$

$$= -\sum_{j=0}^{\infty} \frac{\langle n_k\rangle^j}{(1+\langle n_k\rangle)^{j+1}} \ln\left(\langle n_k\rangle^j\right) + \sum_{j=0}^{\infty} \frac{\langle n_k\rangle^j}{(1+\langle n_k\rangle)^{j+1}} \ln\left((1+\langle n_k\rangle)^{j+1}\right).$$

Taking $y = \frac{\langle n \rangle}{1+\langle n \rangle}$

$$= -\frac{\ln\langle n_k\rangle}{1+\langle n_k\rangle}\sum_{j=0}^{\infty} j y^j + \frac{\ln(1+\langle n_k\rangle)}{1+\langle n_k\rangle}\sum_{j=0}^{\infty}(1+j)y^j.$$

These sums again can be done using (2.1.6). The expression then becomes

$$= -\frac{\ln\langle n_k\rangle}{1+\langle n_k\rangle}\frac{y}{(1-y)^2} + \frac{\ln(1+\langle n_k\rangle)}{1+\langle n_k\rangle}\Big[\frac{1}{1-y} + \frac{y}{(1-y)^2}\Big]$$

$$= -\langle n_k\rangle \ln\langle n_k\rangle + (1+\langle n_k\rangle)\ln(1+\langle n_k\rangle).$$

Finally we put this in (3.2.16) to get the total entropy of a thermal field with m modes as

$$S = \sum_{k=1}^{m}\Big[-\langle n_k\rangle \ln\langle n_k\rangle + (1+\langle n_k\rangle)\ln(1+\langle n_k\rangle)\Big]. \tag{3.2.23}$$

Linking covariance matrices to thermal states and entanglement entropy

We now use *Williamson's theorem*, which states that every positive semi-definite $2n \times 2n$ matrix can be diagonalized via a symplectic transformation to the form

$$\begin{pmatrix} \lambda_1 & & & & & \\ & \ddots & & & & \\ & & \lambda_n & & & \\ & & & \lambda_1 & & \\ & & & & \ddots & \\ & & & & & \lambda_n \end{pmatrix}. \tag{3.2.24}$$

We see that the eigenvalues repeat! We had seen a similar expression for the covariance matrix in (3.2.14). This was to be expected, as the covariance matrix is a $2n \times 2n$ dimensional semi definite matrix, to which Williamson's theorem applies. In the symplectic notation, the CCR's are preserved when the transformation is symplectic. On the other hand, when working in Hilbert spaces and dealing with state vectors etc, unitary transformations preserve CCR's. Nothing physical is changing, only the space in which we work and the kind of vectors change (along with how they transform). But physically both of these transformations represent the same thing,

i.e a symplectic transformation in phase space is equivalent to a unitary transformation in Hilbert space. Every gaussian state is equivalent to a thermal state. Hence (3.2.15) is justified. Using (3.2.15) in (3.2.23), we finally have for a gaussian state, the entropy in terms of the eigenvalues of the covariance matrix as

$$S = \sum_{k=1}^{m} \left[-\left(\lambda_k - \frac{1}{2}\right) \ln\left(\lambda_k - \frac{1}{2}\right) + \left(\lambda_k + \frac{1}{2}\right) \ln\left(\lambda_k + \frac{1}{2}\right) \right]. \tag{3.2.25}$$

3.3 Calculation of entanglement entropy

We now return to (3.1.2) and calculate the entanglement entropy. The Hamiltonian had the form

$$\tilde{H} = \frac{1}{2} \sum_{n=0}^{N-1} \left[p_n^2 + \left(\varphi_{n+1} - \varphi_n\right)^2 + \Lambda \varphi_n^2 \right].$$

We calculate the coupling matrix for a given boundary condition. We will compute the covariance matrix using (3.2.11). We will then form the reduced covariance matrix by tracing out all oscillators but one, calculate its eigenvalues to use them in (3.2.25) and calculate the entropy.

3.3.1 Form of coupling matrix: Boundary conditions

Dirichlet boundary condition

In this boundary condition, we specify the exact value of the field at the boundary. Here we set it to zero. Remember that there are N oscillators in the discrete setting we have. That is $\varphi_0 = \varphi_{N+1} = 0$. Hence K has the form

$$K = \begin{pmatrix} \Lambda+2 & -1 & & & \\ -1 & \Lambda+2 & -1 & & \\ & & \ddots & & \\ & & -1 & \Lambda+2 & -1 \\ & & & -1 & \Lambda+2 \end{pmatrix}. \tag{3.3.1}$$

All the elements not on the diagonal or the diagonals adjacent to the diagonals are zero. We now want to diagonalize this matrix in order to calculate $G = K^{\frac{1}{2}}$. The

eigenvalues and eigenvectors can be found by solving the difference equation $G\mathbf{x} = \lambda\mathbf{x}$ and is done in [appendix B, see (B.1.15), (B.2.4)]. The jth eigenvalue is given by

$$\lambda_j = \Lambda + 4\cos^2\left(\frac{j\pi}{2(N+1)}\right). \tag{3.3.2}$$

Furthermore, the jth component of the kth eigenvector is given by:

$$(x_k)_j = \sqrt{\frac{2}{N+1}}\sin\left(\frac{jk\pi}{N+1}\right). \tag{3.3.3}$$

We hence create a matrix encapsulating all these eigenvectors. We just stack all the eigenvectors, with each eigenvector as one separate column. This matrix then has the elements

$$M_{jm} = \sqrt{\frac{2}{N+1}}\sin\left(\frac{jm\pi}{N+1}\right). \tag{3.3.4}$$

Now, lets go into the eigenbasis. In the eigenbasis, the covariance matrix is given by (3.2.11), i.e

$$\gamma' = \frac{1}{2}\begin{pmatrix} \mathrm{diag}\left(\frac{1}{\lambda_j{}^{\frac{1}{2}}}\right) & 0 \\ 0 & \mathrm{diag}\left(\lambda_j{}^{\frac{1}{2}}\right) \end{pmatrix}. \tag{3.3.5}$$

As before, we switch back to the original basis by $\gamma = M^T\gamma' M$, so we get

$$\gamma = \frac{1}{2}\begin{pmatrix} M^T\mathrm{diag}\left(\frac{1}{\lambda_j{}^{\frac{1}{2}}}\right)M & 0 \\ 0 & M^T\mathrm{diag}\left(\lambda_j{}^{\frac{1}{2}}\right)M \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}. \tag{3.3.6}$$

Now we calculate elements of A and B explicitly. For A, the elements take the form

$$\begin{aligned} A_{lm} &= \frac{1}{2}\left(M^T\mathrm{diag}\left(\frac{1}{\lambda_j{}^{\frac{1}{2}}}\right)M\right)_{lm} = \frac{1}{2}\sum_j M_{jl}\frac{1}{\lambda_j{}^{\frac{1}{2}}}M_{jm} \\ &= \sum_j \frac{1}{\lambda_j{}^{\frac{1}{2}}}\frac{1}{N+1}\sin\left(\frac{jl\pi}{N+1}\right)\sin\left(\frac{jm\pi}{N+1}\right). \end{aligned} \tag{3.3.7}$$

And similarly for B the elements take the form

$$\begin{aligned} B_{lm} &= \frac{1}{2}\left(M^T\mathrm{diag}\left(\lambda_j{}^{\frac{1}{2}}\right)M\right)_{lm} = \frac{1}{2}\sum_j M_{jl}\lambda_j{}^{\frac{1}{2}}M_{jm} \\ &= \sum_j \lambda_j{}^{\frac{1}{2}}\frac{1}{N+1}\sin\left(\frac{jl\pi}{N+1}\right)\sin\left(\frac{jm\pi}{N+1}\right). \end{aligned} \tag{3.3.8}$$

Hence we have the covariance matrix. We now trace out all oscillators except one and look at its entanglement entropy. For ease of calculation and avoid fractions like $\frac{N}{2}$, we instead take a system of $2N$ oscillators and integrate out every oscillator except the Nth one. Note that in all the above expressions, $N \to 2N$. The reduced density matrix can be constructed by manually picking the N, N element of the covariance matrix, i.e:

$$\gamma_{red} = \begin{pmatrix} A_{NN} & 0 \\ 0 & B_{NN} \end{pmatrix}. \tag{3.3.9}$$

We now intend to use the determinant to calculate the eigenvalues of this covariance matrix (which are equal by Williamson's theorem). For a single-mode, from (3.2.25) we get

$$S = \left[-\left(\sqrt{\det\gamma} - \frac{1}{2}\right)\ln\left(\sqrt{\det\gamma} - \frac{1}{2}\right) + \left(\sqrt{\det\gamma} + \frac{1}{2}\right)\ln\left(\sqrt{\det\gamma} + \frac{1}{2}\right)\right]. \tag{3.3.10}$$

In the limit that the determinant term dominates, we get

$$\boxed{S \approx \frac{1}{2}\ln(\det\gamma).} \tag{3.3.11}$$

To find the entropy, we hence calculate the determinant as

$$\det\gamma_{red} = A_{NN}.B_{NN} =$$
$$= \sum_{i=1}^{2N} \frac{1}{\lambda_i{}^{\frac{1}{2}}} \frac{1}{2N+1} \sin^2\left(\frac{i2N\pi}{2N+1}\right). \sum_{j=1}^{2N} \lambda_j{}^{\frac{1}{2}} \frac{1}{2N+1} \sin^2\left(\frac{j2N\pi}{2N+1}\right).$$

Here we can simplify this expression by working in the large N limit where $\sin^2\left(\frac{i.2N.\pi}{2N+1}\right) \approx \sin^2(i\pi) = 0$ for i even and $= 1$ for i odd. Hence now' only the odd terms survive. Renaming the summation over odd numbers and putting the values for the eigenvalues we get

$$\det\gamma_{red} \approx \sum_{k,l=1}^{N} \frac{1}{(2N+1)} \frac{1}{\lambda_i{}^{\frac{1}{2}}}. \sum_{l=1}^{N} \frac{1}{(2N+1)} \lambda_l{}^{\frac{1}{2}}$$

$$\boxed{\implies \det\gamma_{red} \approx \sum_{k,l=1}^{N} \frac{1}{(2N+1)^2} \frac{\sqrt{\Lambda + 4\cos^2\left(\frac{(2l-1)\pi}{2(2N+1)}\right)}}{\sqrt{\Lambda + 4\cos^2\left(\frac{(2k-1)\pi}{2(2N+1)}\right)}}.} \tag{3.3.12}$$

Neumann boundary condition

Before we calculate the entropy using the result derived above, we do the same procedure done above to a different boundary condition and then compare the results. In this boundary condition, we set the derivative of the field zero at the boundary. This implies $\partial_x\varphi = 0 \implies \varphi_0 = \varphi_1$ and $\varphi_N = \varphi_{N+1}$. The resulting form of the K matrix is

$$K = \begin{pmatrix} \Lambda+1 & -1 & & & \\ -1 & \Lambda+2 & -1 & & \\ & & \ddots & & \\ & & -1 & \Lambda+2 & -1 \\ & & & -1 & \Lambda+1 \end{pmatrix}. \tag{3.3.13}$$

The eigenvalues and eigenvectors can again be calculated in a similar way. The eigenvalues are

$$\lambda_j = \Lambda + 4\cos^2\left(\frac{k\pi}{2N}\right). \tag{3.3.14}$$

Note that there is a possibility of $\lambda = 0$ above even for finite N, if $\Lambda = 0$. This was not true for Dirichlet for finite N. The jth component of the kth eigenvector is given by

$$\begin{aligned} (x_k)_j &= \sqrt{\frac{2}{N}}\sin\left(\frac{(2j-1)k\pi}{2N}\right) && \text{for } k = 1, 2, 3\cdots N-1, \\ &= \frac{(-1)^{j-1}}{\sqrt{N}} && \text{for } k = N. \end{aligned}$$

Repeating the same procedure, we get γ_{red} as

$$\det\gamma_{red} = \frac{1}{4N^2}\left[\frac{1}{2\sqrt{\Lambda}} + \sum_{k=1}^{N-1}\frac{1}{\sqrt{\Lambda + 4\cos^2\left(\frac{(2k-1)\pi}{4N}\right)}}\right]\left[\frac{\sqrt{\Lambda}}{2} + \sum_{l=1}^{N-1}\sqrt{\Lambda + 4\cos^2\left(\frac{(2l-1)\pi}{4N}\right)}\right]. \tag{3.3.15}$$

With the form of $\det\gamma_{red}$ for DBC and NBC, we can compute the entanglement entropy for these boundary conditions by using (3.3.11). Given these expressions, we

now show that in this description, entanglement entropy shows different behavior at leading order in different limits of a variable called ζ.

3.3.2 Relative spacing (ζ)

In the continuum limit of the discretized theory, $a \to 0$ and $N \to \infty$. We now look for the different behavior of entanglement entropy when a combination of these parameters is taken in different limits, i.e., we analyze for a crossover in behavior. We look at the quantity relative spacing, which is the spacing between the two lowest-lying modes in the system, scaled by the parameter Λ, i.e.

$$\zeta = \frac{\Delta\lambda}{\Lambda}. \tag{3.3.16}$$

This choice of examining the behavior of entanglement entropy in different limits, specifically in this form of ζ, is unmotivated. Upon computing the entropy, we will see the change in behavior at leading order. We now calculate ζ for various boundary conditions and examine the entanglement entropy.

For DBC, we have (eqn (3.3.2))

$$\lambda_j = \Lambda + 4\cos^2\left(\frac{k\pi}{2(2N+1)}\right).$$

We can see that in the cosine argument, we have $\cos\big(\text{fraction} \times \frac{\pi}{2}\big)$, and the cosine function decreases in that range. This means the lowest lying levels are $k = N$ and $k = N-1$. Therefore ζ is given by

$$\zeta_{DBC} = \frac{\lambda_{2N-1} - \lambda_{2N}}{\Lambda}. \tag{3.3.17}$$

We can see that in large N limit we have

$$\lambda_{2N-1} = \Lambda + 4\cos^2\left(\frac{(2N-1)\pi}{2(2N+1)}\right) = \Lambda + 4\cos^2\left(\frac{\pi}{2} - \frac{\pi}{2N+1}\right) = \Lambda + 4\sin^2\left(\frac{\pi}{2N+1}\right)$$
$$\approx \Lambda + \frac{\pi^2}{N^2}.$$

Calculating similarly for the other term, and putting together we get

$$\zeta_{DBC} = \frac{3\pi^2}{4N^2\Lambda} = \frac{3\pi^2}{4N^2a^2m^2}. \tag{3.3.18}$$

We can do the same for NBC as well, and we get the result

$$\zeta_{NBC} = \frac{\pi^2}{4N^2\Lambda} = \frac{\pi^2}{4N^2a^2m^2}. \tag{3.3.19}$$

Now, in the continuum limit $a \to 0$ and $N \to \infty$. Looking at the denominator of (3.3.18) and (3.3.19), we can see that we have two clear scenarios:

- Rate of increase of $N >$ Rate of decrease of a or m

  $\implies$ $\zeta << 1$ as denominator is rapidly increasing. Note that this actually corresponds to the limit $L = Na \to \infty$, which is the thermodynamic limit.

- Rate of increase of $N <$ Rate of decrease of a or m

  $\implies$ $\zeta >> 1$ as denominator is rapidly decreasing.

We consider these two limits now and calculate entanglement entropy in these limits.

3.3.3 Calculation of entanglement entropy

Small relative spacing

We have shown for both boundary conditions that in small relative separation,

$$\frac{\pi^2}{N^2\Lambda} \ll 1. \tag{3.3.20}$$

- **DBC**

  Since $N \to \infty$, we can replace the sum in (3.3.12) by an integral. We start with looking at the argument of the cosine

$$\frac{(2k-1)\pi}{2(2N+1)} \approx \frac{k\pi}{2N} = \frac{r}{N}, \qquad \frac{r}{N} \in \left[\frac{\pi}{2(2N+1)}, \frac{(2N-1)\pi}{2(2N+1)}\right] \approx \left[\frac{\pi}{4N}, \frac{\pi}{2}\left[1-\frac{1}{2N}\right]\right]$$
$$\approx \left[0, \frac{\pi}{2}\right].$$

Equation (3.3.12) then takes the form

$$\det \gamma_{red} \approx \lim_{N\to\infty} \sum_{\frac{r}{N}=0}^{\frac{\pi}{2}} \frac{1}{N} \frac{1}{\sqrt{\Lambda + 4\cos^2(\frac{r}{N})}} . \sum_{\frac{r}{N}=0}^{\frac{\pi}{2}} \frac{1}{N} \sqrt{\Lambda + 4\cos^2\left(\frac{r'}{N}\right)}.$$

In the limit $N \to \infty$, $\sum \frac{1}{N} \to \int dx$ and $\frac{r}{N} \to x$, the determinant then takes the form

$$\begin{aligned}
&\int_0^{\frac{\pi}{2}} \frac{dx}{\sqrt{\Lambda + 4\cos^2 x}} . \int_0^{\frac{\pi}{2}} dx' \sqrt{\Lambda + 4\cos^2 x'} \\
&= \int_0^{\frac{\pi}{2}} \frac{dx}{\sqrt{\Lambda + 4 - 4\sin^2 x}} . \int_0^{\frac{\pi}{2}} dx' \sqrt{\Lambda + 4 - 4\sin^2 x'} \\
&= \int_0^{\frac{\pi}{2}} \frac{dx}{\sqrt{1 - \frac{4}{\Lambda+4}\sin^2 x}} . \int_0^{\frac{\pi}{2}} dx' \sqrt{1 - \frac{4}{\Lambda+4}\sin^2 x'} \\
&= \int_0^{\frac{\pi}{2}} \frac{dx}{\sqrt{1 - k^2\sin^2 x}} \int_0^{\frac{\pi}{2}} dx' \sqrt{1 - k^2\sin^2 x'}. \qquad (3.3.21)
\end{aligned}$$

The two integrals in (3.3.21) are elliptic integrals with modulus k. Up to leading order, the determinant takes the form [17]

$$\det \gamma_{red} \sim \log \frac{64}{\Lambda}. \qquad (3.3.22)$$

Hence the entropy given by (3.3.11) is

$$\boxed{\lim_{\zeta<<1} S_{DBC} \sim \log\log \frac{64}{\Lambda}.} \qquad (3.3.23)$$

The entropy diverges in the continuum limit and, most importantly, diverges as $\log\log$.

- **NBC**

  Here are condition is different. NBC has the presence of zero modes, i.e., the contribution of the first term in the expression (3.3.15). Now looking at these terms, we see that:

$$\lim_{\substack{\Lambda\to 0 \\ N\to\infty}} \frac{\sqrt{\Lambda}}{N} = 0, \qquad \lim_{\substack{\Lambda\to 0 \\ N\to\infty}} \frac{1}{N\sqrt{\Lambda}} = 0. \qquad (3.3.24)$$

This is true because $\sqrt{\Lambda} \sim a$, and $a \to 0$ slower than $N \to \infty$. We hence have

$$\lim_{\zeta<<1} \det \gamma_{red} = \frac{1}{4N^2}\left[\sum_{k=1}^{N-1} \frac{1}{\sqrt{\Lambda + 4\cos^2\left(\frac{(2k-1)\pi}{4N}\right)}}\right]\left[\sum_{l=1}^{N-1}\sqrt{\Lambda + 4\cos^2\left(\frac{(2l-1)\pi}{4N}\right)}\right].$$

Again, the argument of the cosine has the form

$$\frac{(2k-1)\pi}{4N} \approx \frac{k\pi}{2N} = \frac{r}{N}, \quad \frac{r}{N} \in \left[\frac{\pi}{4N}, \frac{(2N-3)\pi}{4N}\right] \approx \left[\frac{\pi}{4N}, \frac{\pi}{2}\left[1 - \frac{3}{2N}\right]\right] \approx \left[0, \frac{\pi}{2}\right].$$

This expression will now have the same form as before, and we can solve it similarly as we did for DBC. The answer is given by

$$\boxed{\lim_{\zeta<<1} S_{NBC} \sim \log\log\frac{64}{\Lambda}.} \tag{3.3.25}$$

Large relative spacing

We have shown for both boundary conditions that in large relative separation,

$$\frac{\pi^2}{N^2\Lambda} \gg 1 \implies \Lambda \ll \frac{\pi^2}{N}. \tag{3.3.26}$$

- **DBC**

  We go back to equation (3.3.12). In this limit we can assume the same form of $\frac{r}{N}$ and expand the terms as

  $$\Lambda + 4\cos^2\frac{r}{N} \approx \Lambda + 4\Big(1 - \frac{r^2}{2N^2}\Big)^2 \approx \Lambda - \frac{\pi^2}{N^2}. \tag{3.3.27}$$

  But given (3.3.26), this means we can ignore the Λ term. Hence (3.3.12) takes the form

  $$\det \gamma_{red} \approx \frac{1}{(2N+1)^2}\sum_{k=1}^{N}\frac{1}{\cos\left(\frac{(2k-1)\pi}{2(N+1)}\right)}\sum_{l=1}^{N}\cos\left(\frac{(2l-1)\pi}{2(N+1)}\right). \tag{3.3.28}$$

  In order to do this summation, we take the limit $N \to \infty$ (but keeping in mind that it is slower than the limit $\Lambda \to 0$). As before we have

  $$\frac{(2k-1)\pi}{2(2N+1)} \approx \frac{k\pi}{2N} = \frac{r}{N}, \quad \frac{r}{N} \in \left[\frac{\pi}{2(2N+1)}, \frac{(2N-1)\pi}{2(2N+1)}\right] \approx \left[\frac{\pi}{4N}, \frac{\pi}{2}\left[1 - \frac{1}{2N}\right]\right].$$

But here we don't ignore the last $\frac{1}{2N}$ term. In other words we are assuming that the summation index is continuous enough to approximate the sum by an integral, but keeping the N dependence in the limits. Noting that $\sum \frac{1}{N} \to \int dx$ and $\frac{r}{N} \to x$, the determinant then takes the form

$$\det \gamma_{red} \sim \underbrace{\int_0^{\frac{\pi}{2}-\frac{\pi}{4N}} \sec x \, dx}_{\mathcal{I}} \underbrace{\int_0^{\frac{\pi}{2}-\frac{\pi}{4N}} \cos x' \, dx'}_{\mathcal{I}'}. \tag{3.3.29}$$

The second integral is simple, and can be evaluated to be

$$\mathcal{I}' = \int_0^{\frac{\pi}{2}-\frac{\pi}{4N}} \cos x' \, dx' = \sin x' \Big|_0^{\frac{\pi}{2}-\frac{\pi}{4N}} = \cos \frac{\pi}{4N} \approx 1. \tag{3.3.30}$$

The first integral can also be done by a little manipulation as

$$\mathcal{I} = \int_0^{\frac{\pi}{2}-\frac{\pi}{4N}} \sec x \, dx = \int_0^{\frac{\pi}{2}-\frac{\pi}{4N}} \frac{\cos x}{\cos^2 x} \, dx = \int_0^{\frac{\pi}{2}-\frac{\pi}{4N}} \frac{\cos x}{1-\sin^2 x} \, dx. \tag{3.3.31}$$

Now, taking $t = \sin x$, the integral takes the form

$$\mathcal{I} = \int_0^{\cos\frac{\pi}{4N}} \frac{dt}{1-t^2} = \frac{1}{2}\left[\int_0^{\cos\frac{\pi}{4N}} \frac{dt}{1+t} + \int_0^{\cos\frac{\pi}{4N}} \frac{dt}{1-t} \right] = \frac{1}{2} \log \frac{1+\cos\frac{\pi}{4N}}{1-\cos\frac{\pi}{4N}}. \tag{3.3.32}$$

We now use the double angle identity $1 + \cos 2x = 2\cos^2 x$ and simplify the above equation to be

$$\mathcal{I} = \log \cot \frac{\pi}{8N} \approx \log \frac{8N}{\pi}. \tag{3.3.33}$$

Finally, using (3.3.11) we have for DBC

$$\boxed{\lim_{\zeta >> 1} S_{DBC} \sim \log \log N.} \tag{3.3.34}$$

- **NBC**

We go back to equation (3.3.15). Introducing x we get

$$\frac{(2k-1)\pi}{4N} \approx \frac{k\pi}{2N} = \frac{r}{N}, \quad \frac{r}{N} \in \left[\frac{\pi}{4N}, \frac{(2N-3)\pi}{4N} \right] \approx \left[\frac{\pi}{4N}, \frac{\pi}{2}\left[1 - \frac{3}{2N} \right] \right].$$

Following the same prescription as we did for DBC, we get

$$\det \gamma_{red} \sim \left[\frac{1}{N\sqrt{\Lambda}} + \int_0^{\frac{\pi}{2}-\frac{3\pi}{4N}} \sec x \, dx\right]\left[\frac{\sqrt{\Lambda}}{N} + \int_0^{\frac{\pi}{2}-\frac{3\pi}{4N}} \cos x' \, dx'\right].$$

These integrals can be calculated in the exact same way as in the last section.

$$\det \gamma_{red} \approx \left[\frac{1}{N\sqrt{\Lambda}} + \log\frac{8N}{\pi}\right]\left[\frac{\sqrt{\Lambda}}{N} + 1\right] \approx \frac{1}{N\sqrt{\Lambda}}.$$

Using (3.3.11), we can finally find the entropy as

$$\lim_{\zeta>>1} S_{NBC} \sim -\log N\sqrt{\Lambda}. \tag{3.3.35}$$

From these calculations, we see that in the case of Neumann boundary conditions, the leading order term of divergent entanglement entropy switches from a log to log log as we go from large relative spacing to small relative spacing. Since a log log divergence is much slower than a log divergence, the information content in both regimes is different. This crossover can also be observed using other entanglement measures like entanglement spectrum and logarithmic negativity.

This crossover of information content can be understood by the presence of zero modes. Consider large relative spacing. In DBC, the entropy does not diverge even for $\Lambda = 0$, unless $N \to \infty$. So for finite N we have finite entanglement entropy. But for NBC, the entropy diverges as $\Lambda \to 0$ even for finite N. This can be traced back to (3.3.2) and (3.3.14) where for finite N and $\Lambda = 0$, the eigenvalues for NBC can obtain a zero value (and hence called "zero mode") but not for eigenvalues for DBC. This difference essentially comes due to the presence of N in the denominator of the cosine in eigenvalues of NBC and presence of $N+1$ in the denominator of the cosine in eigenvalues of DBC.

The occurrence of zero modes implies that the coupling matrix has a zero eigenvalue in the diagonalized basis. This means that the harmonic term would be absent for one the new co-ordinates, implying the presence of a free particle. Free particles are non-renormalizable and hence cause the divergence of entropy even at finite N. Since a free particle can have any energy, there is ignorance about the exact state of the system which leads to infinite entanglement entropy even at finite N. This also means that under the presence of an effective free particle, correlations span the entire system.

Chapter 4

Entanglement Entropy of a fermionic field

This section will look toward generalizing the scalar entanglement entropy results to a fermionic field. It is also interesting to see if they would also have the crossover in the leading term, as mentioned in chapter 3. Moreover, one can also ask if entanglement for fermionic fields reproduces the area law to the first-order approximation. Most of the current literature mainly focuses on scalar fields. The majority of literature on fermions deals with spin chains rather than fermionic fields, i.e., they work on a lattice where each point represents a fermionic degree of freedom. Fermionic fields are different from spin chains, and we cannot carry over many results. Moreover, the methods used in the last two chapters fail and face some difficulties at specific steps, which we shall now focus on.

The first issue is of discretization of the fermionic fields. Fermionic fields on lattices suffer from the problem of *fermion doubling*. [22, 23, 24] Following the methods of the last two chapters, naive discretization of space-time in the fermionic field theory leads to spurious particles that are unphysical. Since most computations are eventually done on discrete systems, one would also want a proper physical discrete theory. Although this might be excusable in a free field theory, when one is to generalize this method to interacting field theory, it would create problems as the extra fermions

would impact the physical processes (like pair production). We will look at ways to remove these unphysical states to fix this issue. Some standard solutions to this problem, like the Wilson fermion method and the Kogut-Susskind staggered fermions method (commonly used in lattice QCD), will be explained. [22, 24, 25]

The second issue is of using methods from the last two chapters to solve for the entanglement entropy of the Dirac field analogously. Earlier, we had discretized the field and found that it looked like a harmonic chain, which through the knowledge of Gaussian functions, we could calculate the entanglement entropy for. The Dirac equation, by definition, is a first-order differential equation. Hence, its dispersion relation is very different from that of scalar fields. It does not reduce trivially to a set of harmonic oscillators, which we know how to solve. So we look for methods closer to the covariance matrix approach. To calculate the entanglement entropy, we look at Peschel's method [26] of calculating entanglement entropy from correlation functions (alternatively, from the covariance matrix as its elements are precisely the correlation functions). Then, we choose an appropriate Hamiltonian (free from doubling problems as stated above) and calculate the entanglement entropy explicitly. [27]

In this order, let us start looking at these problems above in detail.

4.1 Fermion doubling

Consider the problem of treating fermions on a lattice. A natural place to start would be the Dirac equation and proceeding to discretize it by replacing the spatial derivatives with finite differences. However, as we shall see, that leads to the introduction of unphysical states. It turns out that there is twice the number of fermions in the discrete theory in comparison to the continuum scenario. Here we look at two quantities that explain this doubling, the dispersion relation and the poles of the propagator. Methods in this section mostly follow from [22, 24, 23].

4.1.1 Dispersion relation

Let us try to find the relation between energy and momentum for the continuum and the discrete case. Consider the Dirac equation in 1+1 dimensions (most features of 3+1 are still captured in this example):

$$i\gamma^0\partial_t\psi(x,t) + i\gamma^1\partial_x\psi(x,t) - m\psi(x,t) = 0, \tag{4.1.1}$$

where γ are elements that satisfy the Dirac algebra:

$$\{\gamma_\mu, \gamma_\nu\} \equiv \gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\eta_{\mu\nu}.$$

In the case of 1+1 dimensions, we have $\eta_{\mu\nu} = \text{diag}(+1, -1)$. Let us now look at the Dirac equation in the continuum case.

Continuum case

Solutions of the Dirac equation are positive and negative energy plane waves. To convert this differential eqution to an algebraic equation we hence take the ansatz (considering positive frequency)

$$\psi(x,t) = e^{iEt-ipx}u(p). \tag{4.1.2}$$

Putting (4.1.2) into (4.1.1) we get the equation

$$\left(-\gamma^0 E + \gamma^1 p - m\right) u(p) = 0. \tag{4.1.3}$$

Notice that p takes any real value here. We now look for the dispersion relation, which we can get by "squaring" the Dirac equation. To do this we write $u(p)$ as

$$u(p) = \left(-\gamma^0 E + \gamma^1 p + m\right) u'(p). \tag{4.1.4}$$

Putting (4.1.4) in (4.1.3) we get

$$\left(-\gamma^0 E + \gamma^1 p - m\right)\left(-\gamma^0 E + \gamma^1 p + m\right) u'(p) = 0. \tag{4.1.5}$$

$$\implies \left(\left(-\gamma^0 E + \gamma^1 p\right)^2 - m^2\right) u'(p) = 0$$

$$\implies \left(\gamma^{0^2}E^2 + \gamma^{1^2}p^2 - (\gamma^0\gamma^1 + \gamma^1\gamma^0)Ep - m^2\right)u'(p) = 0.$$

Since we have $\{\gamma_\mu, \gamma_\nu\} = 2\eta_{\mu\nu}$, putting $\mu = \nu = 0$ we get $\gamma^{0^2} = 1$ and similarly putting $\mu = \nu = 1$ we get $\gamma^{0^2} = -1$. Putting $\mu = 0, \nu = 1$ we get that $\gamma^0\gamma^1 + \gamma^1\gamma^0 = 0$. Putting these in the equation above we get

$$\left(E^2 - p^2 - m^2\right)u'(p) = 0.$$

$$\implies p = \pm\sqrt{E^2 - m^2}. \tag{4.1.6}$$

Hence we have two solutions for p given its energy and mass. Let us look at the discretized version now.

Discretized version

In the lattice version of this problem, we replace the spatial derivative in the Dirac equation by a finite difference. Consider now the field on a lattice with separation between the lattice points as a. The Dirac equation will then look like

$$i\gamma^0\partial_t\psi(x,t) + i\gamma^1.\frac{\psi(x+a,t) - \psi(x-a,t)}{2a}\psi(x,t) - m\psi(x,t) = 0. \tag{4.1.7}$$

Now in the lattice, we substitute the same plane wave ansatz (4.1.2) to get

$$\left(-i\gamma^0 E e^{iEt-ipx} + i\gamma^1.\frac{e^{-ip(x+a)} - e^{-ip(x-a)}}{2a}.e^{iEt} - me^{iEt-ipx}\right)u(p) = 0.$$

$$\implies \left(-i\gamma^0 E + i\gamma^1.\frac{e^{-ipa} - e^{+ipa}}{2a} - m\right)u(p) = 0.$$

$$\implies \left(-i\gamma^0 E + i\gamma^1.\frac{-2i\sin pa}{2a} - m\right)u(p) = 0.$$

$$\implies \left(-i\gamma^0 E + \gamma^1.\frac{\sin pa}{a} - m\right)u(p) = 0. \tag{4.1.8}$$

Note here that $p \in [-\frac{\pi}{a}, \frac{\pi}{a}]$. The reason for this can be seen from the fact that this equation is periodic, and we can identify points $p \to p + \frac{2\pi}{a}$. This restricts the momentum to the expression shown, and is frequently called the Brillouin zone. Now to get rid of the matrices we square this equation by replacing $u(p)$ as

$$u(p) = \left(-\gamma^0 E + \gamma^1.\frac{\sin pa}{a} + m\right)u'(p). \tag{4.1.9}$$

Putting (4.1.9) in (4.1.8) and analogously expanding the squares as for the continuous case we get

$$\left(E^2 - \frac{\sin^2 pa}{a^2} - m^2\right) u'(p) = 0.$$

$$\implies \frac{\sin pa}{a} = \pm\sqrt{E^2 - m^2} \tag{4.1.10}$$

This equation has twice as many solutions as (4.1.6). Adding more spatial dimensions duplicates all the states even further. Now to see this explicitly, we go back to how we identify particles in a quantum field theory. Formally, we look at the poles of the propagator of the theory.

4.1.2 Propagator of the lattice field theory

Let us find the propagator in the discretized theory and see the different particles present in the theory. Note that the fermion field operators have canonical anticommutation relations. Note that repeated indices imply summations. We also redefine $\gamma^{mu} \to i\gamma^{mu}$ and $\bar{\psi} = -i\gamma^0\psi^\dagger$ for simpler notation. We have the Dirac action as

$$S = \int d^4x \left[\bar{\psi}\gamma^\mu - \partial_\mu\psi - m\bar{\psi}\psi\right] \tag{4.1.11}$$

We can use integration by parts on the derivative term and let the resultant surface term vanish at the boundary. This gives us the expression

$$S = \int d^4x \left[+\partial_\mu\bar{\psi}\gamma^\mu\psi - m\bar{\psi}\psi\right]$$

Adding both of these and simplifying we get

$$S = -\int d^4x \left[\frac{1}{2}(\bar{\psi}\gamma^\mu\partial_\mu\psi - \partial_\mu\bar{\psi}\gamma^\mu\psi) + m\bar{\psi}\psi\right]. \tag{4.1.12}$$

We now discretize the fermion field. The standard prescription has to be generalized now, and it looks like

$$\partial_\mu\psi(x) \to \frac{\psi(x + a_\mu\hat{\mu}) - \psi(x)}{a_\mu}. \tag{4.1.13}$$

This represents a derivative in the direction denoted by $\hat{\mu}$ direction. Making the space dependence explicit in the equations now, we look at the discretized action as

$$S = -\sum_x \left[\frac{1}{2a_\mu}(\bar{\psi}(x)\gamma^\mu\psi(x + a_\mu\hat{\mu}) - \bar{\psi}(x + a_\mu\hat{\mu})\gamma^\mu\psi(x)) + m\bar{\psi}(x)\psi(x)\right]. \tag{4.1.14}$$

To find the propagator, we look at the path integral. The path integral for fermionic fields reads as

$$\mathcal{Z} = \int D\bar{\psi} D\psi e^{i[S+\sum_x(\bar{\eta}\psi+\bar{\psi}\eta)]}. \tag{4.1.15}$$

Note that η are grassman valued numbers. Now we use the convention $x^0 = \hat{n}_0 a_0$ and $\mathbf{x} = \hat{n}a$. Going to imaginary time ($a_0 \to -ia_4$), the path integral looks like

$$\mathcal{Z} = \int D\bar{\psi} D\psi e^{[S+\sum_x(\bar{\eta}\psi+\bar{\psi}\eta)]}, \tag{4.1.16}$$

where the action looks like (with the definition $\gamma^4 = i\gamma_0$, γ^k redefined as $i\gamma^k$ and $\psi_x = a^{\frac{3}{2}}\psi(x)$)

$$S = -\sum_n \left[\sum_{\mu=1}^{4} \frac{a_4}{2a_\mu}(\bar{\psi}_n\gamma_\mu\psi_{n+\hat{\mu}} - \bar{\psi}_{n+\hat{\mu}}\gamma_\mu\psi_n) + a_4 m\bar{\psi}_n\psi_n\right]. \tag{4.1.17}$$

Note that we have lower indices here as we are in euclidean space. To bring the path integral to a solvable form, one typically writes it as a gaussian integral which can be readily solved, i.e

$$\mathcal{Z} = \int D\bar{\psi} D\psi e^{-\bar{\psi}A\psi+\bar{\eta}\psi+\bar{\psi}\eta}. \tag{4.1.18}$$

The form of A can be deduced by comparing (4.1.18) and (4.1.17). We see it has the form

$$A_{xy} = \sum_{z\mu} \gamma_\mu \frac{a_4}{2a_\mu}(\delta_{x,z}\delta_{y,z+\mu} - \delta_{x,z+\mu}\delta_{y,z}) + a_4 m \sum_z \delta_{x,z}\delta_{y,z}. \tag{4.1.19}$$

The evaluation of this gaussian integral (4.1.18) is straightforward and a similar to what we did in chapter 2 while solving for the reduced density matrix.

$$\mathcal{Z} = \det A e^{\bar{\eta}A^{-1}\eta}.$$

where A^{-1} is the propagator in question. For the action in (4.1.17), we see that the propagator has the form

$$\boxed{S(k) = \frac{m - \sum_\mu i\gamma_\mu \sin(ak_\mu)/a}{m^2 + \sum_\mu \sin^2(ak_\mu)/a^2}.} \tag{4.1.20}$$

In the continuum limit $a \to 0$, we obtain the usual continuum propagator as

$$S(k) = \frac{m - i\gamma k}{m^2 + k^2}. \tag{4.1.21}$$

Comparing the two expressions we can now see how (4.1.20) has more poles than its continuum counterpart. The continuum propagator can be seen to have a pole at $k_4 = i\sqrt{\mathbf{k}^2 + m^2}$. For the discretized propagator, this corresponds to the region near zeros of the sine function at $ak_\mu = 0$. But the sine function also vanishes for other points like $k_A = \frac{\pi_A}{a}$ where π_A can have the from $(\pi, 0, 0, 0), (\pi, \pi, 0, 0), (0, \pi, 0, 0) \cdots$ and so on. The continuum propagator here corresponds to $\pi_A = (0, 0, 0, 0)$. These are the different corners of the Brilloiun zone. The poles of the propagator represent particles. Hence, in the discrete theory the vanishing of sine function at these various π_A contribute extra particles, often called fermion doublers. Note that for d dimensions there are 2^d doubler particles. In the case we have 16 total poles and 15 additional poles.

Hence the naive discretization leads to many problems in the resultant quantum field theory and is inconsistent. The fermion doubling problem originates from the chiral symmetry of the theory and can be related to the axial anomaly as well. Due to a theorem by **Nielson-Ninomiya** [28], one can show that all free fermion theories with chiral symmetry and having an action that is real, local, and translation invariant, *necessarily has fermion doubling*. The proof is topological and uses the fact that the Brillouin zone for the lattice theory is a torus. Due to this, the denominator of the propagator has to go to zero to satisfy periodicity. We will now look at ways to avoid fermion doubling in lattice systems.

4.1.3 Lattice constructions without fermion doubling

In this subsection, we very briefly look at two constructions of a discrete fermionic field theory that do not have the problem of fermion doubling. The first is the Wilson fermion field theory, and the second is the Kogut-Susskind staggered fermion field theory.

4.1.3.1 Wilson's fermion method

In this method, we remove the fermion doublers by introducing "mass terms" (i.e ϕ^2 terms), which increase the fermion doublers's masses to the order of the cutoff. Hence in the continuum limit, the doublers get eliminated from the spectrum of the fermion theory. To see how this happens, we replace the mass term as [22]

$$\sum_x m\bar{\psi}_x\psi_x \to m\bar{\psi}_x\psi_x + \frac{a}{2}\sum_{x\mu}\partial_\mu\bar{\psi}_x\partial_\mu\psi_x. \tag{4.1.22}$$

$$= \left(m + \frac{4}{a}\right)\sum_x m\bar{\psi}_x\psi_x - \frac{1}{2a}\sum_{x\mu}(\bar{\psi}_{x+a\hat{\mu}}\psi_x + \bar{\psi}_x\psi_{x+a\hat{\mu}}). \tag{4.1.23}$$

Doing an analogous calculation, we see that the mass term in the denominator of (4.1.20) gets replaced by

$$\mathcal{M}(k) \equiv m + \frac{1}{a}\sum_\mu(1 - \cos k_\mu a).$$

$$\implies \mathcal{M}(k) = m + \frac{2}{a}\sum_\mu \sin^2\frac{k_\mu a}{2}. \tag{4.1.24}$$

The discrete propagator is hence given by

$$\boxed{S(k) = \frac{\mathcal{M}(k) - \sum_\mu i\gamma_\mu \sin(ak_\mu)/a}{\mathcal{M}(k)^2 + \sum_\mu \sin^2(ak_\mu)/a^2}.} \tag{4.1.25}$$

Since the additional term added is proportional to a, in the continuum limit, it appropriately goes to 0, and the dispersion relation stays the same. The extra Wilson term provides doublers (in the discrete limit) a mass that is proportional to $\frac{1}{a}$. To explicitly see this, let us look at (4.1.24). The roots of $\sum_\mu \sin ak_\mu/a$ in the denominator of the propagator correspond to the doublers. Since the mass correction is a function of the half-angle, each doubler that vanishes in the propagator due to $k_A = (\pi, 0, 0, 0), (\pi, \pi, 0, 0)$ etc, would also contribute to $\sum_\mu \sin ak_\mu/2$ as $\sin\frac{\pi}{2} = 1$. This means that m_A takes the value

$$m_A = m + \frac{2n_A}{a}, \tag{4.1.26}$$

where n_A represents the number of π's in the vector k_A. This approach works well as it gives the correct number of fermions in the continuum limit and can be shown

to give the correct spectra (i.e., particle energies have corrections of order $\mathcal{O}(a)$) for the low energy dynamics one is typically interested in. The doublers with $n_A \neq 0$ become infinitely heavy in the continuum limit, and hence the only state with finite energy becomes the zero corner of the Brillouin zone. The drawback of this method is that it explicitly breaks chiral symmetry (this is also why the Nielson-Ninomiya theorem does not apply here), which can lead to problems such as renormalization of the mass of the resultant fermions. Computations using this method also require heavy computational power, which is why the staggered fermions method is typically used more often.

4.1.3.2 Kogut-Susskind staggered fermions

This method involves eliminating the gamma matrices from the discrete action, which simplifies the action hugely. We start with the discretized action [25, 22] and do the transformations

$$\psi_x = \gamma^x \chi_x, \qquad \bar{\psi}_x = \bar{\chi}_x (\gamma^x)^\dagger \tag{4.1.27}$$

with $\gamma^x \equiv (\gamma_1)^{x_1}(\gamma_2)^{x_2}(\gamma_3)^{x_3}(\gamma_4)^{x_4}$. Note that

$$[(\gamma^x)^\dagger \gamma_\mu \gamma^{x+\mu}]_{\alpha\beta} = [\gamma^x \gamma_\mu (\gamma^{x+\mu})^\dagger]_{\alpha\beta} = \eta_{\mu x}\delta_{\alpha\beta} \tag{4.1.28}$$

where

$$\eta_{1x} = 1, \qquad \eta_{2x} = (-1)^{x_1}, \qquad \eta_{3x} = (-1)^{x_1+x_2}, \qquad \eta_{4x} = (-1)^{x_1+x_2+x_3}.$$

This transformation completely removes the gamma matrices from the action, which now looks like

$$S = -\sum_{\alpha=1}^{4}\left[\sum_{x\mu}\eta_{\mu x}\frac{1}{2}(\bar{\chi}^\alpha_x \chi^\alpha_{x+\hat{\mu}} - \bar{\chi}^\alpha_{x+\hat{\mu}}\chi^\alpha_x) + \sum_x m\bar{\chi}^\alpha_x\chi^\alpha_x\right]. \tag{4.1.29}$$

The labels α are just the spinor labels. They represent internal symmetries, and hence we have four exactly same terms that are being summed. A single one of them is enough to describe a fermion, i.e we take χ and $\bar{\chi}$ as one component fields now. This reduces the particles in the continuum limit from 16 to 4 (as we only take one

component fields instead of four component fields). The overall action does not have the sum over α now. These 4 components are often called "tastes" when these fields are considered in QCD.

We can further reduce the number of particles from 4 to 2 by working on a lattice where we only assign $\bar{\chi}_x$ to even sites and χ_x to the odd ones. A site on the lattice is denoted by the co-ordinates (x_1, x_2, x_3, x_4). The criteria for it to be even or odd is as

$$\epsilon_x = (-1)^{x_1+x_2+x_3+x_4} = \begin{cases} +1, & \text{even} \\ -1, & \text{odd.} \end{cases} \tag{4.1.30}$$

Now we can remove the bar on $\bar{\chi}_x$. This is because sites are classified based on odd and even a function of x (already in the subscript). Looking at the action now, we get

$$S = -\left[\sum_{x\mu} \eta_{\mu x} \frac{1}{2}(\chi_x \chi_{x+\hat{\mu}} - \chi_{x+\hat{\mu}}\chi_x) + \sum_x m\chi_x\chi_x\right]. \tag{4.1.31}$$

Note that χ_x is an anticommuting field, which means we can switch the order of the first term in the above equation and add them. This gives

$$\boxed{S = -\left[\sum_{x\mu} \eta_{\mu x}\chi_x\chi_{x+\hat{\mu}} + \sum_x m\chi_x\chi_x\right].} \tag{4.1.32}$$

For massless fermions, this gives us four "majorana fermions". This method does not break chiral symmetry and is much easier to use in computations, which is why it is typically preferred. Hence we have seen two ways to deal with the "fermion doubling problem".

4.2 Calculation of reduced density matrices from correlation functions

In this section, we review the works of Ingo Peschel in [26] and H. Casini, C. D. Fosco and M. Huerta in [27]. We start with a lattice Hamiltonian of the form

$$\mathcal{H} = \sum_{ij} M_{ij} c_i^\dagger c_j. \tag{4.2.1}$$

We intend to calculate the entanglement entropy for this system with the idea that it will help us deal with the Dirac field. We wish to take an appropriate discretization of the Dirac field (according to the last section) and reduce it to the form above.

The Hamiltonian in (4.2.1)'s eigenstates are are Slater determinants. All averages calculated ahead will be with respect to such eigenfunctions. Then, the correlation matrix (or the covariance matrix) $C_{n,m} = \langle c_n^\dagger c_m \rangle$ is Hermitian. To calculate the entanglement entropy of (4.2.1), we intend to find a form of the density matrix. We know that by Wick's theorem, any high order correlation function can be written as

$$\langle c_n^\dagger c_m^\dagger c_k c_l \rangle = \langle c_n^\dagger c_l \rangle \langle c_m^\dagger c_k \rangle - \langle c_n^\dagger c_k \rangle \langle c_m^\dagger c_l \rangle. \tag{4.2.2}$$

Let us consider subsystem A (degrees of freedom inside S will have the indices i,j). Since averages can be calculated with the help of the density matrix too, we have for the subsystem the restricted correlator matrix as

$$C_{i,j}^A = \mathrm{tr}\Big(\rho c_i^\dagger c_j\Big). \tag{4.2.3}$$

Since these averages must also factor in a similar way as shown in (4.2.2), the density operator must have the form

$$\rho = \mathcal{K} \exp(-\mathcal{H}), \tag{4.2.4}$$

where

$$\mathcal{H} = \sum_{ij} H_{i,j} c_i^\dagger c_j. \tag{4.2.5}$$

Here $\mathcal{H}$ is often called the entanglement Hamiltonian. Going back to chapter 2, we saw the same in the coupled harmonic oscillator and harmonic chain. Since those

Hamiltonians can be brought into a similar form as (4.2.1), we see the same expression for the density operator. To move ahead, as before we diagonalize the density operator by diagonalizing $H_{i,j}$. Suppose the eigenvectors of $H_{i,j}$ are $\phi_k(i)$ with eigenvalues ϵ. Then we can perform a transformation to the fermionic diagonal basis as a_k as

$$c_i = \sum_k \phi_k(i) a_k. \tag{4.2.6}$$

Finally, we have diagonalized the entanglement Hamiltonian and hence the density operator. The entanglement Hamiltonian hence has the form

$$\mathcal{H} = \sum_k \epsilon_k a_k^\dagger a_k \tag{4.2.7}$$

while the density operator looks like

$$\rho = \mathcal{K} \exp\left(- \sum_k \epsilon_k a_k^\dagger a_k \right). \tag{4.2.8}$$

Since the density matrix is traceless, we can use this property to calculate $\mathcal{K}$. Now, the reduced density matrix is given by ρ_A and it looks like

$$\rho_A = \prod_k \rho_k = \prod_k \frac{e^{-\epsilon_l a_k^\dagger a_k}}{1 + e^{-\epsilon_k}}. \tag{4.2.9}$$

The eigenvalues ν_k of C^A and ϵ_l are related by (4.2.2) and (4.2.3). Their relation is as

$$e^{-\epsilon_k} = \frac{\nu_k}{1 - \nu_k}. \tag{4.2.10}$$

Now the total entropy is given by

$$S_A = \sum_k S_k. \tag{4.2.11}$$

The expression for S_k in terms of the eigenvalue ν_k of the operator C^A is given by

$$\boxed{S_k = -(1 - \nu_k)\log(1 - \nu_k) - \nu_k \log(\nu_k).} \tag{4.2.12}$$

Since we are interested in the vacuum state, in the Dirac picture it means that all negative energy states are filled and all positive energy states are empty. We write this as

$$C = \theta(-M). \tag{4.2.13}$$

Clearly this means that $C_{i,j} = 1$ when $M_{i,j} < 0$ and $C_{i,j} = 0$ when $M_{i,j} > 0$. With this set up, we now look at a discrete lattice Hamiltonian from [27] for the Dirac fermion. This is similar to the Majorana staggered fermion expression we saw in (4.1.32). Here we take N lattice sites, with spacing equal to unity. The Hamiltonian reads

$$\mathcal{H} = \frac{-i}{2}\sum_{n=0}^{N-1}(\Psi_n^1\Psi_{n+1}^1 + \Psi_n^2\Psi_{n+1}^2) + im\sum_{n=0}^{N-1}\Psi_n^1\Psi_n^2. \tag{4.2.14}$$

The operators Ψ are fermionic Majorana operators, which means they are real i.e $\Psi_n^i = \Psi_n^{i\,\dagger}$ and satisfy anti-commutation relations. Moreover we work with periodic boundary conditions, i.e $\Psi_N^i = \Psi_0^i$. We now try to look for a transformation that links this discretized Dirac field Hamiltonian to (4.2.1). We now redefine the new fermionic operators as

$$c_{2k} = \frac{1}{2}(\Psi_{2k}^1 + i\Psi_{2k}^2), \qquad c_{2k+1} = \frac{1}{2}(\Psi_{2k+1}^1 - i\Psi_{2k+1}^2). \tag{4.2.15}$$

These new operators also satisfy canonical anti-commutation relations. The final Hamiltonian takes the form

$$\mathcal{H} = \frac{-i}{2}\sum_{n=0}^{N-1}(c_{n+1}^\dagger c_n - c_n^\dagger c_{n+1}^\dagger) + m\sum_{n=0}^{N-1}(-1)^n c_n^\dagger c_n. \tag{4.2.16}$$

Comparing with (4.2.1), we find the form of M_{ij} as

$$M_{ij} = \frac{-i}{2}\Big((\delta(i,j-1) - \delta(i,j+1)) + m\delta(i,j)(-1)^n\Big). \tag{4.2.17}$$

Hence we can now use expressions (4.2.12) and (4.2.11) to numerically find the entropy of the fermionic field.

Chapter 5

Conclusions and further work

This chapter will give a brief description of all the topics discussed till now and covered in this master's project and give a idea for the further work going to be done.

Conclusions

- The role of entanglement in quantum field theory was understood, particularly what it meant for quantum fields to be entangled.
- A possible connection between entropy due to entanglement and Black Hole entropy was discussed. Both were seen to be dependent on area.
- With the goal of calculating the entanglement entropy for the scalar field, we started with toy systems like the coupled harmonic oscillator and the harmonic chain and calculating their entropy. With the help of these results, we calculated the entanglement entropy for scalar fields numerically. Moreover, we also extended the above calculation to space-time with a horizon. Area law was seen to hold in both these examples. One big drawback here was the lack of any analytical results.
- To obtain entanglement entropy for the scalar fields analytically, we used another approach involving the covariance matrix. We established the covariance

matrix's link to entanglement entropy through thermal states(for the ground state of the field), and then we used the covariance matrix method to calculate the entanglement entropy of the scalar field.

- Upon careful analysis of the analytical expression for the entanglement entropy, we found that the entanglement entropy at leading order behaved differently for different boundary conditions. For the case of Neumann boundary conditions, we found that the entanglement entropy diverged as $\log\log$ when $\zeta \ll 1$. In contrast, it diverged as $\log$ when $\zeta \gg 1$, whereas for the Dirichlet boundary condition, the entanglement entropy diverged as $\log\log$ in both the regimes.

- Hence the information content of the field theory in the two regimes of ζ is different. Signatures of this crossover were also seen in other measures of entanglement.

- Finally, we started with the main goal of the project: **generalizing the entanglement entropy calculation for a fermion field**. The reasons to do this were three-fold. First, to see if it is possible to prove the area law using fermionic fields (has not been done in literature). Secondly, try to see if the crossover in the leading term of entanglement entropy is even present for fermionic theories. (try to extend work done by [17]) And lastly, to formulate the Hawking effect for fermions and finding a corresponding temperature.

- Upon starting to do this calculation, it was evident that Dirac equation being first order is a worrying issue. All the calculations done in [chapter 2] used the idea that scalar fields under discretization behave like coupled harmonic oscillators. Since Dirac equation was first order, the structure after discretization was different, and older results from [chapter 2] could not be directly used.

- Moreover, when trying to discretize the Dirac field, we encountered the problem of "fermion doubling", where the discretized version of the Dirac field theory was giving double the number of particles it should (2 per each space-time dimension). This was seen through the extra solutions of the lattice dispersion

relation for p that arise due to the corners of the Brillouin zone (which goes off to infinity in the continuum limit). The same could be seen from the poles of the propagator of the lattice field theory, whose number multiplies by two for each space-time dimension.

- We saw that one of the solutions to this problem was adding certain terms to the action that raised the mass of the extra fermion particles. The extra particles become infinitely heavy in the continuum limit, making the correct fermion state the only one with finite energy.

- Another way to deal with the doubling was to perform a particular transformation that removed gamma matrices from the Dirac action (3+1 dimensional theory) and led to the simplification of the action as it became a sum of 4 identical terms that did not intermix in any way (since the gamma matrices go away). Furthermore, this allowed us to work with only a single component fermion, which greatly reduced the extra solutions. Finally, by breaking the lattice into odd and even sites, we could further reduce the number of these extra solutions and have a lattice theory for fermions that is free of the doubling problem.

- With this out of the way, we looked towards methods similar to those in [chapter 3] for trying to calculate the entanglement entropy for fermions. It was not clear how to generalize the covariance matrix formalism to a system with a Dirac spinors as they have 4 degrees of freedom at each point. Moreover, the gaussianity of the ground state and its thermal nature was what led us to derive (3.2.25), was for the ground state of a scalar field.

- One method of calculating the density matrix using correlation functions in fermionic condensed matter systems was hence studied.

- Construction of the density matrix was done by comparing averages calculated using the density matrices and averages calculated by Wick's theorem (correlation functions). Hence given a matrix with all the different correlation functions

$C_{i,j} = \langle c_i^\dagger c_j \rangle$, we could construct the density matrix ρ and then calculate the entanglement entropy by tracing out degrees corresponding to a subsystem.

- Hence, we could use the correlation functions to calculate the entanglement entropy with the correct choice of a Hamiltonian that leads to the Dirac Hamiltonian in the continuum limit and does not suffer from any fermion doubling problems of the system.

- However, it is not fully clear as of now how the tracing out process in this method corresponds to *real space entanglement*. Work is currently being done on this.

- Lastly, we also saw in detail topics such as cosmological particle creation. This involved studying the time varying harmonic oscillator, quantum fields in expanding space-times, the Unruh effect, and the Hawking radiation.

Further work

Through this masters project, many methods of calculating entanglement entropy were understood. Since a trivial generalization for the entanglement entropy for fermions could not be made from the methods used before, one had to look for other methods. Currently, the correlation function approach is the one that is being worked upon to calculate the entropy. After this calculation, further work on three goals should be possible:

- Showing that entanglement entropy for fermionic fields also follows an area law.

- Investigate the crossover seen in [chapter 3] for a fermionic field and see if it also occurs here.

- Try to formulate the Hawking effect in the same formalism for the fermion field.

Appendices

Appendix A

Cosmological particle creation

In this chapter we look at the phenomena of particle creation in gravitational backgrounds.[29, 8] We start with looking at the simple example of time-dependent harmonic oscillator. It will be that that it has a vacuum state that keeps changing with time, leading to the changing of annihilation operators. The operators at different times are related through the *Bogolyubov transformation*. This change in the vacuum causes a change in the particle description of the theory. Hence a system in vacuum at some time would begin to have particles at another instant of time.

This will be followed by the example of expanding space-time, where now a scalar field is considered in this space-time. It will be shown that this theory also fails to have a vacuum that does not change with time, leading to an inconsistent particle description. Hence a prepared vacuum state at some time fails to be the vacuum state at later times, leading to appearance of particles in a supposedly vacuum state. The operators at each time instance are again linked to each other through Bogolyubov transformations.

This will then be followed by the exploration of the Unruh effect, where an accelerated observer starts to see a thermal spectrum of particles as it starts to accelerate. Using the ideas from the previous sections, one can show that a scalar field in this space-time of an accelerated observer (Rindler space) also fails to have a consistent

vacuum, leading to an appearance of particles that were not there before the acceleration. The particles are observed to have a thermal spectrum, which will be explained in detail.

Finally, we look at the problem of particle creation near Black Holes. It will be shown that most ideas from the Unruh effect can be analogously applied to the Schwarzschild Black Hole. This leads to a observer very far from the Black Hole to see a flux of particles, whose spectrum is thermal. In all of these cases, the Bogolyubov transformation links the annihilation operator in different co-ordinate systems/ at different times, and plays an essential role in the idea of particle creation in their relevant systems.

A.1 Oscillator with variable frequency

We look at the classical oscillator with a twist. We look at at the time independent oscillator with the equation of motion as

$$\ddot{q} + \omega^2(t)q = 0. \tag{A.1.1}$$

Why are we interested in such a system? When dealing with typical scalar fields in quantum field theory, the Klein-Gordan equation in momentum space looks like a simple harmonic oscillator equation. We will see later that gravitational effects influence quantum fields such that the frequency (ω) in the equation of motions becomes times dependent. We now start looking at the time-dependent harmonic oscillator and establish some results.

An example for $\omega(t)$ would be as in (Fig. A.1) (on next page). Finding an exact solution for the differential equation (A.1.1) can be hard for an arbitrary $\omega(t)$. Instead we look at "in" and "out" regimes, i.e

$$\omega = \omega_0 \qquad \forall t < t_0$$

$$\omega_1 \qquad \forall t > t_1$$

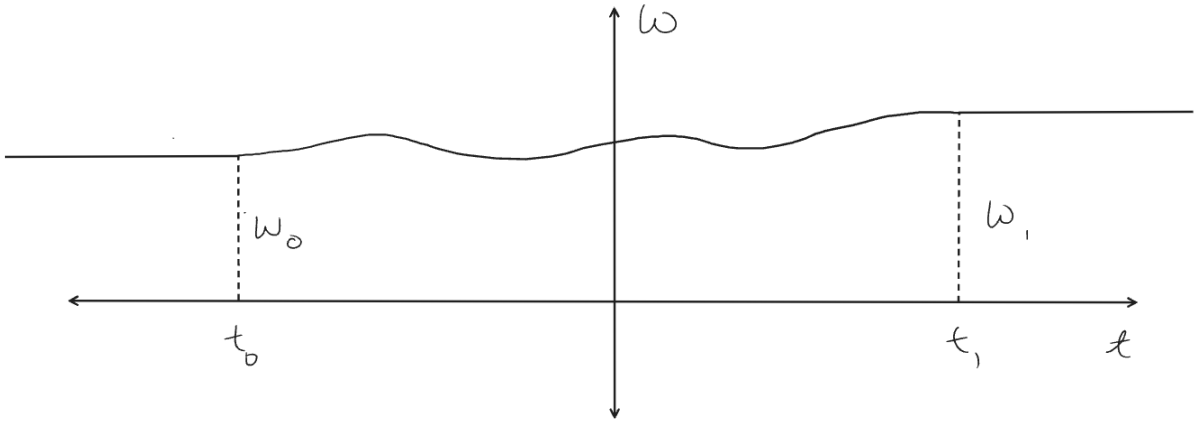


Figure A.1: $\omega(t)$

In these regimes, we already know the solution to the oscillator. It takes the form:

$$q(t) = Ae^{i\omega_0 t} + Be^{-i\omega_0 t} \qquad \forall t < t_0$$

$$q(t) = Ce^{i\omega_1 t} + De^{-i\omega_1 t} \qquad \forall t > t_1.$$

Given the equation of motion (A.1.1), we can write the Lagrangian for it as

$$\mathcal{L} = \frac{\dot{q}^2}{2} - \frac{1}{2}\omega^2(t)q^2.$$

The conjugate momentum is then

$$p = \frac{\partial \mathcal{L}}{\partial \dot{q}} = \dot{q}.$$

The Hamiltonian corresponding to this Lagrangian is

$$\mathcal{H} = \frac{p^2}{2} + \frac{1}{2}\omega^2(t)q^2. \tag{A.1.2}$$

The Hamilton's equations for the above Hamiltonian then reads

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial q} = -\omega^2 q, \qquad \dot{q} = \frac{\partial \mathcal{H}}{\partial p} = p. \tag{A.1.3}$$

Typically these systems do not conserve energy, and physically it stems from the fact that this simple harmonic oscillator has to have variable frequency because of

some form of external driving. Upon quantization of this oscillator, we promote the dynamical variables q and p to operator valued variables and postulate the canonical commutation relations

$$[q(t), p(t)] = i, \qquad [q(t), q(t)] = [p(t), p(t)] = 0. \tag{A.1.4}$$

We then introduce the operators a and $a^\dagger$ as in (3.2.6) as

$$a(t) = \sqrt{\frac{\omega}{2}}\Big(q(t) + \frac{i}{\omega}p(t)\Big), \qquad a^\dagger(t) = \sqrt{\frac{\omega}{2}}\Big(q(t) - \frac{i}{\omega}p(t)\Big). \tag{A.1.5}$$

As we go from the (q, p) basis to $(a, a^\dagger)$ basis, the Hamilton's equations also change form. To find them, we take time derivatives of the new basis variables, $a, a^\dagger$ as

$$\dot{a}(t) = \sqrt{\frac{\omega}{2}}\Big(\dot{q} + \frac{i}{\omega}\dot{p}\Big), \qquad \dot{a}^\dagger(t) = \sqrt{\frac{\omega}{2}}\Big(\dot{q} - \frac{i}{\omega}\dot{p}\Big). \tag{A.1.6}$$

Using (A.1.3) in the above equation we get

$$\dot{a}(t) = \sqrt{\frac{\omega}{2}}\Big(p - i\omega q\Big) = -i\omega\left[\sqrt{\frac{\omega}{2}}\Big(q + \frac{i}{\omega}p\Big)\right] = -i\omega a(t). \tag{A.1.7}$$

and similarly for the other operator. Hence the Hamilton's equations in this new basis take the form

$$\dot{a}(t) = -i\omega a(t), \qquad \dot{a^\dagger}(t) = +i\omega a^\dagger(t). \tag{A.1.8}$$

Let us solve these equations in the case that ω is constant in time.

ω constant

In this case, the differential equation has an easily computable solution as

$$a(t) = a_0 e^{-i\omega t} \equiv a e^{-i\omega t}. \tag{A.1.9}$$

Now we ask what the commutation relations look in the new variables. To do so, we invert equations (A.1.5) as

$$q(t) = \sqrt{\frac{1}{2\omega}}\Big(a e^{-i\omega t} + a^\dagger e^{+i\omega t}\Big), \qquad p(t) = \frac{1}{i}\sqrt{\frac{\omega}{2}}\Big(a e^{-i\omega t} - a^\dagger e^{+i\omega t}\Big). \tag{A.1.10}$$

Putting it into the (A.1.4) we get

$$\frac{1}{i}\sqrt{\frac{\omega}{2}}\sqrt{\frac{1}{2\omega}}\left[ae^{-i\omega t}+a^\dagger e^{+i\omega t}, ae^{-i\omega t}-a^\dagger e^{+i\omega t}\right]=i$$
$$\implies \left[a,a^\dagger\right]=1. \tag{A.1.11}$$

We now wish to rewrite (A.1.10) in a form that will be helpful when generalizing to the general ω case. Looking at $q(t)$ first we get

$$q(t)=\frac{1}{\sqrt{2}}\left(a\frac{e^{-i\omega t}}{\sqrt{\omega}}+a^\dagger\frac{e^{i\omega t}}{\sqrt{\omega}}\right)\equiv\frac{1}{\sqrt{2}}\left(av^*(t)+a^\dagger v(t)\right),$$

where we have defined $v(t)=\frac{e^{i\omega t}}{\sqrt{\omega}}$. Using Hamilton's equation in (A.1.8), we can substitute a and $a^\dagger$ in (A.1.10) to get

$$p(t)=\frac{1}{\sqrt{2}}\left(a\dot{v}^*(t)+a^\dagger\dot{v}(t)\right).$$

Hence we have the expressions

$$q(t)=\frac{1}{\sqrt{2}}\left(av^*(t)+a^\dagger v(t)\right),\qquad p(t)=\sqrt{\frac{1}{2}}\left(a\dot{v}^*(t)+a^\dagger\dot{v}(t)\right). \tag{A.1.12}$$

General ω

Now moving to the case of a general time dependent frequency, the differential equation (A.1.8) will not have a simple solution. It will take the form

$$\frac{da^\dagger(t)}{dt}=+i\omega(t)a^\dagger\implies\log a^\dagger(t)=\int i\omega(t)\,dt$$
$$\implies a^\dagger(t)=a_0^\dagger\exp\left(i\int\omega(t)\,dt\right)\equiv a^\dagger f. \tag{A.1.13}$$

As before, this would mean that

$$q(t)=\frac{1}{\sqrt{2}}\left(a\frac{f^\dagger}{\sqrt{\omega}}+a^\dagger\frac{f}{\sqrt{\omega}}\right)\equiv\frac{1}{\sqrt{2}}\left(av^*(t)+a^\dagger v(t)\right),\ \ p(t)=\frac{1}{\sqrt{2}}\left(a\dot{v}^*(t)+a^\dagger\dot{v}(t)\right) \tag{A.1.14}$$

where we have defined $v(t)=\frac{f}{\sqrt{\omega}}$. It is for this reason $v(t)$ is often called the "mode function". We can now ask what (A.1.1) would imply for the mode function. By plugging the expression of $q(t)$ above into (A.1.1) we get

$$\frac{1}{\sqrt{2}}\left(a\ddot{v}^*(t)+a^\dagger\ddot{v}(t)\right)+\omega^2(t).\frac{1}{\sqrt{2}}\left(av^*(t)+a^\dagger v(t)\right)=0$$

$$\implies \frac{a}{\sqrt{2}}\big(\ddot{v}^*(t)+\omega^2(t)v^*(t)\big)+\frac{a^\dagger}{\sqrt{2}}\big(\ddot{v}(t)+\omega^2(t)v(t)\big)=0.$$

Note that the latter half of this equation is the conjugate of the former. This equation holds for any choice of $v(t)$, meaning the terms in the parenthesis must be zero themselves. This gives us

$$\ddot{v}+\omega^2(t)v=0. \tag{A.1.15}$$

As before, we now evaluate the commutation relations for the general ω case. Starting from (A.1.4) we get

$$\begin{aligned}
&\big[q(t),p(t)\big]=i\\
\implies &\Big[\frac{1}{\sqrt{2}}\big(av^*(t)+a^\dagger v(t)\big),\frac{1}{\sqrt{2}}\big(\dot{a}v^*(t)+\dot{a}^\dagger v(t)\big)\Big]=i\\
\implies &\frac{1}{2}\Big[\big(av^*(t)+a^\dagger v(t)\big),\big(\dot{a}v^*(t)+\dot{a}^\dagger v(t)\big)\Big]=i\\
\implies &\big(\dot{v}v^*-v\dot{v}^*\big)[a,a^\dagger]=2i\\
\implies &[a,a^\dagger]=\frac{2i}{\dot{v}v^*-v\dot{v}^*}.
\end{aligned} \tag{A.1.16}$$

The denominator on the right-hand side is the Wronskian of the solutions $v(t)$ and $v^*(t)$. We now take a slight detour to prove a significant result related to it.

Wronskian

Given a second order differential equation $y''=a(x)y'+b(x)y$ and the two solutions y_1 and y_2, we define the **Wronskian** as

$$W=y_1y_2'-y_1'y_2. \tag{A.1.17}$$

We now calculate the derivative of the Wronskian and substitute the second-order derivatives using the original differential equation as

$$W'=y_1'y_2'+y_1y_2''-y_1'y_2'-y_1''y_2=y_1y_2''-y_1''y_2$$

$$=y_1\big[ay_2'+by_2\big]-y_2\big[ay_1'+by_1\big]=a\big(y_1y_2'-y_2y_1'\big)=aW.$$

This differential equation can be solved easily and gives the Wronskian of the form

$$W=C.e^{\int a\,dx}. \tag{A.1.18}$$

For the differential equation we have in (A.1.15), a(x)=0 so the Wronskian becomes a constant. Since all these solutions are solutions to linear differential equations, any solution upto a multiplicative constant is also a solution. Hence we can normalize the mode functions as we wish and put (A.1.16) as

$$\dot{v}v^* - v\dot{v}^* = 2i, \qquad [a, a^\dagger] = 1. \tag{A.1.19}$$

We have hence canonically quantized the time varying oscillator. We can now postulate the existence of states $|0\rangle, |1\rangle \cdots$ and specially $a|0\rangle = 0$. The vacuum state is defined by $a|0\rangle = 0$, so we invert (A.1.14) to get

$$a = \frac{\dot{v}(t)q(t) - v(t)p(t)}{i\sqrt{2}}. \tag{A.1.20}$$

The choice of the vacuum hence depends on the choice of the mode function $v(t)$. But physically we *expect* the ground state to be unique and not depend on the choice of v. Therefore we try to find such a ground state by imposing a physical condition on it. Since the ground state is a state where the system is at least energy, we can try to find v such that $\langle 0|H|0\rangle$ is minimized. Looking back at (A.1.2), we substitute (A.1.14) as

$$\mathcal{H} = \frac{p^2}{2} + \frac{1}{2}\omega^2(t)q^2,$$
$$\implies \mathcal{H} = \frac{1}{4}\underbrace{\left[a\dot{v}^*(t) + a^\dagger\dot{v}(t)\right]^2}_{I_1} + \frac{1}{4}\omega^2(t)\underbrace{\left[av^*(t) + a^\dagger v(t)\right]^2}_{I_2}.$$

Looking first at I_1 and using (A.1.19) we get

$$I_1 = \left[\dot{v}\dot{v}a^\dagger a^\dagger + \dot{v}\dot{v}^* a^\dagger a + \dot{v}^*\dot{v}aa^\dagger + \dot{v}^*\dot{v}^* aa\right] = \left[\dot{v}^2 a^\dagger a^\dagger + \dot{v}\dot{v}^*(2a^\dagger a + 1) + \dot{v}^{*2}aa\right].$$
$$I_2 = \left[vva^\dagger a^\dagger + vv^* a^\dagger a + v^* vaa^\dagger + v^* v^* aa\right] = \left[v^2 a^\dagger a^\dagger + vv^*(2a^\dagger a + 1) + v^{*2}aa\right].$$

When we take the expectation value in the ground state, all the $a^\dagger a^\dagger$, aa and $a^\dagger a$ terms will go to zero because of orthogonality of states. Hence we have

$$E = \langle 0|H|0\rangle = \frac{|\dot{v}^2| + \omega^2|v|^2}{4}. \tag{A.1.21}$$

The energy clearly a function of time. We first minimize energy at one instance of time $t = t_0$. One possible choice of the mode function that also satisfies (A.1.15) is

$v = q$ and $\dot{v} = p$. We also have the normalization condition $pq^* - qp^* = 2i$. Therefore we have to minimize

$$E = \langle 0|H|0\rangle = \frac{|p^2| + \omega^2|q|^2}{4}.$$

Note that there are two independent parameters in the quantity we wish to minimize. However, we also have the normalization condition, which we can use to eliminate one of the independent variables. However, the form of the normalization condition makes it hard to separate one variable in favor of the other. To use it, we need to change its form to make it usable. We observe that the normalization and energy equation are invariant under the transformation $p \to e^{i\lambda}p$ and $q \to e^{i\lambda}q$. We can use the fact that λ is unconstrained to simplify the form of the normalization equation.If $q = q_1 + q_2$ and $p = p_1 + p_2$ we can see that

$$e^{i\lambda}q = (\cos\lambda + i\sin\lambda)(q_1 + iq_2)$$

$$= (q_1\cos\lambda - q_2\sin\lambda) + i(q_1\sin\lambda + q_2\cos\lambda).$$

We can now demand for the imaginary part to vanish, choosing λ appropriately as

$$\lambda = \arctan\frac{-q_2}{q_1}.$$

This is useful since now that q is real, $q = q^*$ and we can separate the variables in the normalization condition as

$$(p - p^*)q = 2i \implies q = \frac{1}{p_2}.$$

The Energy takes the form

$$H = \frac{1}{4}\Big(p_1^2 + p_2^2 + \frac{\omega^2(t_0)}{p_2^2}\Big).$$

Differentiating with respect to p_1 and p_2 we can now minimize the function. We have

$$p_1 = 0, \qquad 2p_2 - \frac{2\omega^2}{p_2^3} = 0 \implies p_2 = \pm\sqrt{\omega(t_0)}.$$

Hence we have

$$\dot{v}(t_0) = i\sqrt{\omega(t_0)}, \qquad v(t_0) = \frac{1}{\sqrt{\omega(t_0)}}. \tag{A.1.22}$$

Hence the pair v and $\dot{v}$ will define $a, a^\dagger$ such that $E_{\min} = \frac{1}{2}\omega(t_0)$, and we have the instantaneous ground state $|0_{t_0}\rangle$ (because its at time $t = t_0$). Note that if $w^2 < 0$, the minimum does not exist and the energy would be unbounded from below.

A.1.1 In and out states

Let us look back at (Fig. A.1). When $t < t_0, v_{in}(t) = e^{i\omega_0 t}$ and $t > t_1, v_{out}(t) = e^{i\omega_1 t}$. We now ask how the in and the out modes are related.

$e^{\pm i\omega_1 t}$ are a set of plane waves that form a complete basis to the solutions of the equation (A.1.15), any solution to it can be expressed in this basis, i.e any solution can be expressed as a linear superposition of the plane waves. We hence write

$$v_{in}(t) = \alpha e^{i\omega_1 t} + \beta e^{-i\omega_1 t}$$

$$\implies v_{in}(t) = \alpha v_{out} + \beta v_{out}^*. \tag{A.1.23}$$

This relation is an example of a Bogolyubov transformation. But these parameters α, β are not fully free parameters. Again, the normalization condition will impose a constraint on them. We start with (A.1.16) and use the Bogolyubov relation as

$$\dot{v}_{in} v_{in}^* - v_{in}\dot{v}_{in}^* = 2i$$

$$\implies (\alpha i\omega_1 v_{out} - \beta i\omega_1 v_{out}^*)(\alpha^* v_{out}^* + \beta^* v_{out}) + (\alpha^* i\omega_1 v_{out}^* - \beta^* i\omega_1 v_{out})(\alpha v_{out} + \beta v_{out}^*) = 2i$$

$$\implies |\alpha|^2 i\omega_1 + \cancel{\alpha\beta^* i\omega_1 v_{out}^2} - \cancel{\beta\alpha^* i\omega_1 v_{out}^{*\,2}} - |\beta|^2 i\omega_1 + |\alpha|^2 i\omega_1 + \cancel{\alpha^*\beta i\omega_1 v_{out}^{*\,2}} - \cancel{\beta^*\alpha i\omega_1 v_{out}^2} - |\beta|^2 i\omega_1 = 2i$$

$$\implies |\alpha|^2 - |\beta|^2 = \frac{1}{\omega_1}$$

By rescaling $\alpha, \beta \to \sqrt{\omega_1}\alpha, \sqrt{\omega_1}\beta$ we hence get a simple condition on the Bogolyubov coefficients as

$$|\alpha|^2 - |\beta|^2 = 1. \tag{A.1.24}$$

Since the operators a and $a^\dagger$ are composed of v_{in}, we can use (A.1.23) in (A.1.20) for a_{in} as

$$a_{in} = \frac{\dot{v}_{in} q - v_{in} p}{i\sqrt{2}}$$

$$= \frac{(\alpha\dot{v}_{out} + \beta\dot{v}_{out}^*)q - (\alpha v_{out} + \beta v_{out}^*)p}{i\sqrt{2}}$$

$$\implies a_{in} = \alpha a_{out} - \beta a_{out}^\dagger, \qquad a_{in}^\dagger = \alpha^* a_{out}^\dagger - \beta^* a_{out}. \tag{A.1.25}$$

To obtain the a similar relation for a_{out}, we need to eliminate $a^\dagger_{out}$. To do so, we just multiply a_{in} by α^* and $a^\dagger_{in}$ by β and add them to cancel the cross terms. We have

$$\alpha^* a_{in} + \beta a^\dagger_{in} = |\alpha|^2 a_{out} - \cancel{\beta\alpha^* a^\dagger_{out}} + \cancel{\alpha^*\beta a^\dagger_{out}} - |\beta|^2 a_{out} = (|\alpha|^2 - |\beta|^2) a_{out} \overset{(A.1.24)}{=} a_{out}$$

$$\implies a_{out} = \alpha^* a_{in} + \beta a^\dagger_{in}, \qquad a^\dagger_{out} = \alpha a^\dagger_{in} + \beta^* a_{in}. \tag{A.1.26}$$

This means that when $\beta \neq 0$, a_{out} differs from a_{in} and defines different vacuum states through $a|0\rangle = 0$. Hence the vacuum changes in time. To look at this more clearly, this means that if we prepare the system in state $|\psi\rangle = |0_{in}\rangle$ at $t \ll t_0$, and evolve it till time t_1. The quantum state still remains $|0_{in}\rangle$, but after time $t = t_1$ we compare the state to the ground state of the system at that particular time, i.e $|0_{out}\rangle$. The ground states are different, so the out system will no longer be in the ground state. The system will hence be in a superposition of the new $|n_{out}\rangle$. Therefore one will see the system in an excited state. Physically it makes sense as well since a change in frequency of the oscillator corresponds to driving the oscillator. It corresponds to work done on the system leading to the injection or omission of energy and the system's changing energies of states. As before, since the Hamiltonian energy function is time-dependent, so energy is not conserved.

A.2 Scalar field in expanding background

A.2.1 Metric and the action

We now show how gravitational backgrounds influence the equations of motions. We work in the the FRW metric. The metric looks like:

$$ds^2 = g_{\alpha\beta}\, dx^\alpha\, dx^\beta = dt^2 - a^2(t)(\, dx^2 + \, dy^2 + \, dz^2). \tag{A.2.1}$$

This metric looks similar to the Minkowski metric, but with a scale factor in front of the spatial metric part. This metric is an exact solution of the Einstein's equation. We look at a real valued scalar field ϕ, which is minimally coupled to the metric, i.e all contractions that involve the metric are done with the FRW metric defined above

and there is no other term involving the scalar field ϕ and the metric $g_{\alpha\beta}$. Moreover, we work with a free field (i.e no interactions) which has $m \neq 0$. The action for theory is given by

$$\mathcal{S} = \int \sqrt{-g}\, d^3x dt \Big[\frac{1}{2} g^{\alpha\beta}(\partial_\alpha \phi)(\partial_\beta \phi) - \frac{1}{2} m^2 \phi^2\Big]. \tag{A.2.2}$$

Here the $\sqrt{-g}$ is the determinant of the metric $g^{\alpha\beta}$ and ensures that the action is invariant under co-ordinate transformations. Note that standard summation conventions apply here. The corresponding equations of motion corresponding to this action are

$$g^{\alpha\beta}\nabla_\alpha \nabla_\beta \phi + m^2 \phi = 0. \tag{A.2.3}$$

In the flat Minkowski space-time case, this equation had $g^{\alpha\beta} = \eta^{\alpha\beta}$ and this reduced to the well known Klein-Gordan equation we then quantized canonically. But here we would have the $a(t)$ factor complicating the differential equation and finding a mode expansion non-trivial. To have a closer look, we do the following transformation

$$\eta(t) = \int_{t_0}^{t} \frac{dt}{a(t)}. \tag{A.2.4}$$

the metric then looks like

$$ds^2 = a^2(\eta)(d\eta^2 - dx^2 + dy^2 + dz^2). \tag{A.2.5}$$

This metric is similar to the Minkowski metric but up to the factor $a^2(t)$. Metrics like these are called conformally flat because they differ from the flat metric by the factor $a^2(t)$, the conformal factor. We now apply this to the action we have. Conformally equivalent metrics are interesting because they leave the causal structure of the theory invariant. We first calculate the determinant term as

$$\sqrt{-g} = \sqrt{-(a^2(t))(-a^2(t))(-a^2(t))(-a^2(t))} = a^4(t). \tag{A.2.6}$$

Moreover, we can now write the FRW metric in terms of the Minkowski as

$$g^{\alpha\beta} = \frac{1}{a^2}\eta^{\alpha\beta}. \tag{A.2.7}$$

The action hence looks like

$$\mathcal{S} = \frac{1}{2}\int d^3x d\eta \Big[a^2\big[\phi'^2 - (\nabla\phi)^2\big] - a^4(t) m^2 \phi^2\Big].$$

Finally, performing the transformation $a\phi = \chi$ we see that (and noting that prime represents differentiation w.r.t η)

$$\mathcal{S} = \frac{1}{2}\int d^3x d\eta \Big[a^2\Big[\Big(\frac{\chi}{a}\Big)'^2 - \Big(\frac{\nabla\chi}{a}\Big)^2\Big] - a^4 m^2\Big(\frac{\chi}{a}\Big)^2\Big].$$
$$= \frac{1}{2}\int d^3x d\eta \Big[\underbrace{a^2\Big[\Big(\frac{\chi}{a}\Big)'^2\Big]}_{A} - (\nabla\chi)^2 - a^2 m^2\chi^2\Big].$$

We look separately at A. We can see that

$$a^2\Big(\frac{\chi}{a}\Big)'^2 = a^2\Big(\frac{a\chi' - \chi a'}{a^2}\Big)^2 = \chi'^2 + \chi^2\frac{a''}{a} - \Big[\chi^2.\frac{a'}{a}\Big]'.$$

The last term in the equation above is a total derivative and will vanish in the expression for action. Hence we finally get the expression

$$\mathcal{S} = \frac{1}{2}\int d^3x d\eta \Big[\chi'^2 - (\nabla\chi)^2 - \underbrace{\Big(a^2m^2 - \frac{a''}{a}\Big)}_{m_{\text{eff}}}\chi^2\Big]$$

$$\implies \mathcal{S} = \frac{1}{2}\int d^3x d\eta \Big[\chi'^2 - (\nabla\chi)^2 - m_{\text{eff}}\chi^2\Big]. \tag{A.2.8}$$

Where we have called renamed the terms inside the parenthesis as $m_{\text{eff}}(\eta)$. Therefore the dynamics of a scalar field ψ in flat FRW space-time are equivalent to the dynamics of a field χ in Minkowski space-time with an effective mass that depends on the time variable.

A.2.2 Mode expansion and quantization

Let us have a look at the equation of motion

$$\chi'' + \nabla^2\chi + m_{\text{eff}}(\eta)\chi = 0. \tag{A.2.9}$$

We begin with going to the Fourier basis, i.e we substitute

$$\chi(x,\eta) = \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}}\chi_k(\eta)e^{i\mathbf{k}.\mathbf{x}}.$$

We can substitute this in the equation of motion to get

$$\chi_k'' + \underbrace{\big(k^2 + m_{\text{eff}}(\eta)\big)}_{\omega_k^2(\eta)}\chi_k = 0.$$

$$\implies \chi_k'' + \omega_k^2(\eta)\chi_k = 0. \tag{A.2.10}$$

Hence in momentum space, we see that at each point there is a harmonic oscillator whose frequency varies with time i.e a time dependent harmonic oscillator (in comparison to fields in Minkowski space-time where we have *time independent* harmonic oscillators at each point in momentum space). Hence we can now use the results calculated for the time varying harmonic oscillator in last subsection. We can choose a mode function $v_k(\eta)$ and do the mode expansion as shown before as

$$\chi_k(\eta) = \frac{1}{\sqrt{2}}(a_k v_k^*(\eta) + a_k^\dagger v_k(\eta)),$$

$$\implies \chi(x,\eta) = \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}}.\frac{1}{\sqrt{2}}(a_k v_k^* e^{i\mathbf{k}.\mathbf{x}} + a_k^\dagger v_k e^{-i\mathbf{k}.\mathbf{x}}). \tag{A.2.11}$$

Until now, the fields were classical. We can now impose equal time canonical commutation relations for the field operators as

$$[\chi(x_1,\eta), \pi(x_2,\eta)] = [\chi(x_1,\eta), \chi'(x_2,\eta)] = i\delta(x_1 - x_2). \tag{A.2.12}$$

The first equality here can be seen by noting that $\pi = \frac{\partial \mathcal{L}}{\partial \chi'} = \chi'$. Moreover, here we also *demand* that the creation and annihilation operators satisfy canonical commutation relations

$$[a_k, a_{k'}^\dagger] = \delta(k - k'), \qquad [a_k, a_{k'}] = [a_k^\dagger, a_{k'}^\dagger] = 0. \tag{A.2.13}$$

We can ask what (A.2.11) and (A.2.12) mean for the mode functions. We see that

$$[\chi(x_1), \chi'(x_2)] = \int \frac{d^3k d^3k'}{(2\pi)^3} e^{ikx_1} e^{ik'\cdot x_2}.\frac{1}{2}\left[a_k v_k^* + a_{-k}^\dagger v_k, a_{k'} v_k'^* + a_{-k'}^\dagger v_{k'}'\right]$$

$$= \int \frac{d^3k d^3k'}{(2\pi)^3}\frac{e^{ik.x_1}e^{ik'.x_2}}{2}.\left(v_k^* v_k' \underbrace{\left[a_k, a_{-k}^\dagger\right]}_{\delta(k+k')} - v_k v_{k'}'^* \underbrace{\left[a_{-k}^\dagger, a_{k'}\right]}_{\delta(k'+k)}\right)$$

$$= \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}}\frac{e^{ik.(x_1-x_2)}}{2}.\left(v_k^* v_k' - v_k v_{k'}'^*\right) \overset{(A.2.11)}{=} i\delta(x_1 - x_2)$$

$$\implies v_k^* v_k' - v_k v_{k'}'^* = 2i \iff W[v_k, v_k^*] = 2i \quad \text{or} \quad \mathrm{Im}(v_k^* v_k') = 1. \tag{A.2.14}$$

This means that we can quantize the scalar field χ describing quantum fields in an expanding background by promoting a and $a^\dagger$ to operators that satisfy (A.2.13) and

making sure that the mode functions satisfy (A.2.14) and (A.1.15). Here all the focus goes into the choice of the mode functions.

Looking at (A.1.15), we see that the second order equation for $v_k(\eta)$ will give us two independent complex valued solutions. Since we also have the normalization constraint due to quantization in (A.2.14), which is a linear equation relating the complex components of these solutions to each other, we end up with one one independent complex degree of freedom governing the mode functions. Finally, we can observe that multiplying $v_k(\eta)$ by $e^{i\alpha}$ introduces an extra phase, which can be absorbed into the creation and annihilation operators. This then means that the vacuum state changes by a phase. This can be represented by

$$v_k \to v_k e^{i\alpha} \overset{(A.2.11)}{\implies} a \to a e^{-i\alpha} \implies |0\rangle \to e^{-i\alpha} |0\rangle .$$

All states that differ up to a phase are physically equivalent, so we are only left with one real degree of freedom that governs the freedom in choosing the mode function. Hence we have successfully used all the constraints and conditions, but only to find freedom in choosing the mode function. The corresponding real degree of freedom can distinguish between these mode functions. However, since all of these functions satisfy (A.1.15) and (A.2.14), they are all physically equivalent as they give rise to physically equivalent states.

A.2.3 The vacuum

Now that we have the operator a, we can define the vacuum state as $a|0\rangle = 0$. With repeated usage of $a^\dagger$, one can construct the multiparticle states. An excited state $|m_{k_1}, n_{k_2} \cdots\rangle$ with occupation numbers $m, n \cdots$ of the field χ is given by

$$|m_{k_1}, n_{k_2} \cdots\rangle = \frac{1}{\sqrt{m!n! \cdots}} \left[(a^\dagger_{k_1})^m (a^\dagger_{k_2})^n \cdots \right] |0_{k_1}, 0_{k_2} \cdots\rangle .$$

To keep notation simple, we call this $|0\rangle$. Given a mode function, we have the mode expansion and, therefore, the operators a and $a^\dagger$. The operator a *defines* the vacuum state. Hence the mode function's choice invariably changes the vacuum state. The vacuum state is important because it is what the description of the particle is based

on, and a change in it would reflect a change in the type and number of particles present in a particular configuration of the field. We ask, "which mode function will give us the correct physical vacuum?"

Instantaneous energy eigenstates

To find an expression for the mode function, we need to constrain it further, and we do this by demanding that the ground state is a state which minimizes the energy. We do this at a particular time $\eta = \eta_0$. Therefore the statement then becomes "find $v(\eta)$ such that $\langle 0_{\eta_0}| H(\eta_0) |0_{\eta_0}\rangle$ is minimized". This is a question almost identical to what we did in the last subsection with the time-dependent harmonic oscillator in (A.1.22). The results for the appropriate mode function when $\omega_k^2 > 0$ are

$$v_k(\eta_0) = \frac{1}{\sqrt{\omega_k(\eta_0)}}, \qquad v_k'(\eta_0) = i\sqrt{\omega_k(\eta_0)} = i\omega_k(\eta_0)v_k(\eta_0). \tag{A.2.15}$$

Now, when $\omega_k(\eta) =$ constant (for example Minkowski space-time), we get the familiar Minkowski result as

$$v_k(\eta) = \frac{1}{\sqrt{\omega_k}} e^{i\omega_k \eta}.$$

However, in gravitational/expanding backgrounds, ω is a function of time. That means that for each time instance, we have a different v_k. Changing mode functions imply that the creation and annihilation operators also keep changing. This leads to a change in the description of the vacuum and hence the particles. One can now ask how two different creation and annihilation operators coming from these mode functions are related. The relations between the operators are what are called Bogolyubov transformations.

A.2.4 Bogolyubov transformations

Consider two mode functions $v_k(\eta)$ and $u_k(\eta)$. We now wish to write the operator v_k in terms of u_k. Since u_k and u_k^* also form a complete basis, we can use them to write v_k^* as

$$v_k(\eta) = \alpha_k u_k(\eta) + \beta_k u_k^*(\eta). \tag{A.2.16}$$

Since v should be normalized by (A.2.14), we have

$$v^* v' - v v'^* = 2i,$$

$$\implies (\alpha_k^* u_k^* + \beta_k^* u_k)\left(\alpha_k u_k' + \beta_k u_k'^*\right) - (\alpha_k u_k + \beta_k u_k^*)\left(\alpha_k^* u_k'^* + \beta_k^* u_k'\right) = 2i$$

$$\implies |\alpha_k|^2 u_k^* u_k' + \cancel{\alpha_k \beta_k^* u_k' u_k} + \cancel{\beta_k \alpha_k^* u_k'^* u_k^*} + |\beta_k|^2 u_k u_k'^* - |\alpha_k|^2 u_k u_k'^* - \cancel{\alpha_k \beta_k^* u_k' u_k}$$
$$- \cancel{\beta_k \alpha_k^* u_k'^* u_k^*} - |\beta_k|^2 u_k^* u_k' = 2i$$

$$\implies |\alpha_k|^2 \left(u_k^* u_k' - u_k u_k'^*\right) - |\beta_k|^2 \left(u_k^* u_k' - u_k u_k'^*\right) = 2i.$$

But we know that u must also be normalized in the same way. Using this in the above equation, we get

$$|\alpha_k|^2 - |\beta_k|^2 = 1. \tag{A.2.17}$$

These relations are analogous to what we obtained in the last subsection. This relation constraints the coefficients α and β. Looking at the mode expansion (A.2.11) for both the mode functions v and u we find

$$\chi(x,\eta) = \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}} \cdot \frac{1}{\sqrt{2}} (a_k v_k^* + a_{-k}^\dagger v_k) e^{i\mathbf{k}.\mathbf{x}},$$

$$\chi(x,\eta) = \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}} \cdot \frac{1}{\sqrt{2}} (b_k u_k^* + b_{-k}^\dagger u_k) e^{i\mathbf{k}.\mathbf{x}}.$$

Since they are just different expressions for the same quantity, we can equate them. Since they will be equal for any arbitrary x, we can equate the terms in front of the exponential as

$$\left(b_k u_k^* + b_{-k}^\dagger u_k\right) e^{i\mathbf{k}.\mathbf{x}} = \left(a_k v_k^* + a_{-k}^\dagger v_k\right) e^{i\mathbf{k}.\mathbf{x}}. \tag{A.2.18}$$

Using (A.2.16) we look at the RHS as

$$a_k v_k^* + a_{-k}^\dagger v_k = \left(\alpha_k^* u_k^* + \beta_k^* u_k\right) a_k + \left(\alpha_k u_k + \beta_k u_k^*\right) a_{-k}^\dagger$$
$$= \left(\alpha_k^* a_k + \beta_k a_{-k}^\dagger\right) u_k^* + \left(\alpha_k a_{-k}^\dagger + \beta_k^* a_k\right) u_k.$$

Comparing the LHS in (A.2.18) to the equation above, we get

$$\boxed{b_k = \alpha_k^* a_k + \beta_k a_{-k}^\dagger, \qquad b_{-k}^\dagger = \alpha_k a_{-k}^\dagger + \beta_k^* a_k.} \tag{A.2.19}$$

These are the Bogolyubov transformations and the operators a and b here define the two different vacuums, $|0_a\rangle$ and $|0_b\rangle$. As said before, a change in vacuum represents a change in particles. One way to see this explicitly is to look at an average value of the number operator.

A.2.5 Mean particle number

The two vacua define two different particles. We can now ask on average how many "b-particles" (of the field mode χ_k) exist in the "a-vacuum". This would look like

$$\langle N_b \rangle_{0_a} = \langle 0_a | \, N_b \, | 0_a \rangle = \langle 0_a | \, b_k^\dagger b_k \, | 0_a \rangle \, .$$

Here we can use (A.2.19) to write this in terms of a operators as

$$= \langle 0_a | \left(\alpha_k a_k^\dagger + \beta_k^* a_{-k} \right) \left(\alpha_k^* a_k + \beta_k a_{-k}^\dagger \right) | 0_a \rangle = \langle 0_a | \left(|\beta_k|^2 a_{-k} a_{-k}^\dagger \right) | 0_a \rangle \, ,$$

$$\implies \langle N_b \rangle_{0_a} = |\beta_k|^2 \delta^3(0).$$

The appearance of the delta function stems from the commutation relations. It is attributed to the fact that we consider the integral over full space, which has an infinite volume. In a case where we have a finite size of the system, we can then talk about the *number density* of particles in this quantized field mode χ_k as

$$\boxed{\langle n_b \rangle_{0_a} = |\beta_k|^2.} \tag{A.2.20}$$

If we prepare the field in the state $|0_a\rangle$ and look for the number of "b-particles," we will see a finite number of these particles in the vacuum. However, how is this relevant? In the last subsection, we saw that the mode function changes with time for an expanding space-time, which implied that the vacuum state changes with time. If one were to prepare the instantaneous vacuum at a time η_0, then after an infinitesimal amount of time $\eta_0 + \delta\eta$, the original state would not be the vacuum state of the system anymore. As a result, we will see particles with density for a system in that state. This can be attributed to the time-dependent harmonic oscillator (which is what the system boils down to) does not conserve energy, and the energy function is time-dependent. We do not have any faithful time-independent eigenstates that can work as the vacuum state because the Hamiltonian is time-dependent.

A.3 Unruh effect

In this section, we will look at the phenomenon of the Unruh effect and try to explain it using the ideas developed in the past subsections of this appendix. The core idea of the effect is that an accelerated observer in Minkowski space-time observes the ground state of a scalar field to have particles. The particles can be seen to follow a thermal distribution. We start with looking at a co-ordinate system adapted for accelerating observers.

A.3.1 Accelerating observers and the Rindler co-ordinates

Let us go back to special relativity and try to look at the problem of accelerating observers. We would like to see what the world-lines of accelerating observers look like and develop a suitable co-ordinate system for it.

Consider an observer with constant acceleration in x direction. We know that 4-velocity $U^\mu = (u_0, u_1, u_2, u_3)$ has norm -1 for massive particles. This means that

$$-u_0^2 + u_1^2 = -1 \implies u_0^2 - u_1^2 = 1. \tag{A.3.1}$$

We now parametrize u_1 and u_0 as

$$u_0 = \cosh f(\tau), u_1 = \sinh f(\tau). \tag{A.3.2}$$

This gives us the four-acceleration

$$a^\alpha = (\dot{f(\tau)} \sinh f(\tau), \dot{f(\tau)} \cosh f(\tau), 0, 0). \tag{A.3.3}$$

Now we demand that the norm of this 4-acceleration be constant, i.e

$$a^2 = \dot{f(\tau)}^2 (\cosh^2 f(\tau) - \sinh^2 f(\tau)) = \dot{f(\tau)}^2. \tag{A.3.4}$$

This gives us a form for f, i.e $f = k\tau$. Given f, we can now find the corresponding world-lines by integrating the 4-velocity as

$$x^\mu = (\frac{1}{a} \sinh a\tau, \frac{1}{a} \cosh a\tau, 0, 0). \tag{A.3.5}$$

The world-lines of the accelerated observers are hyperbolae. To clearly see this,compute the line element as

$$-t^2 + x^2 = -\frac{1}{a^2}\sinh^2 a\tau + \frac{1}{a^2}\cosh^2 a\tau = \frac{1}{a^2}. \tag{A.3.6}$$

The world-lines correspond to hyperbolae confined in the first and fourth quadrant by $x = y$ and $x = -y$ ((Fig. A.2), on next page) since a^2 is always positive. Higher the acceleration, the smaller would be $\frac{1}{a^2}$, and the graph would come closer to the lines $y = \pm x$.

Now, we want a convenient co-ordinate system for this accelerating object. For example, Minkowski co-ordinates are suitable for objects at rest. An object at rest can be denoted by $x, y, z =$ constant and t which can change. A moving object, in its frame since its is always at rest will always have a fixed position ($x, y, z =$ constant) and the corresponding time co-ordinate will represent proper time, i.e $x^\mu = (\tau, a, b, c)$ for arbitrary constants a,b,c. Hence $x, y, z =$ constant represent static objects. We wish to find a co-ordinate system (η, ρ) such that $\rho =$ constant represents a constantly accelerating object. To do so, we go into the accelerating frame of reference (the *proper frame*) and use co-ordinates (η, ρ) which represent the proper time and proper length. The transformation is much alike to what we saw above and looks like

$$t = \frac{1 + a\rho}{a}\sinh a\eta, \qquad x = \frac{1 + a\rho}{a}\cosh a\eta \tag{A.3.7}$$

$$\implies dt^2 = (d\rho \sinh a\eta + (1 + a\rho)\, d\eta \cosh a\eta)^2, \;\; dx^2 = (d\rho \cosh a\eta + (1 + a\rho)\, d\eta \sinh a\eta)^2.$$

We can now compute the line element in this co-ordinate system as

$$ds^2 = dt^2 - dx^2 = (d\rho \sinh a\eta + (1 + a\rho)\, d\eta \cosh a\eta)^2 - (d\rho \cosh a\eta + (1 + a\rho)\, d\eta \sinh a\eta)^2$$

$$\implies ds^2 = (1 + a\rho)^2\, d\eta^2 - d\rho^2. \tag{A.3.8}$$

This is called the Rindler metric and the co-ordinates (ρ, η) are called Rindler co-ordinates. A few features of this metric and corresponding space-time are written below.

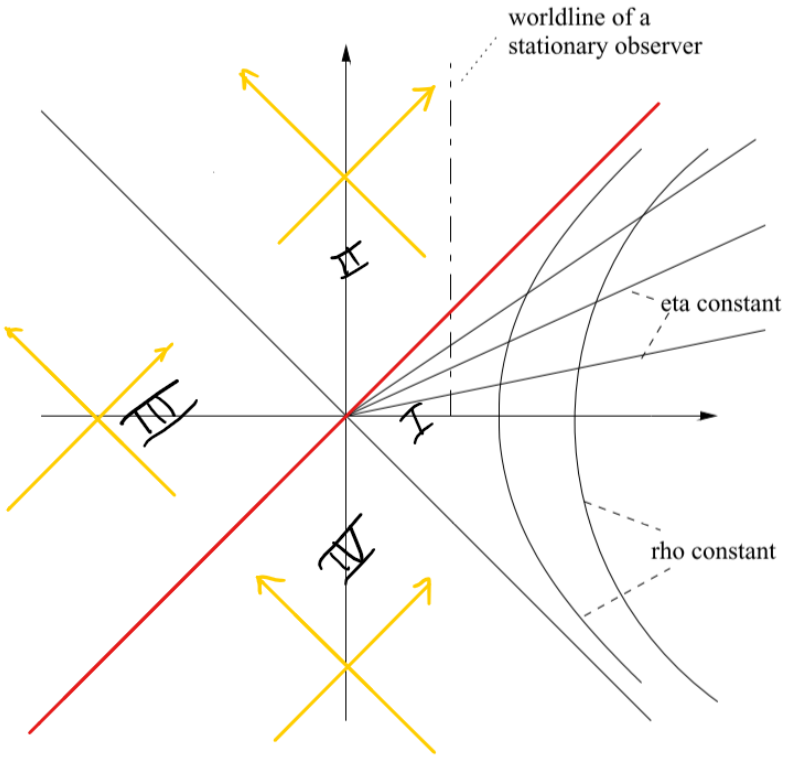


Figure A.2: Rindler co-ordinates

- One can show by substitution that $x^2 - t^2 = \left(\frac{1}{a} + \rho\right)^2$. This means that $\rho =$ constant trajectories trace hyperbolae in the original Minkowski co-ordinates. Connecting this to (A.3.6), $\rho =$ constant trajectories represent accelerating observers with $\rho = \frac{1}{k}$. Hence this is a convenient co-ordinate.

- One can show that $\frac{t}{x} = \tanh a\eta$, which means that $a\eta$ =constant trajectories are straight lines in original Minkowski co-ordinates. When $\rho =$ constant, the metric in terms of proper time can be read as:

$$ds^2 = d\tau^2 = (1 + a\rho_0)^2 \, d\eta^2.$$

  Hence η also acts as a proper time co-ordinate. This is exactly as we wanted in corollary to static observers and Minkowski co-ordinates.

- As shown in (Fig. A.2), all accelerated observers lie in quadrant 1, often called the Rindler wedge. Since light travels along 45-degree lines (shown in yellow),

and the hyperbolas asymptote to $y = \pm x$, the light coming from quadrants 2 and 3 can never reach an observer in region 1. Hence an accelerating observer is causally disconnected to regions 2 and 3. This is an example of an event horizon (this one is called the Rindler horizon), which is a surface (highlighted in red) through which information cannot reach someone outside it. Note that this horizon disappears whenever the object stops accelerating.

A.3.2 Scalar quantum field in Rindler space

Now we put (A.3.8) in a more convenient form. We make the transformation $\xi = \ln(1 + a\rho)$, and the metric then looks like

$$ds^2 = e^{2a\xi}\left(d\eta^2 - d\xi^2\right). \tag{A.3.9}$$

It is evident that the Rindler metric in these co-ordinates is equal to the Minkowski metric multiplied by a space-time function and is therefore conformally flat. We can now ask what a quantum field looks like in this form of the metric in 1+1 dimensions. We look at a massless scalar field that is minimally coupled, i.e., effects of the metric only show up in the co-ordinate invariant measure and the contractions in the Lagrangian. The general action takes the form

$$S[\phi] = \frac{1}{2}\int d^2x\sqrt{-g}g^{\alpha\beta}\partial_\alpha\phi\partial_\beta\phi. \tag{A.3.10}$$

In Minkowski coordinates, the action looks like

$$S[\phi] = \frac{1}{2}\int dx\,dt\left[(\partial_t\phi)^2 - (\partial_x\phi)^2\right]. \tag{A.3.11}$$

We now look at the action in Rindler co-ordinates. One feature which will be of great use is the conformal flatness of the Rindler metric. We observe that if

$$g_{\alpha\beta} \to g'_{\alpha\beta} = \Omega^2(x)g_{\alpha\beta}, \qquad \sqrt{-g} \to \Omega^2(x)\sqrt{-g} \text{ and } g^{\alpha\beta} \to \Omega^{-2}g^{\alpha\beta}. \tag{A.3.12}$$

This means that the action is invariant under conformal transformations as it involves the product of $\sqrt{-g}$ and $g^{\alpha\beta}$. This property of conformal invariance is highly useful

in general. the action in the Rindler metric takes the same form as (A.3.11), but as a function of the Rindler variables:

$$S[\phi] = \frac{1}{2}\int d\xi\, d\eta \left[(\partial_\eta \phi)^2 - (\partial_\xi \phi)^2\right]. \tag{A.3.13}$$

Looking at the equations of motions for both these actions, we get

$$\frac{\partial^2\phi}{\partial t^2} = \frac{\partial^2\phi}{\partial x^2}, \qquad \frac{\partial^2\phi}{\partial \eta^2} = \frac{\partial^2\phi}{\partial \xi^2}. \tag{A.3.14}$$

These have the same form as wave equations. The solutions can be written as superposition of waves that go in both spatial directions. The solutions look like

$$\phi(x,t) = A(t-x) + B(t+x), \qquad \phi(\xi,\eta) = C(\eta-\xi) + D(\eta+\xi). \tag{A.3.15}$$

Proceeding with the mode expansions, we find in the Minkowski metric

$$\phi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \frac{1}{\sqrt{2|k|}} \left(e^{-i|k|t+ikx} a_k + e^{i|k|t-ikx} a_k^\dagger\right), \tag{A.3.16}$$

and in the Rindler metric

$$\phi(\xi,\eta) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \frac{1}{\sqrt{2|k|}} \left(e^{-i|k|\eta+ik\xi} b_k + e^{i|k|\eta-ik\xi} b_k^\dagger\right). \tag{A.3.17}$$

Since the exponentials in these expansions are functions of different variables, their corresponding coefficients (that become operators when quantized) in the general solution of the field will be different. Hence in general, the operators a_k and b_k are different. Consequently the vacua they define would also be different, i.e we have the Minkowski vacuum $a_k |0_M\rangle = 0$ and the Rindler vacuum $b_k |0_R\rangle$ (both of them for all values of k) being different states.

As in the last subsections, we can ask, "Which of these corresponds to the correct/-physical vacuum?". If one were to hop onto an accelerating spaceship and observe the field to be in the Minkowski vacuum, then they would see the Minkowski vacuum $|0_M\rangle$ having particles, i.e., not being the lowest energy state. For observers moving with the accelerated spaceship, the correct vacuum for the fields (the configuration that minimizes the energy) is the Rindler vacuum, $|0_R\rangle$. Hence, the Minkowski vacuum will appear as an excited state. Similarly, if stationary observers observe the

field in a Rindler vacuum, it would be filled with particles.

Hence there is no "correct" vacuum. Its choice is dependent on the situation. This detection of particles in a previously empty (up to quantum fluctuations) space-time upon acceleration is called the Unruh effect. The next step is to find the relation between the different vacuum states defined and the spectrum of the particles observed by the accelerated observer. These relations are precisely the Bogolyubov transformations that were described earlier.

A.3.3 Bogolyubov transformations

To arrive on the relation between the operators a_k and b_k, we need to compare the mode expansions as before. To make this easier, we begin by writing the mode expansion in the light-cone co-ordinates which will decouple x, t or ξ, η and allow for comparison with (A.3.14). For both the co-ordinate systems, we define light-cone co-ordinates as

$$\bar{u}, \bar{v} = t \mp x, \qquad u, v = \eta \mp \xi. \tag{A.3.18}$$

The unbarred co-ordinates will henceforth represent the accelerated frame light-cone co-ordinates and the barred represent the co-ordinates in the unaccelerated frame where the observer is freely falling. Both u and v take take values from $(-\infty, \infty)$. With this transformation, (A.3.7) looks like

$$\bar{u} = -\frac{1}{a}e^{-au}, \qquad \bar{v} = \frac{1}{a}e^{av}. \tag{A.3.19}$$

With these, the field solutions (A.3.15) look like

$$\phi(\bar{u}, \bar{v}) = A(\bar{u}) + B(\bar{v}), \qquad \phi(u, v) = C(u) + D(v). \tag{A.3.20}$$

Using these co-ordinates in the mode expansion, we can decouple the exponentials that were earlier a function of both x, t(or η, ξ for the Rindler case) into exponentials that only depend on these light-cone co-ordinates. The light-cone mode expansion in the unaccelerated frame take the form

$$\phi(\bar{u}, \bar{v}) = \int_0^\infty \frac{d\omega}{\sqrt{2\pi}} \frac{1}{\sqrt{2\omega}} \left(e^{-i\omega\bar{u}} a_\omega + e^{i\omega\bar{u}} a_\omega^\dagger + e^{-i\omega\bar{v}} a_{-\omega} + e^{i\omega\bar{v}} a_{-\omega}^\dagger \right), \tag{A.3.21}$$

and in the Rindler metric

$$\phi(u,v) = \int_0^\infty \frac{d\omega'}{\sqrt{2\pi}} \frac{1}{\sqrt{2\omega'}} \left(e^{-i\omega' u} b_{\omega'} + e^{i\omega' u} b^\dagger_{\omega'} + e^{-i\omega' v} b_{-\omega'} + e^{i\omega' v} b^\dagger_{-\omega'} \right). \quad \text{(A.3.22)}$$

Here ω and ω' are the corresponding momentum variables in the Minkowski frame mode expansion and the Rindler frame mode expansion. We can now compare these expansions to (A.3.20) and see explicit expressions for A, B, C, D as

$$A(\bar{u}) = \int_0^\infty \frac{d\omega}{\sqrt{2\pi}} \frac{1}{\sqrt{2\omega}} \left(e^{-i\omega \bar{u}} a_\omega + e^{i\omega \bar{u}} a^\dagger_\omega \right), \quad B(\bar{v}) = \int_0^\infty \frac{d\omega}{\sqrt{2\pi}} \frac{1}{\sqrt{2\omega}} \left(e^{-i\omega \bar{v}} a_{-\omega} + e^{i\omega \bar{v}} a^\dagger_{-\omega} \right),$$

$$C(u) = \int_0^\infty \frac{d\omega'}{\sqrt{2\pi}} \frac{1}{\sqrt{2\omega'}} \left(e^{-i\omega' u} b_{\omega'} + e^{i\omega' u} b^\dagger_{\omega'} \right), D(v) = \int_0^\infty \frac{d\omega'}{\sqrt{2\pi}} \frac{1}{\sqrt{2\omega'}} \left(e^{-i\omega' v} b_{-\omega'} + e^{i\omega' v} b^\dagger_{-\omega'} \right).$$

To find a relation between the operators a_k and b_k, we compare the mode functions. Since the Rindler mode expansion is only valid in the Rindler wedge, we can only compare the mode functions in that region. Hence for a point in that region, we should have the physical field giving the same value in any co-ordinate system. By equating these expressions for a given mode we would be able to see exactly how these operators are related. To do this, we start with

$$\phi(\bar{u}, \bar{v}) = \phi(\bar{u}, \bar{v}),$$

$$\implies A(\bar{u}) + B(\bar{v}) = C(u) + D(v)$$

$$\implies A(\bar{u}(u)) + B(\bar{v}(v)) = C(u) + D(v)$$

Since the transition from light-cone co-ordinates in Minkowski to Rindler frame does not intermix different momentum modes, we can equate the individual terms. By doing this, we get

$$A(\bar{u}(u)) = C(u), \qquad B(\bar{v}(v)) = D(v).$$

To look at the first part of this equation, we do a fourier transform of both sides of the equation $A(\bar{u}(u)) = C(u)$. This looks like

$$\int_{-\infty}^\infty \frac{du}{\sqrt{2\pi}} e^{i\Omega u} A(\bar{u}(u)) = \int_{-\infty}^\infty \frac{du}{\sqrt{2\pi}} e^{i\Omega u} C(u). \quad \text{(A.3.23)}$$

Looking at the RHS, we see that

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{du}{\sqrt{2\pi}}e^{i\Omega u}C(u) &= \int_{-\infty}^{\infty}\frac{du}{\sqrt{2\pi}}e^{i\Omega u}\int_0^{\infty}\frac{d\omega'}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega'}}\left(e^{-i\omega' u}b_{\omega'}+e^{i\omega' u}b^{\dagger}_{\omega'}\right)\\ &= \int_0^{\infty}\frac{d\omega'}{\sqrt{2\omega'}}\int_{-\infty}^{\infty}\frac{du}{2\pi}\left(e^{-i(\omega'-\Omega)u}b_{\omega'}+e^{i(\omega'+\Omega)u}b^{\dagger}_{\omega'}\right)\\ &= \frac{1}{\sqrt{2\Omega}}\begin{cases}b_{\Omega}, & \text{if } \Omega>0\\ b^{\dagger}_{-\Omega}, & \text{if } \Omega<0\end{cases}\end{aligned} \tag{A.3.24}$$

On the other hand, the LHS can be written as

$$\int_{-\infty}^{\infty}\frac{du}{\sqrt{2\pi}}e^{i\Omega u}A(\bar{u}(u)) = \int_{-\infty}^{\infty}\frac{du}{\sqrt{2\pi}}e^{i\Omega u}\int_0^{\infty}\frac{d\omega}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega}}\left(e^{-i\omega\bar{u}}a_{\omega}+e^{i\omega\bar{u}}a^{\dagger}_{\omega}\right) \tag{A.3.25}$$

$$\begin{aligned}&= \int_0^{\infty}\frac{d\omega}{\sqrt{2\omega}}\int_{-\infty}^{\infty}\frac{du}{2\pi}\left(e^{i\Omega u-i\omega\bar{u}}a_{\omega}+e^{i\Omega u+i\omega\bar{u}}a^{\dagger}_{\omega}\right)\\ &= \int_0^{\infty}\frac{d\omega}{\sqrt{2\omega}}\left(F(\omega,\Omega)a_{\omega}+F(-\omega,\Omega)a^{\dagger}_{\omega}\right).\end{aligned} \tag{A.3.26}$$

Where F is defined as

$$\begin{aligned}F(\omega,\Omega)\equiv\int_{-\infty}^{\infty}\frac{du}{2\pi}\exp\left[i\Omega u-i\omega\bar{u}\right] &= \int_{-\infty}^{\infty}\frac{du}{2\pi}\exp\left[i\Omega u-i\omega\bar{u}\right]\\ &\overset{(A.3.19)}{=}\int_{-\infty}^{\infty}\frac{du}{2\pi}\exp\left[i\Omega u+i\frac{\omega}{a}e^{-au}\right].\end{aligned} \tag{A.3.27}$$

Now, restricting to positive Ω (which means we are only talking about positive momentum modes, as thats the conjugate variable fourier transform brings), we can write b_{Ω} from (A.3.23),(A.3.24) and (A.3.26) as

$$\frac{b_{\Omega}}{\sqrt{2\Omega}} = \int_0^{\infty}\frac{d\omega}{\sqrt{2\omega}}\left(F(\omega,\Omega)a_{\omega}+F(-\omega,\Omega)a^{\dagger}_{\omega}\right)$$

$$\implies b_{\Omega} = \int_0^{\infty}d\omega\left[\underbrace{\sqrt{\frac{\Omega}{\omega}}F(\omega,\Omega)}_{\alpha_{\omega\Omega}}a_{\omega}+\underbrace{\sqrt{\frac{\Omega}{\omega}}F(-\omega,\Omega)}_{\beta_{\omega\Omega}}a^{\dagger}_{\omega}\right]$$

$$\boxed{\implies b_{\Omega} = \int_0^{\infty}d\omega\left[\alpha_{\omega\Omega}a_{\omega}+\beta_{\omega\Omega}a^{\dagger}_{\omega}\right]} \tag{A.3.28}$$

This is the Bogolyubov transformation for the creation and annihilation operators in the case. One difference we can see in comparison to the transformation we've seen

in is that there is an integral over ω. One can think of the transformations we did in the previous subsection as cases where $\alpha_{\omega\Omega}, \beta_{\omega\Omega} \propto \delta(\omega - \Omega)$. We can find expressions for other operators in a similar way. We now look for a constraint equation for the Bogolyubov coefficients similar to (A.2.17). To do so, we start with the commutation relation for b_ω as

$$[b_\Omega, b^\dagger_{\Omega'}] = \delta(\Omega - \Omega'), \tag{A.3.29}$$

LHS:

$$\begin{aligned}
\implies & \int_0^\infty \int_0^\infty d\omega\, d\omega' \Big[\Big(\alpha_{\omega\Omega} a_\omega + \beta_{\omega\Omega} a^\dagger_\omega \Big) \Big(\alpha^*_{\omega'\Omega'} a^\dagger_{\omega'} + \beta^*_{\omega'\Omega'} a_{\omega'} \Big) \\
& \qquad - \Big(\alpha^*_{\omega'\Omega'} a^\dagger_{\omega'} + \beta^*_{\omega'\Omega'} a_{\omega'} \Big) \Big(\alpha_{\omega\Omega} a_\omega + \beta_{\omega\Omega} a^\dagger_\omega \Big) \Big] \\
\implies & \int_0^\infty \int_0^\infty d\omega\, d\omega' \Big[\Big(\alpha_{\omega\Omega}\alpha^*_{\omega'\Omega'} a_\omega a^\dagger_{\omega'} + \beta_{\omega\Omega}\beta^*_{\omega'\Omega'} a^\dagger_\omega a_{\omega'} + \alpha_{\omega\Omega}\beta^*_{\omega'\Omega'} a_\omega a_{\omega'} + \beta_{\omega\Omega}\alpha^*_{\omega'\Omega'} a^\dagger_\omega a^\dagger_{\omega'} \Big) \\
& \qquad - \Big(\alpha_{\omega\Omega}\alpha^*_{\omega'\Omega'} a^\dagger_{\omega'} a_\omega + \beta_{\omega\Omega}\beta^*_{\omega'\Omega'} a_{\omega'} a^\dagger_\omega + \alpha_{\omega\Omega}\beta^*_{\omega'\Omega'} a_{\omega'} a_\omega + \beta_{\omega\Omega}\alpha^*_{\omega'\Omega'} a^\dagger_{\omega'} a^\dagger_\omega \Big) \Big] \\
\implies & \int_0^\infty \int_0^\infty d\omega\, d\omega' \Big[\alpha_{\omega\Omega}\alpha^*_{\omega'\Omega'} \underbrace{[a_\omega, a^\dagger_{\omega'}]}_{\delta(\omega-\omega')} + \beta_{\omega\Omega}\beta^*_{\omega'\Omega'} \underbrace{[a^\dagger_\omega, a_{\omega'}]}_{-\delta(\omega-\omega')} \\
& \qquad + \alpha_{\omega\Omega}\beta^*_{\omega'\Omega'} \underbrace{[a_\omega, a_{\omega'}]}_{0} + \beta_{\omega\Omega}\alpha^*_{\omega'\Omega'} \underbrace{[a^\dagger_\omega, a^\dagger_{\omega'}]}_{0} \Big] \\
\implies & \int_0^\infty d\omega \Big[\alpha_{\omega\Omega}\alpha^*_{\omega\Omega'} - \beta_{\omega\Omega}\beta^*_{\omega\Omega'} \Big]
\end{aligned}$$

Hence, from (A.3.29), we finally get

$$\int_0^\infty d\omega \Big[\alpha_{\omega\Omega}\alpha^*_{\omega\Omega'} - \beta_{\omega\Omega}\beta^*_{\omega\Omega'} \Big] = \delta(\Omega - \Omega') \tag{A.3.30}$$

This is similar to the constraint equation we got in (A.2.17). Again, if $\alpha_{\omega\Omega}, \beta_{\omega\Omega} \propto \delta(\omega - \Omega)$, we would obtain a result similar to (A.2.17).

A.3.4 Mean particle number

We can now ask the number of particles/particle density (with momentum Ω) an accelerated observer sees in the Minkowski vacuum. To do so, we calculate the expectation value

$$\langle N_\Omega \rangle_0 = \langle 0_M | \, N_\Omega \, | 0_M \rangle = \langle 0_M | \, b^\dagger_\Omega b_\Omega \, | 0_M \rangle \, .$$

$$= \langle 0_M| \int_0^\infty d\omega \Big(\alpha^*_{\omega\Omega} a^\dagger_\omega + \beta^*_{\omega\Omega} a_\omega\Big) \int_0^\infty d\omega' \Big(\alpha_{\omega'\Omega} a_{\omega'} + \beta_{\omega'\Omega} a^\dagger_{\omega'}\Big) |0_M\rangle$$

$$= \langle 0_M| \int_0^\infty d\omega \int_0^\infty d\omega' \beta^*_{\omega\Omega}\beta_{\omega'\Omega} a_\omega a^\dagger_{\omega'} |0_M\rangle = \langle 0_M| \int_0^\infty d\omega \int_0^\infty d\omega' \beta^*_{\omega\Omega}\beta_{\omega'\Omega}\delta(\omega-\omega') |0_M\rangle$$

$$\implies \langle N_\Omega\rangle_0 = \int_0^\infty d\omega |\beta_{\omega\Omega}|^2. \tag{A.3.31}$$

Now, to calculate this expression, we use (A.3.30). We can see that upon putting $\Omega = \Omega'$ in the RHS, we generate a $|\beta_{\omega\Omega}|^2$ term, but we still don't know about the $|\alpha_{\omega\Omega}|^2$ term. To calculate this, we will try to look at the expression for $|\alpha_{\omega\Omega}|^2$ and link it to the value of $|\beta_{\omega\Omega}|^2$. Equivalently, this means we need a relation between $F(\omega,\Omega)$ and $F(-\omega,\Omega)$. With that in mind, we start with (A.3.30) in terms of $F(\omega,\Omega)$ and put $\Omega = \Omega'$ to get

$$\int_0^\infty d\omega . \frac{\sqrt{\Omega\Omega'}}{\omega} \Big[F(\omega,\Omega)F^*(\omega,\Omega') - F(-\omega,\Omega)F^*(-\omega,\Omega')\Big] = \delta(\Omega-\Omega').$$

$$\implies \int_0^\infty d\omega . \frac{\Omega}{\omega} \Big[|F(\omega,\Omega)|^2 - |F(-\omega,\Omega)|^2\Big] = \delta(0). \tag{A.3.32}$$

Now, we have a look at (A.3.27) and analyze it carefully. It says

$$F(\omega,\Omega) = \int_{-\infty}^\infty \frac{du}{2\pi} \exp\left[i\Omega u + i\frac{\omega}{a}e^{-au}\right]. \tag{A.3.33}$$

As said before, we wish to find a relation between $F(\omega,\Omega)$ and $F(-\omega,\Omega)$. To retrieve $F(-\omega,\Omega)$ from the equation above, we need

$$\frac{i\omega e^{-au}}{a} \to \frac{-i\omega e^{-au}}{a}.$$

One way to do that is to let $u \to u - \frac{i\pi}{a}$. This can be done looking at this integral in the complex plane. We extend the domain of the variable u to the complex plane as shown in [Fig. A.3]. The original real integral can be thought of as going over the line $u = x, x \in \mathbb{R}$ (denoted by green in the figure). Let us take a rectangular contour Γ with its top edge (T.E in figure) as $u = x, x \in \mathbb{R}$, bottom edge (B.E in figure) as $u = x - i\frac{\pi}{a}, x \in \mathbb{R}$ and the left and right edges (L.E and R.E in figure) as $u = x - \frac{i\pi y}{a}$, where $x \to \pm\infty$ and $y \in [0,1]$.

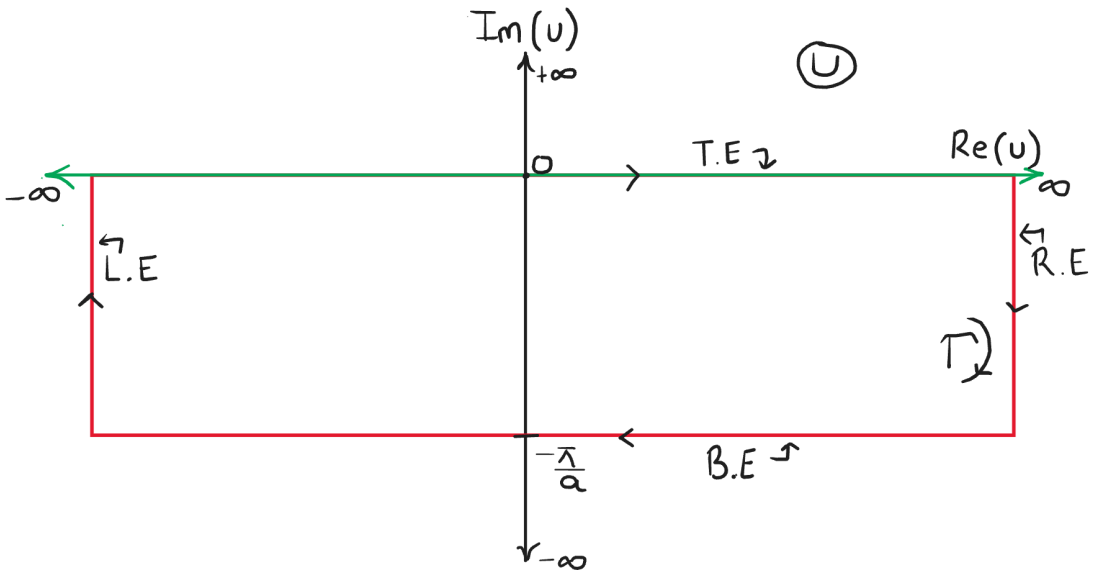


Figure A.3: Contour Γ in the complex u plane.

Then by Cauchy's Integral theorem, the complexified integral in (A.3.33) along Γ is 0 as there are no singularities inside, and the integrand is analytic over this domain. Moreover, one can show that the integrand fully vanishes as the left and right sides of the rectangle go towards infinity (i.e., $x \to \pm\infty$). Hence the integral has equal values on the upper and lower edge of the contour. Hence the real integral in (A.3.33) will have the same value as $u \to u - \frac{i\pi}{a}$. Evaluating the integral now gives

$$F(\omega,\Omega) = \int_{-\infty}^{\infty} \frac{du}{2\pi} \exp\left[i\Omega(u - \frac{i\pi}{a}) + i\frac{\omega}{a}e^{-a(u-\frac{i\pi}{a})}\right]$$

$$\implies F(\omega,\Omega) = \int_{-\infty}^{\infty} \frac{du}{2\pi} \exp\left[i\Omega u + \frac{\pi\Omega}{a} - i\frac{\omega}{a}e^{-au}\right]$$

$$\boxed{\implies F(\omega,\Omega) = F(-\omega,\Omega)\exp\left(\frac{\pi\Omega}{a}\right).} \tag{A.3.34}$$

Using (A.3.34) in (A.3.32), we hence get

$$\int_0^{\infty} d\omega.\frac{\Omega}{\omega}|F(-\omega,\Omega)|^2\Big[\exp\left(\frac{2\pi\Omega}{a}\right) - 1\Big] = \delta(0).$$

$$\implies \int_0^{\infty} d\omega.\frac{\Omega}{\omega}|F(-\omega,\Omega)|^2 = \delta(0)\Big[\exp\left(\frac{2\pi\Omega}{a}\right) - 1\Big]^{-1}.$$

But the LHS in this expression is exactly (A.3.31)! Since $\beta_{\omega\Omega} = \sqrt{\frac{\Omega}{\omega}}F(-\omega,\Omega)$, we have

$$\implies \int_0^\infty d\omega|\beta_{\omega\Omega}|^2 = \int_0^\infty d\omega.\frac{\Omega}{\omega}|F(-\omega,\Omega)|^2 = \delta(0)\Big[\exp\left(\frac{2\pi\Omega}{a}\right)-1\Big]^{-1}.$$

$$\overset{(A.3.31)}{\implies} \langle N_\Omega\rangle_0 = \Big[\exp\left(\frac{2\pi\Omega}{a}\right)-1\Big]^{-1}\delta(0) = n_\Omega\delta(0). \tag{A.3.35}$$

Here $\delta(0)$ represents the infinite volume of space which we work with. Working in a box with a fixed length (called an infrared cutoff) will change this infinity to the finite volume V of the box. Hence n_Ω represents the mean particle density of the mode with momentum Ω. A similar expression can be derived for negative momentum particles.

A.3.5 Unruh temperature

The particle density expression can be seen to be resembling the Bose-Einstein distribution, which is given as

$$n(E) = \Big[\exp\left(\frac{E}{T}\right)-1\Big]^{-1}.$$

Comparing with the expression in (A.3.35), we see that the accelerated observer particles with energy $E = \Omega$ in the Minkowski vacuum seem to follow a Bose-Einstein distribution. The spectrum of particles with temperature

$$T = \frac{a}{2\pi} \quad \text{or} \quad T = \frac{\hbar a}{2\pi c k_b} \tag{A.3.36}$$

in SI units. This is the Unruh effect. Using the Bogolyubov transformations above, one can also conclude that the density matrix corresponding to the Rindler vacuum has a thermal form.

A.4 Hawking radiation

This section explores what happens if we repeat the analysis of the last subsection for Schwarzschild space-time. The Schwarzschild space-time's core feature is the presence

of a Black Hole, and the analogous calculation leads us to conclude that observers far away from the Black Hole see particles emanating from it. The spectrum of these particles is similarly thermal as in the Unruh effect, allowing us to assign a temperature to the Black Hole for a faraway observer.

A.4.1 Scalar field in Schwarzschild space-time

As in the last subsection, we will try to find a set of two co-ordinate frames where both the metrics are conformally flat. Hence in the light-cone co-ordinates, we can equate the decoupled mode function terms and find how operators in these frames are related. Then with the correct physical interpretation, we can conclude that a faraway observer sees particles with a thermal spectrum. We start with the Schwarzschild space-time in 1+1 dimensions, with the metric given as

$$ds^2 = \left(1 - \frac{2M}{r}\right) dt^2 - \left(1 - \frac{2M}{r}\right)^{-1} dr^2.$$

Here M is the mass of the Black Hole. Although usually the metric is written in 3+1 dimensions, we omit the isotropic angular directions. We hope that the simpler calculations in 1+1 dimensions capture the critical features of Black Hole space-time, and these features are preserved in the full 3+1 dimensional case. Given this metric, we look at the minimally coupled scalar field. As before, we try to use the power of conformal invariance and get this metric to be conformally invariant to the Minkowski metric.

Tortoise co-ordinates

We go to the tortoise co-ordinates, a set of co-ordinates commonly used while analyzing the Black Hole in this space-time. In these co-ordinates r^*, a relatively slower The tortoise co-ordinates are defined by (t, r^*) where

$$r^* = r - 2M + 2M \ln\left(\frac{r}{2M} - 1\right).$$

In these co-ordinates, the metric is conformally flat and looks like

$$ds^2 = \left(1 - \frac{2M}{r}\right)\left(dt^2 - dr^{*2}\right).$$

We can clearly see the conformal invariance. Using results from (A.3.12) we can write the action for a scalar field in the tortoise co-ordinates as

$$S[\phi] = \frac{1}{2}\int dr^*\, dt\, \left[(\partial_t\phi)^2 - (\partial_{r^*}\phi)^2\right].$$

As before, we can write its solutions as

$$\phi(r^*, t) = A(t - r^*) + B(t + r^*). \tag{A.4.1}$$

Moving on to the lightcone co-ordinates $u, v = t \mp r^*$, the metric looks like

$$ds^2 = \left(1 - \frac{2M}{r}\right) du\, dv. \tag{A.4.2}$$

Note that the metric is not singular at $r = 2M$ here, as it was in Schwarzschild metric in (t, r) co-ordinates. Finally, in the lightcone co-ordinates the real space solutions to the equations of motion of the scalar field in Schwarzschild spacetime look like

$$\phi(r^*, t) = A(u) + B(v). \tag{A.4.3}$$

Note that the tortoise co-ordinates do not work for $r < 2M$ i.e and they do not cover the entire space-time. We now look for the mode expansion in these co-ordinates. As before, the mode expansion looks like

$$\phi(u, v) = \int_0^\infty \frac{d\omega'}{\sqrt{2\pi}} \frac{1}{\sqrt{2\omega'}} \left(e^{-i\omega' u} b_{\omega'} + e^{i\omega' u} b^\dagger_{\omega'} + e^{-i\omega' v} b_{-\omega'} + e^{i\omega' v} b^\dagger_{-\omega'}\right). \tag{A.4.4}$$

Note the variables convention (like u, v and ω' as the conjuagate variable) is chosen conveniently to illustrate the similarity to the Unruh effect later. In the Rindler co-ordinates, constant ρ physically corresponded to a constantly accelerating observer. Here, constant value of r^* (or equivalently r) also corresponds to an observer accelerating, as to hover a constant distance from the Black Hole, the observer has to accelerate. Physically, this can be seen by the presence of the Black Hole exerting gravitational force on the observer, pulling it inwards. Then to stay at a constant distance from the gravitating object, one has to accelerate against it. Hence $b^\dagger_{\omega'}$ acting on an appropriate vacuum $|0_T\rangle$ would correspond to the state of a particle that is observed by an observer at a constant distance from the Black Hole. Moreover, since

this observer is accelerating, this is similar to the accelerated frame case in the Unruh effect case. This is first of the two frames we look at. Taking inspiration from the last subsection, we now look for an inertial/freely falling reference frame. The second frame we look at will be the Kruskal frame.

Kruskal co-ordinates

Tortoise co-ordinates are ridden with the problem of co-ordinate singularities. They only cover the region of space-time $r \in (2M, \infty)$. However, if we consider a freely falling observer, one can show that it crosses the horizon in finite proper time (the time that the observer measures). This is expected, as we think of space-time as being locally flat at all points (in other words, we think of space-time as a manifold), and the event horizon should be no different. Thus, an observer at this point should be able to move along this flat plane. This means that the region of space-time with $r < 2M$ is physically accessible, and co-ordinates adapted for an inertial observer should cover this region as well. Since the tortoise co-ordinates fail to do so, we choose a set of co-ordinates that do.

Let us say we try to walk around the Earth with a map. Suppose, while traversing, we come across a trench not shown on the map. We naturally conclude that the map is *wrong*, because the physical reality in front of us has to be right. It is the same for co-ordinates. The Schwarzschild and Tortoise co-ordinates are just faulty maps that fail at the horizon since, physically, we expect observers to be able to cross it. The solution is to use a better map that tells us about the trench. One such co-ordinates for the Schwarzschild spacetime are the Kruskal co-ordinates. The co-ordinates will be barred in analogy with the inertial co-ordinates in the last subsection. We start with the light-cone co-ordinates in (A.3.18). In these coordinates, the horizon is at $u = \infty$ or $v = -\infty$. We bring this to a finite co-ordinate value by the transformation

$$\bar{u} = -4M \exp\left(\frac{-u}{4M}\right), \qquad \bar{v} = 4M \exp\left(\frac{v}{4M}\right). \tag{A.4.5}$$

This forces $\bar{u} \in (-\infty, 0)$ and $\bar{v} \in (0, +\infty)$ and the horizon to be at $\bar{u} = 0$ and $\bar{v} = 0$.

If we now rewrite these compactified co-ordinates as $\bar{u}, \bar{v} = \bar{t} \mp \bar{r}$, then $\bar{t}, \bar{r}$ represent the proper time and proper distance measured by a freely falling observer. Writing the metric in these $\bar{u}, \bar{v}$ co-ordinates we get

$$ds^2 = \frac{2M}{r} \exp\left(1 - \frac{r}{2M}\right) d\bar{u} d\bar{v}. \tag{A.4.6}$$

Clearly this metric does not show problems at $r = 2M$. To explore $r < 2M$, we now extend $\bar{u} \in (-\infty, \infty)$ and $\bar{v} \in (-\infty, +\infty)$. Hence in these co-ordinates we can explore the entire space-time and is well adapted for inertial observers. Moreover, comparing (A.4.5) and (A.3.19) we see that the analogy is exact if we set $a = \frac{1}{4M}$. This completes the analogy with the Unruh effect. Finally, from (A.4.6) we can see that the metric is conformally flat. This can be seen more explicitly by going to $\bar{t}, \bar{r}$ co-ordinates and seeing the Minkowski nature. Hence the scalar field in this space-time will have the solutions

$$\phi(\bar{u}, \bar{v}) = A(\bar{u}) + B(\bar{v}). \tag{A.4.7}$$

With this expression, we can finally write the mode expansion for this conformally flat metric as

$$\phi(\bar{u}, \bar{v}) = \int_0^\infty \frac{d\omega}{\sqrt{2\pi}} \frac{1}{\sqrt{2\omega}} \left(e^{-i\omega\bar{u}} a_\omega + e^{i\omega\bar{u}} a_\omega^\dagger + e^{-i\omega\bar{v}} a_{-\omega} + e^{i\omega\bar{v}} a_{-\omega}^\dagger \right). \tag{A.4.8}$$

We can finally compare the two-mode expansions, define the different vacuums and look at the relevant Bogolyubov transformations.

A.4.2 Hawking temperature

The two frames define two different vacuums. The Tortoise co-ordinates vacuum is given by $b_{\omega'} |0_T\rangle = 0$ and the Kruskal vacuum is given by $a_\omega |0_K\rangle = 0$. As in the previous subsection, we can relate these annihilation and creation operators in different frames using Bogolyubov transformations. We now ask, what does an observer far away from the horizon see? To answer that, we need to know what frame the observer is in and what state the field ϕ is in.

From the analogy drawn with Unruh effect, we can immediately see that $|0_M\rangle \leftrightarrow |0_K\rangle$ and $|0_R\rangle \leftrightarrow |0_T\rangle$, and so a faraway observer at constant distance would see a thermal spectrum of particles with temperature $T = \frac{a}{2\pi} = \frac{1}{8\pi M}$. But we can also formally arrive at this result. Looking back at (A.4.2) we had

$$ds^2 = \left(1 - \frac{2M}{r}\right) du\, dv.$$

Note that in the limit $r \gg 2M$, we get back the Minkowski vacuum. Therefore to an observer far away from the Black Hole, the correct vacuum would be $|0_T\rangle$. However, what state is the quantum field in for the faraway observer? It can be shown that for a collapsing star starting in the Minkowski vacuum, the final quantum state of the fields is the $|0_K\rangle$.[8] Moreover, $|0_T\rangle$ can be shown to have infinite energy density at the horizon (even after subtracting the infinite zero-point energies). This means that the quantum fluctuations of the field at the horizon are large and lead to infinite energies, and this vacuum cannot give a good physical picture of the field near the Black Hole. On the other hand, the Kruskal vacuum $|0_K\rangle$ has finite energy density (after subtraction of the zero point energies) and does not suffer from these problems. With this, we formally conclude that a faraway observer will see the Kruskal vacuum full of particles. The average number of particles seen would be given by

$$\langle N_\Omega \rangle_0 = \langle 0_K |\, N_\Omega \,| 0_K \rangle = \langle 0_K |\, b_\Omega^\dagger b_\Omega \,| 0_K \rangle\,. \tag{A.4.9}$$

This integral was precisely calculated in the last section, and the result now can be formally written down with the replacement $a \leftrightarrow \frac{1}{4M}$. The corresponding temperature here is the Hawking temperature and is given by

$$\boxed{T = \frac{1}{8\pi M}.} \tag{A.4.10}$$

Appendix B

Toeplitz matrix eigenspectrum and eigenvalues

B.1 The eigenvalue equation

In this appendix, we will look at the eigenvectors and eigenvalues of the Toeplitz matrix in (3.3.1). A general Toeplitz matrix is given by

$$K = \begin{pmatrix} b & a & & & \\ c & b & a & & \\ & \ddots & \ddots & \ddots & \\ & & c & b & a \\ & & & c & b \end{pmatrix}. \tag{B.1.1}$$

Following [30], we look at its eigenvalue equation $(K - \lambda I)\mathbf{x} = 0$. In its full glory, this looks like

$$\begin{pmatrix} b-\lambda & a & & & \\ c & b-\lambda & a & & \\ & \ddots & \ddots & \ddots & \\ & & c & b-\lambda & a \\ & & & c & b-\lambda \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_n \end{pmatrix} = 0. \tag{B.1.2}$$

Hence we have n equations. We can see that if each $b-\lambda$ term is multiplied by some x_t, then x_{t+1} is multiplied by a and x_{t-1} is multiplied by c. This can be written as

$$cx_{t_1} + (b-\lambda)x_t + ax_{t+1} = 0 \qquad \forall t \text{ such that } 1 \leq t \leq n. \tag{B.1.3}$$

But the 2 equations that correspond to the uppermost and lowermost rows are not the same. The uppermost one has no c term and the lowest one has no a term. This means that $x_0, x_{n+1} = 0$ for (B.1.3) above to fully represent the set of matrix equations given by (B.1.2). We now define $k = t-1$ and divide throughout with a to get

$$x_{k+2} + \left(\frac{b-\lambda}{a}\right) x_{k+1} + \frac{c}{a}x_k = 0, \qquad \forall k \text{ such that } 1 \leq k \leq n., \tag{B.1.4}$$

where $x_0, x_{n+1} = 0$. This equation is a difference equation and is the discrete analogue of a second order homogeneous differential equation $y'' + my' + ny = 0$. While solving the differential equation, we take an exponential ansatz $y = e^{rx}$ to change this differential equation into an algebraic equation. This was only possible because the exponential when differentiated gives itself back. We try to use the same logic for this *difference equation* and write an ansatz $x_k = Cr^k$. The equation then becomes

$$Cr^{k+2} + \left(\frac{b-\lambda}{a}\right).Cr^{k+1} + \frac{c}{a}.Cr^k = 0. \tag{B.1.5}$$

Taking Cr^k common and rejecting the $r = 0$ root (trivial solution) we get

$$r^2 + \left(\frac{b-\lambda}{a}\right) r + \frac{c}{a} = 0. \tag{B.1.6}$$

This quadratic equation can be solved to give the roots

$$r_{1,2} = -\left(\frac{b-\lambda}{2a}\right) \pm \frac{1}{2}\sqrt{\left(\frac{b-\lambda}{a}\right)^2 - \frac{4c}{a}}. \tag{B.1.7}$$

The sum and product of the roots is given by

$$r_1 r_2 = \frac{c}{a}, \qquad r_1 + r_2 = -\left(\frac{b-\lambda}{a}\right). \tag{B.1.8}$$

Hence an arbitrary solution (if the roots are distinct) takes the form

$$x_k = \alpha r_1^k + \beta r_2^k. \tag{B.1.9}$$

We now demand that $x_0 = x_{n+1} = 0$ from (B.1.9) which gives us

$$\alpha + \beta = 0, \qquad \alpha r_1^{n+1} + \beta r_2^{n+1} = 0. \tag{B.1.10}$$

Looking at the second equation we get

$$\left(\frac{r_1}{r_2}\right)^{n+1} = -\frac{\beta}{\alpha} \overset{(B.1.10)}{=} 1, \tag{B.1.11}$$

$$\implies \frac{r_1}{r_2} = \exp\left(\frac{i(2\pi j)}{n+1}\right), \qquad \forall j \text{ such that } 1 \leq j \leq n. \tag{B.1.12}$$

Using the product relation in (B.1.8) and multiplying it with (B.1.12) we get

$$r_1^2 = \frac{c}{a}\exp\left(\frac{i(2\pi j)}{n+1}\right), \tag{B.1.13}$$

$$\implies r_1 = \sqrt{\frac{c}{a}}\exp\left(\frac{i\pi j}{n+1}\right), \qquad \overset{(B.1.8)}{\implies} r_2 = \sqrt{\frac{c}{a}}\exp\left(\frac{-i\pi j}{n+1}\right). \tag{B.1.14}$$

Now using the sum relation in (B.1.8) and the expression for r_1 and r_2 from (B.1.14) we get

$$\lambda = b + a(r_1 + r_2),$$

$$\implies \lambda_j = b + a\sqrt{\frac{c}{a}}\left[\exp\left(\frac{i\pi j}{n+1}\right) + \exp\left(\frac{-i\pi j}{n+1}\right)\right],$$

$$\implies \lambda_j = b + 2\sqrt{ac}\cos\left(\frac{\pi j}{n+1}\right).$$

And hence we have the eigenvalues. For our problem in (3.3.1), we have $a = c = -1$ and $b = \Lambda + 2$. This gives us the form

$$\lambda_j = (\Lambda + 2) + 2\cos\left(\frac{\pi j}{n+1}\right) = \Lambda + 2\left(1 + \cos\left(\frac{\pi j}{n+1}\right)\right),$$

$$\boxed{\lambda_j = \Lambda + 4\cos^2\left(\frac{\pi j}{2(n+1)}\right).} \tag{B.1.15}$$

Note that there are j of them. We now try to calculate the corresponding eigenvectors.

B.2 Calculating the eigenvectors and normalization

Let us look at the eigenvectors. From (B.1.10) we have

$$x_k = \alpha\left(r_1^k - r_2^k\right),$$

$$\overset{\text{(B.1.14)}}{\implies} \alpha\left(\frac{c}{a}\right)^{\frac{k}{2}}\left[\exp\left(\frac{i\pi jk}{n+1}\right) - \exp\left(\frac{-i\pi jk}{n+1}\right)\right],$$

$$\implies x_k = 2i\alpha\left(\frac{c}{a}\right)^{\frac{k}{2}}\sin\left(\frac{jk\pi}{n+1}\right).$$

We now need to be careful with the j and k indices. There are j eigenvalues for the Toeplitz matrix. To each of this eigenvalue, corresponding eigenvector $\vec{x}$ exists. The elements of this eigenvector are denoted by the index k, so the kth component of the jth eigenvector is given by $(x_k)_j$. This is hence given by

$$(x_k)_j = 2i\alpha\left(\frac{c}{a}\right)^{\frac{k}{2}}\sin\left(\frac{jk\pi}{n+1}\right).$$

Since α is just a constant, we can set it to whatever we want, and demand the entire eigenvector to be normalized. For simplicity, we set it to $\alpha = \frac{1}{2i}$ and then write the normalized eigenvector as

$$(x_k)_j = \frac{\sin\left(\frac{jk\pi}{n+1}\right)}{\sqrt{\sum_k \sin^2\left(\frac{jk\pi}{n+1}\right)}}. \tag{B.2.1}$$

Let us calculate the sum in the denominator above. Consider the sum

$$S = \sum_{x=1}^{n}\sin^2(ax),$$

$$\implies \sum_{x=1}^{n}\frac{1-\cos(2ax)}{2} = \frac{n}{2} - \frac{1}{2}\sum_{x=1}^{n}\cos(2ax) = \frac{n}{2} - \frac{1}{2}\sum_{x=1}^{n}\mathrm{Re}\left(e^{2iax}\right). \tag{B.2.2}$$

To calculate this sum, we switch the summation and real sign, and evaluate the resultant geometric progression. This looks like

$$\sum_{x=1}^{n}\mathrm{Re}\left(e^{2iax}\right) = \mathrm{Re}\sum_{x=1}^{n}\left(e^{2iax}\right) = \mathrm{Re}\left(e^{2ia}.\frac{(1-e^{2ian})}{(1-e^{2ia})}\right),$$

$$= \text{Re}\left(e^{2ia}.\frac{e^{ian}(e^{-ian}-e^{ian})}{e^{ia}(e^{-ia}-e^{ia})}\right),$$

$$= \text{Re}\left(e^{ia(n+1)}.\frac{\sin(an)}{\sin a}\right) = \frac{\cos(a(n+1))\sin(an)}{\sin a}.$$

Now going back to (B.2.2) and substituting the expressions obtained above, we get

$$S = \frac{n}{2} - \frac{1}{2}\frac{\cos(a(n+1))\sin(an)}{\sin a}.$$

From (B.2.1), we substitute $a = \frac{j\pi}{n+1}$ and get the value for S as

$$S = \frac{n}{2} - \frac{1}{2}\frac{\cos(j\pi)\sin\left(\frac{j\pi n}{n+1}\right)}{\sin\frac{j\pi}{n+1}}.$$

Now $\cos(j\pi) = (-1)^j$. For the sine term in the numerator, we do the following to get rid of the n

$$\sin\left(\frac{j\pi n}{n+1}\right) = \sin\left(j\pi - \frac{j\pi}{n+1}\right) = (-1)^{j+1}\sin\left(\frac{j\pi}{n+1}\right).$$

With this identity, the sines should cancel. Putting this together, we get

$$S = \frac{n}{2} - \frac{1}{2}\frac{(-1)^j.(-1)^{j+1}\cancel{\sin\frac{j\pi}{n+1}}}{\cancel{\sin\frac{j\pi}{n+1}}} = \frac{n}{2} - \frac{(-1)^{2j+1}}{2},$$

$$\implies S = \frac{n+1}{2}. \tag{B.2.3}$$

With (B.2.3) and (B.2.1), we finally write the fully normalized eigenvector for the Toeplitz matrix as

$$(x_k)_j = \sqrt{\frac{2}{N+1}}\sin\left(\frac{jk\pi}{n+1}\right), \qquad \text{or} \quad x_j = \begin{pmatrix} \sqrt{\frac{2}{N+1}}\sin\left(\frac{j\pi}{n+1}\right) \\ \sqrt{\frac{2}{N+1}}\sin\left(\frac{2j\pi}{n+1}\right) \\ \vdots \\ \vdots \\ \sqrt{\frac{2}{N+1}}\sin\left(\frac{nk\pi}{n+1}\right) \end{pmatrix}, \tag{B.2.4}$$

where x_j is the jth eigenvector. Hence we have found the eigenvalues (B.1.15) and the eigenvectors (B.2.4) for the Toeplitz matrix.

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