Phonon-Electron Equilibriation: A Keldysh Field Theoretic Approach

A Thesis

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Certificate

This is to certify that this dissertation entitled **Phonon-Electron Equilibriation: A Keldysh Field Theoretic Approach** 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 Sagnik Ghosh at Indian Institute of Science Education and Research, Pune under the supervision of Dr. Rajdeep Sensarma, Associate Professor, Department of Theoretical Physics, Tata Institute of Fundamental Research, Mumbai, during the academic year 2020-2021.

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Declaration

I hereby declare that the matter embodied in the report entitled **Phonon-Electron Equilibriation: A Keldysh Field Theoretic Approach**, 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 Dr. Rajdeep Sensarma (TIFR, Mumbai), and the same has not been submitted elsewhere for any other degree.

Sagnik Ghosh

This Thesis is Dedicated to

Dr. Amrita B. Hazra
Veena Shankar Avadhani
&
Team Kalpa

Academic Acknowledgements

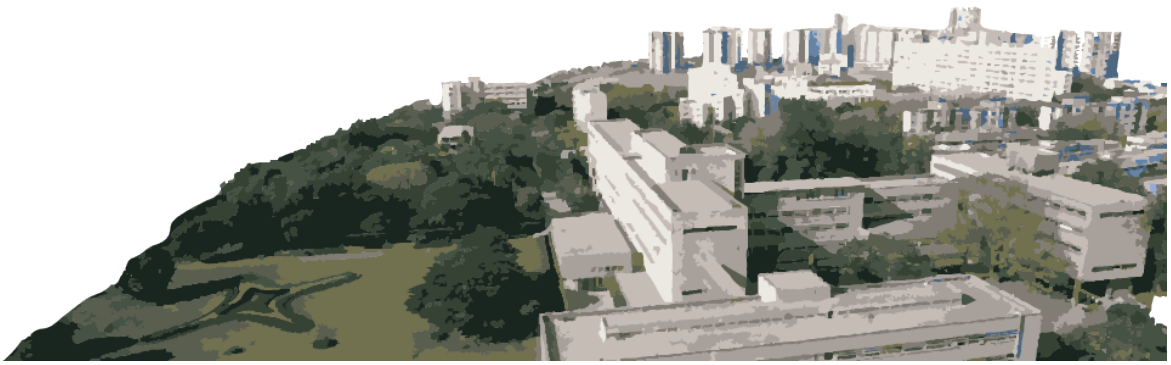
It was July 2019, in Paris, seating near Pont Saint-Michel, me and my good friend Koustav Halder decided to not persue our MS abroad. It was a pre-COVID decision. And a very mature one. I wrote only one application mail for MS. And I wrote it fairly late. I still remember the evening penning it from the Marine Drive, during my last visit to HBCSE, with the anticipation of the opportunity to come back to it again and again for an year!

Rajdeep Sir took me in, but I have not been able return to Marine Drive ever since!

I have met him only once before during the NIUS Physics camp where he was teaching. Like everyone at HBCSE, he was a friendly, caring scientist! In the very first skype meeting post acceptance, he ran me through nukes and corners of the problem statement. I have never taken Quantum Field Theory 2, yet he entrusted me with a project which deals with Keldysh Field Theory at its core. It is only with his push and patience now I know certain things about it.

Anyone who is fairly well versed with the TIFR, is aware that the usual problem lies with difficulty in finding accommodation. Rajdeep Sir, with his utmost care had actually arranged one for me at the Institute! But then the Pandemic happened!

We are blessed that we faced the lockdown in the age of social media. Rajdeep Sir is very vocal on Facebook and I could engage on various



political, social and academic discussions with him over there. It is unfortunately not frequent in Indian Academia to encounter people who shares this spirit. I was fortunate enough to work with one and I only wish, had I been at TIFR, we could have discussed science as well other things at regular intervals! Maybe at a later point, we will meet!

Bijay Sir and Sreejith Sir took utmost care in hosting me at IISER during the whole duration! It is because of their effort and persuasion with the Task Force and the support from Supriya Ma'am (chair MS Committee) I could return in one of the earliest batches of MS students in October, nearly two months before other students could. Very few people ushers this much affection on anybody.

Prof Deepak Dhar has always been my friend, philosopher and guide, since I pursued a semester project with him! He was one of the key person in third year who not only pursued me to exercise, but actually made sure that I do! During the lockdown he kept on checking on me over phone about my academic progress. Since my return he has allowed me to bug him with queries at any possible moment. He also kept me inviting to his home for snacks and never really let me build the homesickness, although it is nearly eight months since I have last stepped out of the campus!

It is an understatement to use the word blessed when I look back at the opportunities I had and the teachers I have got the opportunity to learn from. It is debatable if I have been able to be a good enough student, I am certain that is not so, yet it is because of them, and their support and affection, I have been able to learn whatever I have learnt till now.

Lastly, I end the acknowledgement with Saronyo Da, Mursalin Da and Guru, my lab-mates, without whose support I would not have been able to make any progress whatsoever, especially Mursalin Da, who almost single-handedly answered all my troubles in debugging the bosonic sector. I wish we will all meet one day and come back to our collaboration that we were limited to spend working on only remotely!

May that day come sooner!

Personal Acknowledgements

The Fifth Year Master's Thesis at IISER Pune officially happens over the culminating eight-nine months, but does it really? Can one really judge the last lap of a sprint spanned over five year that isolatedly? Perhaps! But that is injustice.

When I landed at IISER in a similarly overcast August morning as today, I had no plans to stay more than a month or so and was hellbent on joining Presidency College, Calcutta for a B.Sc. in Physics instead. I had always found the BS curriculum in physics very dilute and toned down and was beaming with absolute dissatisfaction eternally. But something nice happened!

We have a fascinating yet extremely underrated system namely the Faculty Advisor over here at IISER. The novice first year me had approached her in the very first month with a request for a return rail ticket to home. She instead took me for a coffee that day and told me about her wonders of why ATP is in abundance as an energy currency. She explained to me what papers are, what a journal is, what summer projects are. She introduced me to TIFR hearing my fascination about physics and wrote me a reco for NIUS Chemistry.

I had found myself into a full blown psychosomatic neuronal failure by the end of second year, owing to "overwork" following a sequence of bad decisions. Dr. Amrita B. Hazra, my faculty advisor, had authority to type out a request to drop courses on behalf of me in the middle of the semester and ask me to sign, without which I probably would have ended up losing an year, maybe my career!

Could there ever be a better college that I would possibly have pursued my degree in? IISER gave me a Mother!

It is also extremely underappreciated how unusually great a Dean Prof. Bhas Bapat is!

Career decisions in my life has always been driven by the idea of approaching well-rounded exceptionalism. I should excel in Physics, but should execute 20 other game changing things on the way too! IISER Pune, like its every student, gave me a national-level stage to execute this! Starting from the Joint Secretaryship at SPIC-MACAY, (which, along with direct contact with maestros of ICM, also gave me some life long friendships to cherish at the COEP!), the now eponymous Hemingway Memorial Debate, The Leadership Conclave and finally the two year stretch of Chief-Editorship at Kalpa, I practically did whatever I wanted whenever I wanted! Veena Shankar Avadhani says I have always lived "a king-sized life." IISER gave me that king-size! IISER also gave me the partner in all these crimes, the great Koustav Halder, who somehow always manages to fundamentally disagree with me yet support me in the act by the end!

It is hard to control the temptation of not writing a king-size acknowledgement of a king-sized journey. But I will control over here! Let this concluding space be reserved for only the most underappreciated ones, with the caveat of not mentioning nearly any of my most favourite people by name!

IISER gave me friends. Social Contacts has never really been my weak suit, so that is unsurprising. What is surprising is when the one with least social skills also turns out to be fairly thought-provoking. Since the days of SPIC MACAY, and throughout the third year, there was a tiny girl who for no good reason chose to hang around with me and again for no good reason let me poke mischief at an ever accelerating rate of precedence. Why? What did she gain? Why was she tolerant? No clue! But never have I ever learnt more things about life, than pondering over how Gopika M would react to certain things; neither have I picked any social fight without wondering how could that possibly affect Gopika M in a positive way. Even though things have not really remained the same, maybe this is a good place to acknowledge that.

That brings us to the conclusion to my attempt of penning a love letter to IISER at the times of Corona! I thank every one who has borne with me, for bearing with me for this long long years!

(The sketch of Main Building is by Samyukhta Ramadurai of BSMS-2018, who sketched it during Mimamsa 2019 for me and has belovedly agreed to let me reuse it here in the very first request.)

Abstract

In this work we develop a non-equilibrium approach to study the time evolution of a coupled electron-phonon many-body system, with electronic initial states driven far-away from the ground states (the Hot Electron problem) to probe its behaviour with regards to thermalisation. The equilibration of "hot electrons", excited to a high energy state either by external electromagnetic waves or by collision with high energy particles, is relevant to a large class of problems, viz. in pump-probe spectroscopy, stability of solid state transistors, response of photodetectors, operation of thermoelectric devices etc. Most previous studies of the "hot electron" problem treat the phonons as a thermal bath whose density matrix (or distribution functions) remain invariant with time. In this project we wish to delve in with the self-consistent time evolution of the coupled system using Schwinger-Keldysh field theory.

We construct an evolution scheme where we assume quassi-static of the electronic sector whereas the phononic sector has been treated preserving is complete non-equilibrium nature. Here we first develop the iteration for phonons and test its dynamics coupling with an Ohmic Bath. Equipped with this we wish to couple this to the system electrons and study their joint dynamics in a self-consitent way.

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Chapter 1

Introduction

A generic system in Condensed Matter Physics consists of a material lattice constituted of atoms (of one or multiple kind) at its each lattice points, which interact with each other in some specified manner.

In the work presented in this thesis, we are interested in studying dynamical behaviour of such an Fermionic Lattice, with one free-electron at each lattice site, interacting with themselves as well as the Lattice Phonons.

For such a system initially the electrons can be assumed to be in the ground state of the Fermi Sea with zero (or with a small but finite) temperature. Then an external interaction is turned on (such as a LASER like in pump-probe experiments or bombardment of high energy charged particles as in the particle detectors), which excites these electrons to very high energy eigenstates, but leaves the phonon sector unaltered to a good approximation.

We are interested in studying how this system of Hot-electrons coupled to the systems of lattice phonons equilibriate.

One interesting question to ask in this respect is the final temperature as a function of the input energy, which can be easily computed from equilibrium statistical mechanics. However, this is an answer at infinite time which is much beyond the usual measurement timescales.

Again, in the experiments described above, there is always some finite energy being injected as an input, and in equilibrium treatment any finite energy has a zero density in the phase space. Hence irrespective of the input energy, at the thermodynamic limit, an equilibrium treatment of the problem will give rise to no temperature rise. However, all the detectors as well as probes are of finite size and they do record a rise in temperature in these experiments. Hence the final answer of the common temperature also becomes a function of the system size.

In this work we seek to develop machinaries for a non-equilibrium treatment of this

problem. In specific we are interested in computing the time scale of equilibration, whether every phonon mode has the same equilibriation timescale, the efficiency of energy transfer at finite time scales involved etc. We wished to study these by setting up a dynamical framework using Keldysh-Schwinger Field Theory[1, 2].

In study of Hot-electron thermalisation it is customary to assume that the electrons thermalise between themselves very quickly[3]. The electrons interact among themselves via a long-range coulomb interaction, which has a thermalisation timescale of the order of femto-seconds. The other relevant timescales reletaed to phenomena one is usually interested in studying (such as electron-phonon interaction, transient dynamics) tends to be of the order of pico-seconds [4]. Hence in study of the mechanism of redistribution of the energy among the phonon degrees of freedom and the approach to a common equilibrium it is usually safe to assume a quassi-static nature of the electrons.

We are interested in investigating the mechanism of this process by keeping into account the non-equilibrium nature of the phonons.

The remainder of this report is structured as follows.

In the following section we briefly review the Two Temperature Model due to Anisimov et. al. [3], which is customary to invoke in study of these systems, which also assumes a quassi-static nature of the phonons and outline some problems it may suffer owing to this assumption.

In the following chapter we review the relevant results of the Keldysh-Schwinger formulation[1, 2] of field theory, required for the study. We briefly summarise some preliminary results for the phononic sector, where we have studied dynamics of non-equilibrium phonons coupled to an ohmic bath. Lastly we trace out the routes to further works and conclude.

1.1 Two Temperature Model

The prototype of the system whose dynamical behaviour we seek to model are studied with Pump-Probe Spectroscopy [3–6]. In these experiments we usually start with a lattice of a suitable material, with an electronic and a phononic sub-lattice. The electron population is then driven away from equilibrium by exciting them to higher momentum levels by shining high frequency photons (The Pump Pulse). To a good approximation the phonons can be assumed to retain their initial equilibrium configuration.

The resulting non-thermal population of electrons usually have an self-equilibrium time scale of 10-100 femto-seconds mediated by the electron electron coulomb scattering. Afterwards, in the time scale of the orders of pico-seconds, the interactions with the phononic sub-lattice plays the primary role as a thermalisation channel.

It is inherently assumed that the el-el interaction as well as the ph-ph interaction mixes the degrees of freedom of the individual sub-systems at time scales much faster than that of the interaction that couples those two. Hence at the time scales comparable to the later it can be assumed that at all times there is a electron temperature (T_e) and a phonon temperature (T_{ph}) at every time step. The action of the coupling is then reduced to updating these two values. Eventually both the sub-system temperature reaches a common equilibrium value and heat diffusion in the system restores to its initial state.

The dynamics of the temperatures of the two sub-systems (T_e, T_{ph}) under the action of the electron-phonon coupling in this model is summarised by the following governing coupled differential equations.

$$\begin{aligned} C_e(T_e)\frac{dT_e}{dt} &= \nabla(\kappa_e \nabla T_e) - G(T_e, T_{ph})\ (T_e - T_{ph}) + S(t) \\ C_{ph}(T_{ph})\frac{dT_{ph}}{dt} &= \nabla(\kappa_{ph} \nabla T_{ph}) + G(T_e, T_{ph})\ (T_e - T_{ph}) \end{aligned} \tag{1.1}$$

Here C_e, C_{ph} denotes the respective heat capacities, κ_e, κ_{ph} stands for the respective thermal conductivities, $G(T_e, T_{ph})$ is the electron phonon coupling that in general depends on both the temperatures and $S(t)$ is the forcing term for the electronic sub-sector, that summarises the contribution of the pulse.

Equations (1.1) can not be solved in closed form in its full generality. But it's application to small systems such as nano-material thin-films allows for certain simplifications. In these systems the temperature becomes spatially uniform at a short time scales [7], so the terms proportional to the temperature gradients can be ignored. The forcing term, $S(t)$ can be traded for choosing a high initial temperature, at which the sub-system settles down after an initial non-equilibrium intermediate dynamics.

The two equations in (1.1) then can be subtracted to obtain,

$$\frac{d}{dt}(T_e - T_{ph}) = -G(T_e, T_{ph})\Big(\frac{1}{C_e(T_e)} + \frac{1}{C_{ph}(T_{ph})}\Big)(T_e - T_{ph}) \tag{1.2}$$

If the heat capacities as well as the interaction term were independent of temperature, then (1.2) could have been integrated to obtain the analytical solution,

$$T_e(t) - T_{ph}(t) = [T_e^0 - T_{ph}^0]e^{-\frac{t}{\tau}} \tag{1.3}$$

which states that the electronic and the phonon temperatures relaxes exponentially two a common temperature with a time scale,

$$\frac{1}{\tau} = G\Big(\frac{1}{C_e} + \frac{1}{C_{ph}}\Big) \tag{1.4}$$

However, this assumption is only true for classical ideal gases. In non-interacting metallic systems phonons and electrons have heat-capacities that varies as power law of the temperature. Yet, in analogy, one can define a local time-scale for these systems,

$$\frac{1}{\tau_{e,ph}} := G(T_e, T_{ph})\Big[\frac{1}{C_e(T_e)} + \frac{1}{C_{ph}(T_{ph})}\Big] \tag{1.5}$$

such that the electron temperature can be modeled with an effective exponential decay,

$$T_e(t) \cong \ T_e^0 e^{-\frac{t}{\tau}} + T_\infty \tag{1.6}$$

where T_∞ is the final common temperature. The quantities in (1.5) can be obtained from ab-initio first principle calculations, such as Density Functional Theory, viz. Forno et al [4]. For some systems like in TiN this approximation is known to replicate closely direct numerical solutions of (1.2).

Inherent to the assumption of *two temperatures* ,

1.2 A change is in order

The two-temperature model inherently assumes instantaneous thermalisation for both the sectors. However, that, especially with regard to the phononic sector is known to not hold good for many scenarios.

Consider a 3 dimensional system of phonons. In this case the phononic phase space volumes varies as k^2dk. If we assume a linear dispersion relation, then the DOS varies as ω^2. Which necessarily means that the low energy phonons has almost negligble scattering, which is contrary to the requirement of assuming instantaneous thermalisation. In general for finite size systems there is no instantaneous process, but an exponetial decay. But for phonons it is possible to get a power-law instead.

Similar scenarios can be argued for the electronic sector. Especially close to the Fermi surface, the electronic sector is known to have almost no effective scattering due to electron-electron interactions, which forms the basis of theories like that of

the Fermi Liquids [8]. With that the validity of instantaneous thermalisation of electronic sectors, especially involving energy scales of the order of Fermi Energy comes to questioning.

No effective scattering near Fermi Surface is hwowever a zero temperature statement. So, at finite temperature probably it can still be assumed that the electrons will exhibit instantaneous self-thermalisation. Hence the validity of this statement becomes a cut-off dependent question. It is not entirely obvious statement that it happens at all energy scales. The approximation has been at use in study and modelling of thermalization for various systems where it exhibits quite reasonable effectiveness. However, Even if the electrons are, Phonons are hardly expected to exhibit instantaneous thermalisation for a spanning range of parameters.

It has been recently shown that both the phonons as well as the fermions when coupled to infinite non-interacting phononic/ fermionic baths, they can exhibit power law decays given there are singularities in the bath spectral functions. [9]. Inherent to the assumption of instantaneous thermalisation lies the assumption of Marcovianity or involvement of memoryless cores. It has been exhibited that following does not hold true for all cases of the scenario we are concerned, especially when we start from arbitrary initial conditions, which is not necessarily a density matrix[10].

In light of that we wish to reopen the quest and set up a general non-equilibrium framework to study the time evolution of the coupled electron-phonon systems in a self-consistent way and revisit some of these questions.

Chapter 2

Theory

2.1 Grassmann Algebra & Coherent States

Consider a single fermionic level, which is spanned by the number states $|0\rangle$ and $|1\rangle$. The annihilation and creation operators, $c, c^\dagger$ are defined by their acion as,

$$\begin{aligned} c\,|0\rangle = 0\,, \quad & c^\dagger\,|1\rangle = |0\rangle\,, \\ c\,|0\rangle = |1\rangle\,, \quad & c^\dagger\,|1\rangle = 0 \end{aligned}$$

It follows that the anticommutator, $\{c, c^\dagger\} = cc^\dagger + c^\dagger c = I$ and that $c^2 = c^{\dagger 2} = 0$. The number operator is defined as,

$$c^\dagger c\,|n\rangle = n\,|n\rangle$$

Individual Fermionic states are parametrized by Grassmann Numbers.

Definition 1 (Grassmann Number)**.** *Let* $\mathbb{G}$ *denote set of Grassmann numbers. Then* $\forall\ \psi, \psi' \in \mathbb{G}$*.*

$$\begin{aligned} &a. \quad \{\psi, \psi'\} = 0 \\ &b. \quad \{\psi, c\} = \{\psi, c^\dagger\} = 0 \end{aligned}$$

It follows from property a. that $\psi^2 = 0,\ \ \forall\ \psi \in \mathbb{G}$. A fermionic left coherent state $|\psi\rangle$ is paramterized using the *Grassmann Field* as,

$$|\psi\rangle = |0\rangle - \psi\,|1\rangle\,, \quad \psi \in \mathbb{G}$$

by construction such a state is an eigenstate to the annihilation operator.

$$\begin{aligned} c\,|\psi\rangle &= c\,|0\rangle - \ c\,\psi\,|1\rangle \\ &= \psi\,|0\rangle = \psi\,|0\rangle - \psi^2\,|1\rangle \\ &= \psi\,|\psi\rangle \end{aligned}$$

Before deriving furthers properties of coherent states it is useful to develop functions and calculus of Grassmann Numbers. Functions of Grassmann Numbers are defined using its Taylor expansion.

Definition 2 (Functions of Grassmann Numbers)**.** *Let f be a map from* $\mathbb{G}$ *to* $\mathbb{G}$*. Then*

$$f(\psi) = f_0 + f_1\psi, \quad f_0, f_1 \in \mathbb{R} \tag{2.1}$$

The definition is naturally generalised to 2 and higher dimensions as follows. Let f be a map from $\mathbb{G}^2$ to $\mathbb{G}$. Then,

$$f(\psi, \psi') = f_{00} + f_{10}\psi + f_{01}\psi' + f_{11}\psi\psi', \quad f_{00}, f_{10}, f_{10}, f_{11} \in \mathbb{R} \tag{2.2}$$

This allows us to introduce the derivatives of Grassmann Numbers in terms of their action on these functions.

Definition 3 (Derivatives of Grassmann Numbers)**.** *Let* $f(\psi)$, $\psi \in \mathbb{G}$ *denote a generic function of Grassmann Number.* $f(\psi) = f_0 + f_1\psi$*. Then the derivative with respect to* ψ *can be defined as map from* $\mathbb{G}$ *to* $\mathbb{G}$ *s.t.*

$$\frac{\partial}{\partial\psi} f(\psi) = f_1$$

Derivatives anti-commute with Grassmann Numbers. Then it follows that derivatives anti-commute with each other. Consider,

$$\begin{aligned} \frac{\partial}{\partial\psi}\frac{\partial}{\partial\psi'} f(\psi, \psi') &= \frac{\partial}{\partial\psi}(f_{01} - f_{11}\psi) = -f_{11} \\ \frac{\partial}{\partial\psi'}\frac{\partial}{\partial\psi} f(\psi', \psi) &= \frac{\partial}{\partial\psi'}(f_{10} + f_{11}\psi') = f_{11} \end{aligned}$$

Ultimately the integrals with respect to Grassmann Numbers are defined as follows,

Definition 4 (Integrals of Grassmann Numbers)**.** *Let $\psi \in \mathbb{G}$. Then the integrals w.r.t. ψ are defined as function from $\mathbb{G}$ to $\mathbb{G}$ such that,*

$$\int d\psi = 0 \quad , \quad \int \psi d\psi = 1$$

The *differentials* anti-commute with each other and Grassmann Numbers. The differential and the Integral map are thus identical for Grassmann Numbers.

Now, since any function of Grassmann Numbers are defined only upto the first order of their Taylor Series, we can rewrite the left coherent state as,

$$\frac{1}{\mathbf{Tr}[\rho_0]}\mathbf{Tr}[U_{-\infty,\infty}U_{\infty,t}\rho_t U_{t-,\infty}] = \mathbb{I} \tag{2.3}$$

$$\begin{aligned} |\psi\rangle &= |0\rangle - \psi\,|1\rangle \\ &= (1 - \psi c^\dagger)\,|0\rangle = e^{-\psi c^\dagger}\,|0\rangle \end{aligned}$$

Similarly the right coherent state is defined as the right eigenstate of creation operator, $c^\dagger$.

$$\begin{aligned} \langle\psi| &= \langle 0|\, e^{-c\bar{\psi}} \\ &= \langle 0| - \langle 1|\,\overline{\psi}, \quad \overline{\psi} \in \mathbb{G} \end{aligned}$$

Here $\overline{\psi}$ is an independent Grassmann Number unrelated to ψ. It follows then, that the coherent states are not orthonormal and their inner product is given by,

$$\begin{aligned} \langle\psi|\psi'\rangle &= (\langle 0| - \langle 1|\,\overline{\psi})(|0\rangle - \psi'\,|1\rangle) \\ &= 1 + \overline{\psi}\psi' = e^{\overline{\psi}\psi'} \end{aligned}$$

The identity can be resolved in terms of the projection operator as follows.

$$\mathbf{I} = \int d\overline{\psi} \int d\psi e^{-\overline{\psi}\psi}\,|\psi\rangle\,\langle\psi| \tag{2.4}$$

Proof. It follows from the definitions that,

$$
\begin{aligned}
&\int d\overline{\psi} \int d\psi \; e^{-\overline{\psi}\psi} \, |\psi\rangle \, \langle\psi| \\
&= \int d\overline{\psi} \int d\psi \; (1 - \overline{\psi}\psi)(|0\rangle - \psi \, |1\rangle)(\langle 0| - \langle 1| \, \overline{\psi}) \\
&= \int d\overline{\psi} \int d\psi \quad - \overline{\psi}\psi(|0\rangle \, \langle 0| + |0\rangle \, \langle 0|) = \int d\overline{\psi} \; \overline{\psi} \; \int d\psi\psi(|0\rangle \, \langle 0| + |0\rangle \, \langle 0|) \\
&= \mathbf{I}
\end{aligned}
$$

□

Definition 5 (Normally ordered operators)**.** *An operator, A is said to be normally ordered if the annihilation operators, c appears at the right of the corresponding creation operator, $c^\dagger$ (if any) in all its additive constituent components.*

Normal Ordered operators are denoted as $: A :$ to distinguish them from the general ones.

Property 1. *Matrix elements of the normally ordered operators are then evaluated as,*

$$
\begin{aligned}
\langle\psi| : A : (c^\dagger, c) \, |\psi'\rangle &=: A : (\overline{\psi}, \psi') e^{\overline{\psi}\psi'} \\
&=: A : (\overline{\psi}, \psi') \, \langle\psi|\psi'\rangle
\end{aligned}
\tag{2.5}
$$

This follows from the definition of Coherent states and the Normal Ordered Operator.

Property 2 (Trace of an Operator)**.** *Trace of an operator can be computed as follows by utilizing the resolution of identity,*

$$
\begin{aligned}
\mathbf{Tr}[O] &= \sum_{n=0,1} \langle n| \, O \, |n\rangle \\
&= \sum_{n=0,1} \int d\overline{\psi} \int d\psi \; e^{-\overline{\psi}\psi} \, \langle n|\psi\rangle \, \langle\psi| \, O \, |n\rangle \\
&= \sum_{n=0,1} \int d\overline{\psi} \int d\psi \; e^{-\overline{\psi}\psi} \, \langle\psi| \, O \, |n\rangle \, \langle n| - \psi\rangle \\
&= \sum_{n=0,1} \int d\overline{\psi} \int d\psi \; e^{-\overline{\psi}\psi} \, \langle\psi| \, O \, |-\psi\rangle
\end{aligned}
\tag{2.6}
$$

The sign here follows from the anti-commutation property of Grassmann Numbers.

2.2 Gaussian Integrals of Grassmann Fields

To what follows in our discussion of the physics, especially in construction of the Path integral and the Green's Functions, which forms the fulcrum of Keldysh Field Theory, the following results related to the (multidimensional) Gaussian Integral plays a relevant role.

Definition 6 (Gaussian Integral of Grassmann Fields)**.** *Let* $\overline{\psi_j}, \psi_j, \overline{\chi_j}, \chi_j \in \mathbb{G}^n, \ \ j \in [1, n]$ *be four mutually independent sets of Grassmann numbers. Let* $A_{ij} \in \mathbf{GL}^n(\mathbb{R})$ *be an invertible* $n \times n$ *matrix. Then the Gaussian Integration of Grassman fields can be parametrically defined as,*

$$\begin{aligned} Z[\overline{\chi}, \chi] &= \int d\overline{\psi_j} \int d\psi_j \ e^{-\sum_{i,j} \overline{\psi_i} A_{ij} \psi_j + \overline{\psi_j} \chi_j + \overline{\chi_j} \psi_j} \\ &= \mathbf{det}(A) e^{-\sum_{i,j} \overline{\chi_i} A^{-1}_{ij} \chi_j} \end{aligned} \tag{2.7}$$

Note that unlike the Gaussian Integration involving c-numbers the determinant of the coefficient matrix appears in the denominator in the formula.

This allows to compute various moments with respect to the Gaussian Distribution summarised by the Wick's theorem.

Theorem 1 (Wick's Theorem for Fermions)**.**

$$\begin{aligned} \langle \psi_a \overline{\psi_b} \rangle &= \frac{1}{Z[0,0]} \frac{\partial^2 Z[\overline{\chi}, \chi]}{\partial \chi_b \partial \overline{\chi}_a} = \ \ A^{-1}_{ab} \\ \langle \psi_a \psi_b \overline{\psi_c \psi_d} \rangle &= \frac{1}{Z[0,0]} \frac{\partial^4 Z[\overline{\chi}, \chi]}{\partial \chi_d \partial \chi_c \partial \overline{\chi}_b \partial \overline{\chi}_a} = -A^{-1}_{ac} A^{-1}_{bd} + A^{-1}_{ad} A^{-1}_{bc} \end{aligned} \tag{2.8}$$

For any odd permutation of the indices the corresponding terms acquire a negative sign as the partial derivatives w.r.t. Grassmann Numbers anti-commute.

2.3 Fermionic Partition Function

We first delve with the non-interacting case. The Hamiltonian for the system is given by,

$$H_0 = \sum_k \epsilon(k) c^\dagger_k c_k \tag{2.9}$$

The energy levels are determined from the system dispersion relation $\epsilon(k) = \frac{k^2}{2m}$ for free fermions [1].

The Keldysh Formulation is formulated upon the idea of time evolution of the density matrix from an initial time $t = t_0$ to $t = \infty$, followed by a backward evolution to $t = \infty$ then back to $t = t_0$ generates the identical state.

The Partition function is then constructed by first discretising the closed time contour into $2N$ many instants and using the resolution of identity to unfoliate the following Identity,

Definition 7 (Fermionic Partition Function)**.**

$$Z = \frac{1}{\mathbf{Tr}[\rho_0]} \int \int \prod_{j=1}^{N} d\overline{\psi_j} d\psi_j \; e^{-i \sum_k \sum_{j=1}^{2N} \overline{\psi_j} G^{-1}_{k,jj} \psi_j} = \mathbb{I} \tag{2.10}$$

where the invertible matrix $G^{-1}_{k,ij}$ has the following form,

$$iG^{-1}_{k,ij} = \left(\begin{array}{ccccc|ccccc} -1 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & -\rho_0(\epsilon_k) \\ 1-i\epsilon_k\delta t & -1 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1-i\epsilon_k\delta t & -1 & \cdots & 0 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 & \cdots & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & \cdots & 1 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & -1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 1+i\epsilon_k\delta t & -1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 1+i\epsilon_k\delta t & -1 \end{array}\right) \tag{2.11}$$

It suffices to sample the momentum only in the first Brillouin zone.

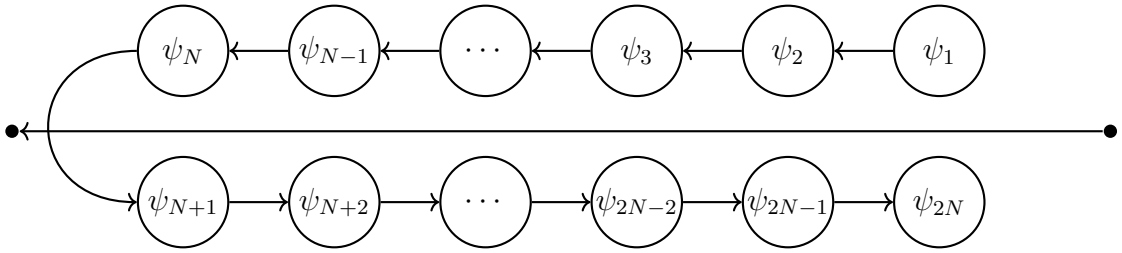
Note that all the momentum levels have independent Matrices. This is a feature of the non-interacting theory that we exploit to write the Partition Functions in the discrete time basis. As we will develop later, these degrees of freedom are mixed as the interaction is turned on.

The argument of the exponent can be rewritten in the continuous notation to define a *Action* function in terms of the Grassmann fields. After suitable normalisation and regularisation of the initial term, in the continum limit we obtain,

[1]Here in we neglect the spin degrees of freedom, since for the results we are concerned with we need to everage over the spins and both results are identical.

$$S[\overline{\psi},\psi] = \int_{-\infty}^{\infty} dt \sum_k \left[\overline{\psi}^{+}(t)(i\partial_t - \epsilon_k)\psi^{+}(t) - \overline{\psi}^{-}(t)(i\partial_t - \epsilon_k)\psi(t)^{-}\right] \tag{2.12}$$

Here the $^{+},^{-}$ fields respectively lives in the forward and the backward contours. Diagrammatically, the fields can be represented on the discretised Keldysh contour as follows,



Which under the $^{+},^{-}$ relabeling becomes,

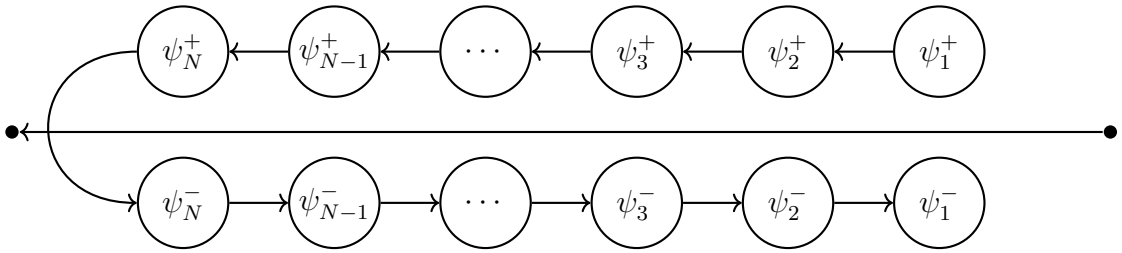


Figure 2.1: Digramatic representation of the time labelling of the Fermionic ψ field in the discrete Keldysh contour. The notion for the $\overline{\psi}$ is analogous. It is worth noting that the when they are relabeled as ψ^+, ψ^-, the ψ^- coordinates are ordered in the opposite way in the backward coordinate. This facilitates the difference in sign of δt in the fourth co-ordinate of (2.11).

It is customary in Keldysh-Schwinger Field theory to do a basis rotation of the equation()for each individual degrees (here the momentum) of freedom. Since the $\overline{\psi}, \psi$ are independent Grassmann Fields, they are needed to be rotated individually.

The following prescription is due to Larkin and Ovchinnikov [11].

$$\begin{aligned} \psi_k^1(t) = (\psi_k^+(t) + \psi_k^-(t))/\sqrt{2} \quad &; \quad \psi_k^2(t) = (\psi_k^+(t) - \psi_k^-(t))/\sqrt{2} \\ \overline{\psi^1}_k(t) = (\overline{\psi^+}_k(t) - \overline{\psi^-}_k(t))/\sqrt{2} \quad &; \quad \overline{\psi^2}_k(t) = (\overline{\psi^+}_k(t) + \overline{\psi^-}_k(t))/\sqrt{2} \end{aligned} \tag{2.13}$$

The Green's Functions of the free field theory (Bare Green's Functions) are thus obtained in the ω domain as,

$$
\begin{aligned}
G_k^{R/A}(\omega) &= \frac{1}{\omega - \epsilon_k \pm i0} \\
G_k^K(\omega) &= -2\pi i \delta(\omega - \epsilon_k)(1 - 2n_F(\epsilon_k)
\end{aligned}
\tag{2.14}
$$

These can be projected onto the time domain using an inverse Fourier Transform,

$$
\begin{aligned}
G_k^R(t,t') &= -i\theta(t-t')e^{-i\epsilon_k(t-t')} \\
G_k^A(t,t') &= \quad i\theta(t'-t)e^{-i\epsilon_k(t-t')} \\
G_k^K(t,t') &= -i\theta(t-t')e^{-i\epsilon_k(t-t')}n_F(\epsilon_k)
\end{aligned}
\tag{2.15}
$$

Following decomposition properties of the Green's Function follows from the expressions in (2.15).

Property 3 (Decomposition of Green's Function (first order))**.** *The Retarded and the Keldysh components of the Green's function have the following decomposition property,*

$$
\begin{aligned}
G_0^R(t,t') &= G_0^R(t,\tau)G_0^R(\tau,t') \;\; \forall \;\; t > \tau > t' \\
G_k^K(t,t') &= G_0^R(t,\tau)G_0^K(\tau,t') \;\; \forall \;\; t > \tau > t'
\end{aligned}
\tag{2.16}
$$

Here the subscript zero denotes free Green's Function. Momentum Indices has been suppressed. The decomposition property of the Advanced Green's function is analogous.

2.4 Interaction

Here in we develop the perturabative theory to treat fermionic interactions using Diagrammatic Techniques. We consider the following momentum space Hamiltonian with a four-fermionic interaction term.

$$
H = \sum_k \epsilon(k) c_k^\dagger c_k + \frac{1}{2}\sum_{k,k',q} u(q) c_k^\dagger c_{k'}^\dagger c_{k+q} c_{k'-q} \tag{2.17}
$$

The action S_{int} corresponding to the interaction term is,

$$
S_{int} = \frac{1}{2}\int_{\mathcal{C}} dt \sum_{k,k',q} u(q)\overline{\psi}_k(t)\overline{\psi}_{k'}(t)\psi_{k+q}(t)\psi_{k'-q}(t) \tag{2.18}
$$

The *total/dressed* Green's Functions can be then defined as various moments of the Path Integral with respect to the total action $S_{tot} = S_0 + S_{int}$,

Definition 8 (Dressed Green's Functions (Fermions))**.** *The various components of the Dressed Green's Functions are defined as,*

$$\begin{pmatrix} G_k^R(t,t') & G_k^K(t,t') \\ 0 & G_k^A(t,t') \end{pmatrix} = G_k^{\alpha\beta}(t,t') = -i \int\int \prod_{j=1}^{N} d\overline{\psi_j} d\psi_j \; \psi_k^{\alpha}(t) \overline{\psi}_k^{\beta}(t') \; e^{i(S_0+S_{int})} \tag{2.19}$$

A series solution for them can be obtained in the following way by expanding the interaction exponential.

For the sake of simplicity we will assume that the interaction strength is independent of the momentum level $u(q) = g$. Various orders in the series then can be labeled using various powers of g.

Consider the first non-trivial order terms in the series. The S_{int} can be rewritten with the Keldysh rotation given by eq(2.13) as,

$$\begin{aligned} S_{int} &= \frac{g}{2} \int_{-\infty}^{\infty} dt \; \sum_{k,k',q} \left[\overline{\psi}_k^+(t) \overline{\psi}_{k'}^+(t) \psi_{k+q}^+(t) \psi_{k'-q}^+(t) - \overline{\psi}_k^-(t) \overline{\psi}_{k'}^-(t) \psi_{k+q}^-(t) \psi_{k'-q}^-(t) \right] \\ &= \frac{g}{2} \int_{-\infty}^{\infty} dt \; \sum_{k,k',q} \left[\overline{\psi^1}_k(t) \overline{\psi^2}_{k'}(t) \psi_{k+q}^2(t) \psi_{k'-q}^2(t) + \overline{\psi^2}_k(t) \overline{\psi^1}_{k'}(t) \psi_{k+q}^1(t) \psi_{k'-q}^1(t) \right. \\ &\qquad + \overline{\psi^2}_k(t) \overline{\psi^1}_{k'}(t) \psi_{k+q}^2(t) \psi_{k'-q}^2(t) + \overline{\psi^1}_k(t) \overline{\psi^2}_{k'}(t) \psi_{k+q}^1(t) \psi_{k'-q}^1(t) \\ &\qquad + \overline{\psi^2}_k(t) \overline{\psi^2}_{k'}(t) \psi_{k+q}^1(t) \psi_{k'-q}^2(t) + \overline{\psi^1}_k(t) \overline{\psi^1}_{k'}(t) \psi_{k+q}^2(t) \psi_{k'-q}^1(t) \\ &\qquad \left. + \overline{\psi^2}_k(t) \overline{\psi^2}_{k'}(t) \psi_{k+q}^2(t) \psi_{k'-q}^1(t) + \overline{\psi^1}_k(t) \overline{\psi^1}_{k'}(t) \psi_{k+q}^1(t) \psi_{k'-q}^2(t) \right] \end{aligned} \tag{2.20}$$

These eight terms can be represented diagrammatically as the following vertices,

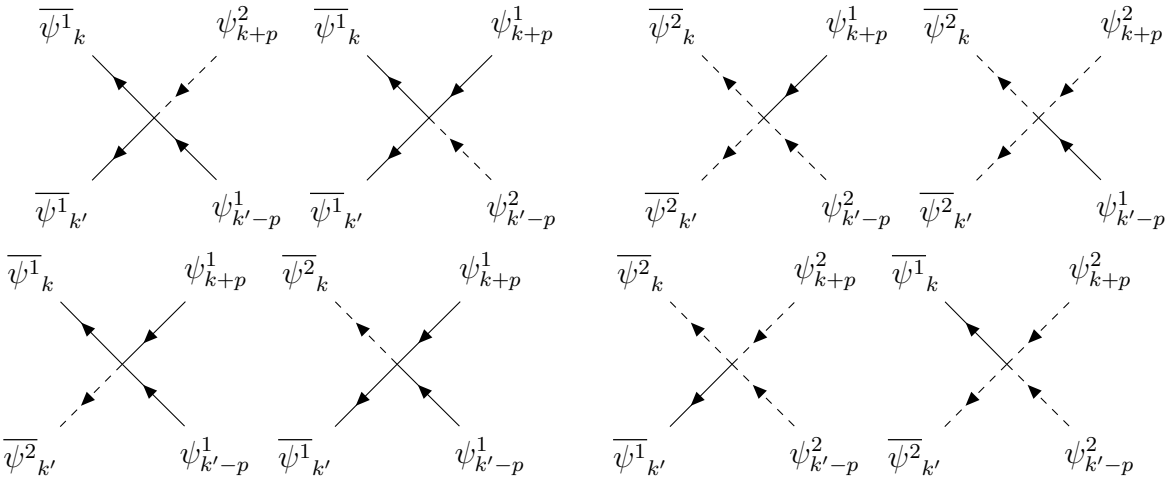


Figure 2.2: Diagrammatic representation of the Vertices of the four-fermionic interaction

where we denote ψ^1 with solid and ψ^2 with dashed lines. However this terms do not contribute in the sum. Their contraction are of the form,

$$\begin{aligned} &< \overline{\psi^1}_k(t)\overline{\psi^2}_{k'}(t)\psi^2_{k+q}(t)\psi^2_{k'-q}(t) + \overline{\psi^2}_k(t)\overline{\psi^1}_{k'}(t)\psi^1_{k+q}(t)\psi^1_{k'-q}(t) > \\ &=< G^K_k(t,t)[G^R_k(t,t) + G^A_k(t,t)] > \\ &= 0 \end{aligned} \tag{2.21}$$

Calculations of the other six terms are similar.

Definition 9 (Irreducible Diagrams)**.** *A diagram of the fields and their contractions is called reducible if there exist an edge such that its removal produces two disconnected components. A diagram is called irreducible if it is not a disconnected and is not reducible.*

Theorem 2. *Only Irreducible and non-loop diagrams have finite contribution to the sum in the Path Integral in computation of the Dressed Greens Functions. Sum of all such diagrams are defined as the Self Energy.*

Similar to the greens functions, the self energies (denoted by Σ) for individual momentum can be written in the ψ_1, ψ_2 basis. It has the following Causality Structure,

$$\Sigma_k(t,t') = \begin{pmatrix} \Sigma^R_k(t,t') & \Sigma^K_k(t,t') \\ 0 & \Sigma^A_k(t,t') \end{pmatrix} \tag{2.22}$$

$\Sigma_k(t,t')$ in general contains fro all other momentum states.

It can be shown then that the complete series solution of for the Dressed Green's Functions can be obtained as,

$$\begin{aligned} G_k(t,t') = G_k^0(t,t') &+ G_k^0(t,t') \circ \Sigma_k(t,t') \circ G_k^0(t,t') \\ &+ G_k^0(t,t') \circ \Sigma_k(t,t') \circ G_k^0(t,t') \circ \Sigma_k(t,t') \circ G_k^0(t,t') \\ &+ \cdots \end{aligned}$$

or,

$$G_k(t,t') = G_k^0(t,t') + G_k^0(t,t') \circ \Sigma_k(t,t') \circ G_k(t,t') \tag{2.23}$$

where $\circ$ denotes component-wise multiplication in the ψ_1, ψ_2 basis as well as a convolution in the time parameter. Equation 2.37 is named after Sir Freeman Dyson. This forms the basis of our endeavour in unraveling the dynamics of the interacting systems.

2.5 Real Scalar Field Theory

In the rest of this chapter we delve with developing similar results for the real scalar field theory which appears as a solution to the Klein-Gordon Equation[12], which is second order in time with an instantaneous infinite source term,

$$(-\partial_t^2 - \nabla^2)\phi_k(x,t) = \delta(t-t') \tag{2.24}$$

Unlike the fermions for which the theory is developed above the bosons are described by the scalar fields (c-numbers). If the underlying bosons have mass then they are described as a solution to a first order equation instead, which is similar to the theory developed above, except that c-numbers commutes unlike the anticommuting Grassmann numbers. This also brings in changes in the Causality structure which will be similar to the theory we develop below.

We are concerned with phonons which are mass less and is described by a real scalar field theory. For the discussion of complex field theory the usueal introduction are [13, 14]. The Keldysh formalism for the same is developed at [2].

In the following section we define the Gaussian Integral for scalar fields and state the wick theorem and then go on to derive the Green's Function and Dyson Equation for the bosonic systems.

2.6 Gaussian Integrals of Real Scalar Fields

Like wise for the Fermions, the idea of Path Integral of bosons are also hinged on the corresponding Gaussian Integrals defined in the following way

Definition 10 (Gaussian Integral of Real Fields)**.** *Let $\phi_j, \chi_j \in \mathbb{R}^n, \quad j \in [1, n]$ be two mutually independent sets of real fields. Let $A_{ij} \in \mathbf{GL}^n(\mathbb{R})$ be an invertible $n \times n$ matrix. Then the Gaussian Integration of Real fields is then parametrically defined as,*

$$\begin{aligned} Z[\chi] &= \int d\phi_j \; e^{-\sum_{i,j} \phi_i A_{ij} \phi_j + \phi_j \chi_j} \\ &= \frac{1}{\mathbf{det}(A)} e^{-\sum_{i,j} \chi_i A^{-1}_{ij} \chi_j} \end{aligned} \tag{2.25}$$

Again, this allows to compute various moments with respect to the Gaussian Distribution summarised by the Wick's theorem.

Theorem 3 (Wick's Theorem for Bosons)**.**

$$\begin{aligned} \langle \phi_a \phi_b \rangle &= \frac{1}{Z[0]} \frac{\partial^2 Z[\chi]}{\partial \chi_b \partial \chi_a} = \quad A^{-1}_{ab} \\ \langle \phi_a \phi_b \phi_c \phi_d \rangle &= \frac{1}{Z[0]} \frac{\partial^4 Z[\chi]}{\partial \chi_d \partial \chi_c \partial \chi_b \partial \chi_a} = A^{-1}_{ac} A^{-1}_{bd} + A^{-1}_{ad} A^{-1}_{bc} \end{aligned} \tag{2.26}$$

Since c-numbers commute, the permutation of indices do not acquire any sign in contrast to the Fermionic Cases.

2.7 Bosonic Partition Function

Again, We start with the non-interacting case. The Hamiltonian for the phonon system is given by,

$$H_0 = \sum_k \omega(k) a^\dagger_k a_k \tag{2.27}$$

The energy levels are determined from the system dispersion relation $\omega(k) = \omega_0 \sqrt{\sin^2(\frac{ka}{2})}$ for acoustic phonons, a being the lattice constant.

$a, a^\dagger$ are the bosonic creation and annihilation operators, which follows the following algebra,

$$a\,|n\rangle = \sqrt{n}\,|n+1\rangle \ , \qquad a^\dagger\,|n+1\rangle = \sqrt{n}\,|n\rangle$$

It follows that the commutator, $[a, a^\dagger] = aa^\dagger - a^\dagger a = I$. The number operator is defined as,

$$a^\dagger a\,|n\rangle = n\,|n\rangle$$

The Partition function is then constructed by first similary discretising the closed time contour into $2N$ many instants and again using the resolution of identity to unfoliate the following Identity,

Definition 11 (Bosonic Partition Function)**.**

$$Z = \frac{1}{\mathbf{Tr}[\rho_0]} \int \prod_{j=1}^{N} d\phi_j \; e^{-i\sum_k \sum_{j=1}^{2N} \phi_j D^{-1}_{k,jj} \phi_j} = \mathbb{I} \tag{2.28}$$

where the invertible matrix $D^{-1}_{k,ij}$ has the following form,

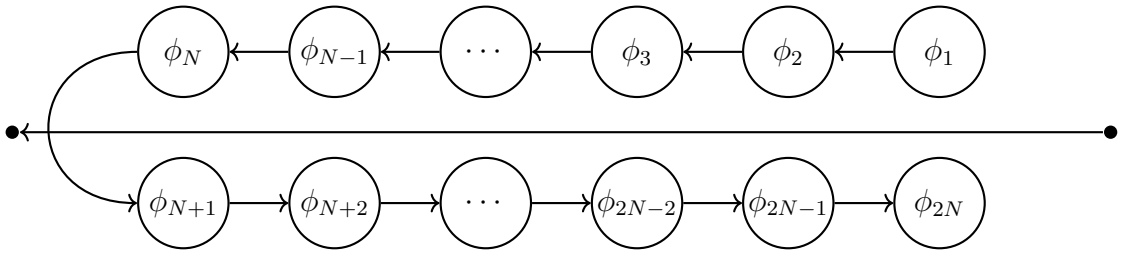
$$\left(\begin{array}{ccccc|ccccc}
-1 & 1-i\omega_k & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & \rho_0(\omega_k) \\
1-i\omega_k\delta t & -1 & 1-i\omega_k & \cdots & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 1-i\omega_k\delta t & -1 & \cdots & 1-i\omega_k & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -1 & 1 & \cdots & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & \cdots & 1 & -1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & 0 & \cdots & -1 & 1+i\omega_k & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 1+i\omega_k\delta t & -1 & 1+i\omega_k \\
0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 1+i\omega_k\delta t & -1
\end{array}\right) \tag{2.29}$$

The momentum is sampled only from the first Brillouin zone.

The argument of the exponent can be rewritten in the continuous notation to define a *Action* function in terms of the Scalar fields. After suitable normalisation and regularisation of the initial term, in the continuum limit we similarly obtain,

$$S[\phi] = \int_{-\infty}^{\infty} dt \sum_k \left[\phi^+(t)(i\partial_t^2 - \omega_k^2)\phi^+(t) - \phi^-(t)(i\partial_t^2 - \omega_k^2)\phi(t)^-\right] \tag{2.30}$$

The $^+$,$^-$ fields respectively lives in the forward and the backward contours. Diagrammatically, the fields can be similarly represented on the discretised Keldysh contour as follows,



Which under the $^+$,$^-$ relabeling becomes,

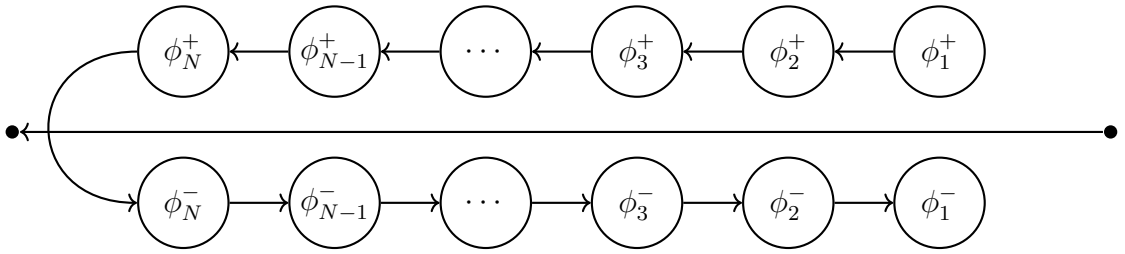


Figure 2.3: Digramatic representation of the time labelling of the Bosonic ϕ field in the discrete Keldysh contour

Then we do the Keldysh rotation to obtain the classical and quantum components of the fields.

$$\phi_k^{cl}(t) = (\phi_k^+(t) + \phi_k^-(t))/2 \quad ; \quad \phi_k^q(t) = (\phi_k^+(t) - \phi_k^-(t))/2 \tag{2.31}$$

The Green's Functions of the free field theory (Bare Green's Functions) are thus obtained in the ω domain as,

$$\begin{aligned} D_k^{R/A}(\omega) &= \frac{1}{(\omega \mp i0)^2 - \omega_k} \\ D_k^K(\omega) &= (1 + 2n_B(\omega_k))[D_k^R(\omega) - D_k^A(\omega)] \end{aligned} \tag{2.32}$$

The last relation is called the *Fluctuation Dissipation Theorem*. The Green's Functions can be projected onto the time domain using an inverse Fourier Transform as,

$$
\begin{aligned}
D_k^R(t,t') &= \frac{1}{2\omega_k}\theta(t-t')\sin[\omega_k(t-t')] \\
D_k^K(t,t') &= -\frac{i}{2\omega_k}\cos[\omega_k(t-t')]\coth\big[\frac{\omega_k}{2\,T_{system}}\big]
\end{aligned}
\tag{2.33}
$$

Following decomposition properties of the Green's Function follows from the expressions in (2.33).

Property 4 (Decomposition of Green's Function (second order))**.** *The Retarded and the Keldysh components of the Green's function have the following decomposition property,*

$$
\begin{aligned}
D_0^R(t,t') &= D_0^R(t,\tau)\overline{D}_0^R(\tau,t') + \overline{D}_0^R(t,\tau)D_0^R(\tau,t') \;\;\forall\;\; t>\tau>t' \\
D_k^K(t,t') &= D_0^R(t,\tau)\overline{D}_0^K(\tau,t') + \overline{D}_0^R(t,\tau)D_0^K(\tau,t') \;\;\forall\;\; t>\tau>t'
\end{aligned}
\tag{2.34}
$$

Here the subscript zero denotes free Green's Function and the bar denotes time derivative with respect to the first index. Momentum Indices has been suppressed here.

2.8 Dyson Equation

The perturbative theory for the bosonic sector is defines in the exact same way as in the case of phonons, modulo the causality. First we define the Dressed Green's Functions of the real scalar field theory.

Definition 12 (Dressed Green's Functions (Bosons))**.** *The various components of the Dressed Green's Functions are defined as,*

$$
\begin{pmatrix} D^K & D^R \\ D^A & 0 \end{pmatrix} = D_k^{\alpha\beta}(t,t') = -\int \prod_{j=1}^{N} d\phi_j \;\phi_k^{\alpha}(t)\phi_k^{\beta}(t')\; e^{i(S_0+S_{int})} \tag{2.35}
$$

The self energies (denoted by Σ) for individual momentum can be written in the ϕ^{cl}, ϕ^{q} basis by summing up the respective irreducible diagrams obtained from contracting the interaction nodes. It has the following Causality Structure for Bosons,

$$
\Sigma_k(t,t') = \begin{pmatrix} 0 & \Sigma^A \\ \Sigma^R & \Sigma^K \end{pmatrix} \tag{2.36}
$$

The complete series solution of for the Dressed Green's Functions is similarly be obtained as,

$$\begin{aligned} D_k(t,t') = D_k^0(t,t') &+ D_k^0(t,t') \circ \Sigma_k(t,t') \circ D_k^0(t,t') \\ &+ D_k^0(t,t') \circ \Sigma_k(t,t') \circ D_k^0(t,t') \circ \Sigma_k(t,t') \circ D_k^0(t,t') \\ &+ \cdots \end{aligned}$$

This in the closed form gives the Bosonic Dyson Equation

$$D_k(t,t') = D_k^0(t,t') + D_k^0(t,t') \circ \Sigma_k(t,t') \circ D_k(t,t') \tag{2.37}$$

Equipped with this results, in the following sections we delve into developing a iterative measure to encapsulate the dynamics of the electron-phonon coupled system in a self consistent way.

Chapter 3

Non interacting Bosons Coupled with Ohmic Bath

In this section we delve in study the dynamical behaviour of the phononic sector as is dictated by the Dyson Equation when it is coupled to an external Ohmic bath.

Before we delve in with our complete system we wished to test the time evolution of the phononic sector under Dyson Equation, when coupled to an external bath, with analytical expressions of self energy.

As is illustrated before, in our alogorithm the non-equilibrium time evolution under the Dyson Equation is kept intact whereas in the electronic sector we have assumed a quassi-static feedback. The results in this chapter were generated to test the behaviour of this sector with a known bath.

For this purpose, we had prepared a 1-d system of non-interacting phonons and had coupled them with an Ohmic bath with an Gaussian Dressing. The Ohmic bath produces closed form expressions for the Keldysh and Retarded component of the self-energy in the ω domain. These then can be projected onto the time domain using an inverse Fourier Transform.

With these analytical expressions in hand, dynamics of the occupation of the system is studied for each individual energy levels, for various bath and system parameters as well as for various interaction strengths. The methods, expressions and the results are summarised below.

3.1 Green's Functions, Self Energies

We start with an 1-dimensional system with 19 equi-seperated momentum modes in the first brillouin zone. It suffices to restrict our discussion in this zone owing to the periodic boundary condition in the configuration space.

Since the photons are described by a real scalar field theory (uncharged bosons), the underlying dynamical equations are second order in time.

It then follows that the bare green's functions are,

$$\begin{aligned} D_k^R(t,t') &= \frac{1}{2\omega_k}\sin[\omega_k(t-t')] \quad \forall \quad t > t' \\ &= 0 \qquad \text{otherwise} \end{aligned} \tag{3.1}$$

The Keldysh Component is,

$$D_k^K(t,t') = -\frac{i}{2\omega_k}\cos[\omega_k(t-t')]\coth\big[\frac{\omega_k}{2\,T_{system}}\big] \tag{3.2}$$

The advanced component is defined as the Hermitian Conjugate of the Retarded one.

$$D_k^R(t,t') = D_k^A(t',t)^c \tag{3.3}$$

It is apparent from equation (3.2) that the Keldysh component is anti-Hermitian.

$$D_k^R(t,t') = -D_{-k}^K(t',t)^c \tag{3.4}$$

Since we work with a Dispersion Relation Symmetric in momentum, for the purposes of this discussion it reduces to,

$$D_K^R(t,t') = -D_k^K(t',t)^c \tag{3.5}$$

Here, we have chosen the thermal $F(\omega_k)$, as we start from a thermal system with temperature T_{system}.

The bath is defined using the bath spectral function $J(\omega)$. The Ohmic Bath has a linear spectral density in ω.

$$J(\omega) = \eta\omega e^{-\frac{\omega^2}{\sigma^2}} \tag{3.6}$$

Here η is a proportionality constant[1], which has the dimension of ω for the second order theory. The Gaussian dressing of the bath is chosen to ensure the convergence

[1]For the purposes of rest of this chapter we set it to 1.

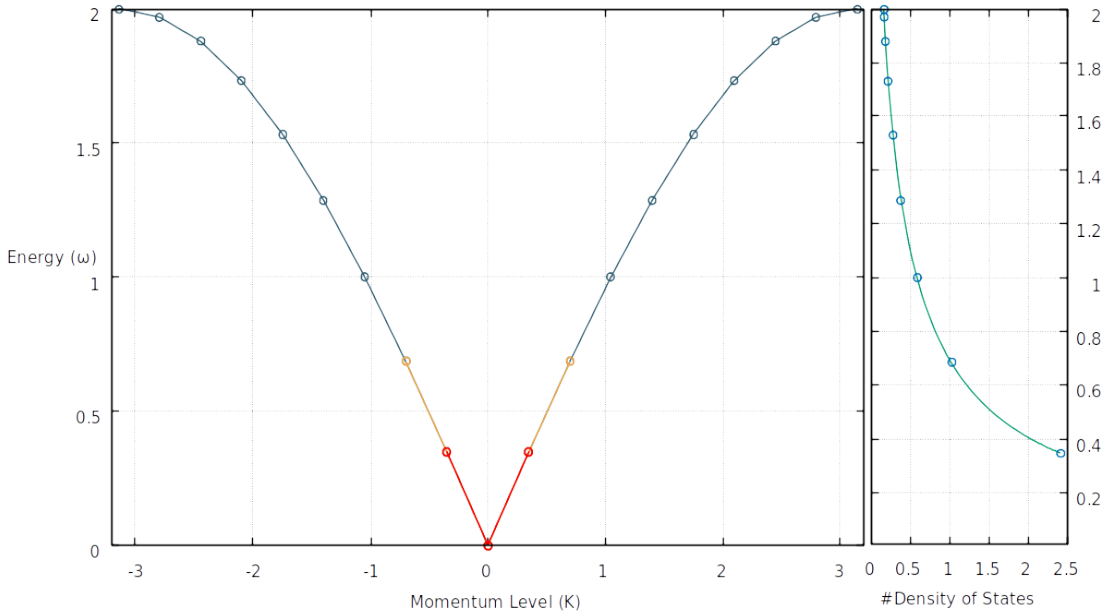


Figure 3.1: Plot of the initial Energy Levels v/s the momentum level in the First Brillioun Zone. The plot in the right shows the initial occupation numbers corresponding to the said energy levels. We are working with acoustic phonons so the dispersion relation is sinusoidal as is given by Eq. (3.9). The occupation number for each energy level is then computed using a Bose Distribution, with $\beta = 1$. For phonons the chemical potential, $\nu = 0$. The bandwidth of the distribution ω_0 is set at 2

of the fourier integrals. The σ gives a measure of the bath bandwidth and is kept fixed at 1 for the purpose of the study. The self energies in the ω domain are obtained as,

$$\Sigma^R(\omega) = \lambda^2 \frac{2}{\sqrt{\pi}} \omega DawsonF\Big(\frac{\omega}{\sqrt{2}\sigma}\Big) - i\lambda^2 \omega \exp(-\frac{\omega^2}{\sigma^2}) \tag{3.7}$$

$$\Sigma^K(\omega) = -i2\lambda^2 \omega \exp(-\frac{\omega^2}{\sigma^2}) \coth\Big(\frac{\omega}{2T_{bath}}\Big) \tag{3.8}$$

Here, T_{bath} is the bath temperature and the Dawson Function, which is obtained as the dressing of the real part of Σ^R from the Kramers–Kronig relation, is defined by,

$$DawsonF(x) = e^{-x^2} \int_0^x e^{y^2} dy$$

The system under our consideration is 1D and consists of 19 phonon modes with the dispersion relation,

$$\omega = \omega_0 \sqrt{\sin^2(\frac{ka}{2})} \tag{3.9}$$

3.2 Iterating the Dyson Equation

The Dyson Equation of the phononic sector have the form,

$$\begin{pmatrix} D^K & D^R \\ D^A & 0 \end{pmatrix} = \begin{pmatrix} D_0^K & D_0^R \\ D_0^A & 0 \end{pmatrix} + \begin{pmatrix} D_0^K & D_0^R \\ D_0^A & 0 \end{pmatrix} \circ \begin{pmatrix} 0 & \Sigma^A \\ \Sigma^R & \Sigma^K \end{pmatrix} \circ \begin{pmatrix} D^K & D^R \\ D^A & 0 \end{pmatrix} \tag{3.10}$$

Here the $\circ$ denotes convolution over corresponding time indices. Component wise the equation can be decomposed into the retarded part,

$$D^R(t,t') = D_0^R(t,t') + \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 D_0^R(t,t_1)\Sigma^R(t_1,t_2)D^R(t_2,t') \tag{3.11}$$

and the Keldysh Part,

$$\begin{aligned} D^K(t,t') = D^K(t,t') &+ \int_{t'}^{0} dt_1 \int_{t'}^{t_1} dt_2 D_0^K(t,t_1)\Sigma^A(t_1,t_2)D^A(t_2,t') \\ &+ \int_{0}^{t} dt_1 \int_{0}^{t'} dt_2 D_0^R(t,t_1)\Sigma^K(t_1,t_2)D^A(t_2,t') \\ &+ \int_{0}^{t} dt_1 \int_{0}^{t_1} dt_2 D_0^R(t,t_1)\Sigma^R(t_1,t_2)D^K(t_2,t') \end{aligned} \tag{3.12}$$

The idea then is to use (3.11), (3.12) to obtain $D^R(t+\epsilon,t'), D^K(t+\epsilon,t')$ iteratively, which can then be fed to the electronic sector to obtain $G_e^k(t+\epsilon,t+\epsilon)$. We first look at the retarded component.

$$\begin{aligned} D^R(t+\epsilon,t') = D_0^R(t+\epsilon,t)\overline{D^R}(t,t') + \overline{D_0^R}(t+\epsilon,t)D^R(t,t') \\ + \int_{t}^{t+\epsilon} dt_1 \int_{t'}^{t_1} dt_2 D_0^R(t+\epsilon,t_1)\Sigma^R(t_1,t_2)D^R(t_2,t') \end{aligned} \tag{3.13}$$

where the bar denotes total derivative w.r.t the first time index. We can now use a two-point Eulerian Quadrature, to approximate the t_1 integral and obtain,

$$\begin{aligned} D^R(t+\epsilon,t') = D_0^R(t+\epsilon,t)\overline{D^R}(t,t') + \overline{D_0^R}(t+\epsilon,t)D^R(t,t') \\ + \frac{\epsilon}{2} D_0^R(t+\epsilon,t) \int_{t'}^{t} dt_2 \Sigma^R(t,t_2)D^R(t_2,t') \end{aligned} \tag{3.14}$$

One of the boundary term in the quadrature drops off, as the equal-time retarded Green's Function being zero. Since it does not depend on $D^R(t+\epsilon, t')$, the iteration is not self-consistent. The iteration equation for $\overline{D^R}(t, t')$ can be obtained by taking derivative w.r.t the first time index of the both sides of eq (3.14).

The equations for the Keldysh Component is similar. The following section summarises the findings of this test.

3.3 Findings

Since the bath spectral function extends to infinite frequencies we expect all modes to thermalise for all parameter values for bath bandwidth and coupling strength.

We compute the imaginary part of the diganoal elements of the Keldysh Component for each energy level. This is related to the occupation number at a particular time t.

As we turn on the bath at time t=0, the bath renormalises the energy levels. Owing to this we expect the $-iD_k^K(t, t)$ to show transient oscillations initially but eventually settle down to its equilibrium value dictated by the Bath Temperature.

We also expect the following behaviour as we vary various parameters.

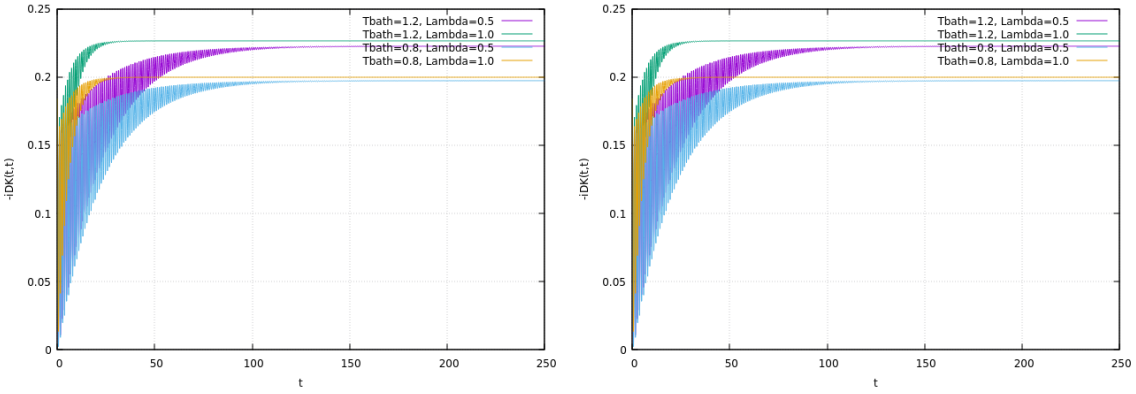
In general a stronger coupling strength is supposed to result in faster damping of the initial oscillations. That is higher λ shows faster timescale of equilibriation.

Bath Bandwidth σ usually does not effectively factor in as long it is not comparable to system bandwidth. That is for a bigger bath bandwidth the system effectively sees it as infinite and shows equivalent timescale of thermalisation.

That is however not true for $\sigma < \omega_0$. In this case the system shows extremely long timescale of thermalisation. The lower energy levels which still has some comparable overlap seems to faster timescale than the higher modes.

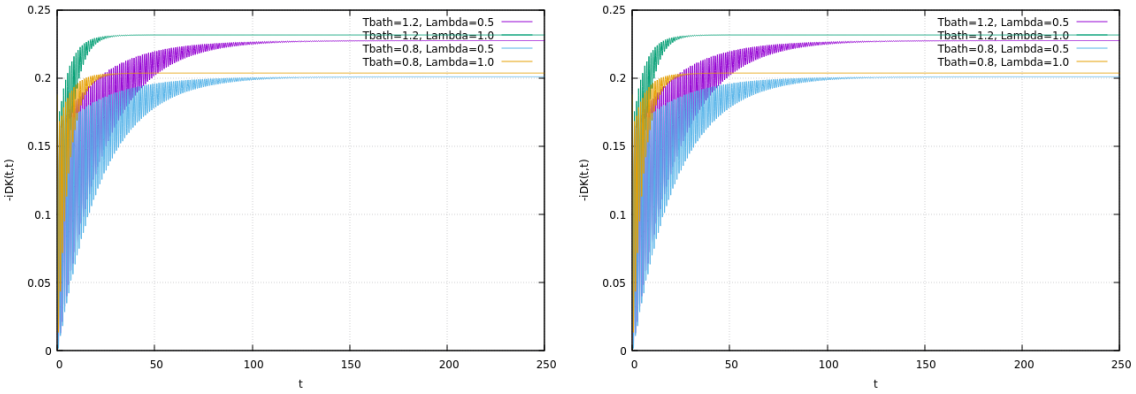
These behaviour of various levels are summarised in the following plots,

The collective behaviour of various levels are summarised in the following plots,



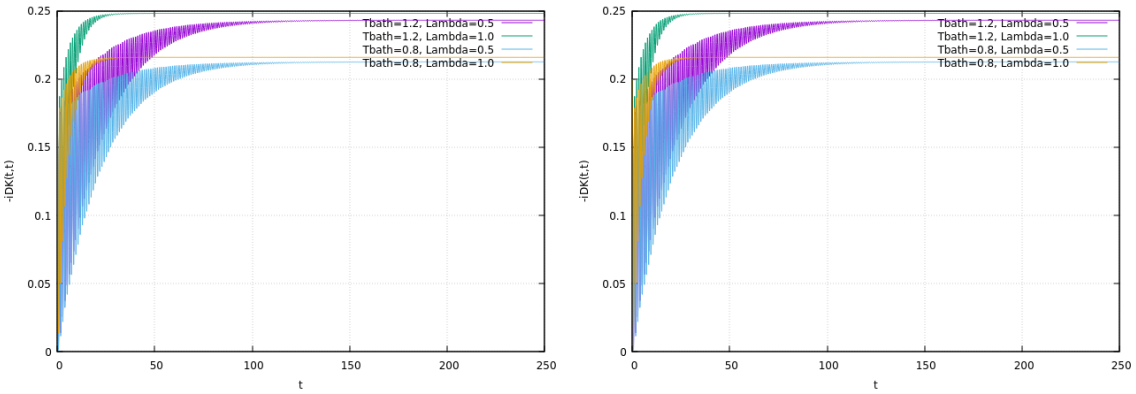
(a) $\sigma = 5$ (b) $\sigma = 10$

Figure 3.2: Plots for $-iD^K(t,t)$ vs t for level=01 of the phononic system for various $\sigma = 10, 5, T_{bath} = 0.8, 1, \lambda = 0.5, 1$



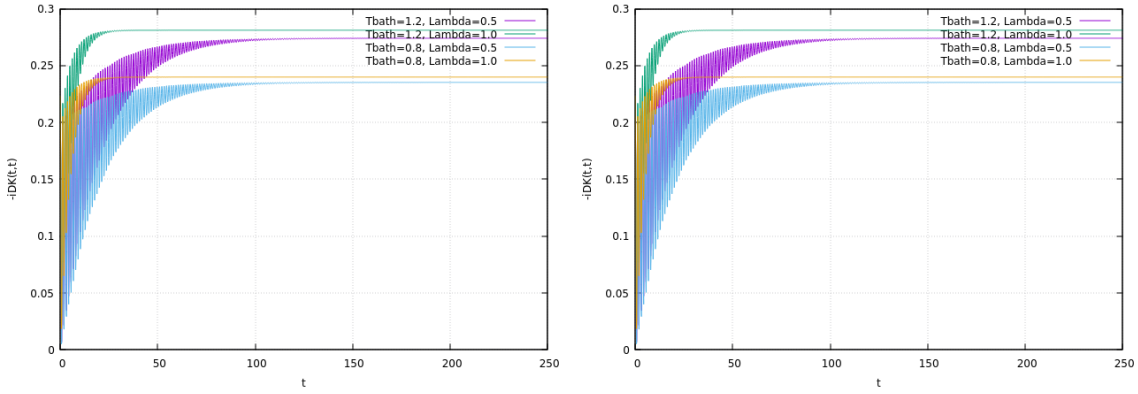
(a) $\sigma = 5$ (b) $\sigma = 10$

Figure 3.3: Plots for $-iD^K(t,t)$ vs t for level=02 of the phononic system for various $\sigma = 10, 5, T_{bath} = 0.8, 1, \lambda = 0.5, 1$



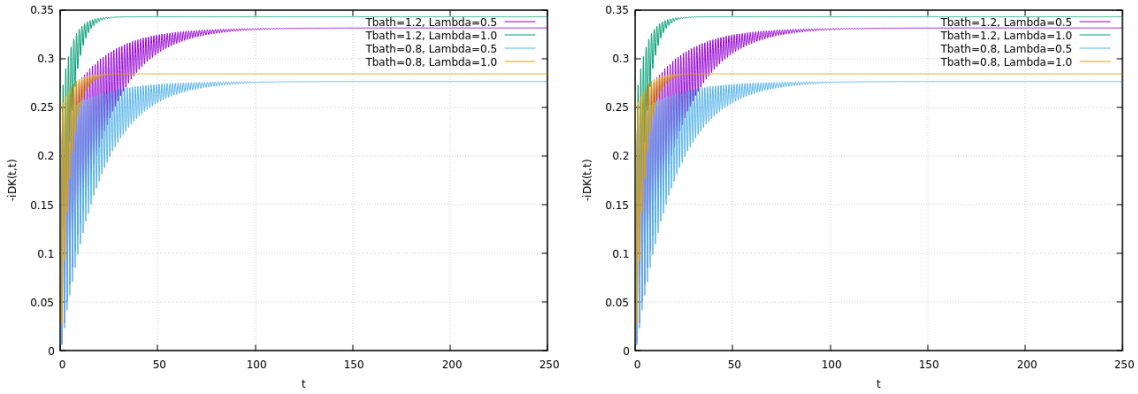
(a) $\sigma = 5$ (b) $\sigma = 10$

Figure 3.4: Plots for $-iD^K(t,t)$ vs t for level=03 of the phononic system for various $\sigma = 10, 5, T_{bath} = 0.8, 1, \lambda = 0.5, 1$



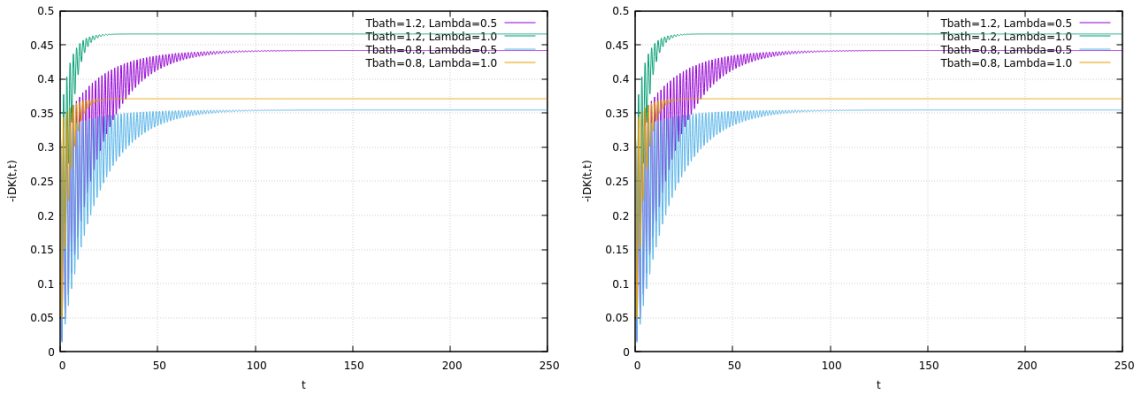
(a) $\sigma = 5$ (b) $\sigma = 10$

Figure 3.5: Plots for $-iD^K(t,t)$ vs t for level=04 of the phononic system for various $\sigma = 10, 5, T_{bath} = 0.8, 1, \lambda = 0.5, 1$



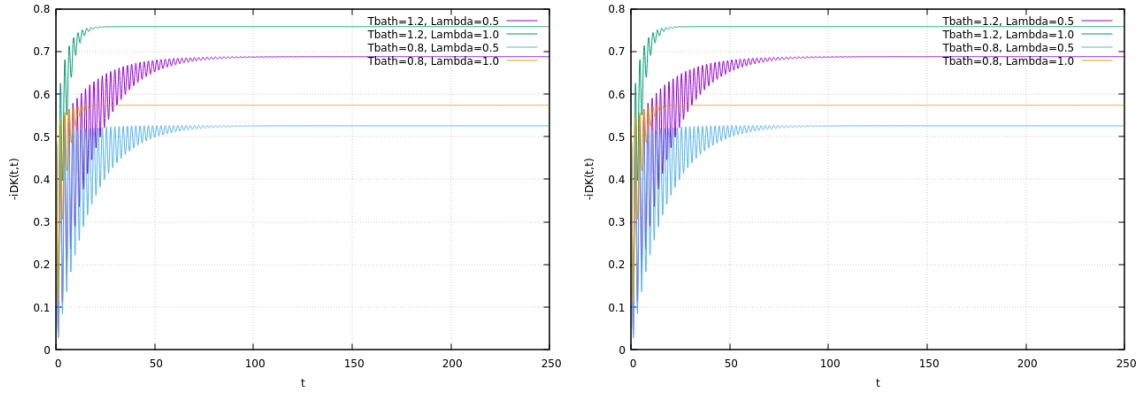
(a) $\sigma = 5$ (b) $\sigma = 10$

Figure 3.6: Plots for $-iD^K(t,t)$ vs t for level=05 of the phononic system for various $\sigma = 10, 5, T_{bath} = 0.8, 1, \lambda = 0.5, 1$



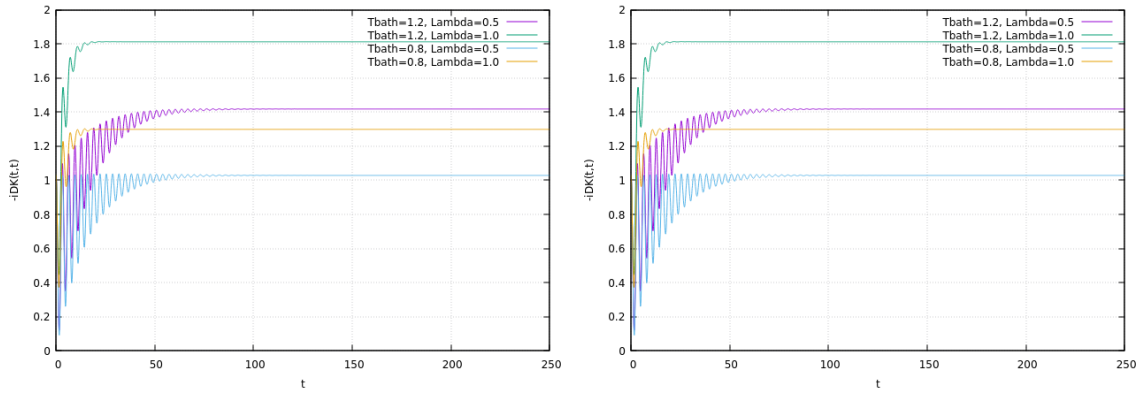
(a) $\sigma = 5$ (b) $\sigma = 10$

Figure 3.7: Plots for $-iD^K(t,t)$ vs t for level=06 of the phononic system for various $\sigma = 10, 5, T_{bath} = 0.8, 1, \lambda = 0.5, 1$



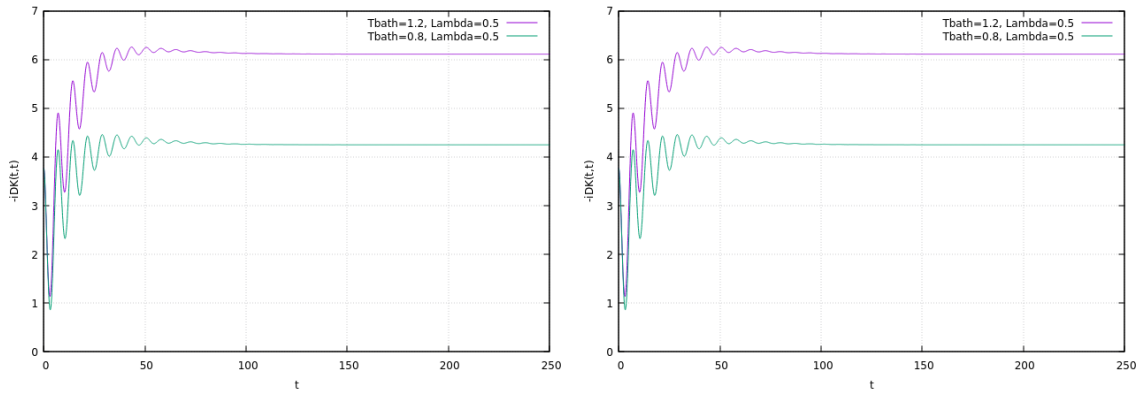
(a) $\sigma = 5$ (b) $\sigma = 10$

Figure 3.8: Plots for $-iD^K(t,t)$ vs t for level=07 of the phononic system for various $\sigma = 10, 5, T_{bath} = 0.8, 1, \lambda = 0.5, 1$



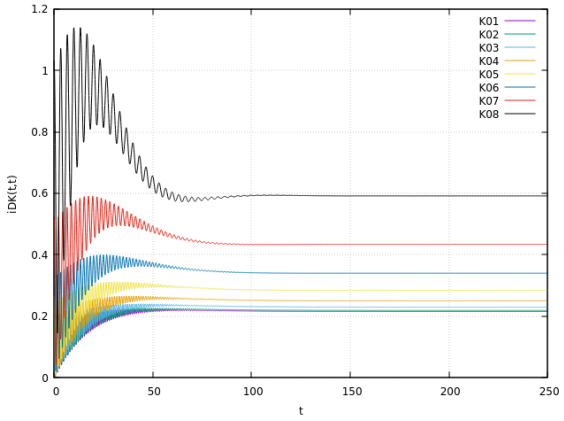
(a) $\sigma = 5$ (b) $\sigma = 10$

Figure 3.9: Plots for $-iD^K(t,t)$ vs t for level=08 of the phononic system for various $\sigma = 10, 5, T_{bath} = 0.8, 1, \lambda = 0.5, 1$

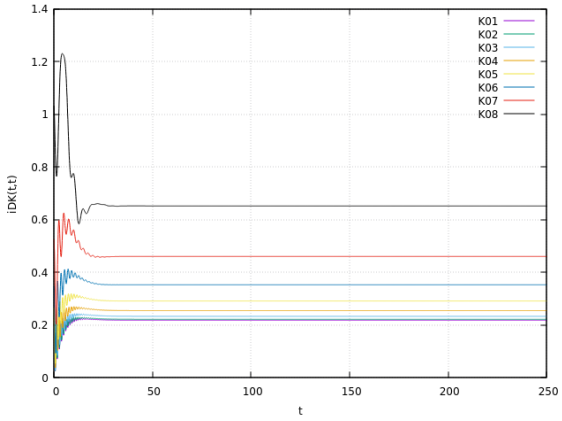


(a) $\sigma = 5$ (b) $\sigma = 10$

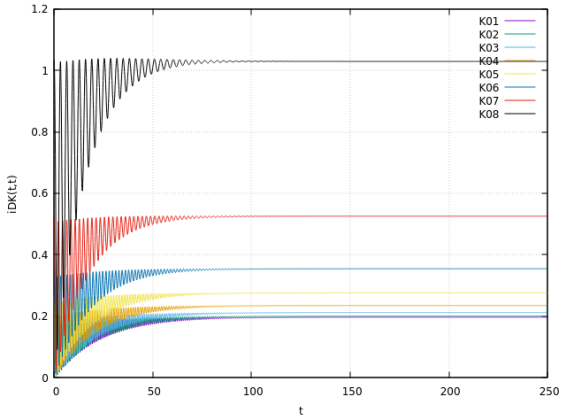
Figure 3.10: Plots for $-iD^K(t,t)$ vs t for level=09 of the phononic system for various $\sigma = 10, 5, T_{bath} = 0.8, 1, \lambda = 0.5, 1$



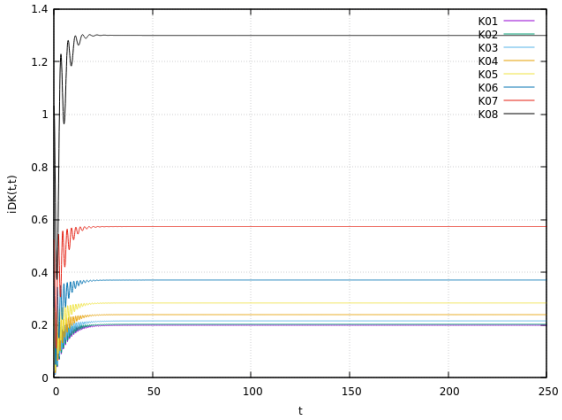
(a) $\sigma = 10, \lambda = 0.5$



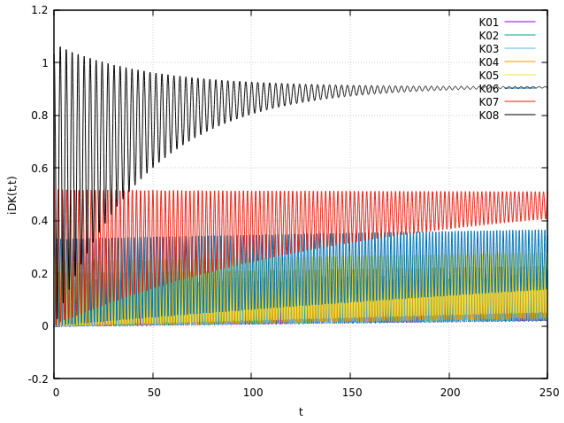
(b) $\sigma = 10, \lambda = 1.0$



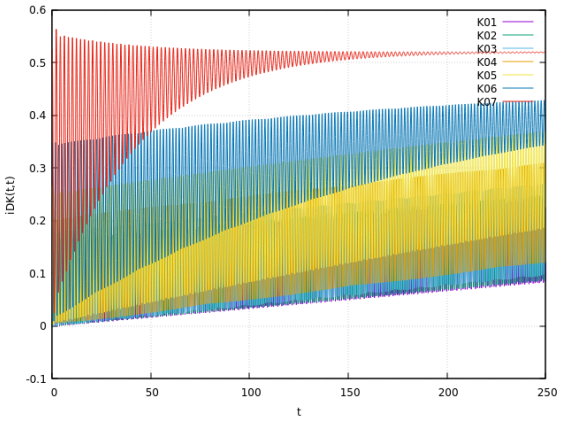
(c) $\sigma = 5, \lambda = 0.5$



(d) $\sigma = 5, \lambda = 1.0$

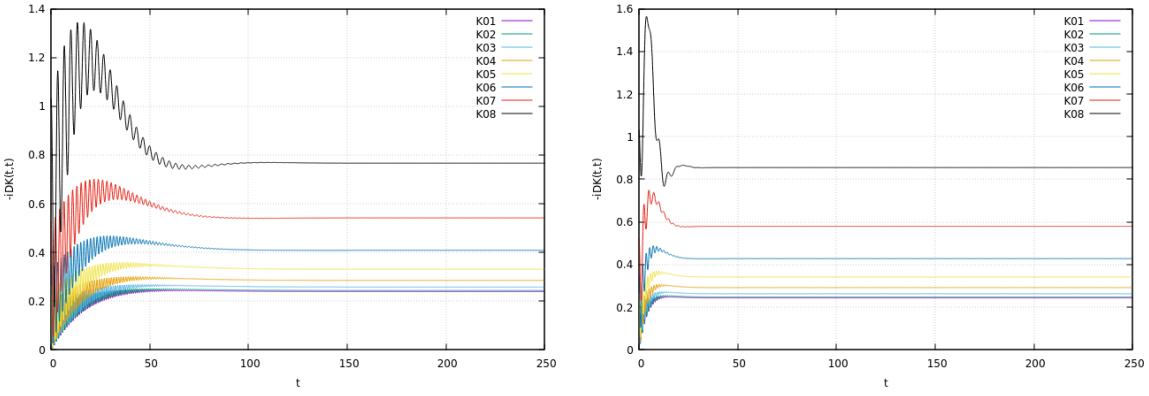


(e) $\sigma = 1, \lambda = 0.5$



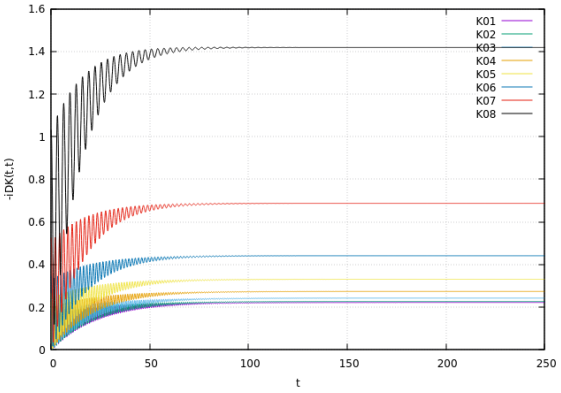
(f) $\sigma = 1, \lambda = 1.0$

Figure 3.11: Plots for $-iD^K(t,t)$ vs t for various levels with $T_{bath} = 0.8$

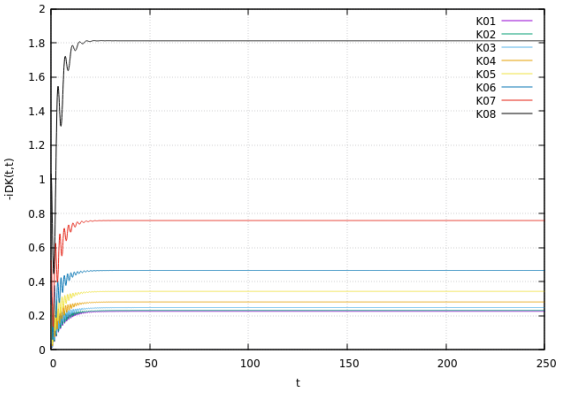


(a) $\sigma = 10, \lambda = 0.5$

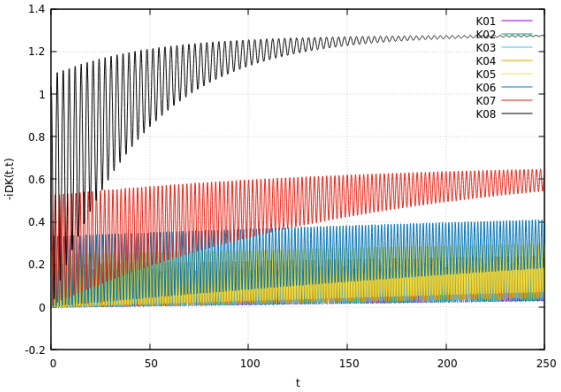
(b) $\sigma = 10, \lambda = 1.0$



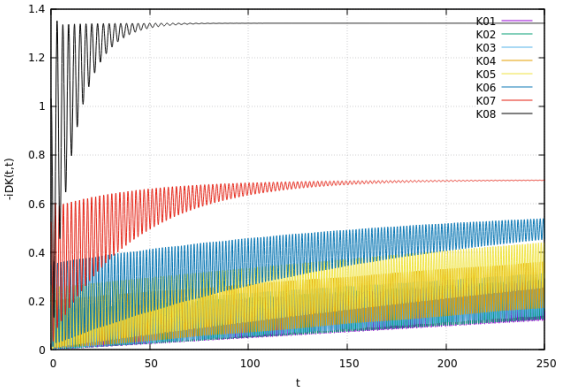
(c) $\sigma = 5, \lambda = 0.5$



(d) $\sigma = 5, \lambda = 1.0$



(e) $\sigma = 1, \lambda = 0.5$



(f) $\sigma = 1, \lambda = 1.0$

Figure 3.12: Plots for $-iD^K(t,t)$ vs t for various levels with $T_{bath} = 1.2$

Chapter 4

Further Work

As discussed in the previous chapter, the non-equilibrium treatment of the phonons using DYson Equation coupled to an Ohmic Bath seems to exhibit to reasonable degrees of accuracy the expectation from such a system coupled to an infinte bath.

In coming days we used to couple this with the Fermionic system where we treat the Fermionic evolution in a quassi-static way and delve into the dynamics of the complete systems.

We are in particular interested in Phonon equilibration because often the measurement in Condensed Matter Experiments are done on the phonons.

Even for finite size and input energy density in experiments like pump-probe usually the involved change in energy and temperature change is very small. The phonon specific heat which varies as T^3 so it gives a very sensitive measurement, as it changes very fast with the temperature.

In case the decay is a power law, that brings in a lot of fundamental changes in the way we see these experiments. The final measure of the system is often the specific heat, in simply in a calorimeter. Existance of a temperature as well as a linear response assumes instantaneous thermalisation which in turn assumes exponential decays.

More importantly the T^3 from the phonons comes from very low momentum modes. Now those one would expect to be very hard to thermalise, due to phase space criterion. One might end up in situations the high energy modes thermalise but the lower ones still exhibit prevalent non-equilibrium features. The boiling question this becomes whether it is possible to recover the behaviour of T^3 heat capacity. These properties can be investigated in a detector specific way.

Analouges of this problem arise owing to the non-thermal behavior of phonons and their mediation in electron equilibriation in Pump-Probe type experiments and can potentially pave routes to unexplored physics.

Enabled with the self consistent framework, we wish to explore at least some of these in the times to come.

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