CHAPTER 1

Review of Greens Functions

1.1 Introduction

The technique of Green’s function is one of the most useful and important tool in the study of various properties of many-body systems. The main advantage of this technique of Green’s function is that it can be calculated easily knowing the Hamiltonian of the system under consideration compared to the direct numerical solution of the Schrodinger equation. It allows one to rigorously formulate the problems and helps one to derive the results exactly which are true generally and which are true only, say, within the framework of perturbation theory. Also, it enables a smooth, easy and convenient transition from zero-temperature case, at which case the calculations are similar to those of Quantum Field Theory, to non-zero temperature case.

We shall use this technique to calculate the relaxation rate of phonons in thermal excitation and then determine the thermal transport coefficient i.e., the thermal conductivity. The Green’s function provides some of the most important physical information such as the ground-state energy and other ther-
modynamic functions, the energy and lifetime of excited states and the linear response to external perturbations [1]. Green’s function is also a convenient means for studying the transport coefficients without explicitly having recourse to setting up transport equations [2]. Since the pioneering technique on Green’s function developed by Matsubara [3], the method has been extensively used in statistical physics [1,2,4], condensed matter physics [5–8], nuclear physics [9,10] and quantum chromodynamics [11]. This technique has also been applied to the study of many physical properties of low-dimensional systems such as carbon nanotubes [12, 13] and graphene [14–17]. We shall briefly describe some of the important properties and discuss how to apply this technique to our problem in this introductory chapter.

1.2 Types of Greens function

The Green’s function used here is the double-time Green’s function applied in condensed matter and statistical mechanics which depend on two operators \( A(t) \) and \( B(t') \) at different times \( t \) and \( t' \) respectively. The basic difference between this Green’s function and the Quantum field theoretical Green’s function is that in the Quantum Field Theory, the average is taken over the lowest vacuum state or the ground state whereas the Green’s function used here is averaged over the grand canonical ensemble [2]. The double-time Green’s function are mainly of four types given below [2,6].

1) The retarded Green’s function defined as

\[
G_R(t, t') = -i\langle[A(t), B(t')]\rangle_\eta \theta(t - t').
\]  

(1.1)

This Green’s function arise from the linear response of a system to external perturbation.
2) The advanced Green’s function defined as

\[ G_A(t, t') = i \langle [A(t), B(t')]_\eta \rangle \theta(t' - t). \]  \hspace{1cm} (1.2)

This advanced Green’s function is the Hermitian conjugate of the retarded Green’s function.

3) The causal Green’s function defined as

\[ G_C(t, t') = -i \langle T_d A(t) B(t') \rangle. \]  \hspace{1cm} (1.3)

This Green’s function is useful for computation of system at absolute zero temperatures [6] and since we will be dealing with systems at finite temperatures, we shall not concentrate on this Green’s function.

Lastly,

4) The thermodynamic Green’s function defined as

\[ G_T(\tau, \tau') = \langle T_d A(\tau) B(\tau') \rangle \]  \hspace{1cm} (1.4)

where \( \tau = it/\hbar \). This Green’s function is found to be most useful for dealing with the properties of systems at finite temperature [6].

The bracket \( \langle \rangle \) in the above equations denotes the average over the grand canonical ensemble i.e., for any operator \( \rho \)

\[ \langle \rho \rangle = \frac{1}{Z} Tr(e^{-\beta(H-\mu N)})\rho \]  \hspace{1cm} (1.5)

where \( Z \) is the partition function for the grand canonical ensemble such that 
\[ Z = Tr(e^{-\beta(H-\mu N)}) \], \( Tr \) denotes the trace of the expression, \( H \) is the Hamiltonian of the system, \( \beta = 1/k_B T \) (\( k_B \) being the Boltzmann constant and \( T \) is the
CHAPTER 1: REVIEW OF GREENS FUNCTIONS

absolute temperature), $\mu^1$ is the chemical potential and $N$ is the number of particles in the system.

The bracket $[ \ ]_\eta$ in equations (1.1) and (1.2) implies that

$$[A(t), B(t')]_\eta = A(t), B(t') + \eta B(t') A(t)$$

where $\eta$ is taken to be +1 or -1 according as the operators A and B are fermi operators or bose operators respectively.

The symbol $T_d$ in equations (1.3) and (1.4) is the time ordering operator defined as

$$\langle T_d A(t) B(t') \rangle = \langle A(t) B(t') \rangle \theta(t - t') + \eta \langle B(t') A(t) \rangle \theta(t' - t)$$

(1.6)

where $\theta(t)$ is the Heaviside step function defined by

$$\theta(t) = \begin{cases} 1, & t > 0 \\ 0, & t < 0. \end{cases}$$

(1.7)

In fact, all the Green’s function are related and in our work we will be finding the thermal response of a system from the thermodynamic Green’s function. So, we will consider the relationship between the retarded and thermodynamic Green’s function in the succeeding sections which is helpful in finding the response to external perturbation. Let us first discuss the important properties of the thermodynamic Green’s function.

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1For bosons $\mu = 0$ and since we will be dealing with study of thermal transport by phonons, we shall assume that $\mu = 0.$
1.3 Thermodynamic Green’s function

The thermodynamic Green’s function is also called the Matsubara Green’s function or the imaginary time Green’s function. From the definition of the thermodynamic Green’s function given by equation (1.4), we can establish its three important properties [18]. Firstly, it is a function of time difference only, i.e., \( G(\tau, \tau') = G(\tau - \tau') \) which can be easily verified by expanding the operators in Heisenberg representation and using the cyclic property of trace (i.e., \( Tr(ABC) = Tr(BCA) = Tr(CAB) \)) as shown below:

\[
G(\tau, \tau') = \frac{1}{Z} Tr\{e^{(-\beta + \tau)H}A(0)e^{-\tau H}e^{\tau' H}B(0)e^{-\tau' H}\}
\]

\[
= \frac{1}{Z} Tr\{e^{-\beta H}e^{(\tau - \tau')H}A(0)e^{-(\tau - \tau')H}B(0)\}
\]

\[
= G(\tau - \tau') \tag{1.8}
\]

Secondly, it converges only if \(-\beta < (\tau - \tau') < \beta\) for \(\tau > \tau'\) and \(-\beta < (\tau' - \tau) < \beta\) for \(\tau' > \tau\). And, thirdly, using the cyclic property of trace, we can show that

\[
G(\tau + \beta) = \eta G(\tau), \quad \text{for } -\beta < \tau < 0. \tag{1.9}
\]

Thus, the Green’s function \(G(\tau)\) can be expanded as a Fourier series with periodicity \(\beta\) in the interval \(-\beta < \tau < 0\) as

\[
G(\tau) = \sum_{l=-\infty}^{+\infty} G(i\omega_l)e^{2\pi il\tau\beta} \tag{1.10}
\]
with the Fourier coefficients $G(i\omega_l)$ given by

$$G(i\omega_l) = \frac{1}{2\beta} \int_{-\beta}^{+\beta} G(\tau)e^{-i\omega_l\tau} d\tau$$  \hspace{1cm} (1.11)

where $l$ is an integer and

$$\omega_l = \begin{cases} 2l\pi/\beta\hbar, & \text{for bosons} \\ (2l+1)\pi/\beta\hbar, & \text{for fermions} \end{cases}$$  \hspace{1cm} (1.12)

### 1.4 Connection between Retarded and Thermodynamic Green’s Functions

The physical quantities or the response of a system to any external disturbance can be expressed in terms of correlation functions of some operators appropriate to the problem. This correlation function is evaluated in terms of the retarded Green’s function or the thermodynamic Green’s function. Thus, with the knowledge of Green’s function we can determine the response of external stimuli such as the thermal transport coefficient (i.e., thermal conductivity) in response to the thermal disturbance. To find the relationship between the retarded and thermodynamic Green’s function let us first consider the spectral representation of the two Green’s function following Zubarev [2]. From equation (1.1), we have

$$G_R(t, t') = -i\mathcal{F}_{AB}(t, t')\theta(t - t') + i\mathcal{F}_{BA}(t, t')\theta(t - t')$$  \hspace{1cm} (1.13)

where

$$\mathcal{F}_{AB}(t, t') = \langle A(t)B(t') \rangle$$  \hspace{1cm} (1.14)
are the time correlation functions. These time correlation functions depend on time only through \((t - t')\) (which can be shown by expanding the operators in Heisenberg representation and using the cyclic property of trace). This means that the retarded Green’s function \(G_R(t, t')\) does not depend explicitly on time but only through \((t - t')\). This result also holds good for the thermodynamic Green’s function.

Let us now define a function \(J(\omega)\) known as spectral density function as

\[
J(\omega) = \frac{1}{Z} \sum_{\nu \nu'} e^{-\beta E_\nu} \langle \nu | A(0) | \nu' \rangle \langle \nu' | B(0) | \nu \rangle \delta( E_\nu - E_{\nu'} - \hbar \omega) \tag{1.16}
\]

where \(|\nu\rangle\) and \(E_\nu\) are the eigenstates and the corresponding energies of the Hamiltonian, \(H\). Then, the two correlation functions can be written in terms of this spectral density function as

\[
F_{BA}(t) = \int_{-\infty}^{+\infty} J(\omega) e^{i \omega t} d\omega \tag{1.17}
\]

and

\[
F_{BA}(t) = \int_{-\infty}^{+\infty} J(\omega) e^{\beta \hbar \omega + i \omega t} d\omega. \tag{1.18}
\]

Now, the Fourier transform of the retarded Green’s function \(G_R(t)\) is given by

\[
G_R(\sigma) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\sigma t} G_R(t) dt
= -\frac{i}{2\pi} \int_{-\infty}^{+\infty} e^{-i\sigma t} [F_{AB}(t) - F_{BA}(t)] \theta(t) dt
= -\frac{i}{2\pi} \int_{-\infty}^{+\infty} d\omega (1 - e^{\beta \hbar \omega}) J(\omega) \int_{-\infty}^{+\infty} dte^{i(\omega - \sigma)t} \theta(t). \tag{1.19}
\]
We can write the Heaviside step function $\theta(t)$ in the integral form as

$$
\theta(t) = \frac{i}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{-ixt}}{x + ie} dx.
$$

(1.20)

The integral in equation (1.20) has a pole at $x = -ie$ which lies in the lower half of the complex-plane. Using contour integration, it can be verified that this integral is equal to unity and closed in the lower half-plane for $t > 0$ while it vanishes for $t < 0$. Thus, the retarded Green’s function is analytic in the lower half-plane due to the presence of the $\theta$-function.

Now in equation (1.19), the integral

$$
\int_{-\infty}^{+\infty} dt e^{i(\omega - \sigma)t} \theta(t) = \frac{i}{2\pi} \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dt \frac{e^{i(\omega - \sigma - x)t}}{x + ie}
$$

$$
= i \int_{-\infty}^{+\infty} dx \frac{\delta(x + \sigma - \omega)}{x + ie} \left[ \text{since } \delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ixt} dt \right]
$$

$$
= \frac{i}{-\sigma + \omega + ie}
$$

(1.21)

Then, using equation (1.21) in equation (1.19), we have

$$
G_R(\sigma) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} (e^{i\beta\omega} - 1) J(\omega) \frac{d\omega}{\sigma - \omega - ie}.
$$

(1.22)

Now, the thermodynamic Green’s function equation (1.11) can be written as

$$
G(i\omega) = \frac{1}{2\beta} \int_{-\beta}^{0} G(\tau < 0) e^{-i\omega\tau} d\tau + \frac{1}{2\beta} \int_{0}^{\beta} G(\tau > 0) e^{-i\omega\tau} d\tau
$$

$$
= \frac{1}{2\beta} \int_{-\beta}^{0} \int_{-\infty}^{+\infty} \theta(-t) J(\omega) e^{i\omega t - i\omega\tau + \beta\omega} d\tau d\omega
$$

$$
+ \frac{1}{2\beta} \int_{-\beta}^{0} \int_{-\infty}^{+\infty} \theta(t) J(\omega) e^{i\omega t - i\omega\tau} d\tau d\omega
$$

(1.23)
The integral representation of $\theta(-t)$ is given by

$$\theta(-t) = \frac{i}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{-ixt}}{x - ie} dx$$  \hspace{1cm} (1.24)$$

Using equations (1.20) and (1.24), we obtain from equation (1.23)

$$G(i\omega) = \frac{i}{4\pi\beta} \int_{-\beta}^{0} \int_{-\infty}^{+\infty} \left[ \int_{-\infty}^{+\infty} \frac{e^{i(\omega-x)t}}{x - ie} dx \right] e^{-ih\omega_\tau + \beta h \omega} J(\omega) d\tau d\omega$$

$$+ \frac{i}{4\pi\beta} \int_{0}^{\beta} \int_{-\infty}^{+\infty} \left[ \int_{-\infty}^{+\infty} \frac{e^{i(\omega-x)t}}{x + ie} dx \right] e^{-ih\omega_\tau} J(\omega) d\tau d\omega$$

$$= \frac{1}{2\beta} \int_{-\beta}^{0} \int_{-\infty}^{+\infty} e^{i(\omega-ie)t} e^{-ih\omega_\tau + \beta h \omega} J(\omega) d\tau d\omega$$

$$- \frac{1}{2\beta} \int_{0}^{\beta} \int_{-\infty}^{+\infty} e^{i(\omega+ie)t} e^{-ih\omega_\tau} J(\omega) d\tau d\omega$$  \hspace{1cm} (1.25)$$

Putting $t = -i\hbar \tau$ in the above equation, we have

$$G(i\omega) = -\frac{1}{2\beta} \int_{-\infty}^{+\infty} d\omega J(\omega) e^{\beta h \omega} \left[ \int_{-\beta}^{0} e^{i(h(\omega-\omega_\tau+i\omega_\tau))} d\tau \right]$$

$$- \frac{1}{2\beta} \int_{-\infty}^{+\infty} d\omega J(\omega) \left[ \int_{0}^{\beta} e^{i(h(\omega+\omega_\tau-i\omega_\tau))} d\tau \right]$$

$$= -\frac{1}{2\beta h} \int_{-\infty}^{+\infty} d\omega J(\omega) e^{\beta h \omega} \frac{1 - e^{-\beta h \omega}}{\omega - ie - i\omega_\tau}$$

$$- \frac{1}{2\beta h} \int_{-\infty}^{+\infty} d\omega J(\omega) \frac{e^{\beta h \omega} - 1}{\omega + ie - i\omega_\tau}$$

$$= -\frac{1}{\beta h} \int_{-\infty}^{+\infty} d\omega J(\omega) \frac{e^{\beta h \omega} - 1}{\omega - i\omega_\tau}$$  \hspace{1cm} (1.26)$$

where we have neglected the $ie$ term in the above equation as $e$ is a positive
infinitesimal quantity. Comparing equations (1.22) and (1.26), we have

\[ G_R(\sigma) = \frac{\beta \hbar}{2\pi} G(i\omega_l) \]  

only if \( i\omega_l = \sigma - i\epsilon \) is satisfied, where \( \epsilon \) is a positive infinitesimal number.

Here, \( G(i\omega_l) \) is a function of discrete variable \( i\omega_l \) (as defined by equation (1.12)) whereas \( G_R(\sigma) \) is a function of continuous variable \( \sigma \). The function \( G_R(\sigma) \) is analytic in the lower half of the \( \sigma \)-plane and equation (1.27) suggest that the two Green’s function are identical at the infinite set of points for which the thermodynamic green’s function is defined. Thus, the function \( G_{i\omega_l} \) can be analytically continued into the whole of the \( \sigma \)-plane by simply replacing the discrete variable \( i\omega_l \) by the continuous variable \( \sigma - i\epsilon \). Hence, we can obtain the retarded Green’s function from the thermodynamic Green’s function by analytic continuation using relation (1.27). Thus, the response of a system to external disturbance can be expressed in terms of the thermodynamic Green’s function, or rather its Fourier transform. This Fourier transform can then be evaluated using the Wicks theorem and the powerful Feynman diagram technique. For this, we have to establish a new kind of Perturbation expansion for the Green’s function which is discussed in the next section.

### 1.5 Perturbation expansion of Thermodynamic Green’s function

Green’s function can be obtained from the equation of motion [2–4, 19] or from the straightforward use of the perturbation technique [1, 5, 7]. We are using in this thesis the perturbation technique along with the powerful diagrammatic
Chapter 1: Review of Greens Functions

technique. We consider a system which is described by a Hamiltonian $H$ given by

$$H = H_0 + H_A$$

where $H_0$ and $H_A$ are respectively the unperturbed Hamiltonian and the perturbed Hamiltonian of the system. We define an operator $S$ by using the relation

$$S(\beta_1, \beta_2) = e^{H_0 \beta_1} e^{-H(\beta_1 - \beta_2)} e^{-H_0 \beta_2}$$

We observe that this operator $S(\beta_1, \beta_2)$ is not unitary but it satisfies the group property

$$S(\beta_1, \beta_2) S(\beta_2, \beta_3) = S(\beta_1, \beta_3)$$

and the boundary condition

$$S(\beta_1, \beta_1) = 1.$$ 

Now,

$$\frac{\partial}{\partial \beta} S(\beta, \beta') = \frac{\partial}{\partial \beta} \left[ e^{H_0 \beta} e^{-H(\beta - \beta')} e^{-H_0 \beta'} \right]$$

$$= e^{H_0 \beta} \left[ H_0 - H \right] e^{-H(\beta - \beta')} e^{-H_0 \beta'}$$

$$= -e^{H_0 \beta} H_A e^{-H_0 \beta} e^{H_0 \beta} e^{-H(\beta - \beta')} e^{-H_0 \beta'}$$

$$= -\tilde{H}_A(\beta) S(\beta, \beta')$$

where

$$\tilde{H}_A(\beta) = e^{H_0 \beta} H_A e^{-H_0 \beta}$$

11
is an operator in the interaction representation.

Now, integrating equation (1.32) from $\beta_0$ to $\beta$, we obtain

$$S(\beta, \beta_0) - S(\beta_0, \beta_0) = -\int_{\beta_0}^{\beta} \tilde{H}_A(\beta') S(\beta', \beta_0) d\beta'$$

$$\Rightarrow S(\beta, \beta_0) = 1 - \int_{\beta_0}^{\beta} \tilde{H}_A(\beta') S(\beta', \beta_0) d\beta'$$

(1.34)

Then, by iteration, we can write the above equation as

$$S(\beta, \beta_0) = 1 + (-1)^1 \int_{\beta_0}^{\beta} \tilde{H}_A(\beta') d\beta' + (-1)^2 \int_{\beta_0}^{\beta} d\beta' \int_{\beta_0}^{\beta'} d\beta'' \tilde{H}_A(\beta') \tilde{H}_A(\beta'')$$

$$+ \cdots$$

(1.35)

Now, let us consider the third term in the above expansion (1.35). It may be rewritten as

$$\int_{\beta_0}^{\beta} d\beta' \int_{\beta_0}^{\beta'} d\beta'' \tilde{H}_A(\beta') \tilde{H}_A(\beta'') = \frac{1}{2} \int_{\beta_0}^{\beta} d\beta' \int_{\beta_0}^{\beta'} d\beta'' \tilde{H}_A(\beta') \tilde{H}_A(\beta'')$$

$$+ \frac{1}{2} \int_{\beta_0}^{\beta} d\beta'' \int_{\beta_0}^{\beta} d\beta' \tilde{H}_A(\beta') \tilde{H}_A(\beta'')$$

(1.36)

The last term in the above equation is obtained by reversing the order of integration. That is, we can write
where the step function \( \theta(\beta) \) is introduced because the operators \( H_A \) do not commute at different times (i.e., at different values of \( \beta \)). Then, we can introduce the time-ordering operator and rewrite equation (1.37) in a more compact form as

\[
\int_{\beta_0}^{\beta} d\beta' \int_{\beta_0}^{\beta''} d\beta'' H_A(\beta') H_A(\beta'') = \frac{1}{2} \int_{\beta_0}^{\beta} d\beta' \int_{\beta_0}^{\beta''} d\beta'' [\tilde{H}_A(\beta') \tilde{H}_A(\beta'') \theta(\beta' - \beta'')] + \tilde{H}_A(\beta'') H_A(\beta') \theta(\beta'' - \beta').
\] (1.37)

Thus, we can readily generalize this result and put the expansion of \( S \) finally as

\[
S(\beta, \beta_0) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{\beta_0}^{\beta} d\beta_1 \ldots \int_{\beta_0}^{\beta} d\beta_n \mathcal{T}_d [\tilde{H}_A(\beta_1) \ldots \tilde{H}_A(\beta_n)].
\] (1.39)

Thus, equation (1.39) give an iterated series. Putting \( \beta_0 = 0 \) in equation (1.39), we have

\[
S(\beta) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{0}^{\beta} d\beta_1 \ldots \int_{0}^{\beta} d\beta_n \mathcal{T}_d [\tilde{H}_A(\beta_1) \ldots \tilde{H}_A(\beta_n)].
\] (1.40)

Now, the thermodynamic Green’s function can be written as

\[
G_T(\tau) = \langle \mathcal{T}_d A(\tau) B^\dagger(0) \rangle
\]

\[
= \frac{1}{Z} Tr[e^{-\beta H} e^{\tau H} A(0) e^{-\tau H} B^\dagger(0)]
\]

\[
= \frac{Tr[e^{-\beta H_0} S(\beta) S^\dagger(\tau) A(\tau) S(\tau) B^\dagger(0)]}{Tr[e^{-\beta H_0} e^{\beta H_0} e^{-\beta H}]}.
\]
\[ \begin{align*}
\langle T_d S(\beta) \tilde{A}(\tau) \tilde{B}^\dagger(0) \rangle_o &= \langle \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\beta_1 \ldots \int_0^\beta d\beta_n \tilde{H}_A(\beta_1) \ldots \tilde{H}_A(\beta_n) \rangle \\
\langle \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\beta_1 \ldots \int_0^\beta d\beta_n \ldots \langle T_d \tilde{H}_A(\beta_1) \ldots \tilde{H}_A(\beta_n) \rangle \rangle
\end{align*} \] (1.43)
entering the vertex corresponds to that of the creation operator and the line leaving the vertex corresponds to that of the annihilation operator. The number \( n \) gives the order of interaction. These diagrams can be connected or disconnected diagrams. A disconnected diagram is one which can be divided into two or more parts which are not connected either by one of the vertices or by a line (e.g. Figure 1.1 (a)) while a connected diagram is one which cannot be separated (e.g. Figure 1.1 (b)). All the disconnected diagrams can be discarded as the contribution from the denominator gives disconnected diagrams which cancel with the disconnected diagrams in the numerator and hence only the connected diagrams in the numerator are left. Thus, we can finally write the thermodynamic Green’s function as

\[
G_T(\tau) = \langle T_d \tilde{A}(\tau) \tilde{B}^\dagger(0) \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\beta_1 \ldots \int_0^\beta d\beta_n \tilde{H}_A(\beta_1) \ldots \tilde{H}_A(\beta_n) \rangle_c
\]

where the suffix \( c \) indicates that the average should be evaluated for the connected diagrams only. This equation (1.45) is called the Feynman-Dyson Perturbation expansion and is the basic equation for the diagrammatic analysis of the Green’s functions.
References


