I. QUANTUM FIELDS

Like a classical field, a quantum field is a continuous function of position. However, in the language of second quantisation it is a field *operator*. This implies that it is subject to quantum fluctuations and that it in general does not commute with other operators.

The “first quantisation"corresponds to the transformation

$$E \rightsquigarrow i\hbar\partial_t, \quad p \rightsquigarrow \hat{p} = -i\hbar\partial_t$$

Additionally the classical Poisson Bracket is replace by the commutator:

$$\{p_i, q_j\}_{\mathrm{PB}} = \delta_{ij} \rightsquigarrow [\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

The “second quantisation"is the next step we require to describe macroscopic systems, quasiparticles, dynamic response of quantum systems as well as collective behaviour and broken-symmetry phase transitions.

The classical Hamiltonian for a string is

$$H = \int \mathrm{d}x \left\{ \frac{T}{2}(\nabla_x\phi)^2 + \frac{1}{2\rho}\pi^2 \right\}$$

which we can quantise by enforcing the following commutator

$$[\phi(x), \pi(y)] = i\hbar\delta(x-y)$$

hence the procedure of second quantisation is quite similar to what we did during our initial quantum mechanics courses, however, the algebra that we will come to do is quite different. In many-body physics the relevant operator is the quantum field operator $\psi(x)$, the *annihilation* operator whose hermitian conjugate is the *creation* operator, $\psi^\dagger(x)$.

The Pauli exclusion principle, which only holds for fermions, can be boiled down to the simple difference in how these field operators commute for the two different particle types:

$$\begin{aligned} \left[\psi(x), \psi^\dagger(y)\right] &= \delta(x-y) \quad \text{Bosons} \\ \left\{\psi(x), \psi^\dagger(y)\right\} &= \delta(x-y) \quad \text{Fermions} \end{aligned}$$

The operators operate on a state within *Fock-Space*, which is the many-particle generalisation of Hilbert Space (it is a tensor product of Hilbert Spaces). The *Fock-Vacuum* is the state in which there are no particles, which is denoted $|0\rangle$. Upon this zero-particle state we can create particles and make many-particle states

$$|x_1, x_2, \ldots, x_N\rangle = \psi^\dagger(x_N)\ldots\psi^\dagger(x_1)\,|0\rangle$$

A. Collective Modes

Consider now a one-dimensional chain of particles, whose position is expressed by their equilibrium position plus some displacement $x_j = x_j^0 + \phi_j$. Let us now couple neighbouring sites by imposing the following Hamiltonian

$$\begin{aligned} \hat{H} &= \sum_j \left[\frac{\pi_j^2}{2m} + \frac{m\omega^2}{2}\left(\phi_j - \phi_{j+1}\right)^2 \right] \\ &= \sum_j \left[\frac{\pi_j^2}{2m} + \frac{m\omega^2}{2}\phi_j\left(2\phi_j - \phi_{j+1} - \phi_{j-1}\right) \right] \end{aligned}$$

where $[\phi_i, \pi_j] = \delta_{ij}$. The generator of the discrete translational symmetry (from one lattice point to another) is the crystal momentum, which hence commutes with the Hamiltonian. Translational symmetry always implies that we should Fourier transform, however, in the case of a discrete translational symmetry the Fourier transform becomes a Fourier series:

$$\begin{aligned} \phi_j &= \frac{1}{\sqrt{N}}\sum_q e^{iqR_j}\phi_q \\ \pi_j &= \frac{1}{\sqrt{N}}\sum_q e^{iqR_j}\pi_q \end{aligned}$$

where $R_j = ja$ is the site of the j^{th} vertex. By applying these Fourier series to the Hamiltonian we obtain

$$\begin{aligned} H &= \sum_q \left[\frac{1}{2m}\pi_q\pi_{-q} + \frac{m\omega_q^2}{2}\phi_q\phi_{-q} \right] \\ &\qquad\qquad \omega_q \equiv 4\omega^2\sin^2\left(\frac{qa}{2}\right) \end{aligned}$$

We can diagonalise this by means of a unitary transformation

$$\begin{pmatrix} \pi_q \\ \phi_q \end{pmatrix} = \begin{pmatrix} -i\sqrt{\frac{m\omega_q\hbar}{2}} & i\sqrt{\frac{m\omega_q\hbar}{2}} \\ \sqrt{\frac{\hbar}{2m\omega_q}} & \sqrt{\frac{\hbar}{2m\omega_q}} \end{pmatrix} \begin{pmatrix} a_q \\ a_q^\dagger \end{pmatrix}$$

from which we obtain

$$H = H_{\mathrm{CM}} + \sum_{q\neq 0}\hbar\omega_q\left(a_q^\dagger a_q + \frac{1}{2}\right)$$

where we have condensed the collective motion of the centre-of-mass into

$$H_{\mathrm{CM}} = \frac{1}{2m}\pi_0^2$$

Hence we see that the interaction between neighbouring atoms in a chain results in bosonic quasiparticles which are referred to as *phonons*.

B. Thermodynamic Limit

Generally it is quite useful to be able to convert sums into integrals and in some cases integrals into sums. An example of a case in which this is possible is if we are summing over the different momenta of phonons in a lattice; this is a *sum* because the momenta are discrete, however, in the thermodynamic limit the difference between adjacent momenta becomes smaller and smaller because $\Delta q = \frac{2\pi}{L}$ where L is the length of the chain (or volume in higher dimensions). The thermodynamic limit corresponds to letting $L \rightsquigarrow \infty$ which allows us to replace

$$\sum_{\boldsymbol{q}} [\cdots] \rightsquigarrow L \int_0^{\frac{2\pi}{a}} \frac{\mathrm{d}q}{2\pi} [\cdots]$$

In d-dimensions this would be

$$\sum_{\boldsymbol{q}} [\cdots] \rightsquigarrow L^d \int_0^{\frac{2\pi}{a}} \frac{\mathrm{d}^d\boldsymbol{q}}{(2\pi)^d} [\cdots]$$

An application hereof would be to calculate the zero-point energy of phonons in a three-dimensional harmonic crystal. Similarly to what we found in one-dimension the energy is

$$H = \sum_{\boldsymbol{q}} \hbar\omega_{\boldsymbol{q}} \left(\hat{n}_{\boldsymbol{q}} + \frac{1}{2} \right)$$

so the zero-point energy is

$$E_0 = \sum_{\boldsymbol{q}} \frac{\hbar\omega_{\boldsymbol{q}}}{2} \xrightarrow{\text{Thermodynamic Limit}} L^3 \int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^3} \frac{\hbar\omega_{\boldsymbol{q}}}{2}$$

Solving this expression after substituting in for $\omega_{\boldsymbol{q}}$ we get

$$E_0 \approx N\hbar\omega_0 \times 1.19$$

so the zero-point energy per unit cell is a finite number, but a macroscopic number for the entire material.

C. The Continuum Limit

By letting the lattice spacing go towards zero $a \to 0$ we increase the size of the Brillouin zone to infinity and we would treat q as a continuous variable. However, this limit brings with it a divergence; the zero point energy scales with length in one-dimension

$$E_0 = \frac{L\hbar c}{2\pi\varepsilon^2}$$

II. CONSERVED PARTICLES

A general second quantised many-body Hamiltonian can be written as

$$H = \int \mathrm{d}^3x \left[\psi^\dagger(x) \left(-\frac{\hbar^2}{2m}\mathcal{L}\{+\}\, U(x) \right) \psi(x) + \frac{1}{2} \int \mathrm{d}^3x'\; V(x-x') \,{:}\rho(x)\rho(x'){:} \right]$$

where we have introduced the *normal ordering operator*, which takes an expression and tells you that you need to convert it into a form where the annihilation operators are on the right, and the creation operators are on the left. For instance

$${:}\psi(x)\psi(y)^\dagger{:} \; = \zeta\psi(y)^\dagger\psi(x)$$

where ζ is one for bosons and minus one for fermions.

A. Coleman's Notation

Henceforth Coleman uses a notation that needs some getting used to, but it simplifies expressions significantly and is quite well defined. Let $1 = (\boldsymbol{x}_1, \boldsymbol{k}_1, t_1, \sigma_1)$ i.e all relevant numbers that we would index with a 1. This allows us to write

$$[\psi(1), \psi(2)]_\pm = [\psi^\dagger(1), \psi^\dagger(2)]_\pm = 0$$
$$[\psi(1), \psi^\dagger(2)]_\pm = \delta(1-2)$$

where $[\cdot\,,\cdot]_\pm$ is the anti-commutator for bosons $(+)$ and the commutator for fermions $(-)$.

B. Field Operators in Different Bases

Suppose we have two bases $\{|r\rangle\}$ and $\{|\tilde{s}\rangle\}$. The (unitary) transformation that takes us from one basis to the other:

$$|\tilde{s}\rangle = \sum_r \langle r|\tilde{s}\rangle\, |r\rangle$$

tells us about the transformation between field operators:

$$a_{\tilde{s}} = \langle \tilde{s}|\psi\rangle = \sum_r \langle \tilde{s}|r\rangle \underbrace{\langle r|\psi\rangle}_{\psi_r}$$

This also works for continuous bases, such as the position and momentum bases:

$$\psi(x) = \int \mathrm{d}q\;\; \langle x|q\rangle\, c_q = \frac{1}{\sqrt{L}} \int \mathrm{d}q\; e^{-iqx} c_q$$

where $\langle x|q\rangle$ is normalised with $L^{-\frac{1}{2}}$ in one dimension. All observables are hermitian operators, which implies there exists a basis in which they are diagonal, thus for example Hamiltonian operators can always be diagonalised;

$$H = \sum_{\ell} \varepsilon_\ell \, \psi_\ell^\dagger \psi_\ell$$

we will quite often see that this diagonal basis is the momentum basis; in cases where the Hamiltonian is translationally invariant, however, this is not always the case and sometimes it is quite difficult to find the basis in which a Hamiltonian (or any operator) is diagonal.

1. *Bogoliubov Transformation*

Suppose we have **bosonic** operators a and $a^\dagger$, such that $[a, a^\dagger] = 1$, if we change basis

$$b = ua + va^\dagger$$

for $u, v \in \mathbb{C}$, it must be the case that

$$[b, b^\dagger] = \left(|u|^2 - |v|^2\right)[a, a^\dagger] = 1$$

hence that $|u|^2 - |v|^2 = 1$, this is satisfied by

$$\begin{aligned} u &= e^{i\theta_1}\cosh\beta \\ v &= e^{i\theta_2}\sinh\beta \end{aligned}$$

where θ_1 and θ_2 are free variables.

Similarly for **fermionic** operators, where we have $\{a, a^\dagger\} = 1$, we require that

$$|u|^2 + |v|^2 = 1$$

which is satisfied for

$$\begin{aligned} u &= e^{i\theta_1}\cos\phi \\ v &= e^{i\theta_2}\sin\phi \end{aligned}$$

again with θ_1 and θ_2 as free variables.

C. Field Operators as Creation and Annihilation Operators

We previously discussed the Fock Space, and that creation and annihilation operators can take us from one state in Fock Space to another, this is naturally true in all bases, which means we should denote the Fock State slightly differently from what we did previously. The only relevant quantity is the number of fermions or bosons in each state:

$$\begin{aligned} |n_1, n_2, \ldots, n_\ell, \ldots\rangle &= \prod_\ell \frac{(\psi_\ell^\dagger)^{n_\ell}}{\sqrt{n_\ell!}}\,|0\rangle\,, \quad \text{bosons} \\ |n_1, n_2, \ldots, n_r\rangle &= (\psi_r^\dagger)^{n_r}\cdots(\psi_1^\dagger)^{n_r}\,|0\rangle\,, \quad \text{fermions} \end{aligned}$$

for bosons the numbers n_ℓ are non-negative integers, however, for fermions the Pauli exclusion principle prevents there from being more than one fermion in the same quantum state, which implies that the fermionic occupation numbers can only be $n_r \in \{0, 1\}$.

The wave function of the N-particle state $\Psi_S(t)$ is the overlap with:

$$\begin{aligned} \Psi_S(x_1, x_2, \ldots, x_N, t) &= \langle x_1, x_2, \ldots, x_N|\Psi_S(t)\rangle \\ &= \langle 0|\psi(x_1)\psi(x_2)\cdots\psi(x_N)|\Psi_S(t)\rangle \end{aligned}$$

note that the statistics is already encoded into this wavefunction due to the fact that we enforced the (anti-)commutation relations for the field operators. This means we never need to think about Slater-determinants again.

D. Interactions

Classically the interaction potential of a continuous plasma of particles is given by

$$V = \frac{1}{2}\int \mathrm{d}^3x\mathrm{d}^3x'\; V(x - x')\rho(x)\rho(x')$$

however if we were to just put hats on the densities, then one-particle states would interact with themselves. Thus, the correct form of the second quantised interaction is the above form minus the self interactions:

$$\begin{aligned} \hat{V} &= \frac{1}{2}\int \mathrm{d}^3x\mathrm{d}^3x'\; V(x - x')\hat{\rho}(x)\hat{\rho}(x') - \frac{1}{2}\int \mathrm{d}^3x\; V(0)\hat{\rho}(x) \\ &= \frac{1}{2}\int \mathrm{d}^3x\mathrm{d}^3x'\; V(x - x')\,\vdots\hat{\rho}(x)\hat{\rho}(x')\vdots \end{aligned}$$

It is worth mentioning that

$$\hat{V}\,|x_1, x_2, \ldots, x_N\rangle = \sum_{i<j} V(x_i - x_j)\,|x_1, x_2, \ldots, x_N\rangle$$

so the state $|x_1, x_2, \ldots, x_N\rangle$ is an eigenstate of the second quantised interaction potential, with eigenvalues of the classical interaction. Writing this in the momentum basis gives us quite a bit more insight. That is, we would like to Fourier transform

$$\hat{V} = \frac{1}{2}\int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}' V(\boldsymbol{x}-\boldsymbol{x}')\hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}^\dagger(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x})$$

Using that

$$\boxed{\psi_\sigma(\boldsymbol{x}) = \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}\ c_{\boldsymbol{k}\sigma}e^{i\boldsymbol{k}\cdot\boldsymbol{x}}}$$

And Fourier transforming the potential, $V(\boldsymbol{x}-\boldsymbol{x}') = \int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^3}V(\boldsymbol{q})e^{i\boldsymbol{q}\cdot(\boldsymbol{x}-\boldsymbol{x}')}$, we obtain

$$\hat{V} = \frac{1}{2}\underbrace{\int \frac{\mathrm{d}^3\boldsymbol{k}_1}{(2\pi)^3}\frac{\mathrm{d}^3\boldsymbol{k}_2}{(2\pi)^3}\frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^3}}_{\int_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{q}}} V(\boldsymbol{q})c^\dagger_{\boldsymbol{k}_1+\boldsymbol{q}}c^\dagger_{\boldsymbol{k}_2-\boldsymbol{q}}c_{\boldsymbol{k}_2}c_{\boldsymbol{k}_1}$$

however, if we would include the possibility that the two interacting particles have different spin this would become

$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma'}\int_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{q}} V(\boldsymbol{q})c^\dagger_{\boldsymbol{k}_1+\boldsymbol{q},\sigma}c^\dagger_{\boldsymbol{k}_2-\boldsymbol{q},\sigma'}c_{\boldsymbol{k}_2,\sigma'}c_{\boldsymbol{k}_1,\sigma}$$

Thus this is a process where we begin with two particles; with momentum $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ respectively, that are scattered by the potential to particles with momentum $\boldsymbol{k}_1+\boldsymbol{q}$ and $\boldsymbol{k}_2-\boldsymbol{q}$ respectively. We can represent this interaction with the following Feynman Diagram:

Figur 1: *Feynman Diagram for a simple scattering process*

3.8: Identical conserved particles in thermal equilibrium – maybe put that

III. SIMPLE EXAMPLE OF SECOND QUANTISATION

A. Jordan-Wigner Transformation

Let us now consider a spin-$\frac{1}{2}$ system, which will soon become a system containing many spin-$\frac{1}{2}$ particles. If we think of the spin-down state as $|0\rangle$ and the spin-up state as $|1\rangle$ then we can construct raising and lowering operators that take us from one to the other

$$|0\rangle = f\,|1\rangle\,, \qquad |1\rangle = f^\dagger\,|0\rangle$$

Using this we can construct one-particle spin operators

$$S_x = \frac{1}{2}(f^\dagger + f)$$
$$S_y = \frac{1}{2i}(f^\dagger - f)$$

these are just the spin-raising and lowering operators we know from other Quantum Mechanics courses. However, an issue arises when we want to look at multi-particle states; in these the fermionic operators from different Hilbert spaces *anti*-commute, whereas the spin operators commute. The solution to this is described by the Jordan-Wigner transformation where we add an additional phase operator:

$$S^z_j = f^\dagger_j f_j - \frac{1}{2}$$
$$S^+_j = f^\dagger_j e^{i\pi\hat{\phi}_n}$$
$$S^-_j = f_j e^{-i\pi\hat{\phi}_n}$$

where

$$\hat{\phi}_n \equiv \sum_{\ell<j}\hat{n}_\ell$$

Some useful identities here are that

$$\begin{aligned}
\left\{f_j, e^{i\pi\hat{n}_j}\right\} &= 0, && f_j e^{i\pi\hat{n}_j} = -f_j \\
\left\{e^{i\hat{\phi}_j}, f^{(\dagger)}_\ell\right\} &= 0, && \text{for } l<j \\
\left[e^{i\hat{\phi}_j}, f^{(\dagger)}_\ell\right] &= 0, && \text{for } l\geq j
\end{aligned}$$

where $f^{(\dagger)}_\ell$ means the identity works both for the raising and lowering operators. This transformation allows us to write magnetic Hamiltonians in forms that make them far easier to read. For instance the one-dimensional Heisenberg model,

$$H = -J\sum\left(S^x_jS^x_{j+1} + S^y_jS^y_{j+1}\right) - J_z\sum S^z_jS^z_{j+1}$$

can be written as

$$H = \sum_k \omega_k s^\dagger_k s_k - J_z\sum_j n_j n_{j+1}$$

where also have Fourier transformed and defined

$$\omega_k = J_z - J\cos ka$$

B. Hubbard Model

The nearest-neighbour Hubbard model describes localised electrons on a lattice, that can hop from one site to one of its neighbouring sites. By beginning with the real-space Hamiltonian that describes this, together with electron-electron interactions and Fourier transforming we obtained the Hubbard model Hamiltonian

$$H = \sum_{\boldsymbol{k}\sigma} \varepsilon_{\boldsymbol{k}}$$

where

$$\varepsilon_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y + \cos k_z) + \varepsilon$$

and t is the hopping constant and ε is the energy associated with being on one of the sites. Additionally U is the electron-electron interaction energy at the same site (hence the requirement for the spins to be opposite).

C. Fluid of non-interacting fermions, thermal equilibrium

The thermodynamics of a fluid of fermions is described by Fermi-liquid-theory, which for instance can be used to describe metals.

The free energy is a central quantity as we can use it to calculate different (measurable) quantities, such as entropy, pressure and density. For a single particle the free energy is described by the *single-free-energy-functional*

$$F = -2k_BTV \int_{\boldsymbol{k}} \ln\left[1 + \exp\left(-\beta(E_{\boldsymbol{k}} - \mu)\right)\right]$$

In thermal equilibrium the number of fermions in a state with momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$ is given by the Fermi-Dirac distribution

$$n_{\boldsymbol{k}} = f_{\mathrm{FD}}(E_{\boldsymbol{k}} - \mu), \qquad f_{\mathrm{FD}}(x) = \frac{1}{e^{\beta x} + 1}$$

the low-temperature limit of the Fermi-Dirac distribution is a Heaviside $\Theta(\mu - E_{\boldsymbol{k}})$. In this limit the ground state is the state where all electrons are below the Fermi-level ($\varepsilon_F = \lim_{T\to 0}\mu(T) = \frac{\hbar k_F^2}{2m}$):

$$|\psi_G\rangle = \prod_{|\boldsymbol{k}|<k_F,\sigma} c^\dagger_{\boldsymbol{k}\sigma}\,|0\rangle$$

The ground state density of a Fermi gas is given by the number of occupied states divided by the volume of the Fermi-surface:

$$\langle\rho\rangle = \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}\sigma}\langle c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}\rangle = 2\int_{|\boldsymbol{k}|<k_F}\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3} = \frac{2}{(2\pi)^3}V_{\mathrm{FS}}$$

where

$$V_{\mathrm{FS}} = \frac{4\pi k_F^3}{3} = \left(\frac{4\pi}{3}\right)\left(\frac{3m\varepsilon_F}{\hbar^2}\right)^{\frac{3}{2}}$$

hence

$$\langle\rho\rangle = \frac{1}{3\pi^2}\left(\frac{3m\varepsilon_F}{\hbar^2}\right)^{\frac{3}{2}}$$

Some other important quantities are

$$P = -\frac{\partial F}{\partial V} = -2k_BT\int_{\boldsymbol{k}}\ln\left[1 + \exp\left(-\beta(E_{\boldsymbol{k}} - \mu)\right)\right]$$

$$N = -\frac{\partial F}{\partial \mu} = 2\int_{\boldsymbol{k}} f(E_{\boldsymbol{k}} - \mu)$$

IV. GREEN'S FUNCTIONS

A. Interaction Picture

|X|c|c|

gr!50 Picture	States	Operators
gr!10 S	$i\partial_t\,|\psi_S\rangle = H\,|\psi_S\rangle$	Constant
gr!10 H	Constant	$-i\partial_t O_H = [H, O_H]$
gr!10 I	$i\partial_t\,|\psi_I\rangle = V_I\,|\psi_I\rangle$	$-i\partial_t O_I = [H_0, O_I]$

As shown in the table above, it is both operators and states that evolve in the interaction picture, however, the states evolve only according to the perturbation, V_I, whereas operators evolve according to the unperturbed Hamiltonian. Another way of seeing this is that we have moved all trivial time evolution on to the operators, such that we only need to worry about the potential's action on the state.

The time-evolution operator in the interaction picture is $U_I(t) = e^{iH_0t}e^{-iHt}$, which has the following action

$$|\psi_I(t)\rangle = U_I(t)\,|\psi_I(0)\rangle$$

more generally

$$|\psi_I(t)\rangle = S_I(t,t')\,|\psi_I(t')\rangle\,, \quad S_I(t,t') = U_I(t)U_I^\dagger(t')$$

The time-evolution operator $S_I(t,t')$ will be used shortly to generate free-single-particle Green's functions, so this operator will play a central role in this section. Note that because $i\partial_t U_I(t) = V_I(t)U_I(t)$ we have that

$$i\partial_{t_2}S_I(t_2,t_1) = V_I(t_2)S_I(t_2,t_1)$$

B. Time-ordering operator

The time-ordering operator, T, allows us to write time-evolution operators in a very compact way. The time-ordering operator takes a product of time-dependent operators and orders them such that *later times are to the right*, such that when the operators operate on a ket, they will operate chronologically:

$$T\left\{O_1(t_1)O_2(t_2)\cdots O_N(t_N)\right\} = \zeta^p O_{p_1}(t_{p_1})\cdots O_{p_N}(t_{p_N})$$

where again ζ is minus one for fermions and positive one for bosons and $t_{p_N} < t_{p_{N-1}} < \cdots < t_{p_1}$ and p is the parity of the permutation (whether it's an even or an odd permutation).

Using the time-ordering operator we can now express the time-evolution operator quite simply:

$$S_I(t_2,t_1) = T\left[\exp\left(-i\int_{t_1}^{t_2} \mathrm{d}t\; V_I(t)\right)\right]$$

C. Driven harmonic oscillator

Consider now a (bosonic) harmonic oscillator

$$H_0 = \omega\left(b^\dagger b + \frac{1}{2}\right)$$

to which we apply the following perturbation

$$V(t) = \bar{z}(t)b + b^\dagger z(t)$$

where $z, \bar{z} \in \mathbb{C}$ are independent complex functions of time. In the case that we apply a force $H = H_0 - f(t)\hat{x}$ the z functions would be equal:

$$z(t) = \bar{z}(t) = \frac{f(t)}{\sqrt{2m\omega}}$$

The inner product between the ground state at $t = -\infty$ and $t = \infty$ defines a functional of z and $\bar{z}$, and is related to the probability of the perturbation exciting the ground state. This functional is given by

$$\mathcal{S}[\bar{z}, z] = \langle -\infty|\infty\rangle = \langle 0|U_I(\infty)U_I^\dagger(-\infty)|0\rangle$$

which, using the time-ordered expression we obtained previously can be written as

$$\mathcal{S}[\bar{z}, z] = \langle T\exp\left(-i\int_{-\infty}^{\infty} \mathrm{d}t\;\left[\bar{z}(t)b(t) + b^\dagger(t)z(t)\right]\right)\rangle_0$$

A general property of time-evolution property is the propagation identity:

$$S(t_2,t_1) = S(t_2,t_i)S(t_i,t_1)$$

Thus we can break $S(\infty,-\infty)$ up into small bites propagating from some t to $t+\Delta t$:

$$\begin{aligned} S(\infty,-\infty) &= S(\infty,\infty-\Delta t)S(\infty-\Delta t,\infty-2\Delta t) \\ &\quad\cdots S(\Delta t,0)S(0,-\Delta t)\cdots S(-\infty+\Delta t,-\infty) \end{aligned}$$

Over these small intervals of time we can approximate the integral $\int_t^{t+\Delta t} f(t')\mathrm{d}t' \approx f(t)\Delta t$. Let us consider $S(t,-t)$ and split it up into N pieces as described above, then we let $N\to\infty$ and $t\to\infty$:

$$S(t,-t) = e^{A_N - A_N^\dagger}e^{A_{N-1}-A_{N-1}^\dagger}\cdots e^{A_1 - A_1^\dagger}$$

where

$$\begin{aligned} A_j &\equiv -i\bar{z}(t_j)b(t_j)\Delta t, \qquad t_j \equiv t\left(\frac{2j}{N} - 1\right) \\ A_j^\dagger &\equiv iz(t_j)b^\dagger(t_j)\Delta t \end{aligned}$$

due to the fact they A_j and $A_j^\dagger$ are operators they will not commute with each other, so normal ordering Equation IV C is not quite trivial, however, we can use

$$e^{\hat{\alpha}+\hat{\beta}} = e^{\hat{\beta}}e^{\hat{\alpha}}e^{[\hat{\alpha},\hat{\beta}]/2}, \qquad e^{\hat{\alpha}}e^{\hat{\beta}} = e^{\hat{\beta}}e^{\hat{\alpha}}e^{[\hat{\alpha},\hat{\beta}]}$$

which only holds if $[\hat{\alpha},[\hat{\alpha},\hat{\beta}]] = [\hat{\beta},[\hat{\alpha},\hat{\beta}]] = 0$. Using this we can write

$$S(t,-t) = e^{-\sum_j A_j^\dagger}e^{\sum_j A_j}\exp\left(-\sum_{j\geq k}[A_j, A_k^\dagger]\left(1 - \frac{1}{2}\delta_{jk}\right)\right)$$

The commutator

$$[A_j, A_k^\dagger] = \bar{z}(t_j)z(t_k)\Delta t^2 e^{-i\omega(t_j - t_k)}$$

where we've used that H_0 is the simple harmonic oscillator which means that $b(t) = be^{-i\omega t}$. Note that $[A_j, A_k^\dagger] \in \mathbb{C}$, so the operator part of $S(t,-t)$ is in the first two exponentials. However, note that the lowering operator on the vacuum state* gives zero, so

$$e^{\sum_j A_j}|0\rangle = e^{\sum_j 0}|0\rangle = |0\rangle$$

---

* we are taking the expectation value with respect to the vacuum state $\langle\cdot\rangle_0$.

therefore $\langle e^{-\sum_j A_j^\dagger} e^{\sum_j A_j} \rangle_0 = 1$:

$$\langle S(t,-t)\rangle_0 =$$
$$\exp\left(-\sum_{j,k} \Delta t^2 \bar{z}(t_j)\Theta(t_j - t_k)e^{-i\omega(t_j-t_k)}z(t_k)\left(1-\delta_{jk}\right)\right)$$

in the limit where $N \to \infty$ and hence $\Delta t \to 0$ we obtain integrals, however, the term with δ_{jk} only has one sum and a Δt^2, which implies that it dies in the limit where $\Delta t \to 0$. Thus we are left with

$$\langle S(t,-t)\rangle_0 =$$
$$\exp\left(-\int_{-t}^{t} \mathrm{d}t'\mathrm{d}t''\ \bar{z}(t')\Theta(t'-t'')e^{-i\omega(t'-t'')}z(t'')\right)$$

we are interested in the limit where $t \to \infty$, in which case we obtain our generating functional:

$$\mathcal{S}[\bar{z},z] = \exp\left(-\int_{-\infty}^{\infty} \mathrm{d}t'\mathrm{d}t''\ \bar{z}(t')G(t'-t'')z(t'')\right)$$

where $G(t'-t'')$ is our first example of a Green's function:

$$G(t'-t'') \equiv \Theta(t'-t'')e^{-i\omega(t'-t'')}$$

D. Wick's theorem

We now have two identities that describe $\mathcal{S}[\bar{z},z]$: Equations IV C and IV C. If we expand up to linear order in $\bar{z}$ and z, we obtain:

$$(-i)^2\int_{-\infty}^{\infty} \mathrm{d}t'\mathrm{d}t''\ \bar{z}(t')\langle T\left\{b(t')b^\dagger(t'')\right\}\rangle_0 z(t'') + \mathcal{O}(\bar{z}^2,z^2)$$
$$= -i\int_{-\infty}^{\infty} \mathrm{d}t'\mathrm{d}t''\ \bar{z}(t')G(t'-t'')z(t'')$$

hence

$$G(t'-t'') = -i\langle T\left\{b(t')b^\dagger(t'')\right\}\rangle_0$$

note that the terms $\langle T\{b(t)\}\rangle_0$ and $\langle T\left\{b^\dagger(t)\right\}\rangle_0$ are both zero, because of the fact that we are taking an expectation value. Similarly, to second order we would have

$$G(t_1,t_2,t_3,t_4) = \langle T\left\{b(t_1)b(t_2)b^\dagger(t_3)b^\dagger(t_4)\right\}\rangle_0$$

and so on. Wick's theorem tells us how we can take these many-body Green's functions and decompose them into products of single-particle Green's functions. **Wick's Theorem:**

$$G(1,\dots,n;1',\dots,n') = \sum_P \prod_r \zeta^P G(r - P'_r)$$

where the ζ has been included so that this result also holds for fermions. For fermions the derivation is very similar, except that we must treat the source and sink terms $\bar{z} \to \overline{\eta}$ and $z \to \eta$ as *Grassman-numbers*, which anti-commute with each other and with field operators.

In reality Wick's theorem is more general than what is given above; Wick's theorem refers to general products of operators that can be contracted by means of the time-ordering and normal-ordering operators. However, in this course we only used Wick's theorem in the context of Green's functions (and later response functions).

E. Gell-Mann-Low Theorem

The Gell-Mann-Low theorem relates a time-ordered expectation value in the Heisenberg picture to a time-ordered expectation value in the interaction picture, provided that the perturbation is turned on and off adiabatically:

$$\langle\phi|T\left\{A(t_1)B(t_2)\cdots\right\}|\phi\rangle_H$$
$$= \frac{\langle -\infty|TS(\infty,-\infty)A(t_1)B(t_2)\cdots|-\infty\rangle_I}{\langle -\infty|S(\infty,-\infty)|-\infty\rangle}$$

where the state $|-\infty\rangle$ is well known $|-\infty\rangle_H = |-\infty\rangle_I$. Using this we can relate full interacting Green's functions to non-interaction Green's functions.

F. Useful quantities calculable from Green's functions

The expectation value of the density operator can be written as a Green's function:

$$\langle\phi|\hat{\rho}(\boldsymbol{x},t)|\phi\rangle = \sum_\sigma \langle\phi|\hat{\psi}^\dagger_\sigma(\boldsymbol{x},t)\hat{\psi}_\sigma(\boldsymbol{x},t)|\phi\rangle$$
$$= -(2S+1)\lim_{\delta\to0^+} \langle\phi|T\hat{\psi}(\boldsymbol{x},t)\hat{\psi}^\dagger(\boldsymbol{x},t-\delta)|\phi\rangle$$
$$= -(2S+1)\lim_{\delta\to0^+} G(\boldsymbol{x}=\boldsymbol{0},t=-\delta)$$
$$= -i(2S+1)G(\boldsymbol{0},0^-)$$

Similarly, we can calculate the expectation value of the kinetic energy:

$$\langle\phi|\hat{T}(\boldsymbol{x})|\phi\rangle = -\sum_{\sigma}\frac{\hbar^2}{2m}\langle\phi|\psi^\dagger_\sigma(\boldsymbol{x})\mathcal{L}\{\}\,x\psi_\sigma(\boldsymbol{x})|\phi\rangle$$

$$\frac{\hbar^2\mathcal{L}\{\}\,x}{2m}(2S+1)\left.\langle\phi|T\psi(\boldsymbol{x},0^-)\psi^\dagger(\boldsymbol{x}',0)|\phi\rangle\right|_{\boldsymbol{x}=\boldsymbol{x}'}$$

$$\frac{=i(2S+1)\hbar^2\mathcal{L}\{\}}{2m}G(\boldsymbol{x},0^-)_{\boldsymbol{x}=0}$$

subsection

VII. ZERO-TEMPERATURE FEYNMAN DIAGRAMS

The generating function for fermions $\mathcal{S}[\overline{\eta},\eta]$ can by written diagrammatically as

$$\mathcal{S}[\overline{\eta},\eta] = \exp\left(-i\overline{\eta}\qquad\eta\right)$$

where we have associated

$$\int \mathrm{d}1\mathrm{d}2\,\overline{\eta}(2)G(2-1)\eta(1) = \overline{\eta}\quad\eta$$

Note that

$$i^2\ln\mathcal{S}[\overline{\eta},\eta]\eta(2)\delta\overline{\eta}(1) = G(1-2) = 1\quad 2$$

A general expectation value of the form

$$\langle\phi|T\mathcal{S}[\overline{\eta},\eta]F[\psi^\dagger,\psi]|\phi\rangle$$

can be shown to be equal to

$$F\left[i\zeta\eta,i\overline{\eta}\right]\exp\left(-i\overline{\eta}\quad\eta\right)$$

if we now set $F[\psi^\dagger,\psi] = T\exp\left(-i\int\mathrm{d}t\,V[\psi^\dagger,\psi]\right)$ we obtain the *interacting generator*:

$$\mathcal{S}_I[\overline{\alpha},\alpha] = \exp\left(i^{n-1}\int_{-\infty}^{\infty}\mathrm{d}t\,V\left[\zeta\alpha,\overline{\alpha}\right]\right)\times \exp\left(-i\overline{\eta}\quad\eta\right)$$

where $\alpha=\eta$ and $\overline{\alpha}=-i\overline{\eta}$.

In processes where two particles scatter of each other at once, such as the Coulomb interaction, we have that

$$i^{n-1}V\left[\zeta\alpha,\overline{\alpha}\right] = \frac{i}{2}\int\mathrm{d}^3x\mathrm{d}^3x'\;V(x-x')\alpha(x)\alpha(x')\overline{\alpha}(x')\overline{\alpha}(x)$$

where $iV(x-x')$ is the two-particle scattering amplitude. The scattering process is depicted by

$\frac{1}{2}$

Which gives us

$$\mathcal{S}_I[\overline{\alpha},\alpha] = \exp\left(\qquad\qquad\right)\times \exp\left(-i\overline{\eta}\quad\eta\right)$$

This should be thought of in terms of the exponential function's power series. The lowest nonzero (nontrival) term is

$$\frac{1}{2}\left(\qquad\qquad\right)\left(-i\overline{\eta}\quad\eta\right)^2$$

$$=\qquad\qquad+$$

A. Linked-Cluster Theorem

The linked-cluster theorem states that

$$\ln\mathcal{S}_I[\overline{\alpha},\alpha] = \sum\{\text{linked}-\text{cluster diagrams}\}$$

which can be shown by making identital(commuting) copies of $\mathcal{S}_I$ and using the identity that

$$\ln\mathcal{S}_I = \lim_{n\to 0}\left[\frac{\mathcal{S}_I^n-1}{n}\right]$$

The linked cluster diagrams are all connected diagrams, so the dumbbell and oyster diagram are of order α^0, next are single particle propagators with α and $\overline{\alpha}$ at the ends, then come two-particle propagators etc. But there are *not* products of diagrams, as these are not linked.

A similar statement can be made about the full two-particle Green's function:

$$G(2-1) = {}^2\ln\mathcal{S}_I[\overline{\alpha},\alpha]\alpha(1)\delta\overline{\alpha}(2)\Big|_{\alpha,\overline{\alpha}=0} = \sum\{\text{two}-\text{leg diagrams}\}$$

and similarly

$$G(1,2;3,4) = \sum\{\text{four}-\text{legged diagrams}\}$$

B. Feynman Rules in Momentum Space

1. Fermions with four-momentum, k, and spin σ: $\equiv G^0_\sigma(k)$
2. Interaction lines with four-momentum, q: $\equiv iV(q)$
3. Conserve spin and four-momentum at each vertex; incoming and outgoing momenta are equal and spins cannot be flipped
4. Multiply by $(-1)^F(2S+1)^F$ where F is the number of fermion loops.
5. If there are any "same-time"fermion-loops, i.e ones that loop back on themselves, include (a) convergence factor(s), $e^{ik_n 0^+}$
6. For each *internal* four-momentum, k, integrate $\int \frac{\mathrm{d}^4 k}{(2\pi)^4}$
7. Divide by the symmetry factor, p, of the diagram and multiply by VT (volume times time-interval)

Tabel I: *Feynman Rules in Momentum Space, as per Bruus & Flensberg*

C. Hartree-Fock energy

The Hartree-Fock shift in the ground-state energy of an interacting electron gas to first order is given by

$$E_g = E_0 + i\mathcal{V}\left(\qquad\qquad + \qquad \right)$$

Using Feynman's momentum-space rules we can write the energy shift out, noting that $p = 2$ for both diagrams:

$$\Delta E_{\mathrm{HF}} = \frac{i\mathcal{V}}{2}\int \frac{\mathrm{d}^4k\mathrm{d}^4k'}{(2\pi)^8} e^{i(\omega+\omega')\delta} \Big[\left(-\left[2S+1\right]\right)^2\left(iV_{\boldsymbol{q}=\mathbf{0}}\right) + \left(-\left[2S+1\right]\right)\left(iV_{\boldsymbol{k}=\boldsymbol{k}'}\right)\Big] \times G(k)G(k')$$

where $k = (\boldsymbol{k}, \omega)$ and similarly for k'. It is only the Green's functions that depend on the frequencies, so let us integrate those away

$$\langle c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}\rangle = -i\int \frac{\mathrm{d}\omega}{2\pi} G(k)e^{i\omega\delta} = f_{\boldsymbol{k}} = \Theta(k_F - |\boldsymbol{k}|)$$

giving us

$$\Delta E_{\mathrm{HF}} = \frac{i\mathcal{V}}{2}(2S+1)\int_{\boldsymbol{k}\boldsymbol{k}'}\left[(2S+1)\,V_{\boldsymbol{q}=\mathbf{0}} - V_{\boldsymbol{k}-\boldsymbol{k}'}\right] f_{\boldsymbol{k}} f_{\boldsymbol{k}'}$$

Unfortunately the $\boldsymbol{q} = \mathbf{0}$ term is infinite, but the book argues that we can neglect this, which means the first order approximation of the ground-state energy of an electron gas with interactions taken into account can be written as

$$\frac{E_g}{\mathcal{V}} = (2S+1)\left(\int_{\boldsymbol{k}} \frac{\hbar^2 k^2}{2m} f_{\boldsymbol{k}} - \frac{1}{2}\int_{\boldsymbol{k}\boldsymbol{k}'} f_{\boldsymbol{k}} f_{\boldsymbol{k}'} \frac{e^2}{\varepsilon_0(\boldsymbol{k}-\boldsymbol{k}')^2}\right)$$

carefully evaluating these integrals gives us

$$\frac{E_g}{\rho\mathcal{V}} = \frac{3}{5}\varepsilon_F - \frac{3}{4\pi}\frac{e^2 k_F}{4\pi\varepsilon_0}$$

D. Exchange correlation

Due to the Pauli Exclusion Principle we expect that if we know an electron has a charge distribution $\rho(x)$, then another electron will have a low probability of being there where $\rho(x)$ is at its maximum. It is useful to consider the equal-time density correlation function:

$$C_{\sigma\sigma'}(\boldsymbol{x}-\boldsymbol{x}') = \langle\phi_0|{:}\hat{\rho}_\sigma(\boldsymbol{x})\hat{\rho}_\sigma(\boldsymbol{x}'){:}|\phi_0\rangle$$

It turns out that we can relate this to the Hartree-Fock energy (first order approximation of the correction due to interactions of the energy of an electron gas), because

$$\begin{aligned}\langle\phi_0|V|\phi_0\rangle =& \frac{1}{2}\sum_{\sigma\sigma'}\int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}'\; V(\boldsymbol{x}-\boldsymbol{x}')\times \\ & \langle\phi_0|{:}\hat{\rho}_\sigma(\boldsymbol{x})\hat{\rho}_\sigma(\boldsymbol{x}'){:}|\phi_0\rangle \\ =& \frac{1}{2}\sum_{\sigma\sigma'}\int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}'\; V(\boldsymbol{x}-\boldsymbol{x}')C_{\sigma\sigma'}(\boldsymbol{x}-\boldsymbol{x}')\end{aligned}$$

By removing the potential part of the dumbbell and oyster diagrams, we can hence obtain a diagrammatic expression for the correlation function

$$C_{\sigma\sigma'}(\boldsymbol{x}-\boldsymbol{x}') = -\left[\left(\qquad\qquad\right) + \left(\qquad\qquad\right)\delta_{\sigma\sigma'}\right]$$

which we can write out explicitly

$$\begin{aligned}C_{\sigma\sigma'}(\boldsymbol{x}-\boldsymbol{x}') =& -\big[(-G(\mathbf{0},0^-))^2 - \\ & \delta_{\sigma\sigma'}G(\boldsymbol{x}-\boldsymbol{x}',0^-)G(\boldsymbol{x}'-\boldsymbol{x},0^-)\big] \\ =& \rho_0^2 + \delta_{\sigma\sigma'}G(\boldsymbol{x}-\boldsymbol{x}',0^-)G(\boldsymbol{x}'-\boldsymbol{x},0^-)\end{aligned}$$

We can evaluate the Green's function

$$\begin{aligned}G(\boldsymbol{r},0^-) &= \int_{\boldsymbol{k}} G(\boldsymbol{k},0^-) = i\int_{\boldsymbol{k}} f_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \\ &= i\int \frac{\mathrm{d}k}{2\pi^2}\frac{k\sin kr}{r} = i\rho_0 P(k_F r)\end{aligned}$$

where

$$P(x) = 3\left(\frac{\sin x - x\cos x}{x^3}\right)$$

which is an even function, therefore the two Green's functions are equal.

$$C_{\sigma\sigma'}(r) = \rho_0^2\left(1 - \delta_{\sigma\sigma'}\left[P(k_F r)\right]^2\right)$$

E. Self-energy

The full Green's function of a fermion in an interacting environment can be written as an infinite sum of terms that depend on the free Green's function to higher and higher order. However, it is possible to express this infinite sum in terms of a recurring term, the self-energy, which allows us to evaluate the sum exactly, just as one can do for geometric series. The self-energy is the sum of all scattering processes that cannot be separated into disconnected diagrams by cutting a single propagator.

Denote the full Green's function as

$$G(k) =$$

and the self energy as

$$\Sigma(\boldsymbol{k},\omega) =$$

then

$$= \qquad\qquad +$$

Which algebraically would be written as

$$G(\boldsymbol{k},\omega) = G^0(\boldsymbol{k},\omega) + G^0(\boldsymbol{k},\omega)\Sigma(\boldsymbol{k},\omega)G(\boldsymbol{k},\omega)$$

which is a *Dyson Equation* and solving it yields

$$G(\boldsymbol{k},\omega) = \frac{1}{\omega - \varepsilon_{\boldsymbol{k}} - \Sigma(\boldsymbol{k},\omega)}$$

Generally, the self-energy can have be $\Sigma \in \mathbb{C}$, where the real part corresponds to a shift in the energy levels ("renormalised energy"), whereas the imaginary part gives the electrons a lifetime.

1. *Hartree-Fock Self-Energy*

The lowest order terms in the self energy are the so-called Hartree-Fock self-energy terms:

$$\Sigma_{\mathrm{HF}}(\boldsymbol{p},\omega) = \qquad\qquad +$$

However, if these are the only terms in the self-energy that we include, then the full Green's function also includes diagram's where we've replace the fermion lines above by either of the diagrams above. This nested behaviour is what allows us to include orders up to infinity, even if we don't include the entire expression for Σ.

F. Response Functions

We will now consider Hamiltonians of the form

$$H(t) = H_0 + H_s(t)$$

where $H_s(t) = -A(t)f(t)$ for some operator A and some complex function $f(t)$. These can for instance be the spin-density operator and the magnetic field or charge density and an external electric field. We can go from the Interaction picture to the Heisenberg picture by

$$A_H(t) = U^\dagger(t)A_I(t)U(t)$$

where $U(t) = S_I(t,-\infty)$ from before. By evaluating $U(t)$ up to linear order in the perturbation we obtain

$$A_H(t) = A_I(t) - i\int_{-\infty}^{t} \mathrm{d}t'\ [A_I(t), H_s(t')] + \mathcal{O}(H_s^2)$$

which, first of all gives us a result from linear response theory:

$$\langle A\rangle(t) = \langle A\rangle_0 - i\int_{-\infty}^{t} \mathrm{d}t'\ \langle[A_I(t), H_s(t')]\rangle_0$$

where here $\langle\cdot\rangle_0$ is the equilibrium average with respect to the unperturbed Hamiltonian, H_0. If we now plug in our expression for $H_s(t)$ we get

$$\begin{aligned}\delta\langle A\rangle(t) &= i\int_{-\infty}^{t} \mathrm{d}t'\ \langle[A_I(t), A_I(t')]\rangle_0 f(t') \\ &= \int_{-\infty}^{\infty} \mathrm{d}t'\ \chi(t-t')f(t')\end{aligned}$$

where we've defined the dynamical susceptibility

$$\chi(t-t') = i\langle[A_I(t), A_I(t')]\rangle_0\Theta(t-t')$$

1. *Magnetic Susceptibility of Non-Interacting Electron Gas*

The relation between magnetisation and an external magnetic field is

$$M(x) = \int \mathrm{d}^4x' \, \underline{\chi}(x - x')B(x')$$

where the susceptibility tensor is given by

$$\left(\underline{\chi}\right)_{i,j}(x) = i\mu_B^2 \langle [\sigma_i(x), \sigma_j(0)] \rangle_0$$

which we can Fourier transform:

$$\chi_{ij}(q) = i\mu_B^2 \int \mathrm{d}^4x \, \langle [\sigma_i(x), \sigma_j(0)] \rangle_0 \Theta(t) e^{-iq\cdot x}$$

The susceptibility is related to the time-ordered susceptibility through $\chi_{ij}(\boldsymbol{q}, \nu) = -i\chi_{ij}^T(\boldsymbol{q}, \nu + i\delta)$ where the latter is given by

$$\chi_{ij}^T(q) = \mu_B^2 \left[\sigma_j \qquad\qquad \sigma_i \right]$$

$$= -2\mu_B^2 \delta_{ij} \int_{\boldsymbol{k}} \left[\frac{1}{\omega + \nu - \tilde{\varepsilon}_{\boldsymbol{k}+\boldsymbol{q}}} \frac{1}{\omega - \tilde{\varepsilon}_{\boldsymbol{k}}} \right]$$

where $\tilde{\varepsilon}_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} - i\delta \mathrm{sgn}(\varepsilon_{\boldsymbol{k}})$ and $k = (\boldsymbol{k}, \omega)$. Performing the calculation gives us the *dynamical spin susceptibility*:

$$\chi(\boldsymbol{q}, \nu + i\delta) = 2\mu_B^2 \int_{\boldsymbol{k}} \frac{f_{\boldsymbol{k}+\boldsymbol{q}} - f_{\boldsymbol{k}}}{\nu - (\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}}) + i\delta}$$

where $f_{\boldsymbol{k}}$ still is the zero-temperature limit of the Fermi-Dirac Distribution. In the $\nu \to 0$ limit we obtain the *static susceptibility*, which tells us about the response to a spatially (but not temporally) varying magnetic field, in which case we obtain

$$\chi(\boldsymbol{q}) = 2\mu_B^2 N(0) F\left(\frac{q}{2k_F}\right),$$
$$F(x) = \frac{1 - x^2}{4x} \ln\left|\frac{1+x}{1-x}\right| + \frac{1}{2}$$

VIII. NON-ZERO-TEMPERATURE MANY-BODY PHYSICS

Non-zero-temperature many-body physics begins with the recognition that the time-evolution operator $U(t) = \exp(-itH)$ and the quantum mechanical partition function $\hat{\rho} \sim e^{-\beta H}$ are identical if we treat t as an imaginary number:

$$t \to -i\beta$$

Using this we can express the partition function in terms of the imaginary-time-evolution operator:

$$Z = \mathrm{Tr}\, U(-i\beta)$$

and we can do the same with thermal-equilibrium expectation values:

$$\langle A \rangle = \frac{\mathrm{Tr}\,[U(-i\beta)A]}{\mathrm{Tr}\,[U(-i\beta)]}$$

It turns out that the machinery that we developed for zero-temperature many-body physics can be generalised to non-zero-temperature many-body physics, simply by letting $t \to -i\tau$ where the imaginary-time parametre $\tau \in [0, \beta]$. For instance, operators in the Heisenberg picture would be:

$$A_H(\tau) = e^{\tau H} A e^{-\tau H}$$

and the creation and annihilation operators in the free-particle Hamiltonian $H = \sum_k \varepsilon_k c_k^\dagger c_k$ are described by means of their Heisenberg equation of motion:

$$\frac{\partial c_k}{\partial \tau} = [H, c_k] = -\varepsilon_k c_k$$
$$\frac{\partial c_k^\dagger}{\partial \tau} = [H, c_k^\dagger] = \varepsilon_k c_k^\dagger$$

which tells us that $c_k(\tau) = e^{-\varepsilon_k \tau} c_k$ and $c_k^\dagger(\tau) = e^{\varepsilon_k \tau} c_k^\dagger$. Note that even though $(c_k^\dagger)^\dagger = c_k$ it is *not* the case that $(c_k^\dagger(\tau))^\dagger = c_k(\tau)$ – i.e they are not hermitian conjugates.

We also have the (imaginary-)time-ordering operator, which has exactly the same effect as the regular time-ordering operator, which allows us to write

$$U(\tau) = T \exp\left[-\int_0^\tau \mathrm{d}\tau \, V_I(\tau)\right]$$
$$S(\tau_2, \tau_1) = T \exp\left[-\int_{\tau_1}^{\tau_2} \mathrm{d}\tau \, V_I(\tau)\right]$$

$S(\beta, 0)$ is of particular interest, because this tells us about the change in the Helmholtz free energy, and can be expressed in terms of the full partition function, Z, and the free partition function, Z_0:

$$\frac{Z}{Z_0} = e^{-\beta\Delta F} = \langle T \exp\left[-\int_0^\beta \mathrm{d}\tau \, V_I(\tau)\right] \rangle$$

In imaginary-time many-body physics it is the partition function that is the generator of (imaginary-time) Green's functions, which makes sense because we just saw that Z is related to $S(\beta, 0)$ (time-evolution operator over the entire τ interval), which corresponds to $S(\infty, -\infty)$ which was the generator for real-time Green's functions. We will denote imaginary time Green's functions as $\mathcal{G}(\tau)$.

A. Imaginary-Time Green's Functions

The imaginary-time Green's function is defined as

$$\begin{aligned}\mathcal{G}_{\lambda\lambda'}(\tau-\tau') &= -\langle T\ \psi_\lambda(\tau)\psi^\dagger_{\lambda'}(\tau')\rangle \\ &= -\mathrm{Tr}\left[e^{-\beta(H-F)}\psi_\lambda(\tau)\psi^\dagger_{\lambda'}(\tau')\right]\end{aligned}$$

where we have assumed that H is invariant under temporal translations, such that $\mathcal{G}(\tau,\tau') = \mathcal{G}(\tau-\tau')$, which is often the case. Additionally, it is often the case that the quantum number λ is conserved (for example very often spin is not flipped by H), in which case $\mathcal{G}_{\lambda\lambda'}(\tau-\tau') = \delta_{\lambda\lambda'}\mathcal{G}_\lambda(\tau-\tau')$.

For non-interacting particles $H = \sum_\lambda \xi_\lambda \psi^\dagger_\lambda \psi_\lambda$, where $\xi_\lambda = \varepsilon_\lambda - \mu$ the equal-time expectation value of the fields is

$$\langle \psi^\dagger_\lambda \psi_{\lambda'}\rangle = \delta_{\lambda\lambda'}\begin{cases} n(\xi_\lambda) & \text{Bosons} \\ f_{\mathrm{FD}}(\xi_\lambda) & \text{Fermions}\end{cases}$$

and we have that $\langle \psi_{\lambda'}\psi^\dagger_\lambda\rangle = \delta_{\lambda\lambda'} - \langle \psi^\dagger_\lambda \psi_{\lambda'}\rangle$, which tells us that

$$\mathcal{G}_\lambda(\tau) = -e^{-\xi_\lambda\tau}\begin{cases}(1+n(\xi_\lambda))\Theta(\tau) + n(\xi_\lambda)\Theta(-\tau) & \mathrm{B} \\ (1-f_{\mathrm{FD}}(\xi_\lambda))\Theta(\tau) - f_{\mathrm{FD}}(\xi_\lambda)\Theta(\tau) & \mathrm{F}\end{cases}$$

Due to the fact that our imaginary-time parametre, τ, spans from 0 to β the behaviour of imaginary-time Green's functions are slightly different from real-time Green's functions. For instance it can be shown that for $-\beta < \tau < 0$ we have

$$\mathcal{G}_\lambda(\tau+\beta) = \zeta\mathcal{G}_\lambda(\tau)$$

where as usual ζ is negative one for fermions and positive one for bosons

B. Matsubara Representation

The (anti-)periodicity of the Green's functions implies that we can decompose them into an infinite sum of complex exponentials. The *Matsubara Frequencies* are defined as

$$\begin{aligned}\nu_n &= \frac{2\pi n}{\beta}, && \text{Bosons} \\ \omega_n &= \frac{\pi(2n+1)}{\beta}, && \text{Fermions}\end{aligned}$$

we choose these so that

$$\begin{aligned}e^{i\nu_n(\tau+\beta)} &= e^{i\nu_n\tau} \\ e^{i\omega_n(\tau+\beta)} &= -e^{i\omega_n\tau}\end{aligned}$$

Now, using these we can decompose the Green's functions:

$$\mathcal{G}_{\lambda\lambda'} = \frac{1}{\beta}\begin{cases}\sum_n \mathcal{G}_{\lambda\lambda'}(i\nu_n)e^{-i\nu_n\tau} & \text{Bosons} \\ \sum_n \mathcal{G}_{\lambda\lambda'}(i\omega_n)e^{-i\omega_n\tau} & \text{Fermions}\end{cases}$$

where

$$\mathcal{G}_{\lambda\lambda'}(i\alpha_n) = \int_0^\beta \mathrm{d}\tau\ G_{\lambda\lambda'}(\tau)e^{i\alpha_n\tau}$$

for some Matsubara frequency α_n. Using this we can calculate the Matsubara representation Green's functions for free particles:

$$\begin{aligned}\mathcal{G}_\lambda(i\omega_n) &= -\int_0^\beta \mathrm{d}\tau\ e^{(i\omega_n-\xi_\lambda)\tau}(1-f_{\mathrm{FD}}(\xi_\lambda)) \\ &= \frac{-1}{i\omega_n-\xi_n}\frac{e^{(i\omega_n-\xi_\lambda)\beta}-1}{e^{-\beta\xi_\lambda}+1} \\ &= \frac{1}{i\omega_n-\xi_\lambda}\end{aligned}$$

where we have used that $e^{i\omega_n\beta} = -1$. Similarly for bosons we get

$$\mathcal{G}_\lambda(i\nu_n) = \frac{1}{i\nu_n-\xi_\lambda}$$

note how closely the zero and non-zero temperature Green's functions are related to each other.

C. Contour-Integral Method

The first important point to make is that the distribution functions have first order poles with weight $\frac{\zeta}{\beta}$ at the Matsubara frequencies:

$$\begin{aligned}\lim_{z\to i\omega_n}(z-i\omega_n)f(z) = \lim_{z\to i\omega_n}\frac{z-i\omega_n}{1+e^{z\beta}} &\approx \lim_{z\to i\omega_n}\frac{z-i\omega_n}{\beta\,(i\omega_n-z)} \\ &= -\frac{1}{\beta}\end{aligned}$$

and similarly for bosons. Now, consider a sum of the form

$$\frac{1}{\beta}\sum_n F(i\omega_n)$$

for some function $F(z)$ that tends to zero faster than $\frac{1}{|z|}$. Let γ be a circular path in the Argand plane with centre at the origin and radius ∞. If the integrand converges towards zero quickly enough, then the contour integral along γ must be zero, which implies that the sum of all residues is zero. Suppose $F(z)$ has poles at z_i

and $f_{\mathrm{FD}}(z)$ has poles at $i\omega_n$ as previously established, then it must be the case that

$$0 = \oint_\gamma \frac{\mathrm{d}z}{2\pi i} F(z) f_{\mathrm{FD}}(z) = \sum_i \mathrm{Res}\left[F(z_i) f_{\mathrm{FD}}(z_i)\right] + \sum_n \mathrm{Res}\left[F(i\omega_n) f_{\mathrm{FD}}(i\omega_n)\right]$$

which gives us

$$\frac{1}{\beta}\sum_n F(i\omega_n) = \sum_i f_{\mathrm{FD}}(z_i)\,\mathrm{Res}\left[F(z_i)\right]$$

it is essential that $F(z)$ and $f_{\mathrm{FD}}(z)$ don't have any common poles. However, quite often $F(z)$ will have poles along the real axis, whereas $f_{\mathrm{FD}}(z)$ has poles on the imaginary axis, which avoids this problem.

Consider the following response function

$$\begin{aligned}\chi_0(\boldsymbol{q},\tau) &= -\frac{1}{\mathcal{V}}\langle T\,\rho(\boldsymbol{q},\tau)\rho(-\boldsymbol{q},0)\rangle \\ &= \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}\sigma} \mathcal{G}_{0,\sigma}(\boldsymbol{k}+\boldsymbol{q},\tau)\mathcal{G}_{0,\sigma}(\boldsymbol{k},-\tau)\end{aligned}$$

where we obtained Equation VIII C with Wick's theorem. Now it is beneficial to Fourier transform, such that we are left with

$$\chi_0(\boldsymbol{q},\nu_\ell) = \frac{1}{\beta}\sum_{\omega_n}\frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}\sigma}\mathcal{G}_{0,\sigma}(\boldsymbol{k}+\boldsymbol{q}, i\omega_n + i\nu_\ell)\mathcal{G}_{0,\sigma}(\boldsymbol{k}, i\omega_n)$$

we know the form of $\mathcal{G}_{0,\sigma}$:

$$\mathcal{G}_{0,\sigma}(\boldsymbol{k},z) = \frac{1}{z-\xi_{\boldsymbol{k}}}$$

hence our $F(z)$ has two simple poles and converges to 0 faster than $\frac{1}{z}$. Hence we can use the contour-integral method, which tells us that

$$\chi_0(\boldsymbol{q}, i\nu_\ell) = \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}\sigma}\left(\frac{f_{\mathrm{FD}}(\xi_{\boldsymbol{k}+\boldsymbol{q}}) - f_{\mathrm{FD}}(\xi_{\boldsymbol{k}})}{\xi_{\boldsymbol{k}+\boldsymbol{q}} - \xi_{\boldsymbol{k}} - i\nu_\ell}\right)$$

This Matsubara susceptibility is related to the regular susceptibility by an analytic continuation; $i\nu_\ell \to \omega + i\delta$, which means we have obtained quite a powerful result by not doing a lot of complicated maths.

We can do something very similar for bosons, where we use bosonic Matsubara frequencies, and we just need to be careful because there is a factor minus one that we didn't need to take into account in the fermionic case.

D. Generating Functional and Wick's Theorem

We can develop Wick's theorem in the same fashion as we developed it for zero temperature, however, the difference is that the integrals no longer go from $-\infty$ to ∞ but rather from 0 to β, and we replace $\mathcal{S}_I[\bar{\eta},\eta] \to \frac{Z[\bar{\eta},\eta]}{Z_0}$. Similarly to before we will consider

$$\begin{aligned}H_0 &= \sum_\lambda \varepsilon_\lambda \psi^\dagger_\lambda \psi_\lambda \\ V(\tau) &= -\sum_\lambda \left[\bar{\eta}_\lambda(\tau)\psi_\lambda + \psi^\dagger_\lambda \eta(\tau)\right]\end{aligned}$$

plugging this into our expression for Z we obtain

$$\frac{Z[\bar{\eta},\eta]}{Z_0} = \exp\left(-\sum_\lambda \int_0^\beta \mathrm{d}\tau_1 \mathrm{d}\tau_2\, \bar{\eta}(\tau_1)\mathcal{G}_\lambda(\tau_1-\tau_2)\eta_\lambda(\tau_2)\right)$$

where

$$\mathcal{G}_\lambda(\tau_1-\tau_2) = -\langle T\psi_\lambda(\tau_1)\psi^\dagger_\lambda(\tau_2)\rangle$$

By taking various functional derivatives of our new generating functional, we can derive an imaginary-time Wick's theorem

$$\mathcal{G}(1,2,\ldots,n;n',\cdots,2',1') = \sum_P \prod_{r=1}^{n} (-1)^P \mathcal{G}(r-P'_r)$$

which looks identical to the zero-temperature version, except that we use τ instead of t. Now we can also relate the full partition function the non-interacting partition function by means of a Feynman Diagram expansion;

$$Z = Z_0 \sum\{\mathrm{unlinked\ Feynman-Diagrams}\}$$

And the shift in the *Helmholtz Free Energy*

$$\Delta F = F - F_0 = -\frac{1}{\beta}\sum\{\mathrm{linked\ Feynman-Diagrams}\}$$

The Feynman rules for imaginary time diagrams are very similar to those we had in Table I. However, now it is the Matsubara Green's functions that we obtain, and interaction lines are $-V(q)$ instead of $iV(q)$.

E. Electron in a Disordered Potential

In real physical systems the atoms in a lattice are not located in a perfectly periodic grid, and there are often other types of impurities, for instance a different atom, with different properties placed in the midst of the other atoms perturbing the crystal structure and characteristics.

Let us consider the following Hamiltonian:

$$H = \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}} + V_{\text{disorder}}$$
$$V_{\text{disorder}} = \int \mathrm{d}^3\boldsymbol{x}\, U(\boldsymbol{x})\psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x})$$

where $U(\boldsymbol{x})$ is the potential due to the impurities:

$$U(\boldsymbol{x}) = \sum_j \mathcal{U}_j(\boldsymbol{x} - \boldsymbol{R}_j)$$

where $\boldsymbol{R}_j$ is the location of the j^{th} impurity. We're not interested in a specific example, where we know exactly where all the impurities are, but rather a general result, where we've averaged over all impurity positions. Hence we're interested in the impurity averaged Green's function, which we will denote by $\overline{\mathcal{G}(\boldsymbol{k},\boldsymbol{k}',i\omega_n)}$. First let us denote

$$\delta U(x) = U(x) - \overline{U(x)} = U(x) - \mu$$

hence it is only the fluctuation in $U(x)$ that is important; the averaged value just readjusts the chemical potential. Hence we can use the following potential

$$V = \int_{\boldsymbol{k}\boldsymbol{k}'} \delta U_{\boldsymbol{k}-\boldsymbol{k}'} c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}'} =$$

Note that the impurity average of δU is zero, therefore the first order term in our expansion for $\overline{\mathcal{G}(\boldsymbol{k},\boldsymbol{k}',i\omega_n)}$ will be zero; we must go to second order

$$\overline{\mathcal{G}(\boldsymbol{k},\boldsymbol{k}',i\omega_n)} = \mathcal{G}_0(\boldsymbol{k},\boldsymbol{k}',i\omega_n)\delta_{\boldsymbol{k},\boldsymbol{k}'} + \mathcal{G}_0(\boldsymbol{k}) \int_{\boldsymbol{k}_1} \mathcal{G}_0(\boldsymbol{k}_1)\overline{\delta U_{\boldsymbol{k}-\boldsymbol{k}_1}\delta U_{\boldsymbol{k}_1-\boldsymbol{k}'}} G_0(\boldsymbol{k}')$$

we can show that

$$\overline{\delta U_{\boldsymbol{k}-\boldsymbol{k}_1}\delta U_{\boldsymbol{k}_1-\boldsymbol{k}'}} = \delta(\boldsymbol{k}-\boldsymbol{k}')n_I\,|u(\boldsymbol{k}-\boldsymbol{k}_1)|^2$$

where n_I is the density of impurities and $u(\boldsymbol{q})$ are the Fourier coefficients of the impurity potential. We obtain a Dyson Equation, which allows us to write the full Green's function in terms of the impurity-free Green's function and a self-energy:

$$\mathcal{G}(\boldsymbol{k},\boldsymbol{k}') = \frac{1}{i\omega - \xi_{\boldsymbol{k}} - \Sigma(\boldsymbol{k})}$$

where

$$\Sigma(\boldsymbol{k}) = n_I \int_{\boldsymbol{k}_1} \frac{|u(\boldsymbol{k}-\boldsymbol{k}_1)|^2}{i\omega_n - \xi_{\boldsymbol{k}_1}} \approx -\frac{i\mathrm{sgn}(\omega_n)}{2\tau}$$

where we've defined the scattering rate $\tau \equiv 2\pi n_I u_0^2$ and we've assumed that the Fourier coefficients $u(\boldsymbol{k}-\boldsymbol{k}_1)$ are dominated by the constant part, u_0. This gives us

$$\mathcal{G}(\boldsymbol{k},i\omega_n) = \frac{1}{i\omega - \xi_{\boldsymbol{k}} + i\frac{\mathrm{sgn}(\omega_n)}{2\tau}}$$

which tells us that the impurity gives rise to electron-lifetimes; or equivalently the existence of impurities in metals gives rise to a resistivity, just as one might expect.

F. Electron-Phonon Coupling

Let us consider a system of phonons and electrons that coupled through an interaction given by $V_{\mathrm{e-ph}}$;

$$H_{\mathrm{ph}} = \sum_{\boldsymbol{q}\lambda} \omega_{\boldsymbol{q}\lambda}\left(a^\dagger_{\boldsymbol{q}\lambda}a_{\boldsymbol{q}\lambda} + \frac{1}{2}\right)$$
$$H_{\mathrm{e}} = \sum_{\boldsymbol{k}\sigma} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}$$
$$V_{\mathrm{e-ph}} = \int \mathrm{d}^3\boldsymbol{x}\,(-e\hat{\rho}(x))\sum_j U_{\mathrm{ion}}(\boldsymbol{x}-\boldsymbol{R}_j)$$

In the low-temperature limit we can expect the displacement $R_j - R_j^0$ to be sufficiently small that we can approximate the ion-potential up to first order:

$$U_{\mathrm{ion}}(\boldsymbol{x}-\boldsymbol{R}_j) = U_{\mathrm{ion}}(\boldsymbol{x}-\boldsymbol{R}_j^0) - \nabla_{\boldsymbol{x}}U_{\mathrm{ion}}(\boldsymbol{x}-\boldsymbol{R}_j^0)\cdot\boldsymbol{u}_j$$

where $\boldsymbol{u}_j = \boldsymbol{R}_j - \boldsymbol{R}_j^0$. The first term is a periodic potential, which tells us that to zeroth order in $\boldsymbol{u}_j$ the eigenfunctions are Bloch-waves. The vector $\boldsymbol{u}_j$ can be written as

$$\boldsymbol{u}_j = \sum_{\boldsymbol{q}\lambda} \bar{\varepsilon}_\lambda e^{-i\boldsymbol{q}\cdot\boldsymbol{R}_j^0}\frac{\ell_{\boldsymbol{q}\lambda}}{\sqrt{2}}\left(a_{\boldsymbol{q}\lambda} + a^\dagger_{-\boldsymbol{q}\lambda}\right)$$

the quantity $a+a^\dagger$ is related to the displacement (recall the harmonic oscillator), and the displacement of the j^{th} atom is related to the phonon-displacement because phonons are waves in the periodic lattice structure. The quantity $\ell_{\boldsymbol{q}\lambda} = \sqrt{\frac{\hbar}{2mN\omega_{\boldsymbol{q}\lambda}}}$ is the so-called *magnetic-length.* Hence, the interaction up to first order is given by

$$V_{\mathrm{e-ph}} = \sum_{\boldsymbol{q}\boldsymbol{k}\lambda} g_{\boldsymbol{q}\lambda}c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}}\left[a_{\boldsymbol{q}\lambda} + a^\dagger_{-\boldsymbol{q}\lambda}\right]$$

where the electron-phonon coupling constant, $g_{\boldsymbol{q}\lambda}$ is given by

$$g_{\boldsymbol{q}\lambda} = \begin{cases} Cq\ell_{\boldsymbol{q}\lambda} & \lambda: \text{ longitudinal} \\ 0 & \lambda: \text{ transversal} \end{cases}$$

at each vertex we write $(ig_{\boldsymbol{q}\lambda})$ as this is the coupling-constant, which means that we should expand in terms of g.

The non-interacting Green's functions are

$$\mathcal{G}^0(\boldsymbol{k}, i\omega_n) = \frac{1}{i\omega_n - \xi_{\boldsymbol{k}}}$$
$$\mathcal{D}^0(\boldsymbol{q}, i\nu_n) = \frac{2\omega_{\boldsymbol{q}}}{(i\nu_n)^2 - \omega_{\boldsymbol{q}}^2}$$

This interaction is quite similar to the Coulomb interaction, however, the propagation speed is lower than that of photons, which tells us that the electron-phonon interaction is always delayed. In some materials at low temperature this can lead to attractive forces between electrons, such that they form Cooper-pairs; superconductors.

If we now just consider the lowest order contribution to the self-energy:

$$\Sigma(k) =$$

which is

$$\Sigma(\boldsymbol{k}, i\omega_\ell) = \sum_{\boldsymbol{q},n} \frac{-g_{\boldsymbol{q}\lambda}^2}{\beta} \left(\frac{1}{i\omega_\ell - i\nu_n - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}}} \right) \times \left[\frac{1}{i\nu_n - \omega_{\boldsymbol{q}}} - \frac{1}{i\nu_n + \omega_{\boldsymbol{q}}} \right]$$

where I've written the phonon propagator out. Performing the contour-integral we obtain

$$\Sigma(\boldsymbol{k}, z) = \sum_{\boldsymbol{q}} g_{\boldsymbol{q}}^2 \left[\frac{1 + n_{\boldsymbol{q}} - f_{\boldsymbol{k}-\boldsymbol{q}}}{z - (\varepsilon_{\boldsymbol{k}-\boldsymbol{q}} + \omega_{\boldsymbol{q}})} + \frac{n_{\boldsymbol{q}} + f_{\boldsymbol{k}-\boldsymbol{q}}}{z - (\varepsilon_{\boldsymbol{k}-\boldsymbol{q}} - \omega_{\boldsymbol{q}})} \right]$$

at zero-temperature we can neglect the Bose-Einstein distribution. The first term in the self-energy corresponds to virtual phonon emission by an electron, whereas the second term corresponds to virtual phonon emission by a hole.

The real part of this energy contributes to the renormalised energy through the self-consistent equation

$$\varepsilon_{\boldsymbol{k}}^* = \varepsilon_{\boldsymbol{k}} + \mathrm{Re}\,(\Sigma(\boldsymbol{k}, \varepsilon_{\boldsymbol{k}}^*))$$

whereas the imaginary part contributes to the decay rate of the electron, which by means of the Cauchy-Dirac relation can be shown to give

$$\Gamma_{\boldsymbol{k}} = 2\pi \sum_{\boldsymbol{q}} g_{\boldsymbol{q}}^2 \left[(1 + n_{\boldsymbol{q}} - f_{\boldsymbol{k}-\boldsymbol{q}})\delta(\varepsilon_{\boldsymbol{k}} - (\varepsilon_{\boldsymbol{k}-\boldsymbol{q}} + \omega_{\boldsymbol{q}})) + (n_{\boldsymbol{q}} + f_{\boldsymbol{k}-\boldsymbol{q}})\delta(\varepsilon_{\boldsymbol{k}} - (\varepsilon_{\boldsymbol{k}-\boldsymbol{q}} - \omega_{\boldsymbol{q}})) \right]$$

which is reminiscent of something one may obtain from Fermi's Golden Rule.

IX. FLUCTUATION-DISSIPATION THEOREM AND LINEAR RESPONSE THEORY

A. Classical Harmonic Oscillator

The differential equation that describes a classical harmonic oscillator

$$m(\ddot{x} + \omega_0^2 x) + \eta\dot{x} = f(t)$$

can be solved by means of a Fourier transform

$$x(\omega) = \chi(\omega) f(\omega), \qquad \chi(\omega) = \frac{1}{m(\omega_0^2 - \omega^2) - i\omega\eta}$$

if we now denote $\chi = \chi' + i\chi''$ for $\chi', \chi'' \in \mathbb{R}$ (which we will do for this entire section) then

$$\chi''(\omega) = \frac{\omega\eta}{m^2(\omega_0^2 - \omega^2)^2 + \omega^2\eta^2} = \omega\eta\, |\chi(\omega)|^2$$

In the classical example we can relate this imaginary part to the noice spectrum, just as we will do for the quantum mechanical case:

$$S(\omega) = \langle |x(\omega)|^2 \rangle = \frac{2k_B T}{\omega} \chi''(\omega)$$

B. Fluctuations and Dissipation in a Quantum World

We can derive a fluctuation-dissipation theorem in quantum mechanics by means of spectral decomposition. Let us first consider a correlation function $S(t - t') = \langle A(t)A(t') \rangle$ and consider the eigenbasis of the full Hamiltonian $H\,|\lambda\rangle = E_\lambda\,|\lambda\rangle$:

$$S(t - t') = \langle A_H(t) A_H(t') \rangle = \sum_\lambda \langle\lambda| e^{-\beta(H-F)} A_H(t) A_H(t') |\lambda\rangle$$
$$= \sum_{\lambda\lambda'} e^{-\beta(E_\lambda - F)}\, \langle\lambda| A_H(t) |\lambda'\rangle \langle\lambda'| A_H(t') |\lambda\rangle$$

distributing the time-dependence from the operators to the states we get

$$S(t-t') = \sum_{\lambda\lambda'} e^{-\beta(E_\lambda - F)} \left| \langle\lambda|A|\lambda'\rangle\right|^2 e^{-i(E_{\lambda'}-E_\lambda)(t-t')}$$

which we can quite easily Fourier transform, because the only time-dependence is in the exponential

$$S(\omega) = \sum_{\lambda\lambda'} e^{-\beta(E_\lambda - F)} \left|A_{\lambda\lambda'}\right|^2 2\pi\delta(E_{\lambda'} - E_\lambda - \omega)$$

Similarly, for the retarded response function $\chi_R(t-t') = i\langle[A(t), A(t')]\rangle\Theta(t-t')$ we obtain

$$\chi_R(t) = i\sum_{\lambda\lambda'} e^{\beta F}\left(e^{-\beta E_\lambda} - e^{-\beta E_{\lambda'}}\right)\left|A_{\lambda\lambda'}\right|^2 e^{-i(E_{\lambda'}-E_\lambda)t}\Theta(t)$$

and Fourier transforming

$$\chi_R(\omega) = \underbrace{\sum_{\lambda\lambda'} e^{\beta F}\left(e^{-\beta E_\lambda} - e^{-\beta E_{\lambda'}}\right)\left|A_{\lambda\lambda'}\right|^2}_{\Upsilon} \frac{1}{(E_{\lambda'}-E_\lambda) - \omega - i\delta}$$

where we've included a convergence factor in the Fourier transformation. We have that $\chi_R(\omega) = \chi(\omega + i\delta)$ so if we denote $\chi(\omega + i\delta) = \chi'(\omega) + i\chi''(\omega)$ we get that

$$\chi(\omega + i\delta) = \Upsilon\left(\mathcal{P}\frac{1}{(E_{\lambda'}-E_\lambda) - \omega} + i\pi\delta\left[(E_{\lambda'}-E_\lambda) - \omega\right]\right)$$

Note that

$$\chi'(\omega) = \int \frac{d\omega'}{\pi}\mathcal{P}\frac{1}{\omega' - \omega}\chi''(\omega')$$

which tells us that

$$\chi(z) = \int \frac{d\omega'}{\pi}\frac{1}{\omega' - z}\,\chi''(\omega')$$

which is a *Kramers-Kroning relation.*

Using our expressions for $S(\omega)$ and $\chi''(\omega)$ we can show that

$$S(\omega) = 2\hbar(1 + n_{\mathrm{B}}(\hbar\omega))\chi''(\omega)$$

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