Title

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Contents

Chapter 1

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TODO before the lectures note, there are some content are from slides
topics

1. quantum harmonic oscillator

2. creation and annihilation operators

3. Fock space

4. real space wave functions

5. coherent state

6. propagator

goals

1. QM warm-up

2. do some Gaussian integrals

3. change some basis

As a warm-up, consider the QHO in one-dimension.

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$
$$[\hat{x}, \hat{p}] = i\hbar$$

in position basis, $\hat{p} = -i\hbar\partial_x$. check

$$\begin{aligned}[\hat{x}, \hat{p}]\, f\left(x\right) &= -i\hbar x\partial_x f + i\hbar\partial_x\left(xf\right) \\ &= -i\hbar x\partial_x f + i\hbar f + i\hbar x\partial_x f \\ &= i\hbar f\end{aligned}$$

In position basis, the eigenvalues satisfy

$$-\frac{\hbar^2}{2m}\partial_x^2\phi\left(x\right) + \frac{1}{2}m\omega^2 x^2\phi\left(x\right) = E\phi\left(x\right)$$

We can, however, solve it algebraically (without going to the position basis). First, let's adopt some dimensionless coordinates. We know $[\hat{H}] = [\hbar\omega]$; write

$$\hat{H} = \frac{\hbar\omega}{2}\left(\frac{m\omega}{\hbar}\hat{x}^2 + \frac{1}{m\hbar\omega}\hat{p}^2\right)$$

Define

$$\hat{X} = \sqrt{\frac{m\omega}{\hbar}}\hat{x}, \quad \hat{P} = \frac{1}{\sqrt{m\hbar\omega}}\hat{p}$$

Then

$$\left[\hat{X}, \hat{P}\right] = \sqrt{\frac{m\omega}{\hbar}}\frac{1}{\sqrt{m\hbar\omega}}\left[\hat{x}, \hat{p}\right] = i$$

Let's now define

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\hat{X} - i\hat{P}\right), \quad \hat{a} = \frac{1}{\sqrt{2}}\left(\hat{X} + i\hat{P}\right)$$

which gives

$$\hat{a}^\dagger\hat{a} = \frac{1}{2}\left(\hat{X} - i\hat{P}\right)\left(\hat{X} + i\hat{P}\right) = \frac{1}{2}\left(\hat{X}^2 + \hat{P}^2 + i\left[\hat{X}, \hat{P}\right]\right)$$
$$\hat{H} = \frac{\hbar\omega}{2}\left(\hat{X}^2 + \hat{P}^2\right) = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

This gives a convenient way to construct the spectrum. First, check

$$\left[\hat{a}, \hat{a}^\dagger\right] = \frac{1}{2}\left[\hat{X} + i\hat{P}, \hat{X} - i\hat{P}\right] = \frac{1}{2}i\left[\hat{P}, \hat{X}\right] - \frac{1}{2}i\left[\hat{X}, \hat{P}\right] = 1$$

So, if $\hat{H}|E\rangle = E|E\rangle$, we have

$$\begin{aligned}
\hat{H}\left(\hat{a}^\dagger|E\rangle\right) &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hat{a}^\dagger|E\rangle \\
&= \hbar\omega\left(\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \frac{1}{2}\hat{a}^\dagger\right)|E\rangle \\
&= \hbar\omega\left(\hat{a}^{\dagger 2}\hat{a} + \hat{a}^\dagger + \frac{1}{2}\hat{a}^\dagger\right)|E\rangle \\
&= \hat{a}^\dagger\left(\hat{H} + \hbar\omega\right)|E\rangle \\
&= \hat{a}^\dagger\left(E + \hbar\omega\right)|E\rangle \\
&= \left(E + \hbar\omega\right)\left(\hat{a}^\dagger|E\rangle\right)
\end{aligned}$$

which means $\hat{a}^\dagger|E\rangle$ is another eigenstate with energy $E + \hbar\omega$. This relates the different eigenstates. We just need to find the ground state. Since

$$\langle\phi|\hat{a}^\dagger\hat{a}|\phi\rangle = \|\hat{a}|\phi\rangle\|^2 \geq 0, \quad \forall|\phi\rangle$$

If $\hat{a}$ has a null vector, then it will be the ground state. Let's just posit such a state exist, i.e.,

$$\exists|0\rangle \quad \text{s.t.} \quad \hat{a}|0\rangle = 0$$

Then the eigen spectrum is given by

$$\left\{|n\rangle; E_n = \hbar\omega\left(n + \frac{1}{2}\right)\right\}$$

We can also find the matrix elements of $\hat{a}, \hat{a}$ in this eigen basis. Recall

$$|n+1\rangle = \mathcal{N}\hat{a}^\dagger|n\rangle$$

where $\mathcal{N} \in \mathbb{R}^+$ is the normalization factor. Also, from the preceding discussion we have

$$\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle$$

The normalization is then

$$\begin{aligned}
1 = \langle n+1|n+1\rangle &= \mathcal{N}^2\langle n|\hat{a}\hat{a}^\dagger|n\rangle \\
&= \mathcal{N}^2\langle n|\left(\hat{a}^\dagger\hat{a} + 1\right)|n\rangle \\
&= (n+1)\mathcal{N}^2
\end{aligned}$$

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

similar argument gives $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$. In a matrix picture.

$$\hat{a}^\dagger = \begin{bmatrix} l0 & & & & \\ 1 & 0 & & & \\ & \sqrt{2} & 0 & & \\ & & \sqrt{3} & 0 & \\ & & & \ddots & \ddots \end{bmatrix}, \quad \hat{a} = \begin{bmatrix} l0 & 1 & & & \\ & 0 & \sqrt{2} & & \\ & & 0 & \sqrt{3} & \\ & & & 0 & \ddots \\ & & & & \ddots \end{bmatrix}$$

This is a "number" basis. We call it the Fock space. It's separable (but infinite dimensional). We are only left with showing $\hat{a}|0\rangle = 0$ *TODO-UNKNOWN-WORD* solution. To do so, let's go back to the position basis. Recall

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\hat{X} + i\hat{P}\right) = \frac{1}{\sqrt{2}}\left(X + i\left(-i\frac{\partial}{\partial X}\right)\right) = \frac{1}{\sqrt{2}}\left(X + \frac{\partial}{\partial X}\right)$$

$$\hat{a}|\phi_0\rangle = 0$$

$$\left(X + \frac{\partial}{\partial X}\right)\phi_0(X) = 0$$

$$\int \frac{d\phi_0(X)}{\phi_0(X)} = -\int X dX$$

$$\phi_0(X) = \mathcal{N} e^{-X^2/2}$$

Which is a Gaussian. Recall $X = \sqrt{\frac{m\omega}{\hbar}} x$,

$$\phi_0(x) = \mathcal{N} e^{-m\omega x^2/(2\hbar)}$$

To get the normalization,

$$1 = \int_{-\infty}^{\infty} |\phi_0(x)|^2 \, dx = \mathcal{N}^2 \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar} dx$$

$$= \mathcal{N}^2 \sqrt{\frac{\hbar}{2m\omega}} \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar} \exp\left(-\left(\sqrt{\frac{\hbar}{2m\omega}} x\right)^2 /2\right) d\left(\sqrt{\frac{\hbar}{2m\omega}} x\right)$$

$$= \mathcal{N}^2 \sqrt{\frac{\hbar}{2m\omega}} \sqrt{2\pi}$$

$$\mathcal{N} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/(2\hbar)}$$

Side note: Gaussian integration

$$\int_{-\infty}^{\infty} e^{-ax^2/2} dx = \sqrt{\frac{2\pi}{a}}, \quad a > 0$$

A standard discussion will next introduce the real-space wave function of the excited states through the Hermite polynomial. Let's try to avoid that!

1.1 coherent state

We have seen that the creation and annihilation operators provides a simple way to analyze the QHO. Let's now take these as the "coordinates" for our problem. Recall position basis $\hat{x}|x\rangle = x|x\rangle$. Similarly, we consider the eigenstates of the form

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle; \quad \alpha \in \mathbb{C}$$

E.g., The ground state $\hat{a}|0\rangle = 0|0\rangle = 0$. To solve for the eigenstate, write

$$|\alpha\rangle = \sum_{n=0} C_n(\alpha) |n\rangle$$

Then,

$$
\begin{aligned}
\hat{a}|\alpha\rangle &= \sum_{n=0} C_n\left(\alpha\right) \hat{a}|n\rangle \\
&= \sum_{n=0} C_n\left(\alpha\right) \sqrt{n}|n-1\rangle \\
&= \sum_{n=0} C_{n+1}\left(\alpha\right) \sqrt{n+1}|n\rangle
\end{aligned}
$$

versus

$$
\alpha|\alpha\rangle = \sum_{n=0} C_n\left(\alpha\right) \alpha|n\rangle
$$

we conclude

$$
C_{n+1}\left(\alpha\right) = \frac{\alpha C_n\left(\alpha\right)}{\sqrt{n+1}} = \frac{\alpha^2 C_{n-1}\left(\alpha\right)}{\sqrt{(n+1)\,n}} = \cdots = \frac{\alpha^{n+1} C_0\left(\alpha\right)}{\sqrt{(n+1)!}}
$$

Note: $|\alpha\rangle$ is a superposition of $\{|n\rangle\}$. It's not an energy eigenstate (unless $\alpha = 0$).

We have

$$
|\alpha\rangle = C_0\left(\alpha\right) \sum_{n=0} \frac{\alpha^n}{\sqrt{n!}}|n\rangle
$$

Normalization:

$$
1 = \langle\alpha|\alpha\rangle = |C_0\left(\alpha\right)|^2 \sum_{m,n=0} \frac{\left(\alpha^*\right)^m \alpha^n}{\sqrt{m!}\sqrt{n!}} \langle m|n\rangle
$$

$$
= |C_0\left(\alpha\right)|^2 \sum_{m=0} \frac{|\alpha|^{2m}}{m!}
$$

$$
= |C_0\left(\alpha\right)|^2 e^{|\alpha|^2}
$$

$$
C_0\left(\alpha\right) = e^{-|\alpha|^2/2}
$$

$$
|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0} \frac{\alpha^n}{\sqrt{n!}}|n\rangle
$$

This looks almost like the exponential! Recall

$$
|n\rangle = \frac{\hat{a}^\dagger}{\sqrt{n}}|n-1\rangle = \frac{\hat{a}^{\dagger 2}}{\sqrt{n\left(n-1\right)}}|n-2\rangle = \cdots = \frac{\hat{a}^{\dagger n}}{\sqrt{n!}}|0\rangle
$$

So,

$$
\begin{aligned}
|\alpha\rangle &= e^{-|\alpha|^2/2} \sum_{n=0} \frac{\alpha^n \hat{a}^{\dagger n}}{\sqrt{n!}\sqrt{n!}}|0\rangle \\
&= e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger}|0\rangle
\end{aligned}
$$

Chapter 2

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topics:

1. QHO: displacement operator and propagator

2. Phonons: from QHO to second quantization

 goals

1. continue with our QM warm-up

2. introduce the propagator, Green function

3. free phonons as our first "many-body" bosonic problem

2.1   QHO

Recall the QHO Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\hat{X} + i\hat{P}\right)$$

$$\hat{X} = \sqrt{\frac{m\omega}{\hbar}}\hat{x}$$

$$\hat{P} = \frac{1}{\sqrt{m\hbar\omega}}\hat{p}$$

Coherent states are labeled by $\alpha \in \mathcal{C}$

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$$

Displacement operator: unitary to rotate between coherent states, let

$$\hat{D}\left(\alpha\right) = e^{\alpha\hat{a}^{\dagger} - \alpha^{*}\hat{a}}$$

where $\alpha\hat{a}^{\dagger} - \alpha^{*}\hat{a}$ is anti-Hermitian.

Baker-Campbell-Hausdorff formula: for $[\hat{A}, \hat{B}]$ central ($[\hat{A}, \hat{B}]$ commutes with both $\hat{A}\&\hat{B}$)

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A} + \hat{B} + \frac{1}{2}\left[\hat{A}, \hat{B}\right]}$$

By BCH, and noting $\left[\alpha\hat{a}^{\dagger}, -\alpha^{*}\hat{a}\right] = |\alpha|^{2}$ is central,

$$e^{\alpha\hat{a}^{\dagger}}e^{-\alpha^{*}\hat{a}} = e^{\alpha\hat{a}^{\dagger} - \alpha^{*}\hat{a}}e^{\left[\alpha\hat{a}^{\dagger}, -\alpha^{*}\hat{a}\right]/2}$$

$$\hat{D}\left(\alpha\right) = e^{\alpha\hat{a}^{\dagger} - \alpha^{*}\hat{a}} = e^{-|\alpha|^{2}/2}e^{\alpha\hat{a}^{\dagger}}e^{-\alpha^{*}\hat{a}}$$

Check

$$\hat{D}\left(\alpha\right)|0\rangle = e^{-|\alpha|^{2}/2}e^{\alpha\hat{a}^{\dagger}}e^{-\alpha^{*}\hat{a}}|0\rangle = e^{-|\alpha|^{2}/2}e^{\alpha\hat{a}^{\dagger}}|0\rangle = |\alpha\rangle$$

"Displacement"? compute (also using BCH formula)

$$\begin{aligned}
\hat{D}^{\dagger}\left(\alpha\right)\hat{a}\hat{D}\left(\alpha\right) &= e^{-\alpha\hat{a}^{\dagger} + \alpha^{*}\hat{a}}\hat{a}e^{\alpha\hat{a}^{\dagger} - \alpha^{*}\hat{a}} \\
&= \hat{a} + \left[-\alpha\hat{a}^{\dagger} + \alpha^{*}\hat{a}, \hat{a}\right] \\
&= \hat{a} + \alpha
\end{aligned}$$

$$\hat{D}^{\dagger}\left(\alpha\right)\hat{a}^{\dagger}\hat{D}\left(\alpha\right) = \hat{a}^{\dagger} + \alpha^{*}$$

E.g., 1. Average energy

$$\begin{aligned}
\langle\alpha|\hat{H}|\alpha\rangle &= \langle 0|\hat{D}^{\dagger}\left(\alpha\right)\hbar\omega\left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}\right)\hat{D}\left(\alpha\right)|0\rangle \\
&= \langle 0|\hbar\omega\left(\left(\hat{a}^{\dagger} + \alpha^{*}\right)\left(\hat{a} + \alpha\right) + \frac{1}{2}\right)|0\rangle \\
&= \frac{\hbar\omega}{2} + \hbar\omega\langle 0|\left(\hat{a}^{\dagger}\hat{a} + \hat{a}^{\dagger}\alpha + \alpha^{*}\hat{a} + |\alpha|^{2}\right)|0\rangle \\
&= \hbar\omega\left(|\alpha|^{2} + \frac{1}{2}\right)
\end{aligned}$$

Not an eigenstate, and has a continuously adjustable average energy.

E.g., 2. Expectation values for $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$

$$\alpha = \langle\alpha|\left(\hat{X} + i\hat{P}\right)|\alpha\rangle = \frac{1}{\sqrt{2}}\langle\alpha|\hat{X}|\alpha\rangle + \frac{i}{\sqrt{2}}\langle\alpha|\hat{P}|\alpha\rangle$$

It's natural for us to parametrize the complex variable

$$\alpha = \frac{1}{\sqrt{2}}\left(X_{\alpha} + iP_{\alpha}\right), X_{\alpha}, P_{\alpha} \in \mathbb{R}$$

and simply the expectation values

$$X_\alpha = \langle \alpha | \hat{X} | \alpha \rangle = \sqrt{\frac{m\omega}{\hbar}} \langle \alpha | \hat{x} | \alpha \rangle$$

$$P_\alpha = \langle \alpha | \hat{P} | \alpha \rangle = \frac{1}{\sqrt{m\hbar\omega}} \langle \alpha | \hat{P} | \alpha \rangle$$

In particular, the ground state for the shifted Hamiltonian

$$\hat{H}' = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 (\hat{x} - x_0)^2$$

will be the coherent state $\hat{D}(\sqrt{\frac{m\omega}{\hbar}} x_0) |0\rangle$.

E.g., 3. Composition of displacement operator

We can think of $\hat{D}(\alpha)$ as a "displacement" in the phase space. It is natural to look how such transformation compose.

$$
\begin{aligned}
\hat{D}(\alpha) \hat{D}(\beta) &= e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}} e^{\beta \hat{a}^\dagger - \beta^* \hat{a}} \\
&= e^{(\alpha+\beta)\hat{a}^\dagger - (\alpha^* + \beta^*)\hat{a}} e^{\left[\alpha \hat{a}^\dagger - \alpha^* \hat{a}, \beta \hat{a}^\dagger - \beta^* \hat{a}\right]/2} \\
&= \hat{D}(\alpha + \beta) e^{\frac{1}{2}\left(-\alpha^* \beta [\hat{a}, \hat{a}^\dagger] - \alpha \beta^* [\hat{a}^\dagger, \hat{a}]\right)} \\
&= \hat{D}(\alpha + \beta) e^{(\alpha\beta^* - \alpha^*\beta)/2} \\
&= \hat{D}(\alpha + \beta) e^{i\text{Im}(\alpha\beta^*)}
\end{aligned}
$$

Note:

$$\hat{D}(\alpha) \hat{D}(-\alpha) = \hat{D}(0) = I \quad \Rightarrow \quad \hat{D}^\dagger(\alpha) = \hat{D}(-\alpha)$$

Overlap between coherent states: we now see that coherent states are *not* orthogonal:

$$
\begin{aligned}
\langle \alpha | \beta \rangle &= \langle 0 | \hat{D}^\dagger(\alpha) \hat{D}(\beta) | 0 \rangle \\
&= \langle 0 | \hat{D}(-\alpha + \beta) | 0 \rangle e^{-i\text{Im}(\alpha\beta^*)} \\
&= e^{-|\alpha - \beta|^2/2} e^{-i\text{Im}(\alpha\beta^*)} \\
&= e^{-\left(|\alpha|^2 + |\beta|^2\right)/2} e^{\alpha^* \beta}
\end{aligned}
$$

we usually say they form an over-complete basis.

Resolution of identity

$$
\begin{aligned}
\int d^2\alpha \langle n | \alpha \rangle \langle \alpha | m \rangle &= \int d^2\alpha \frac{(\alpha^*)^n \alpha^m}{\sqrt{n!m!}} e^{-|\alpha|^2} \\
&= \delta_{nm} \int d^2\alpha \frac{|\alpha|^{2n}}{n!} e^{-|\alpha|^2} \\
&= \pi \delta_{nm} \int d^2 r \frac{r^{2n}}{n!} e^{-r^2} \\
&= \pi \delta_{nm}
\end{aligned}
$$

$$I = \frac{1}{\pi} \int d^2\alpha |\alpha\rangle\langle\alpha|$$

Now, the coherent states are not (generally) energy eigenstates, so they evolve under time:

$$e^{-i\hat{H}t/\hbar}|\alpha\rangle = \sum_{n=0} |n\rangle\langle n|\alpha\rangle e^{-i\omega t\left(n+\frac{1}{2}\right)}$$

$$= \sum_{n=0} |n\rangle \frac{\alpha^n}{\sqrt{n!}} e^{-i\omega t\left(n+\frac{1}{2}\right)}$$

$$= e^{-i\omega t/2} \sum_{n=0} |n\rangle \frac{\left(\alpha e^{-i\omega t}\right)^n}{\sqrt{n!}}$$

$$= |\alpha e^{-i\omega t}\rangle e^{-i\omega t/2}$$

And we can define the propagator

$$K\left(\beta,\alpha;t\right) = \langle\beta|e^{-i\hat{H}t/\hbar}|\alpha\rangle$$

$$= e^{-i\omega t/2}\langle\beta|\alpha e^{-i\omega t}\rangle$$

$$= e^{-i\omega t/2}e^{-\left(|\alpha|^2+|\beta|^2\right)/2}\exp\left(\alpha e^{-i\omega t}\beta^*\right)$$

2.2   Propagator and Green's function

Why worry about the propagator?

Level 1: It allows us to solve for the general dynamics. Suppose we have an initial state $|\phi\rangle$. Its time evolution in Schrodinger's picture is

$$|\phi\left(t\right)\rangle = e^{-i\hat{H}t/\hbar}|\phi\rangle$$

If we specify our initial state in some basis, and suppose we have pre-computed the propagator in that basis, then we can readily compute the time evolved state through a "matrix multiplication".

energy basis

$$|\phi\rangle = \sum_{n=0} |n\rangle\langle n|\phi\rangle = \sum_{n=0} |n\rangle\phi_n$$

$$e^{-i\hat{H}t/\hbar} = \sum_{n=0} |n\rangle\langle n|e^{-in\omega t}e^{-i\omega t/2}$$

$$|\phi\left(t\right)\rangle = \sum_{n=0} |n\rangle\phi_n e^{-in\omega t}e^{-i\omega t/2}$$

Coherent states

$$|\phi\rangle = \int \frac{d^2\alpha}{\pi}|\alpha\rangle\langle\alpha|\phi\rangle = \int \frac{d^2\alpha}{\pi}|\alpha\rangle\phi\left(\alpha\right)$$

$$|\phi\left(t\right)\rangle = \int \frac{d^2\alpha d^2\beta}{\pi^2}|\beta\rangle\langle\beta|e^{-i\hat{H}t/\hbar}|\alpha\rangle\phi\left(\alpha\right)$$

$$= \int \frac{d^2\beta}{\pi}|\beta\rangle \int \frac{d^2\alpha}{\pi}K\left(\beta,\alpha;t\right)\phi\left(\alpha\right)$$

$$= \int \frac{d^2\beta}{\pi}|\beta\rangle\phi\left(\beta;t\right)$$

position basis

$$K\left(x',x;t\right) = \langle x'|e^{-i\hat{H}t/\hbar}|x\rangle$$

$$|\phi\rangle = \int dx|x\rangle\langle x|\phi\rangle = \int dx|x\rangle\phi\left(x\right)$$

$$\phi\left(x',t\right) = \langle x'|t\rangle = \int dxK\left(x',x;t\right)\phi\left(x\right)$$

Level 2: It allows us to probe what are the excitations above the ground state, which are really what we are interested in (a system permanently stuck in the ground state has no dynamics and hence no physics). Start with the ground state $|\Omega\rangle$, we can consider doing two things.

1. perturbing the system by an operator (e.g., your finger)

2. time evolution for some time

We can do it in two orders: $e^{-i\hat{H}t/\hbar}\hat{f}|\Omega\rangle$ versus $\hat{f}e^{-i\hat{H}t/\hbar}|\Omega\rangle$. How colse are these two states? We can measure their overlap

$$\langle\Omega|e^{i\hat{H}t/\hbar}\hat{f}^\dagger e^{-i\hat{H}t/\hbar}\hat{f}|\Omega\rangle = e^{i\omega_\Omega t}\langle\Omega|\hat{f}^\dagger e^{-i\hat{H}t/\hbar}\hat{f}|\Omega\rangle$$

where $\langle\Omega|\hat{f}^\dagger e^{-i\hat{H}t/\hbar}\hat{f}|\Omega\rangle$ is a "propagator" in some basis.

Notes

1. Some of you may already recognize we are really talking about an auto-correlation ffunction in the Heisenberg picture, which is simply a "Green's function"

2. How to extract the energies of the excitation? Fourier transform! We will be using that extensively later

Level 3: It allows us to treat perturbations to our system. The time-evolution operator solves the equation

$$\left(i\hbar\partial_t - \hat{H}\right)e^{-i\hat{H}t/\hbar} = 0$$

$$K\left(x;t\right) = \langle x|e^{-i\hat{H}t/\hbar}|0\rangle$$

$$\left(i\hbar\partial_t - \hat{H}\left(x,\partial_x,\partial_x^2\right)\right)K\left(x;t\right) = 0$$

Now let's define

$$\Theta\left(t\right) = \begin{cases} 1, & t > 0 \\ 0, & t \leq 0 \end{cases}$$

$$G\left(x;t\right) = \frac{1}{i\hbar}\Theta\left(t\right)K\left(x;t\right)$$

where $\Theta(t)$ is known as the Heaviside step function.

$$\frac{d}{dx}\Theta\left(x\right) = \delta\left(x\right)$$

Note: consider the integral with $a < b$

$$\int_a^b dx\,\Theta\left(x - x_0\right)f\left(x\right) = \begin{cases} F\left(b\right) - F\left(a\right), & x_0 < a < b \\ F\left(b\right) - F\left(x_0\right), & a \leq x_0 \leq b \\ 0, & a < b < x_0 \end{cases}$$

$$\frac{d}{dx_0}\int_a^b dx\,\Theta\left(x - x_0\right)f\left(x\right)$$
$$= \begin{cases} 0, & x_0 \notin [a,b] \\ -f\left(x_0\right), & x_0 \in [a,b] \end{cases}$$
$$= -\int_a^b dx\,\delta\left(x - x_0\right)f\left(x\right)$$

These manipulation make sense when the "function" are used to weight an integral. One usually thinks of them as "distribution" method.

Now let's compute

$$\left(i\hbar\partial_t - \hat{H}\left(x, \partial_x, \partial_x^2\right)\right)G\left(x,t\right)$$
$$= \frac{1}{i\hbar}\left(i\hbar\partial_t - \hat{H}\left(x, \partial_x, \partial_x^2\right)\right)\left(\Theta\left(t\right)K\left(x;t\right)\right)$$
$$= \left(\partial_t\Theta\left(t\right)\right)K\left(x,t\right) + \frac{1}{i\hbar}\Theta\left(t\right)\left(i\hbar\partial_t - \hat{H}\left(x, \partial_x, \partial_x^2\right)\right)K\left(x;t\right)$$
$$= \delta\left(t\right)K\left(x;t\right)$$
$$= \delta\left(t\right)K\left(x;0\right)$$
$$= \delta\left(t\right)\delta\left(x\right)$$

I.e., G solves the differential equation

$$\left(i\hbar\partial_t - \hat{H}\left(x, \partial_x, \partial_x^2\right)\right)G\left(x,t\right) = \delta\left(t\right)\delta\left(x\right)$$

It provides the basis for solving the more general inhomogeneous equation. If we have both space and time translation invariance (not true for QHO)

$$\left(i\hbar\partial_t - \hat{H}\left(x, \partial_x, \partial_x^2\right)\right)G'\left(x,t\right) = f\left(x,t\right)$$

$$G'\left(x,t\right) = \int dx'\,dt'\,G\left(x - x', t - t'\right)f\left(x', t'\right)$$

Notes:

1. This is *THE* mathematical meaning of a "Green function"

2. In physics, the meaning and usage of "Green functions" and "propagator" are kind of messed up

3. As discussed in "level 2", when we say "Green function" in our context we really refer to some correlation function

When does such an inhomogeneous equation show up? Imagine a perturbation to the system:

$$\hat{H} = \hat{H}_0 + \hat{V}$$

$$\left(i\hbar\partial_t - \hat{H}\right)|\Psi\rangle = 0$$

$$\left(i\hbar\partial_t - \hat{H}_0\right)|\Psi\rangle = \hat{V}|\Psi\rangle$$

An "inhomogeneous" equation "solved" by the bare Green's function!

Of course, the true story is (much) more complicated than that. Anyway this suggests the bare Green functions from the starting point for solving the perturbed system. This is the general theme of perturbative quantum many-body theory.

2.3 Free phonons

So, we have started our "many-body" course with exactly one particle in a harmonic trap. Let's now see how we can build from there and go to a "many-body" setup. We set $\hbar = 1$ from now on.

Note: this will be a review for those of you who have taken solid state / quantum statistics mechanics.

Consider a collection of atoms, with their real-space coordinates denoted by $\vec{R}_i; i = 1, \cdots, V; V \propto$ volume. The atoms will have some mutual repulsion / attraction, and we suppose they have a collective elastic energy $\mathcal{V}$. The physical origin of all these energy can be complicated, e.g., maybe it contains electronic contribution (since the electronic ground state energy would depend on the atom locations). We don't worry about the "microscopic" details here. Instead, let's just suppose a stable minimum energy configuration exists, and we study the deviation from the equilibrium.

$$\vec{R}_i = \vec{R}_i^\circ + \vec{u}_i$$

$$\mathcal{V}\left(\left\{\vec{R}_i\right\}\right) \approx \mathcal{V}\left(\left\{\vec{R}_i^\circ\right\}\right) + \frac{1}{2}\sum_{i,j,\alpha,\beta}\frac{\partial^2\mathcal{V}}{\partial R_i^\alpha \partial R_j^\beta}u_i^\alpha u_j^\beta + O\left(u^3\right)$$

The index $alpha, \beta$ go through $1, \cdots, d$. Note: terms linear in u vanish at equilibrium.

Now, we can go quantum mechanical. The Hamiltonian is

$$\hat{H} = \sum_{i,\alpha} \frac{\hat{p}_i^{\alpha 2}}{2m_i} + \frac{1}{2} \sum_{i,j,\alpha,\beta} \hat{u}_i^{\alpha} \left(\frac{\partial^2 \mathcal{V}}{\partial R_i^{\alpha} \partial R_j^{\beta}} \right) \hat{u}_j^{\beta}$$

Here $\hat{p}_i^{\alpha}$ and $\hat{u}_i^{\alpha}$ are conjugate variables $\left[\hat{u}_i^{\alpha}, \hat{p}_j^{\beta} \right] = i\delta_{\alpha\beta}\delta_{ij}$. The masses m_i could be different for different i. Let's first rescale

$$\hat{\pi}_i^{\alpha} = \frac{\hat{p}_i^{\alpha}}{\sqrt{m_i}}; \quad \hat{\phi}_i^{\alpha} = \hat{u}_i^{\alpha} \sqrt{m_i}$$

which preserves the canonical commutation relation

$$\left[\hat{\phi}_i^{\alpha}, \hat{\pi}_j^{\beta} \right] = i\delta_{\alpha\beta}\delta_{ij}$$

Define

$$D_{ij}^{\alpha\beta} = \frac{1}{\sqrt{m_i m_j}} \frac{\partial^2 \mathcal{V}}{\partial R_i^{\alpha} \partial R_j^{\beta}}$$

which is called the "dynamical matrix"

$$\hat{H} = \frac{1}{2} \sum_{i,\alpha} \hat{\pi}_i^{\alpha 2} + \frac{1}{2} \sum_{i,j,\alpha,\beta} \hat{\phi}_i^{\alpha} D_{ij}^{\alpha\beta} \hat{\phi}_j^{\beta}$$

such a Hamiltonian can be solved by diagonalizing the dynamical matrix, which is real symmetric (and hence unitary). I.e., there exists an orthogonal matrix O

$$ODO^T = \text{diag} \left\{ \left(\omega_1^1\right)^2, \left(\omega_1^2\right)^2, \left(\omega_2^3\right)^2, \left(\omega_2^1\right)^2, \left(\omega_2^2\right)^2, \left(\omega_2^3\right)^2, \cdots, \left(\omega_V^3\right)^2 \right\}$$

here, we have used the stability assumption to write the eigenvalues as $\omega_i^2 \geq 0$. This is a "one-particle" diagonalization: we have so far only considered the dynamical matrix of size $d \cdot V$. But as is typical for such non-interacting problem, it's basically the same as solving the "many-body" problem. To see why, let's first transform the operators by the matrix

$$\hat{\Pi}_i^{\alpha} = O_{ij}^{\alpha\beta} \hat{\pi}_j^{\beta}, \quad \hat{\Phi}_i^{\alpha} = O_{ij}^{\alpha\beta} \hat{\phi}_j^{\beta}$$

where repeated indices are summed.

Chapter 3

lec03 202200211

topics:

1. free phonons: solving with (without) and with (without) invariance

2. acoustic versus optical phonons

3. finite temperature: density matrix

goals

1. getting used to Fourier transformation and canonical transformation

2. lightning review of quantum statistics mechanics

recall we have the phonon Hamiltonian

$$hatH = \frac{1}{2} \prod_{i,\alpha} (\hat{\pi}_i^\alpha)^2 + \frac{1}{2} \sum_{i,j,\alpha,\beta} \hat{\phi}_i^\alpha D_{ij}^{\alpha\beta} \hat{\phi}_j^\beta$$

which we claim is diagonalized by

$$ODO^T = \text{diag} \{\omega_1^\alpha, \omega_2^\alpha, \cdots \}, \quad \omega_i^\alpha \geq 0.$$

This basis rotation induces one on the the operators

$$\hat{\Pi}_i^\alpha = O_{ij}^{\alpha\beta} \hat{\pi}_j^\beta, \quad \hat{\Phi}_i^\alpha = O_{ij}^{\alpha\beta} \hat{\phi}_j^\beta$$

we can verify

$$\begin{aligned}
\left[\hat{\Phi}_i^\alpha, \hat{\Phi}_j^\beta \right] &= O_{il}^{\alpha r} O_{jm}^{\beta s} \left[\hat{\phi}_l^r, \hat{\phi}_m^s \right] \\
&= i O_{il}^{\alpha r} O_{jm}^{\beta s} \delta_{lm} \delta_{rs} \\
&= i O_{il}^{\alpha r} \left(O^T \right)_{lj}^{r\beta} \\
&= i \left(OO^T \right)_{ij}^{\alpha\beta} \\
&= i \delta_{ij} \delta_{\alpha\beta}
\end{aligned}$$

all other commutators vanish.

Note: we simply asserted that we are free to perform a linear transformation on the $\hat{\pi}$ and $\hat{\phi}$. But it may be more pleasing to show that there exists a unitary operator (acting on the Hilbert space) which transforms the operators in the way described. This is usually called a canonical transformation and is generated by a bilinears of $\hat{a}$&$\hat{a}^\dagger$.

As such, the transformed Hamiltonian reads

$$\hat{H}' = \frac{1}{2}\sum_{i,\alpha}\left(\hat{\Pi}_i^\alpha\right)^2 + (\omega_i^\alpha)^2\left(\hat{\Phi}_i^\alpha\right)^2$$
$$= \sum_{i,\alpha}\omega_i^\alpha\left(\hat{a}_i^{\alpha\dagger}\hat{a}_i^\alpha + \frac{1}{2}\right)$$

The compound index $i\alpha$ can be viewed as a collective mode index. The Hamiltonian is simply $d \cdot V$ decoupled QHO, and the Hilbert space is now recognized with the tensor product of the $d \cdot V$ Fock spaces associated with them.

Summary: The diagonalization of the one-particle "dynamical matrix" gives us the frequencies of the "normal modes". This is the same as the classical problems. The quantum part simply comes from quantizing each of the individual harmonic oscillator, and recognizing they each come with a Fock space. The same is true for "free fermions", e.g., tight-binding models or even BdG mean-field.

So far, we have not assumed anything about the phonon problem except that we keep only up to quadratic terms. This is sometimes called a "harmonic approximation".

Let's now go to the more conventional solid-state setup and assume we have lattice translation symmetry of a crystal, i.e., $D_{ij}^{\alpha\beta}$ depends only on the distance between the equilibrium positions $\delta_{\vec{R}} = \vec{R}_j - \vec{R}_i$. To this end, let's switch notation slightly $D_{ij}^{\alpha\beta} \to D_{\vec{R}\vec{R}'}^{\alpha\beta}$.

Here, we let $\vec{R}, \vec{R}'$ denote unit cell coordinates. There could be multiple atoms inside each unit cell, and we group all degrees of freedom inside a unit cell (spatial dimensions times number of atoms inside a unit cell) in the indices α, β.

Note: This is a very solid-state-specific kind of worry. If you don't want to worry about that, then don't. Our approach works in the same way anyway.

The presence of (lattice) translation implies (crystal) momentum is a good quantum number. In other words, the eigenstates of the Hamiltonian can be labeled by their momenta. In our context, that's just a verbal of saying we can

Block-diagonalize the dynamical matrix upon Fourier transform. Explicitly

$$\frac{1}{V}\sum_{\vec{R},\vec{R}'}D^{\alpha\beta}_{\vec{R}\vec{R}'}e^{-i\vec{q}\cdot\vec{R}}e^{-i\vec{q}'\cdot\vec{R}'}$$

$$\stackrel{\delta_{\vec{R}}=\vec{R}'-\vec{R}}{=}\frac{1}{V}\sum_{\vec{R},\delta_{\vec{R}}}D^{\alpha\beta}_{\delta_{\vec{R}}}e^{-i\vec{q}\cdot\vec{R}}e^{-i\vec{q}'\cdot\left(\vec{R}+\delta_{\vec{R}}\right)}$$

$$=\sum_{\delta_{\vec{R}}}D^{\alpha\beta}_{\delta_{\vec{R}}}e^{-i\vec{q}'\cdot\delta_{\vec{R}}}\frac{1}{V}\sum_{\vec{R}}e^{-i\left(\vec{q}+\vec{q}'\right)\cdot\vec{R}}$$

$$=\sum_{\delta_{\vec{R}}}D^{\alpha\beta}_{\delta_{\vec{R}}}e^{i\vec{q}\cdot\delta_{\vec{R}}}\delta\left(\vec{q}+\vec{q}'\right)$$

$$D^{\alpha\beta}_{\vec{q}}=\sum_{\delta_{\vec{R}}}D^{\alpha\beta}_{\delta_{\vec{R}}}e^{i\vec{q}\cdot\delta_{\vec{R}}}=\left(D^{\alpha\beta}_{-\vec{q}}\right)^{*}$$

Note that the "Fourier transform" is nothing other than a unitary transformation. More explicitly, define the unitary matrix

$$U^{\alpha\beta}_{\vec{q}\vec{R}}=\frac{1}{\sqrt{V}}e^{i\vec{q}\cdot\vec{R}}\delta_{\alpha\beta}$$

check

$$\left(U^{\dagger}U\right)^{\alpha\beta}_{\vec{R},\vec{R}'}=\frac{1}{V}\sum_{q}e^{-i\vec{q}\cdot\vec{R}'}e^{i\vec{q}\cdot\vec{R}}\delta_{\alpha\beta}=\delta\left(\vec{R}-\vec{R}'\right)\delta_{\alpha\beta}$$

The block diagonalization of D suggests we should transform

$$\hat{\phi}^{\alpha}_{i}D^{\alpha\beta}_{ij}\hat{\phi}^{\beta}_{j}=\hat{\phi}^{T}\cdot D\cdot\hat{\phi}$$

$$=\left(\hat{\phi}^{T}U^{T}\right)\cdot\left(U^{*}DU^{\dagger}\right)\cdot\left(U\hat{\phi}\right)$$

$$=\sum_{\vec{q},\vec{q}'}\hat{\phi}^{\alpha}_{\vec{q}}D^{\alpha\beta}_{\vec{q}}\delta\left(\vec{q}+\vec{q}'\right)\hat{\phi}^{\beta}_{\vec{q}'}$$

$$=\sum_{\vec{q}}\hat{\phi}^{\alpha}_{\vec{q}}D^{\alpha\beta}_{\vec{q}}\hat{\phi}^{\beta}_{-\vec{q}}$$

where

$$\hat{\phi}^{\alpha}_{\vec{q}}=\frac{1}{\sqrt{V}}\sum_{\vec{R}}e^{i\vec{q}\cdot\vec{R}}\hat{\phi}^{\alpha}_{\vec{R}}$$

similarly,

$$\hat{\pi}^{\alpha}_{\vec{q}}=\frac{1}{\sqrt{V}}\sum_{\vec{R}}e^{i\vec{q}\cdot\vec{R}}\hat{\pi}^{\alpha}_{\vec{R}}$$

Note that the pairing between $\vec{q}$ and $-\vec{q}$ is natural for a couple of reasons

1. $\hat{\phi}_{\vec{q}}^{\alpha\dagger} = \frac{1}{\sqrt{V}} \sum_{\vec{R}} e^{-i\vec{q}\cdot\vec{R}} \hat{\phi}_{\vec{R}}^{\alpha} = \hat{\phi}_{-\vec{q}}^{\alpha}$

2. $\hat{t}_{\vec{a}} \hat{\phi}_{\vec{q}}^{\alpha} \hat{t}_{\vec{a}}^{-1} = \frac{1}{\sqrt{V}} \sum_{\vec{R}} e^{i\vec{q}\cdot\vec{R}} \hat{\phi}_{\vec{R}+\vec{a}}^{\alpha} = e^{-i\vec{q}\cdot\vec{a}} \hat{\phi}_{\vec{q}}^{\alpha}$, where $\hat{t}_{\vec{a}}$ is lattice translation by $\vec{a}$

So $\hat{\phi}_{\vec{q}}^{\alpha}$ and $\hat{\phi}_{-\vec{q}}^{\alpha}$ transform in opposite way under translation, and they have to appear in pairs to keep the Hamiltonian translation invariant. (Same story for non-FFLO superconductors: pairing $\sim \Delta C_{\vec{q}}^{\dagger} C_{-\vec{q}}^{\dagger}$)

Let's finish diagonalizing the Hamiltonian. First note that the Fourier transform is complex, so it's unitary (instead of orthogonal). This leads to a slightly different commutation relation.

$$
\begin{aligned}
\left[\hat{\phi}_{\vec{q}}^{\alpha}, \hat{\pi}_{\vec{q}'}^{\beta} \right] &= \frac{1}{V} \sum_{\vec{R},\vec{R}'} e^{i\vec{q}\cdot\vec{R}} e^{i\vec{q}'\cdot\vec{R}'} \left[\hat{\phi}_{\vec{R}}^{\alpha}, \hat{\pi}_{\vec{R}'}^{\beta} \right] \\
&= \frac{1}{V} \sum_{\vec{R},\vec{R}'} e^{i\vec{q}\cdot\vec{R}} e^{i\vec{q}'\cdot\vec{R}'} i\delta\left(\vec{R} - \vec{R}'\right) \delta_{\alpha\beta} \\
&= \frac{i\delta_{\alpha\beta}}{V} \sum_{\vec{R}} e^{i(\vec{q}+\vec{q}')\cdot\vec{R}} \\
&= i\delta\left(\vec{q} + \vec{q}'\right) \delta_{\alpha\beta}
\end{aligned}
$$

i.e., the canonical conjugate pairs are $\hat{\phi}_{\vec{q}}^{\alpha} \& \hat{\pi}_{-\vec{q}}^{\alpha}$. The transformed Hamiltonian is now

$$
\hat{H} = \frac{1}{2} \sum_{\vec{q}} \left(\sum_{\alpha} \hat{\pi}_{\vec{q}}^{\alpha} \hat{\pi}_{-\vec{q}}^{\alpha} + \sum_{\alpha\beta} \hat{\phi}_{\vec{q}}^{\alpha} D_{\vec{q}}^{\alpha\beta} \hat{\phi}_{-\vec{q}}^{\beta} \right)
$$

We further diagonalize the block

$$
S_{\vec{q}}^{\dagger} D_{\vec{q}} S_{\vec{q}} = \mathrm{diag}\left\{ \left(\omega_{\vec{q}}^{1}\right)^{2}, \left(\omega_{\vec{q}}^{2}\right)^{2}, \cdots \right\}
$$

and transform $\hat{\pi}_{\vec{q}}^{\alpha}$ and $\hat{\phi}_{\vec{q}}^{\alpha}$ accordingly. This leads to

$$
\hat{H} = \frac{1}{2} \sum_{\vec{q},\alpha} \left(\hat{\Pi}_{\vec{q}}^{\alpha} \hat{\Pi}_{-\vec{q}}^{\alpha} + \left(\omega_{\vec{q}}^{\alpha}\right)^{2} \hat{\Phi}_{\vec{q}}^{\alpha} \hat{\Phi}_{-\vec{q}}^{\beta} \right)
$$

we should now define the creation and annihilation operators

$$
\hat{a}_{\vec{q}}^{\alpha} = \left(\sqrt{\omega_{\vec{q}}^{\alpha}} \hat{\Phi}_{\vec{q}}^{\alpha} + \frac{i}{\sqrt{\omega_{\vec{q}}^{\alpha}}} \hat{\Pi}_{\vec{q}}^{\alpha} \right) / \sqrt{2}
$$

$$
\hat{a}_{\vec{q}}^{\alpha\dagger} = \left(\sqrt{\omega_{\vec{q}}^{\alpha}} \hat{\Phi}_{-\vec{q}}^{\alpha} - \frac{i}{\sqrt{\omega_{\vec{q}}^{\alpha}}} \hat{\Pi}_{-\vec{q}}^{\alpha} \right) / \sqrt{2}
$$

As usual, let's check

$$
\left[\hat{a}_{\vec{q}}^{\alpha}, \hat{a}_{\vec{q}}^{\alpha\dagger} \right] = \frac{1}{2} \left[\hat{\Phi}_{\vec{q}}^{\alpha}, -i\hat{\Pi}_{-\vec{q}}^{\alpha} \right] + \frac{1}{2} \left[i\hat{\Pi}_{\vec{q}}^{\alpha}, \hat{\Phi}_{-\vec{q}}^{\alpha} \right] = 1
$$

Anticipating the answer, let's compute

$$\hat{a}_{\vec{q}}^{\alpha\dagger}\hat{a}_{\vec{q}}^{\alpha} = \frac{1}{2}\left(\omega_{\vec{q}}^{\alpha}\hat{\Phi}_{-\vec{q}}^{\alpha}\hat{\Phi}_{\vec{q}}^{\alpha} + i\hat{\Phi}_{-\vec{q}}^{\alpha}\hat{\Pi}_{\vec{q}}^{\alpha} - i\hat{\Pi}_{-\vec{q}}^{\alpha}\hat{\Phi}_{\vec{q}}^{\alpha} + \hat{\Pi}_{-\vec{q}}^{\alpha}\hat{\Phi}_{\vec{q}}^{\alpha}/\omega_{\vec{q}}^{\alpha}\right)$$

$$\hat{a}_{-\vec{q}}^{\alpha\dagger}\hat{a}_{-\vec{q}}^{\alpha} = \frac{1}{2}\left(\omega_{\vec{q}}^{\alpha}\hat{\Phi}_{\vec{q}}^{\alpha}\hat{\Phi}_{-\vec{q}}^{\alpha} + i\hat{\Phi}_{\vec{q}}^{\alpha}\hat{\Pi}_{-\vec{q}}^{\alpha} - i\hat{\Pi}_{\vec{q}}^{\alpha}\hat{\Phi}_{-\vec{q}}^{\alpha} + \hat{\Pi}_{\vec{q}}^{\alpha}\hat{\Phi}_{-\vec{q}}^{\alpha}/\omega_{\vec{q}}^{\alpha}\right)$$

where we have used $\omega_{\vec{q}}^{\alpha} = \omega_{-\vec{q}}^{\alpha}$ as $D_{\vec{q}}^{\alpha\beta} = \left(D_{-\vec{q}}^{\alpha\beta}\right)^{*}$.
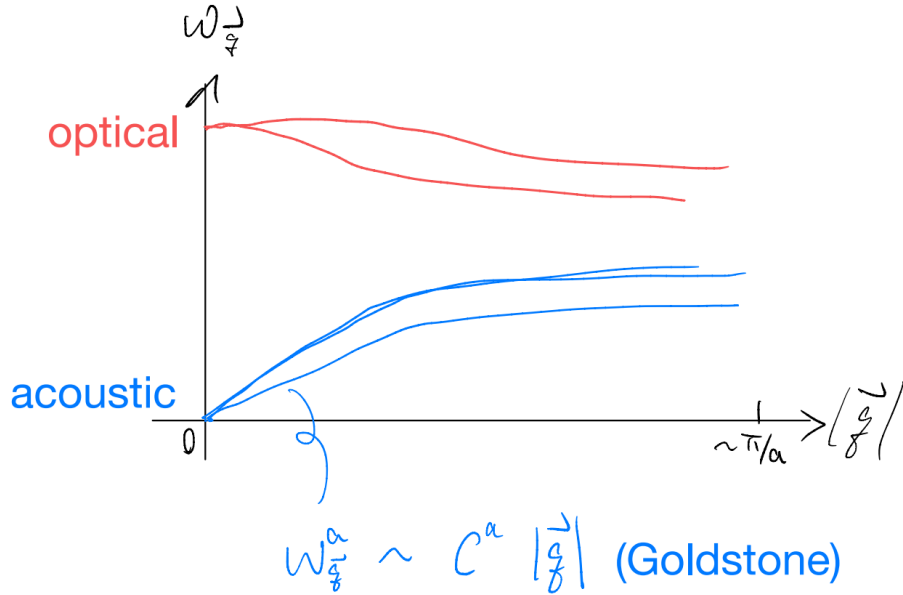
$$\hat{a}_{\vec{q}}^{\alpha\dagger}\hat{a}_{\vec{q}}^{\alpha} + \hat{a}_{-\vec{q}}^{\alpha\dagger}\hat{a}_{-\vec{q}}^{\alpha}$$

$$=\omega_{\vec{q}}^{\alpha}\hat{\Phi}_{\vec{q}}^{\alpha}\hat{\Phi}_{-\vec{q}}^{\alpha} + \hat{\Pi}_{\vec{q}}^{\alpha}\hat{\Pi}_{-\vec{q}}^{\alpha}/\omega_{\vec{q}}^{\alpha} + \frac{i}{2}\left[\hat{\Phi}_{-\vec{q}}^{\alpha},\hat{\Pi}_{\vec{q}}^{\alpha}\right] + \frac{i}{2}\left[\hat{\Phi}_{\vec{q}}^{\alpha},\hat{\Pi}_{-\vec{q}}^{\alpha}\right]$$

$$=\omega_{\vec{q}}^{\alpha}\hat{\Phi}_{\vec{q}}^{\alpha}\hat{\Phi}_{-\vec{q}}^{\alpha} + \hat{\Pi}_{\vec{q}}^{\alpha}\hat{\Pi}_{-\vec{q}}^{\alpha}/\omega_{\vec{q}}^{\alpha} - 1$$

$$\hat{H} = \frac{1}{2}\sum_{\alpha}\left(\hat{\Pi}_{0}^{\alpha 2} + \omega_{0}^{\alpha 2}\hat{\Phi}_{0}^{\alpha 2}\right) + \sum_{\alpha,\vec{q}:q>0}\left(\hat{\Pi}_{\vec{q}}^{\alpha}\hat{\Pi}_{-\vec{q}}^{\alpha} + \omega_{\vec{q}}^{\alpha 2}\hat{\Phi}_{\vec{q}}^{\alpha}\hat{\Phi}_{-\vec{q}}^{\alpha}\right)$$

$$= \frac{1}{2}\sum_{\alpha}\left(\hat{\Pi}_{0}^{\alpha 2} + \omega_{0}^{\alpha 2}\hat{\Phi}_{0}^{\alpha 2}\right) + \sum_{\alpha,\vec{q}:q>0}\omega_{\vec{q}}^{\alpha}\left(\hat{a}_{\vec{q}}^{\alpha\dagger}\hat{a}_{\vec{q}}^{\alpha} + \hat{a}_{-\vec{q}}^{\alpha\dagger}\hat{a}_{-\vec{q}}^{\alpha} + 1\right)$$

$$= \frac{1}{2}\sum_{\alpha}\left(\hat{\Pi}_{0}^{\alpha 2} + \omega_{0}^{\alpha 2}\hat{\Phi}_{0}^{\alpha 2}\right) + \sum_{\alpha,\vec{q}:q\neq 0}\omega_{\vec{q}}^{\alpha}\left(\hat{a}_{\vec{q}}^{\alpha\dagger}\hat{a}_{\vec{q}}^{\alpha} + \frac{1}{2}\right)$$

Notice that we have treated $\vec{q} = 0$ differently. This is more than a formality (e.g. we would have double counted if we simply group the sums for $\vec{q}$ and $-\vec{q}$). Physically, having crystal momentum of $\vec{q} = \vec{0}$ implies

1. we specify a distortion of the atoms within one unit cell

2. we copy the distortion everywhere

One specific distortion we can obtain in this way is to shift every atom by the same amount in the same direction. Such uniform distortion is simply a center of mass motion, which should not cost any elastic energy.

In other words, we expect the lowest frequencies at $\vec{q} = \vec{0}$ to be 0. We have as many of them as the spatial dimension d. In fact, we can say something stronger: a nearly uniform distortion should, by similar reasoning, takes very little energy. We can make the energy cost as small as we wish by taking $|\vec{q}| \to 0$. This implies we have d branches of low-lying phonon modes radiating out from the Γ point ($\vec{q} = \vec{0}$). There are called "acoustic phonons". There existence is a consequence of the spontaneously broken global continuous translation symmetry when we, say, go from a liquid of the same atoms to a crystal. They can be identified as examples of Goldstone modes. Recall, however, that in our current treatment the α index ranges beyond $1, 2, \cdots, d$ if we have multiple atoms per unit cell. We argued the lowest d eigenvalues of $D_{\vec{q}}^{\alpha\beta}$ will be 0, but we don't really have a constraint for the rest. These will generically have a finite frequency, and they are referred to as the "optical phonons".

$$\omega_{\vec{q}}^{a} \sim C^{a} \left|\frac{\vec{q}}{\delta}\right| \text{ (Goldstone)}$$

Goldstone modes: $\omega_{vecq}^{\alpha} \sim C^{\alpha}|\vec{q}|$

Anyway, we can finally write the phonon Hamiltonian as (CM abbreviate for Classical Mechanics)

$$\hat{H} = \sum_{\alpha=1}^{d} \frac{\hat{\Pi}_{CM}^{\alpha 2}}{2M} + \sum_{\alpha,\vec{q}:q\neq 0} \omega_{\vec{q}}^{\alpha} \left(\hat{a}_{\vec{q}}^{\alpha\dagger} \hat{a}_{\vec{q}}^{\alpha} + \frac{1}{2} \right)$$

This isn't really any different from what we have without assuming translation symmetry! All we have gained is a more refined understanding on how the "modes" are organized with respect to the conserved crystal momentum.

Let's end this part by spending a bit of time thinking about the eigenstates, and then also what happens at finite temperature (as a quantum statistics mechanics review).

3.1   Q stat mech review

For simplicity, let's drop the CM motion piece. The phonon Hamiltonian is then

$$\hat{H} = \sum_{\vec{q},\alpha} \omega_{\vec{q}}^{\alpha} \left(\hat{a}_{\vec{q}}^{\alpha\dagger} \hat{a}_{\vec{q}}^{\alpha} + \frac{1}{2} \right)$$

Each of the number operators $\hat{n}_{\vec{q}} = \hat{a}_{\vec{q}}^{\dagger} \hat{a}_{\vec{q}}$ commutes with the Hamiltonian, and so the eigenstates are simply labeled by them

$$\hat{H}| \left\{ n_{\vec{q}}^{\alpha} \right\} \rangle = \sum_{\vec{q},\alpha} \omega_{\vec{q}}^{\alpha} \left(n_{\vec{q}}^{\alpha} + \frac{1}{2} \right) | \left\{ n_{\vec{q}}^{\alpha} \right\} \rangle$$

The constant $\omega_{\vec{q}}^\alpha/2$ in the Hamiltonian is problematic for two reasons

1. It's shared by all states, but physical processes can only probe energy differences between states

2. It scales with the number of atoms inside. If we wish to take a continuum limit, it diverges

It is customary to simply drop that overall constant in the Hamiltonian. So far, we have focused on the eigenstates. At zero temperature, we can simply state that the system is in the lowest energy state. At finite temperatures, however, we expect states within an energy scale of $k_B T$ to be "populated". This is reflected in the density matrix.

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{\mathcal{Z}}$$

$$\mathcal{Z} = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right)$$

$$\beta = \frac{1}{k_B T}$$

$$\mathrm{Tr}\left(\hat{\rho}\right) = 1$$

Expectation value for a physical observable is then given by

$$\left\langle \hat{A} \right\rangle = \mathrm{Tr}\left(\hat{\rho} \hat{A}\right)$$

For our free phonon problem, we know all the eigenstates and one can evaluate explicitly

$$\mathcal{Z}\left(\beta\right) = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) = \sum_{\{n_{\vec{q}}^\alpha\}} \langle \{n_{\vec{q}}^\alpha\} | e^{-\beta \hat{H}} | \{n_{\vec{q}}^\alpha\}\rangle$$

$$= \sum_{\{n_{\vec{q}}^\alpha\}} \exp\left(-\beta \sum_{\vec{q},\alpha} \omega_{\vec{q}}^\alpha n_{\vec{q}}^\alpha\right)$$

$$= \sum_{\{n_{\vec{q}}^\alpha\}} \prod_{\vec{q},\alpha} \exp\left(-\beta \omega_{\vec{q}}^\alpha n_{\vec{q}}^\alpha\right)$$

$$= \prod_{\vec{q},\alpha} \sum_{n_{\vec{q}}^\alpha=0}^{\infty} \exp\left(-\beta \omega_{\vec{q}}^\alpha n_{\vec{q}}^\alpha\right)$$

$$= \prod_{\vec{q},\alpha} \frac{1}{1 - \exp\left(-\beta \omega_{\vec{q}}^\alpha\right)}$$

$$\Rightarrow \ln \mathcal{Z}\left(\beta\right) = -\sum_{\vec{q},\alpha} \ln\left(1 - e^{-\beta \omega_{\vec{q}}^\alpha}\right)$$

To find, e.g., the energy expectation value we notice

$$\langle H \rangle = \frac{\text{Tr}\left(\hat{H}\rho\right)}{\mathcal{Z}} = -\partial_\beta \ln \mathcal{Z}\left(\beta\right)$$

That's an awesome trick. What about computing some other expectation values? It's *tempting* to imaging generalizing

$$\mathcal{Z}\left(\beta, J\right) = \text{Tr}\left(e^{-\beta\hat{H}+J\hat{O}}\right)$$

$$\partial_J \ln \mathcal{Z}\left(\beta, J\right) = \frac{\partial_J \text{Tr}\left(e^{-\beta\hat{H}+J\hat{O}}\right)}{Z\left(\beta, J\right)} \stackrel{?}{=} \frac{\text{Tr}\left(\hat{O}e^{-\beta\hat{H}+J\hat{O}}\right)}{Z\left(\beta, J\right)}$$

$$\partial_J \ln \mathcal{Z}\left(\beta, J\right)|_{J=0} \stackrel{?}{=} \frac{\text{Tr}\left(\hat{O}e^{-\beta\hat{H}}\right)}{Z\left(\beta, J\right)} = \left\langle\hat{O}\right\rangle$$

BUT $\hat{H}\&\hat{O}$ may not commute! The manipulation above is faulty in general. Nevertheless, the spirit above is great. We just need a more sophisticated formalism to make it work. That requires time-ordering, generating functional, path integral etc. More later.

In any case, we have completely solved the free phonon problem, in the sense that for any observables we would want to compute, we have a way of doing so (by rotating to the decoupled QHO basis).

But let's pretend we are experimentalists. How do we even get to get to find the coupling coefficients etc in the first place? Without that, how do we find out the phonon frequencies etc? The natural approach is to perturb the system, and watches how it responds, e.g., If you have a guitar string, you probe its
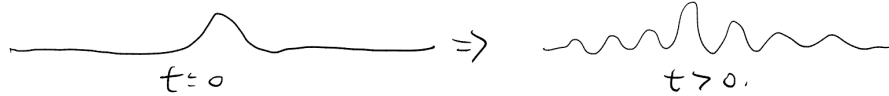
frequency by plucking with you fingers, Too bad our fingers are too big for the microscopic crystal! Instead, we probe phonons with other tools, like photon, or more indirectly through electrons in the solid. E.g. We generally expect the equilibrium position of the atoms to shift depending on the electronic state. So, we can use the electron as our "phonon pick"!

To that end, let's now introduce the electron, a fermion.
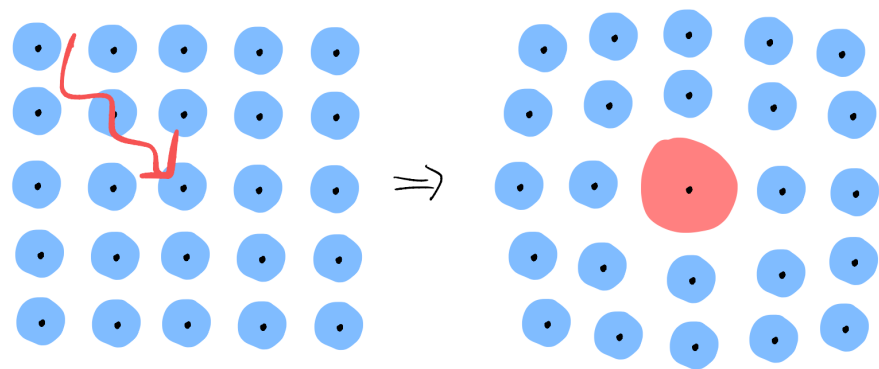
Chapter 4

lec04 202200216

topics

1. particle statistics

2. localized electrons

3. Heisenberg picture

4. Green's and spectral functions: a primer

 Goals

1. relate particle statistics to (anti-)commutation of second quantized operators

2. sharpening connection of Green's functions vs excitations

 Reminder: PS1 due coming Fri $1:30\text{pm} - \varepsilon$

4.1   particle statistics

We have mentioned on and off that phonon problem is a bosonic one. Recall from QM that boson vs fermion is a question about particle exchange statistics. In the so-called "first quantized" wave function, a two-particle wave function depends on two coordinate variables

$$\Psi\left(x_1, x_2\right) = \langle x_1, x_2 | \Psi \rangle$$

"Particle statistics" refers to what happen if we decide to relabel the two indistinguishable particles

$$\Psi\left(x_1, x_2\right) = \begin{cases} \Psi\left(x_2, x_1\right); & \text{boson} \\ -\Psi\left(x_2, x_1\right); & \text{fermion} \end{cases}$$

Generalization to an N-particle state is similar, noticing any permutation is a product of pair-wise exchanges. For our purpose, we just assert without any justification that one can relate the state with one boson at x_1 and one at x_2 can be identified with

$$|x_1, x_2\rangle = \hat{b}_{x_1}^\dagger \hat{b}_{x_2}^\dagger |0\rangle$$

where $\hat{b}^\dagger$ is the creation operator we have written down countless time already from QHO. In essence, we associate to each point x in space a QHO. The vacuum $|0\rangle$ is then the joint vacuum of all these QHO's.

Notes:

1. but (if) space is continuous, then we have uncountably many QHO's even in a finite volume of space! That sounds sick. That is sick. But that's okay.

2. We have implicitly promoted the single-particle wave function $\delta(x)$ to an operator $\hat{b}_x^\dagger$. That's why this is called "second quantization".

3. implicitly, we have defined an object which maps space to quantum operators: $\vec{r} \to \hat{b}_x^\dagger$. Such maps are called "fields". (E.g., think about electric field $\vec{r} \to \vec{E}\vec{r}$. Our fields here are quantum mechanical in that they do not have simple point-wise multiplication but instead canonical commutation). Whence the name "QFT"

Now, back to particle statistics. We have, for bosons,

$$\Psi_B(x_1, x_2) = \langle 0|\hat{b}_{x_1}^\dagger \hat{b}_{x_2}^\dagger |0\rangle = \langle 0|\hat{b}_{x_2}^\dagger \hat{b}_{x_1}^\dagger |0\rangle = \Psi_B(x_2, x_1)$$

So the exchange sign of $+1$ is really the commutation of among the creation(annihilation) operators. It is then natural to guess what should happen for fermions:

$$\Psi_F(x_1, x_2) = \langle 0|\hat{c}_{x_1}^\dagger \hat{c}_{x_2}^\dagger |0\rangle = -\langle 0|\hat{c}_{x_2}^\dagger \hat{c}_{x_1}^\dagger |0\rangle = \Psi_F(x_2, x_1)$$

This implies the fermionic creation and annihilation operators should satisfy canonical anti-commutation relations. Let $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$. For fermions

$$\{\hat{c}_x, \hat{c}_y\} = \left\{\hat{c}_x^\dagger, \hat{c}_y^\dagger\right\} = 0$$

$$\left\{\hat{c}_x^\dagger, \hat{c}_y\right\} = \delta(x - y)$$

$$\{\hat{c}_x, \hat{c}_x\} = \left\{\hat{c}_x^\dagger, \hat{c}_x^\dagger\right\} = 0 \quad \Rightarrow \quad \hat{c}_x^2 = \hat{c}_x^{\dagger 2} = 0$$

Note: we take these as the practical definition for the "second-quantized" operators. One can also do it in the traditional way of making very explicit connections to the Hilbert space of symmetrized / anti-symmetrized wave functions. Schematically, The "first quantized" description focus on each particle sector individually. The "second quantized" description focus on how to relate the different sectors. In particular, we have a natural relation between the ground

Fock space =

n-particle sector of (anti-)symmetrized wave functions
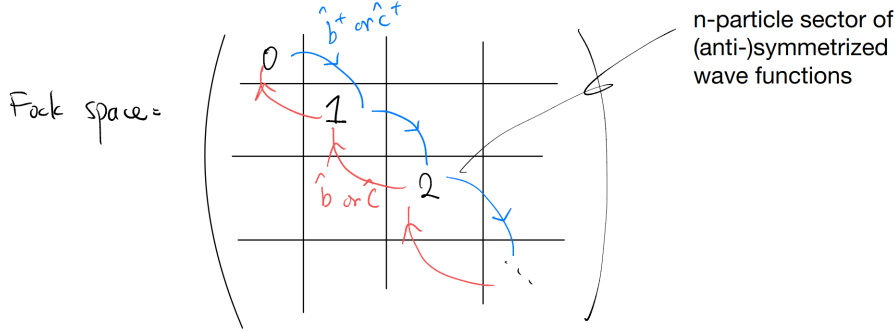
state and a state in the n-particle sector. Consider putting n particles (bosons or fermions) into n "orbitals" $\phi_1, \phi_2, \cdots, \phi_n$

$$\Phi^{\phi_1,\phi_2,\cdots,\phi_n}_{x_1,x_2,\cdots,x_n} \xrightarrow{\text{sym}} \hat{b}^\dagger_{\phi_1} \hat{b}^\dagger_{\phi_2} \cdots \hat{b}^\dagger_{\phi_n} |0\rangle \quad \text{bosons}$$

$$\Phi^{\phi_1,\phi_2,\cdots,\phi_n}_{x_1,x_2,\cdots,x_n} \xrightarrow{\text{anti}-\text{sym}} \hat{c}^\dagger_{\phi_1} \hat{c}^\dagger_{\phi_2} \cdots \hat{c}^\dagger_{\phi_n} |0\rangle \quad \text{fermions}$$

where we assume the "orbitals" are distinct and orthogonal. (i.e., we are considering a canonical transformation on the defining modes of the system).

The above is rather schematic. In practice there are some factors of $\sqrt{n!}$ etc. if one wants to relate first and second quantization. We won't cover that here (usually covered in advanced QM), see e.g. Coleman Chapter-3 for more details.

Final note: so is QHO bosonic?

It depends. IF you have exactly one particle, there is no exchange and hence no statistics. If you have multiple particles, then the statistics is an "intrinsic" aspect of the problem in the sense that it defines the many-body Hilbert space, whereas being a QHO is "kinematic" in the sense that it's just characterizing the Hamiltonian acting on the Hilbert space. E.g.,

1. Phonons: the momenta and displacements of different atoms commute, so we have a bosonic problem to start with. In the "harmonic approximation" we have a collection of coupled QHO

2. Electronic quantum Hall: we have fermions to start with, but the B-field enters the single particle problem as a spatially varying gauge field. That also leads to the QHO Hamiltonian for the single particle problem. But now the raising / lowering operators act between different *fermionic* modes that could be empty or filled

P.S. We can certainly have bosonic operators in a fermionic Hilbert space: combining an even number of fermionic operators leads to bosonic ones. For those of you have prefer a math-oriented language, the operator algebra is Z_2-graded and we have even=bosonic and odd=fermionic.

P.P.S. We can even have effectively fermionic operators in a bosonic Hilbert space. That's the wonder of topological order...

4.2   Localized electrons

Let us now consider our very first electronic problem. Consider as a warm-up an electronic Hamiltonian

$$\hat{H} = \varepsilon \left(\hat{c}_\uparrow^\dagger \hat{c}_\downarrow + \hat{c}_\downarrow^\dagger \hat{c}_\uparrow \right) \quad \text{manybody}$$

$$= \left(\hat{c}_\uparrow^\dagger, \hat{c}_\downarrow^\dagger \right) \begin{pmatrix} 0 & \varepsilon \\ \varepsilon & 0 \end{pmatrix} (\hat{c}_\uparrow, \hat{c}_\downarrow) \quad \text{singleparticle}$$

Let's consider writing out the matrix elements in the Fock space

$$\hat{H}|0\rangle = \varepsilon \left(\hat{c}_\uparrow^\dagger \hat{c}_\downarrow + \hat{c}_\downarrow^\dagger \hat{c}_\uparrow \right) |0\rangle = 0$$

$$\hat{H}\hat{c}_\uparrow^\dagger|0\rangle = \varepsilon \left(\hat{c}_\uparrow^\dagger \hat{c}_\downarrow + \hat{c}_\downarrow^\dagger \hat{c}_\uparrow \right) \hat{c}_\uparrow^\dagger|0\rangle$$

$$= \varepsilon \left(\hat{c}_\uparrow^\dagger \hat{c}_\downarrow \hat{c}_\uparrow^\dagger + \hat{c}_\downarrow^\dagger \hat{c}_\uparrow \hat{c}_\uparrow^\dagger \right) |0\rangle$$

$$= \varepsilon \left(-\hat{c}_\uparrow^\dagger \hat{c}_\uparrow^\dagger \hat{c}_\downarrow + \hat{c}_\downarrow^\dagger \left(1 - \hat{c}_\uparrow^\dagger \hat{c}_\uparrow \right) \right) |0\rangle$$

$$= \varepsilon \left(0 + \hat{c}_\downarrow^\dagger - \hat{c}_\downarrow^\dagger \hat{c}_\uparrow^\dagger \hat{c}_\uparrow \right) |0\rangle$$

$$= \varepsilon \left(0 + \hat{c}_\downarrow^\dagger - 0 \right) |0\rangle$$

$$= \varepsilon \hat{c}_\downarrow^\dagger|0\rangle$$

$$\hat{H}\hat{c}_\downarrow^\dagger|0\rangle = \varepsilon \left(\hat{c}_\uparrow^\dagger \hat{c}_\downarrow + \hat{c}_\downarrow^\dagger \hat{c}_\uparrow \right) \hat{c}_\downarrow^\dagger|0\rangle = \varepsilon \hat{c}_\uparrow^\dagger|0\rangle$$

$$\hat{H}\hat{c}_\uparrow^\dagger\hat{c}_\downarrow^\dagger|0\rangle = \varepsilon \left(\hat{c}_\uparrow^\dagger \hat{c}_\downarrow + \hat{c}_\downarrow^\dagger \hat{c}_\uparrow \right) \hat{c}_\uparrow^\dagger\hat{c}_\downarrow^\dagger|0\rangle = 0$$

$$\hat{H} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon & 0 \\ 0 & \varepsilon & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

in the basis $\left\{ |0\rangle, \hat{c}_\uparrow^\dagger|0\rangle, \hat{c}_\downarrow^\dagger|0\rangle, \hat{c}_\uparrow^\dagger\hat{c}_\downarrow^\dagger|0\rangle \right\}$ ($\left\{ \hat{c}_\uparrow^\dagger|0\rangle, \hat{c}_\downarrow^\dagger|0\rangle \right\}$ is single-particle basis). We know the single-particle eigenstates are

$$\varepsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} = \pm \varepsilon \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$

It is natural to "rotate" in the eigenbasis

$$\hat{c}_+^\dagger = \frac{1}{\sqrt{2}} \left(\hat{c}_\uparrow^\dagger + \hat{c}_\downarrow^\dagger \right), \quad \hat{c}_-^\dagger = \frac{1}{\sqrt{2}} \left(\hat{c}_\uparrow^\dagger - \hat{c}_\downarrow^\dagger \right)$$

we may check

$$\begin{cases} \left\{ \hat{c}_{\pm}^{\dagger}, \hat{c}_{\pm} \right\} = \frac{1}{2} \left\{ \hat{c}_{\uparrow}^{\dagger} \pm \hat{c}_{\downarrow}^{\dagger}, \hat{c}_{\uparrow} \pm \hat{c}_{\downarrow} \right\} = \frac{1}{2} \left(1 \pm 0 \pm 0 + 1 \right) = 1 \\ \left\{ \hat{c}_{+}^{\dagger}, \hat{c}_{-} \right\} = \frac{1}{2} \left\{ \hat{c}_{\uparrow}^{\dagger} + \hat{c}_{\downarrow}^{\dagger}, \hat{c}_{\uparrow} - \hat{c}_{\downarrow} \right\} = \frac{1}{2} \left(1 + 0 - 0 - 1 \right) = 0 \end{cases}$$

$$\Rightarrow \begin{cases} \left\{ \hat{c}_{\alpha}^{\dagger}, \hat{c}_{\beta} \right\} = \delta_{\alpha\beta} \\ \left\{ \hat{c}_{\alpha}^{\dagger}, \hat{c}_{\beta}^{\dagger} \right\} = \{ \hat{c}_{\alpha}, \hat{c}_{\beta} \} = 0 \end{cases}$$

Using which we have

$$\hat{H} = \varepsilon \hat{c}_{+}^{\dagger} \hat{c}_{+} - \varepsilon \hat{c}_{-}^{\dagger} \hat{c}_{-}$$

We can schematically draw the spectrum as $(\varepsilon > 0)$

Side note: The calculation above can be readily generalized. Consider some Hamiltonian defined over N fermionic modes:

$$\hat{H} = \sum_{\alpha,\beta=1}^{N} \hat{c}_{\alpha}^{\dagger} h_{\alpha\beta} \hat{c}_{\beta}$$

Here, h is a Hermitian matrix and can be diagonalized by a unitary

$$h_{\alpha\beta} = \sum_i U_{\alpha i} \varepsilon_i \left(U^{\dagger} \right)_{i\beta}$$

$$\hat{H} = \sum_i \left(\sum_{\alpha} \hat{c}_{\alpha}^{\dagger} U_{\alpha i} \right) \varepsilon_i \left(\sum_{\beta} \left(U^{\dagger} \right)_{i\beta} \hat{c}_{\beta} \right)$$

$$= \sum_i \varepsilon_i \hat{c}_i^{\dagger} \hat{c}_i \quad \text{canonical transformation}$$

(c.f. the phonon discussion)

Back to the two mode problem: this is again an exactly solved problem, which is in a way similar to the QHO / free phonon. We know all the eigenstates and eigen-energies. Yet, it is natural to ask how we can probe the "physics" of the system. Suppose we start with the ground state ($t > 0$):

$$|\Omega\rangle = \hat{c}_-^\dagger|0\rangle = \frac{1}{\sqrt{2}}\left(\hat{c}_\uparrow^\dagger - \hat{c}_\downarrow^\dagger\right)|0\rangle$$

Recall our discussion on propagator / correlation functions / Green's functions. Let us compare

1. create an up electron: $\hat{c}_\uparrow^\dagger$

2. evolution for time t: $e^{-i\hat{H}t}$

$$e^{-i\hat{H}t}\hat{c}_\uparrow^\dagger|\Omega\rangle \quad \text{vs} \quad \hat{c}_\uparrow^\dagger e^{-i\hat{H}t}|\Omega\rangle$$

$$G_{\uparrow\uparrow}(t) = -i\langle\Omega|e^{i\hat{H}t}\hat{c}_\uparrow e^{-i\hat{H}t}\hat{c}_\uparrow^\dagger|\Omega\rangle$$

where $e^{i\hat{H}t}\hat{c}_\uparrow e^{-i\hat{H}t}$ is the conjugate action of time evolution on an operator. We claimed

1. Such functions contains important dynamical info about the system

2. It is natural to interpret it as a specific kind of correlation function

Let us now introduce these ideas more systematically

Heisenberg picture

So far, we have introduced time evolution of a quantum system through the evolution operator $\hat{U} = e^{-i\hat{H}t}$, which satisfies

$$i\partial_t\hat{U} = \hat{H}\hat{U}$$

Implicitly, we know that if a state satisfies the Schrodinger equation

$$i\partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

then its time evolution can be expressed simply as

$$|\Psi(t)\rangle = \hat{U}|\Psi(0)\rangle = e^{-i\hat{H}t}|\Psi(0)\rangle$$

$$i\partial_t|\Psi(t)\rangle = i\partial_t\left(\hat{U}|\Psi(0)\rangle\right) = \left(i\partial_t\hat{U}\right)|\Psi(0)\rangle = \hat{H}\left(\hat{U}|\Psi(0)\rangle\right) = \hat{H}|\Psi(t)\rangle$$

Now imagine computing some observables as the state evolves

$$A(t) = \langle\Psi(t)|\hat{A}|\Psi(t)\rangle = \langle\Psi(0)|\hat{U}^\dagger\hat{A}\hat{U}|\Psi(0)\rangle$$

It's simply a mater of interpretation to say that the operator is evolving $\hat{A} \to \hat{U}^\dagger \hat{A} \hat{U}$, and we compute its expectation value with respect to a fixed state $|\Psi\rangle(0)$. This perspective is called the "Heisenberg picture".

$$\text{Schrodinger} \begin{cases} |\Psi(0)\rangle_S \to |\Psi(t)\rangle_S = \hat{U}|\Psi(0)\rangle_S \\ \hat{A}_S \to \hat{A}_S \end{cases}$$

$$\text{Heisenberg} \begin{cases} |\Psi\rangle_H \to |\Psi\rangle_H \\ \hat{A}_H(0) \to \hat{A}_H(t) = \hat{U}^\dagger \hat{A}_H(0) \hat{U} \end{cases}$$

Here we assume the operator is time-independent in the Schrodinger picture. We can also check explicitly what is the equation governing the time evolution of Heisenberg-picture operators:

$$\begin{aligned} i\partial_t \hat{A}_H(t) &= i\partial_t \left(\hat{U}^\dagger \hat{A}_H(0) \hat{U} \right) \\ &= -\hat{H}\hat{A}_H(t) + \hat{A}_H(t)\hat{H} \\ &= \left[\hat{A}_H(t), \hat{H} \right] \end{aligned}$$

In fact, nothing in the check above demands that we use the actual Hamiltonian! One can imagine picking a "convenient" part of the actual Hamiltonian in defining the dynamics of the operators. Correspondingly, however, the state vectors are *not* static since we are not using the actual Hamiltonian. In this hybrid picture, both the operators and the state evolve. This is called the "interaction picture"; more later.

Note: for those of you who know quantum optics, think about rotating wave approximation.

4.3 One-particle Green's function: a first example

In the following, we keep the subscript S vs H implicit. Whenever we write a time dependence for an operator, it is understood that we are in the Heisenberg picture.

Back to our example. Recall we were comparing

$$\hat{c}_\uparrow^\dagger e^{-i\hat{H}t}|\Omega\rangle \quad \text{vs} \quad e^{-i\hat{H}t}\hat{c}_\uparrow^\dagger|\Omega\rangle$$

where

$$\hat{H} = \varepsilon \left(\hat{c}_\uparrow^\dagger \hat{c}_\downarrow + \hat{c}_\downarrow^\dagger \hat{c}_\uparrow \right)$$

$$|\Omega\rangle = \frac{1}{\sqrt{2}} \left(\hat{c}_\uparrow^\dagger - \hat{c}_\downarrow^\dagger \right) |0\rangle$$

In Heisenberg picture, we have defined

$$G_{\uparrow\uparrow}(t) = -i\langle\Omega|e^{i\hat{H}t}\hat{c}_\uparrow e^{-i\hat{H}t}\hat{c}_\uparrow^\dagger|\Omega\rangle$$

$$= -i\langle\Omega|\hat{c}_\uparrow(t)\,\hat{c}_\uparrow^\dagger(0)\,|\Omega\rangle$$

which can be interpreted as a (quantum) auto-correlation function: we create an electron at time $t = 0$, and then annihilate it at time t. We are measuring correlation across time. Yet, this is *NOT* by itself a physical observable! We cannot understand it as the expectation value of some Hermitian operator. Nevertheless, "unphysical" expressions of such form provides the basis for computing actual observables. As one first check, let us investigate how $G(t)$ reflects the energy scale of the problem. Noticing

$$\hat{H} = \varepsilon\hat{c}_+^\dagger\hat{c}_+ - \varepsilon\hat{c}_-^\dagger\hat{c}_-$$

$$\hat{c}_\pm^\dagger = \frac{1}{\sqrt{2}}\left(\hat{c}_\uparrow^\dagger \pm \hat{c}_\downarrow^\dagger\right)$$

we first note that time evolution for $\hat{c}_\pm^\dagger$ is simple. In the Heisenberg picture,

$$i\partial_t\left(\hat{c}_\pm^\dagger(t)\right) = \left[\hat{c}_\pm^\dagger(t), \hat{H}\right]$$

$$= \hat{U}^\dagger\left[\hat{c}_\pm^\dagger, \pm\varepsilon\hat{c}_\pm^\dagger\hat{c}_\pm\right]\hat{U}$$

$$= \hat{U}^\dagger\left(\pm\varepsilon\hat{c}_\pm^\dagger\right)\left[\hat{c}_\pm^\dagger, \hat{c}_\pm\right]\hat{U}$$

$$= \hat{U}^\dagger\left(\pm\varepsilon\hat{c}_\pm^\dagger\right)\left(2\hat{c}_\pm^\dagger\hat{c}_\pm - 1\right)\hat{U}$$

$$= \mp\varepsilon\hat{c}_\pm^\dagger(t)$$

$$\hat{c}_\pm^\dagger(t) = \hat{c}_\pm^\dagger(0)e^{\pm i\varepsilon t}$$

With the blue symbols denoting Heisenberg picture and the red symbols Schrodinger picture. Noticing $\hat{c}_\uparrow^\dagger(t) = \frac{1}{\sqrt{2}}\left(\hat{c}_+^\dagger(t) + \hat{c}_-^\dagger(t)\right)$,

$$G_{\uparrow\uparrow}(t) = -i\langle\Omega|\hat{c}_\uparrow(t)\,\hat{c}_\uparrow^\dagger(0)\,|\Omega\rangle$$

$$= -\frac{i}{2}\langle\Omega|\left(\hat{c}_+(t) + \hat{c}_-(t)\right)\left(\hat{c}_+^\dagger(0) + \hat{c}_-^\dagger(0)\right)|\Omega\rangle$$

$$= -\frac{i}{2}\langle 0|\hat{c}_-\left(\hat{c}_+e^{-i\varepsilon t} + \hat{c}_-e^{i\varepsilon t}\right)\left(\hat{c}_+^\dagger + \hat{c}_-^\dagger\right)\hat{c}_-^\dagger|0\rangle$$

$$= -\frac{i}{2}\langle 0|\hat{c}_-\hat{c}_+e^{-i\varepsilon t}\hat{c}_+^\dagger\hat{c}_-^\dagger|0\rangle$$

$$= -\frac{i}{2}e^{-i\varepsilon t}\langle 0|\left(1 - \hat{c}_+^\dagger\hat{c}_+\right)\left(1 - \hat{c}_-^\dagger\hat{c}_-\right)|0\rangle$$

$$= -\frac{i}{2}e^{-i\varepsilon t}$$

How to interpret this?
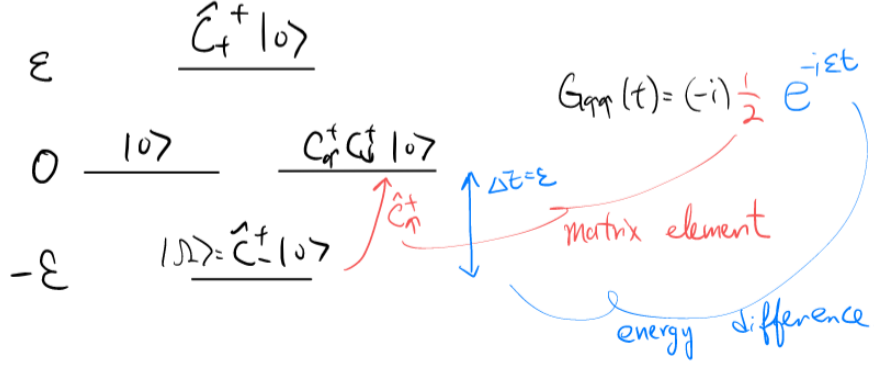
4.4 One-particle Green's function and spectral Lehmann representation

Our "single-site" example is designed to be simple (simple enough to solve everything exactly). Interestingly, the physical picture derived from above is actually very general, as we will see now.

Suppose we have an electronic problem with some many-body Hamiltonian $\hat{H}$ and the ground state $|\Omega\rangle$. We consider the one-particle Green's function as defined above:

$$G_{\alpha\alpha}\left(t\right) = -i\langle\Omega|\hat{c}_\alpha\left(t\right)\hat{c}_\alpha^\dagger\left(0\right)|\Omega\rangle_H$$
$$= -i\langle\Omega|e^{i\hat{H}t}\hat{c}_\alpha e^{-i\hat{H}t}\hat{c}_\alpha^\dagger|\Omega\rangle_S$$

where we use one subscript to denote if the expression is understood in the Heisenberg or Schrodinger picture.

To probe the dynamics, it is natural to go to the eigenbasis of the Hamiltonian. We insert a complete set of basis

$$G_{\alpha\alpha}\left(t\right) = -i\sum_n e^{iE_\Omega t}\langle\Omega|\hat{c}_\alpha|n\rangle_S e^{-iE_n t}\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle_S$$
$$= -i\sum_n \left|\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle_S\right|^2 e^{-i(E_n - E_\Omega)t}$$

where $\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle_S$ is the matrix element and $e^{-i(E_n - E_\Omega)t}$ is the energy difference. This is practically identical to what we had, but we now know neither the matrix element nor the excitation energy (i.e., energy difference from the ground state)!

Importantly, the many-body spectrum is dense! Remember the number of quantum states scales exponentially with the system size $\dim(\mathcal{H}) \sim 2^V$.

Chapter 5

lec05 202200218

Topics

1. Spectral function

2. (Thought) experiment on spectroscopy

3. The zoo of Green's functions

4. Impurity-phonon coupling

Goals

1. developing intuition about Green's and spectral functions

2. Appreciating how they relate to physical problems

3. Applying the techniques to a less trivial and physically relevant problem

5.1 Spectral function

Last time, we were considering a "one-particle" Green's function in a general quantum many-body problem

$$G_{\alpha\alpha}(t) = (-i) \langle \Omega | \hat{c}_\alpha(t) \hat{c}_\alpha^\dagger(0) | \Omega \rangle_H$$
$$= (-i) \sum_n \left| \langle n | \hat{c}_\alpha^\dagger | \Omega \rangle \right|^2 e^{-i(E_n - E_\Omega)t}$$

$$\Delta E_n = (E_n - E_\Omega) \geq 0$$

where n labels the complete (but unknown) eigenstates of the Hamiltonian. We will continue analyzing how much information we can gain from considering such expressions. We would want to understand the excitation energies. However, in general it is hopeless to try to resolve each of the frequencies. Instead, we should

think of a distribution of frequencies, and prominent features will be "peaks" with some widths. This can be done systematically by Fourier transform with respect to time t

$$G_{\alpha\alpha}(\omega) \stackrel{?}{=} \int_{-\infty}^{\infty} dt\, G_{\alpha\alpha}(t)\, e^{i\omega t}$$

$$= -i \sum_n \int_{-\infty}^{\infty} \left| \langle n | \hat{c}_\alpha^\dagger | \Omega \rangle \right|^2 e^{i(\omega - \Delta E_n)t}$$

But there's a serious issue: the integrand is oscillating as we attempt to Fourier transform with $t \to \pm\infty$. Clearly this is an artifact of our mathematical treatment: we don't know if our universe existed or will exist all the way to $t = \pm\infty$!

Here, let us do two things to circumvent the problem

1. In our thought experiment, we always let the system evolve forward in time when we evaluate the auto-correlation. In other words, we restrict ourselves to $t \geq 0$

2. we won't be able to access $t \to +\infty$ anyway. Let's "damp" the contribution by adding a convergence factor $e^{-\eta t}$ to the integrand, taking $\eta \to 0^+$

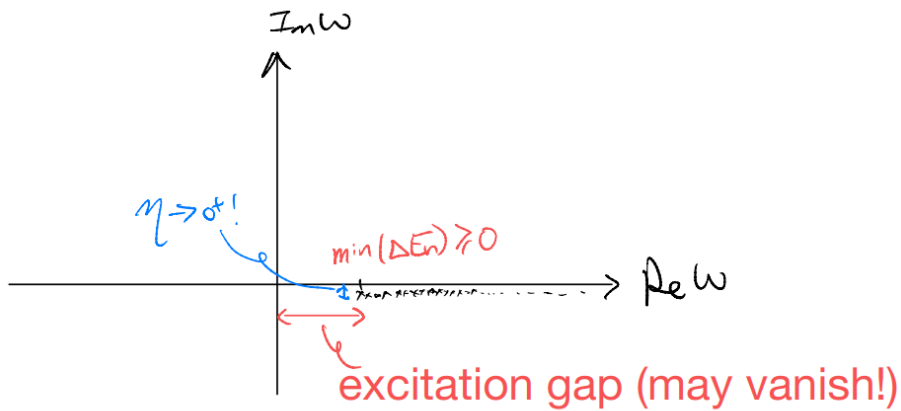$$G_{\alpha\alpha}(\omega) = \lim_{\eta \to 0^+} (-i) \int_0^\infty dt\, G_{\alpha\alpha}(t)\, e^{i\omega t} e^{-\eta t}$$

$$= \lim_{\eta \to 0^+} (-i) \sum_n \left| \langle n | \hat{c}_\alpha^\dagger | \Omega \rangle \right|^2 \int_0^\infty e^{i(\omega - \Delta E_n + i\eta)t}$$

$$= \lim_{\eta \to 0^+} \sum_n \frac{(-i) \left| \langle n | \hat{c}_\alpha^\dagger | \Omega \rangle \right|^2}{i\,(\omega - \Delta E_n + i\eta)} \left(e^{-\eta(+\infty)} - 1 \right)$$

$$= \lim_{\eta \to 0^+} \sum_n \frac{\left| \langle n | \hat{c}_\alpha^\dagger | \Omega \rangle \right|^2}{\omega - \Delta E_n + i\eta}$$

Notes:

1. this explains the convention of attaching $(-i)$ to the definition of $G_{\alpha\alpha}(t)$

2. $G_{\alpha\alpha}(\omega)$ as a function over ω has a (dense) series of poles at $\omega = \Delta E_n - i\eta$

But this is still not something we can measure directly! The matrix element $\left| \langle n | \hat{c}_\alpha^\dagger | \Omega \rangle \right|^2$ is physical: it corresponds to the transition probability of the ground state to some excited state when we add an electron to it. But energy information is hidden in the location of the poles which we displaced below the real line by a sleight of hand. We now claim that, in fact one can identify a "spectral function", closely related to actual experiments, from the frequency-space Green's function:
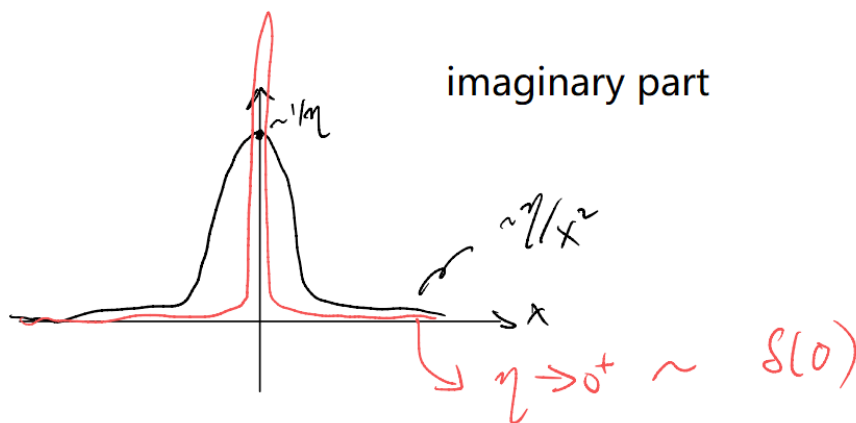
$$A_{\alpha\alpha}(\omega) = \frac{-1}{\pi} \mathrm{Im}\left[G_{\alpha\alpha}(\omega) \right] = \sum_n \left| \langle n | \hat{c}_\alpha^\dagger | \Omega \rangle \right|^2 \delta\left(\omega - \Delta E_n \right)$$

where $\left| \langle n | \hat{c}_\alpha^\dagger | \Omega \rangle \right|^2$ is the matrix element and $\delta \left(\omega - \Delta E_n \right)$ is the density of states. We will give a "lousy" derivation here first; will revisit later. Noticing

$$\frac{1}{x + i\eta} = \frac{x}{x^2 + \eta^2} - i \frac{\eta}{x^2 + \eta^2}$$

We will handle the real part later. The imaginary part looks like

Normalization:

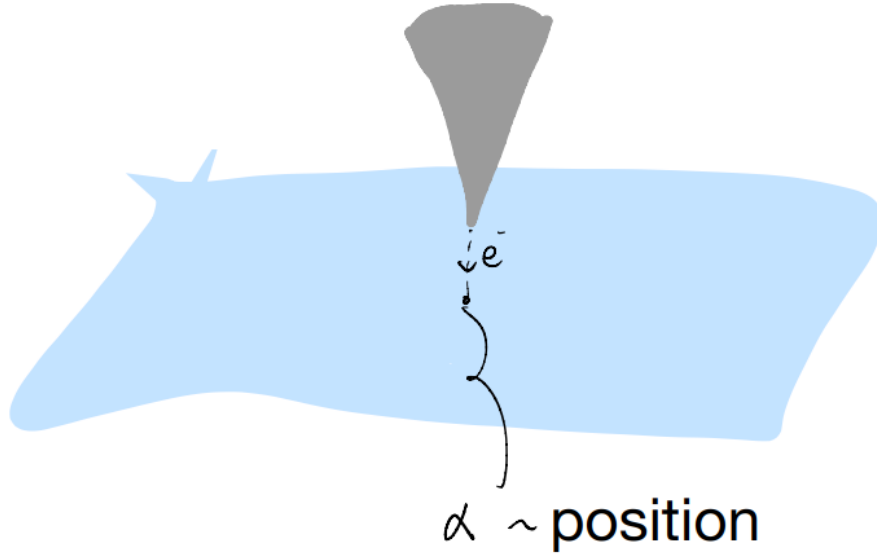$$\int_{-\infty}^{\infty} dx \frac{\eta}{x^2 + \eta^2} = \pi$$

$$\Rightarrow \lim_{\eta \to 0^+} \text{Im} \left[\frac{1}{x + i\eta} \right] = -\pi \delta \left(0 \right)$$

This gives

$$A_{\alpha\alpha}(\omega) = \frac{-1}{\pi} \lim_{\eta\to0^+} \operatorname{Im} \sum_n \frac{\left|\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle\right|^2}{\omega - \Delta E_n + i\eta}$$

$$= \sum_n \left|\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle\right|^2 \delta(\omega - \Delta E_n)$$

where $\left|\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle\right|^2 \delta(\omega - \Delta E_n)$ is the probability of finding the system in the $|n\rangle$ eigenstate when we add an electron $\hat{c}_\alpha^\dagger$ to the ground state $|\Omega\rangle$ with energy ω matching ΔE_n. How can we measure a quantity like that?

STM: trying to add electrons to the sample (approx. in the ground state at low temperature)

$\alpha \sim$ position

But STM doesn't only try to add electrons! The tip also tries to "pull" electrons out of the sample, i.e., remove electron from the ground state, Similarly for ARPES

Clearly, there are many more things one can do. We are only starting to see the tip of the iceberg.
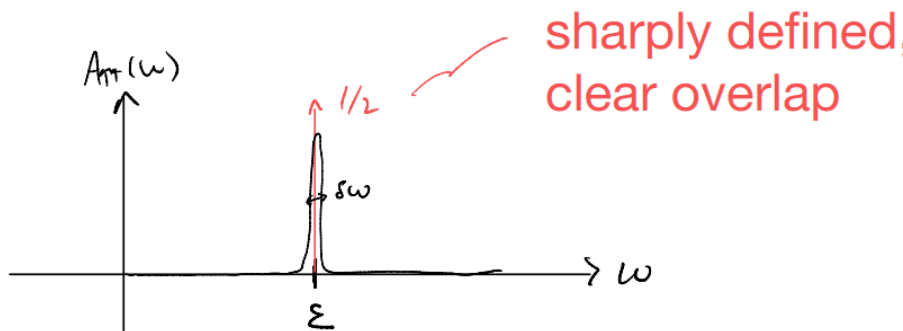
5.2   Ground state deduction: a thought experiment

Now, let's imagine plotting this spectral function. First, let us revert to our simple "single-orbital" example

$$\hat{H} = \varepsilon\left(\hat{c}_\uparrow^\dagger\hat{c}_\downarrow + \hat{c}_\downarrow^\dagger\hat{c}_\uparrow\right)$$
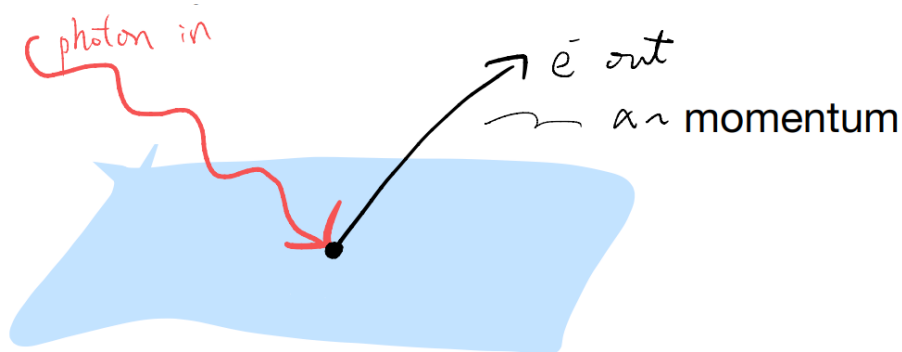
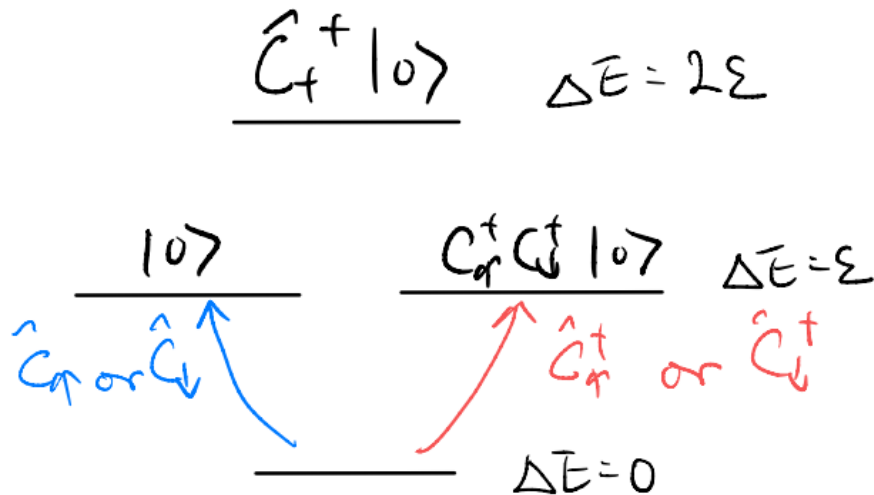$$G_{\uparrow\uparrow}(t) = -i\frac{1}{2}e^{-i\varepsilon t}$$

$$A_{\uparrow\uparrow}(t) = \frac{1}{2}\delta(\omega - \varepsilon)$$

If this was an experimental result, how would we interpret it? There is a sharp "resonance" when we try to add an up electron with energy ε to the ground state. The overlap is $\frac{1}{2}$. Suppose we can do similar experiments and measure $A_{\downarrow\downarrow}(\omega)$, as well as those associated with electron electron removal
we will conclude:

1. Adding $\hat{c}_{\uparrow}^{\dagger}$: sharp resonance with weight $\frac{1}{2}$

2. Adding $\hat{c}_{\downarrow}^{\dagger}$: sharp resonance with weight $\frac{1}{2}$

3. Removing $\hat{c}_{\uparrow}$: sharp resonance with weight $\frac{1}{2}$

4. Removing $\hat{c}_{\downarrow}$: sharp resonance with weight $\frac{1}{2}$

Further, IF we know the relevant Hilbert space is one orbital with spin-$\frac{1}{2}$ electrons, we can conclude

$$\hat{C}_\uparrow^\dagger |0\rangle \qquad \Delta E = 2\varepsilon$$

$$|0\rangle \qquad\qquad \hat{C}_\uparrow^\dagger \hat{C}_\downarrow^\dagger |0\rangle \qquad \Delta E = \varepsilon$$

$$\hat{C}_\uparrow \text{ or } \hat{C}_\downarrow \qquad\qquad \hat{C}_\uparrow^\dagger \text{ or } \hat{C}_\downarrow^\dagger$$

$$\Delta E = 0$$

(a) We can both add and remove electron from the ground state, it must have 1 electron

(b) The one electron is in some half-half state between spins up and down (equal weights above)

$$|\Omega\rangle = \frac{1}{\sqrt{2}} \left(\hat{c}_\uparrow^\dagger + e^{i\phi} \hat{c}_\downarrow^\dagger \right) |0\rangle$$

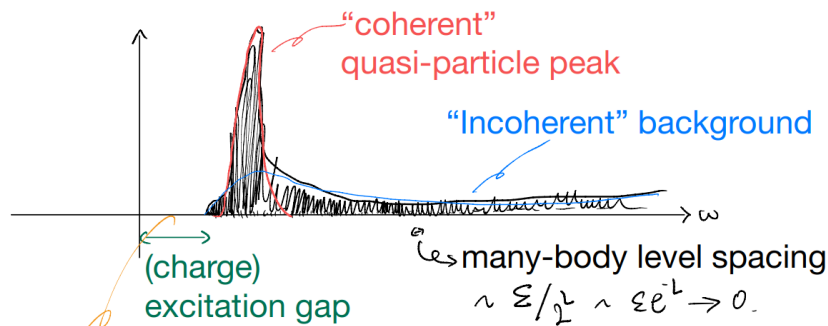i.e., we know the ground state up to an undetermined phase!
   Notes:

1. We assumed above that we can choose to tunnel spin up versus down electrons independently. This is a kind of "resolution", giving "spin-resolved" spectral function (e.g., spin-polarized STM tips). If we don't have such spin resolution, we can only conclude (a) but not (b). More resolved means more knowledge

2. For such a "small" system, one can imagine cooking up fancier measurements to "better resolve" the system. That's in the spirit of quantum tomography. We don't usually have the luxury of such measurement capability in many-body quantum systems so we won't go further down there.

Let us next imagine plotting the spectral function for a general interacting many-body Hamiltonian
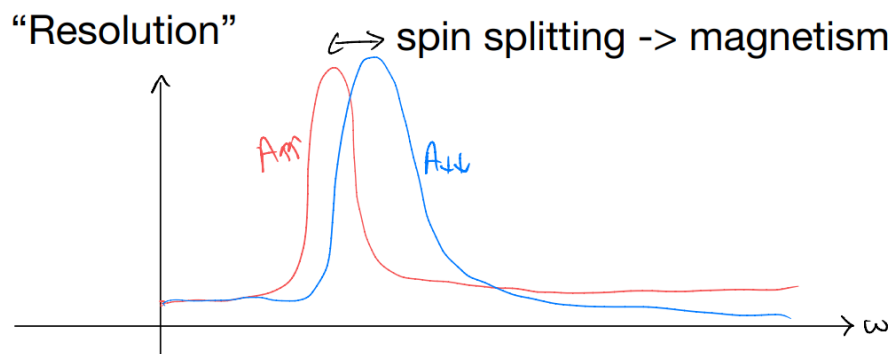
$$A_{\alpha\alpha}(\omega) = \sum_n \left| \langle n | \hat{c}_\alpha^\dagger | \Omega \rangle \right|^2 \delta(\omega - \Delta E_n)$$

Strange situations: featureless over the energy range. If such a spectrum is observed, it suggests either

$$A_{\alpha\alpha}(\omega) = \sum_n |\langle n | c_\alpha^\dagger | \Omega \rangle|^2 \, \delta(\omega - \Delta E_n)$$

"coherent"
quasi-particle peak

"Incoherent" background

ω

(charge)
excitation gap

$\hookrightarrow$ many-body level spacing
$\sim \varepsilon/2^L \sim \varepsilon e^{-L} \to 0.$

There may be excitations here too! Just no
matrix element. E.g., magnons

"Resolution" $\hookrightarrow$ spin splitting -> magnetism

$A_{\uparrow\uparrow}$

$A_{\downarrow\downarrow}$

ω

1. the excitations cannot be understood as quasi-particles

2. quasi-particles exist, but they have poor overlap with the physical electrons

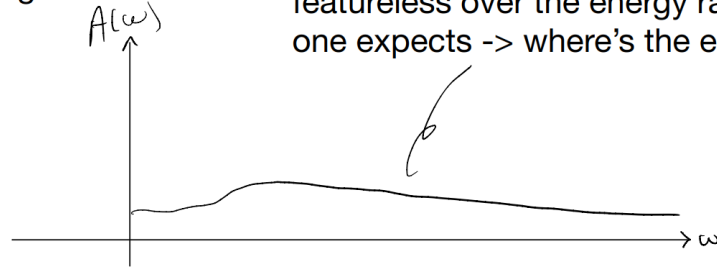Either will be very interesting! But beyond our scope...

5.3   A peek of the iceberg

In the above, we chose in an ad hoc manner to consider the real-time Green's function

$$G_{\alpha\alpha}(t) = (-i) \langle \Omega | \hat{c}_\alpha(t) \, \hat{c}_\alpha^\dagger(0) | \Omega \rangle$$

"dispersion"

Strange situations…

$A(\omega)$

featureless over the energy range
one expects -> where's the electron?
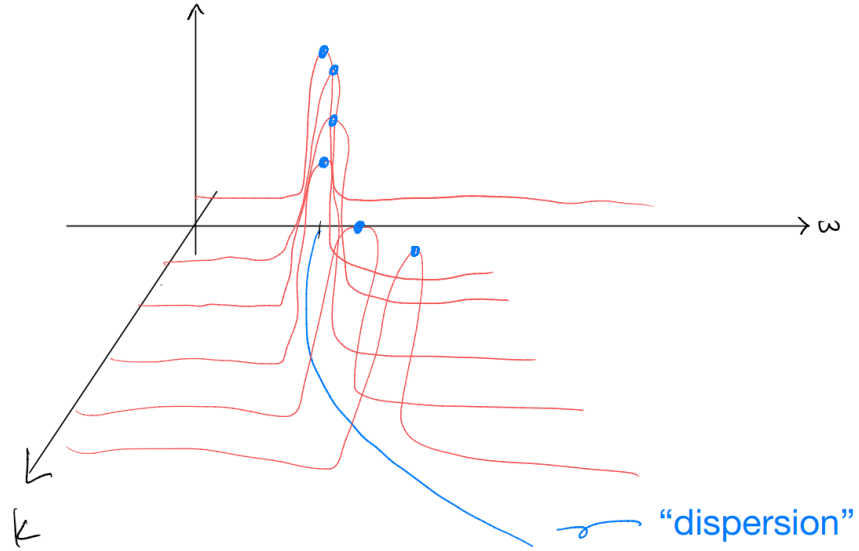
Since our ground state will have a some finite density of electrons to start with, it will be equally natural to consider, e.g.,

$$G'_{\alpha\alpha}(t) = (-i)\langle\Omega|\hat{c}^\dagger_\alpha(t)\,\hat{c}_\alpha(0)|\Omega\rangle$$

which contains information about electron removal from $|\Omega\rangle$.

In addition, we don't necessarily have to commit to the "diagonal" form with matched indices. E.g., if α denotes spatial indices, it would be natural to consider

$$G_{xy}(t,t') = (-i)\langle\Omega|\hat{c}_x(t)\,\hat{c}^\dagger_y(t')|\Omega\rangle$$

Our commitment above on $t > 0$ is also a bit ad hoc anyway. We should be free ask what happens if we compute "negative time" correlation function, at least as a theoretical gadget. Also, why not do something more than single electron addition (removal)? E.g.,

$$G''_{\alpha\alpha\gamma\delta}(t_1, t_2, t_3, t_4) = (-i)\langle\Omega|\hat{c}_\alpha(t_1)\,\hat{c}_\beta(t_2)\,\hat{c}^\dagger_\gamma(t_3)\,\hat{c}^\dagger_\delta(t_4)|\Omega\rangle$$

These discussions suggest that there is a huge zoo of possible "Green's functionS" to consider, and we need a way to organize them, e.g., fix some ordering on the time of "insertions", etc.

Such generalized Green's functions appear under different considerations, and we may want to give them different names, Nevertheless, they are all variations on the same tune, much like Schubert's trout quintet! More later...

5.4 Impurity phonon coupling

So far, we have discussed

1. QHO: coherent states, displacement operator,...

2. Free phonons: collection of decoupled QHOs

3. Localized electrons: a primer into "spectroscopy"

Let us now integrate all these into one single problem: how could we use electrons to probe phonons?
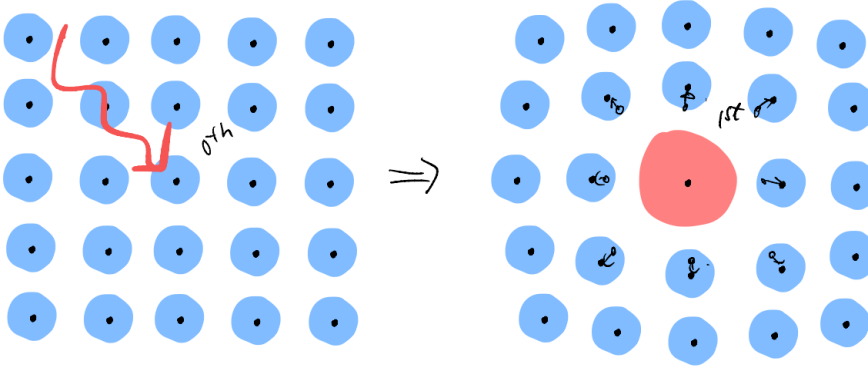
Similar to before, let us consider a single-site electronic problem:

$$\hat{H}_e = \sum_{i=1}^{N} \varepsilon_i \hat{c}_i^\dagger \hat{c}_i$$

let us interpret the index i as labeling some relevant orbitals $s, p, d, \cdots$ and for concreteness we suppose there are N relevant orbitals in our problem. We also consider the free phonon Hamiltonian

$$\hat{H}_{ph} = \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q$$

where we have dropped the zero-point energy for simplicity, and take a single branch with uniform masses.

Let us suppose the electronic Hamiltonian describes the electronic states of an impurity located at the origin. The size and shape of the electron cloud surrounding our impurity depends in general on the orbital index i. This, in turn, affect the equilibrium position of the neighboring atoms, e.g., a "fatter" electron cloud will push the neighboring atoms further away. We claim this coupling can be modelled as

$$\hat{H}_{e-ph} = \sum_{i,q} \hat{c}_i^\dagger \hat{c}_i M_{iq} \left(\hat{a}_q + \hat{a}_q^\dagger \right)$$

We will see why in the next class.

Chapter 6

lec06 20220223

Topics

1. impurity-phonon coupling

2. zero-temperature solution

3. impurity spectral function

Goals

1. Applying the techniques to a less trivial and physically relevant problem

2. Appreciating how we could probe phonons with electrons

Last time, we began introducing an impurity-phonon problem:

$$\hat{H} = \underbrace{\sum_{i=1}^{N} \varepsilon_i \hat{c}_i^\dagger \hat{c}_i}_{\hat{H}_e} + \underbrace{\sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q}_{\hat{H}_{ph}} + \underbrace{\sum_{i,q} \hat{c}_i^\dagger \hat{c}_i M_{iq} \left(\hat{a}_q + \hat{a}_q^\dagger \right)}_{\hat{H}_{e-ph}}$$

It describes a system of an electronic impurity, whose state (occupancy of the orbitals indexed by i) affects the phonon through the last electron-phonon interaction term $\hat{H}_{e-ph}$. We will first sketch why $\hat{H}_{e-ph}$ takes the stated form.

Recall that our phonon Hamiltonian resulted from an expansion of the elastic potential energy about the equilibrium

$$\hat{H}_{ph} = \sum_{r\alpha} \frac{\hat{p}_r^{\alpha 2}}{2m} + \frac{1}{2} \sum_{r,r'} \left. \frac{\partial^2 \mathcal{V}}{\partial R_r \partial R_{r'}} \right|_0 \left(\hat{R}_r - R_{r,0} \right) \left(\hat{R}_{r'} - R_{r',0} \right)$$

$$\hat{u}_r = \hat{R}_r - R_{r,0}$$

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where $\hat{R}_r$ is the actual position, $R_{r,0}$ is the equilibrium position and $\hat{u}_r$ is the deviation from the equilibrium. As discussed, the equilibrium positions are now dependent on the electronic state

$$R_{r,0} \to R_{r,0} + \delta R^i_{r,0}$$

where we expect $\delta R_{r,0} \approx 0$ for r far from the impurity. To leading order, this leads to an i-dependent change of the phonon Hamiltonian

$$\delta \hat{H}^i_{ph} \sim - \sum_{r,r'} \left. \frac{\partial^2 \mathcal{V}}{\partial R_r \partial R_{r'}} \right|_0 \hat{u}_r \left(\delta R^i_{r'} \right) + \delta E^i$$
$$= \sum_r \left(M^i \right)_r \hat{u}_r + \delta E^i$$

where the first term is linear in $\hat{u}_r$ and δE^i absorbs the electronic energies ε_i (*TODO strange expression*). We should now recast the operators into the phonon creation and annihilation $\hat{a}^\dagger_q$ and $\hat{a}_q$.

$$\begin{cases} \hat{a}_q = \frac{1}{\sqrt{2}} \left(\sqrt{m\omega_q}\hat{u}_q + \frac{i}{\sqrt{m\omega_q}}\hat{p}_q \right) \\ (\hat{a}_{-q})^\dagger = \frac{1}{\sqrt{2}} \left(\sqrt{m\omega_q}\hat{u}_q - \frac{i}{\sqrt{m\omega_q}}\hat{p}_q \right) \end{cases}$$

$$\Rightarrow \hat{u}_q = \frac{\hat{a}_q + \hat{a}^\dagger_q}{\sqrt{2m\omega_q}}$$

where we used

$$\hat{u}^\dagger_{-q} = \hat{u}_q$$

$$\hat{p}^\dagger_{-q} = \hat{p}_q$$

as one can see from the Fourier transform

$$\hat{u}_q = \frac{1}{\sqrt{V}} \sum_r e^{iq \cdot r} \hat{u}_r$$

$$\hat{u}_r = \frac{1}{\sqrt{V}} \sum_q e^{-iq \cdot r} \hat{u}_q$$

This gives the electron-dependent correction

$$\delta\hat{H}_{ph}^i = \sum_r M_r^i \hat{u}_r$$

$$= \sum_r M_r^i \frac{1}{\sqrt{V}} \sum_q e^{-iq\cdot r} \frac{\hat{a}_q + \hat{a}_{-q}^\dagger}{\sqrt{2m\omega_q}}$$

$$= \sum_q \underbrace{\frac{1}{\sqrt{2m\omega_q}} \left(\frac{1}{\sqrt{V}} \sum_r M_r^i e^{-iq\cdot r} \right)}_{} \left(\hat{a}_q + \hat{a}_{-q}^\dagger \right)$$

$$= \sum_q M_q^i \left(\hat{a}_q + \hat{a}_{-q}^\dagger \right)$$

$$= \sum_q \left(M_q^i \hat{a}_q + M_{-q}^i \hat{a}_q^\dagger \right)$$

let us further assert that $M_r^i = M_{-r}^i$ such that $M_q^i = M_{-q}^i$

$$\Rightarrow \delta\hat{H}_{ph}^i = \sum_q M_q^i \left(\hat{a}_q + \hat{a}_q^\dagger \right)$$

Altogether, we have the impurity-phonon Hamiltonian (c.f. Mahan Chapter-4)

$$\hat{H} = \underbrace{\sum_{i=1}^N \varepsilon_i \hat{c}_i^\dagger \hat{c}_i}_{\hat{H}_e} + \underbrace{\sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q}_{\hat{H}_{ph}} + \underbrace{\sum_{i,q} \hat{c}_i^\dagger \hat{c}_i M_{iq} \left(\hat{a}_q + \hat{a}_q^\dagger \right)}_{\hat{H}_{e-ph}}$$

Note: is this a good approximation? Not necessarily. One should recognize what we have done above is quite schematic, and there are many possible reasons to object to our treatment, e.g.,

1. The shift in equilibrium position is probably not as simple as what we have assumed. E.g., the shift may not be simply the sum of the individual orbital contribution

2. There is no particular reason why terms like $\hat{c}_i^\dagger \hat{c}_j \left(\hat{a}_q + \hat{a}_q^\dagger \right) + h.c.$ are absent

There are valid concerns. It's important to realize that, here, we are simply trying to motivate a toy model which is not crazy (doesn't mean it is directly applicable to any real problem). In particle, we will not dwell into details like the form of the coefficients M_q^i etc. Those are important for really modelling an actual system. But our goal is simply to show how such problems could be approached, and from this illustrates relevant aspects of the one-particle Greens' function and spectral function.

6.1   Exact solution

We have discussed how the problems of free phonons and localized electrons are both exactly soluble. In our current problem, we have introduced a coupling between the two. Generally speaking, we cannot find exact solutions for such coupled problem. But we will now see that our toy model is really designed to remain exactly soluble.

To this end, let us introduce $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$ being the electron number for the i-th orbital. It satisfies

$$\hat{n}_i^2 = \hat{c}_i^\dagger \hat{c}_i \hat{c}_i^\dagger \hat{c}_i = \hat{c}_i^\dagger \left(1 - \hat{c}_i^\dagger \hat{c}_i \right) \hat{c}_i = \hat{c}_i^\dagger \hat{c}_i = \hat{n}_i$$

$$\Rightarrow \operatorname{eig}\left(\hat{n}_i \right) = 0 \quad \text{or} \quad 1$$

Also, notice that $[\hat{n}_i, \hat{n}_j] = 0$. We can write the Hamiltonian as

$$\hat{H} = \sum_{i=1}^{N} \varepsilon_i \hat{n}_i + \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q + \sum_{i,q} \hat{n}_i M_{iq} \left(\hat{a}_q + \hat{a}_q^\dagger \right)$$

We see readily that

$$\left[\hat{H}, \hat{n}_i \right] = 0, \quad \forall i = 1, \cdots, N$$

As such, the electron numbers are good quantum numbers, and we can decompose the full Hilbert space into the 2^N sectors labeled by

$$(n_1, n_2, \cdots, n_N) = (0, 0, \cdots, 0), (1, 0, \cdots, 0), \cdots, (1, 1, \cdots, 1)$$

For simplicity, let us denote one such "configuration" by $\{n_i\}$. The Hamiltonian restricted to one such sector becomes

$$
\begin{aligned}
\hat{H} \Big|_{\{n_i\}} &= \sum_{i=1}^{N} \varepsilon_i n_i + \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q + \sum_q \left(\sum_i n_i M_{iq} \right) \left(\hat{a}_q + \hat{a}_q^\dagger \right) \\
&= \sum_{i=1}^{N} \varepsilon_i n_i + \sum_q \omega_q \left(\hat{a}_q^\dagger + \frac{1}{\omega_q} \sum_i n_i M_{iq} \right) \left(\hat{a}_q + \frac{1}{\omega_q} \sum_i n_i M_{iq} \right) \\
&\quad - \sum_q \frac{1}{\omega_q} \left(\sum_i n_i M_{iq} \right)^2
\end{aligned}
$$

where we have used the usual trick of "completing square" $((a+b)^2 = a^2 + b^2 + 2ab)$

In this restricted Hilbert space, the Hamiltonian acts only on the phonons. In addition, it contains only up to quadratic terms for the phonons, and so it remains exactly solvable. To construct the eigenstates, let us recall the displacement operator.

$$\hat{D}_q \left(\alpha \right) = e^{\alpha \hat{a}_q^\dagger - \alpha^* \hat{a}_q}$$

$$\Rightarrow \hat{D}_q(\alpha)\,\hat{a}_q\hat{D}_q^\dagger(\alpha) = \hat{a}_q - \alpha$$

$$\Rightarrow \hat{D}_q(\alpha)\,\hat{a}_q^\dagger\hat{D}_q^\dagger(\alpha) = \hat{a}_q^\dagger - \alpha^*$$

Recall that M_{iq} is real (TODO why), this gives

$$\left[\prod_q \hat{D}_q\left(\frac{1}{\omega_q}\sum_i n_i M_{iq}\right)\right]\left(\hat{H}\Big|_{\{n_i\}}\right)\left[\prod_q \hat{D}_q^\dagger\left(\frac{1}{\omega_q}\sum_i n_i M_{iq}\right)\right]$$

$$= \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q + \sum_{i=1}^{N}\varepsilon_i n_i - \sum_q \frac{1}{\omega_q}\left(\sum_i n_i M_{iq}\right)^2$$

where the first term is equivalent to the original phonon Hamiltonian, and other terms are just a number. We may define the energy

$$\Delta(\{n_i\}) = \sum_{i=1}^{N}\varepsilon_i n_i - \sum_q \frac{1}{\omega_q}\left(\sum_i n_i M_{iq}\right)^2$$

where the first term is the non-interacting orbital energy and the second term is the effective density-density interaction mediated by the phonons!

Note: this expression is slightly different from Mahan's who (somehow) assumed there is exactly one electron on the impurity, and so wrote $n_i n_j = n_i \delta_{ij}$.

As such, we now know all the eigenstates and energy of our Hamiltonian. They can be labeled by two sets of integers

1. $\{n_i\}$: occupation of the $i = 1, \cdots, N$ electronic orbitals

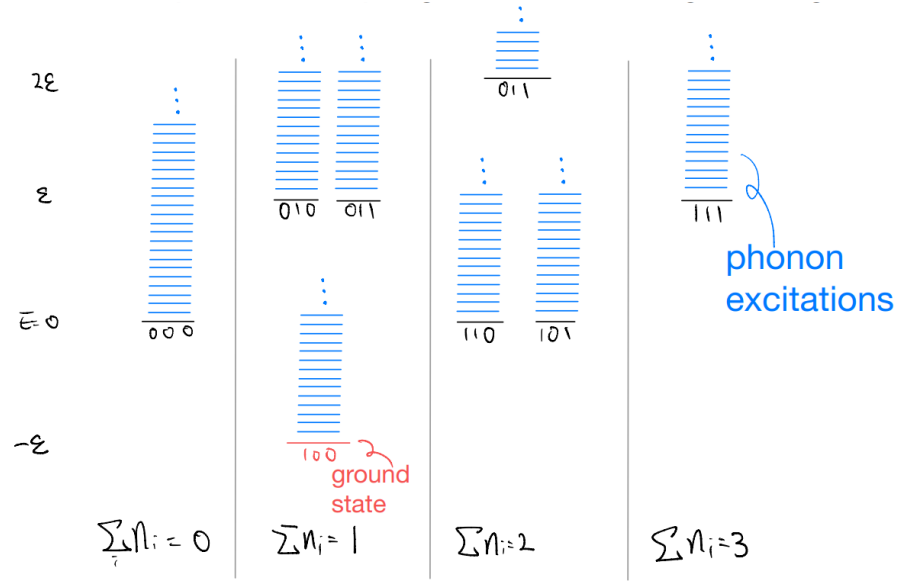2. $\{m_q\}$: number of quanta in each of $q = 1, \cdots, V$ phonon modes

The energy is

$$|\{n_i\},\{m_q\}\rangle: \quad \Delta(\{n_i\}) + \sum_q \omega_q m_q$$

It may be instructive to sketch an energy level diagram corresponding to our solution. To illustrate the ideas, suppose we have three electronic orbitals in our problem, and they have "bare" orbital energy of $-\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = \varepsilon > 0$
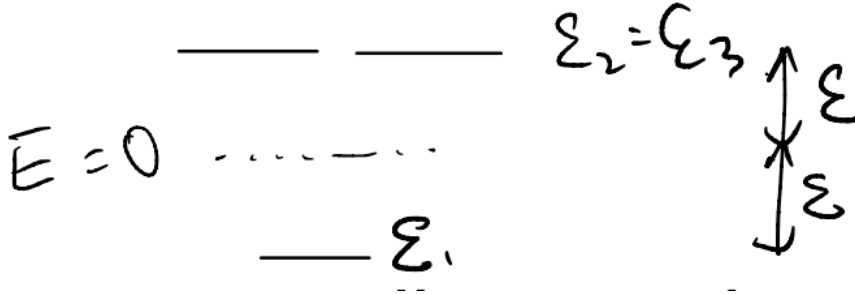
Without electron-phonon coupling, we have the eigen-energies

phonon
excitations

ground
state

3ε ε $E=0$ $-\varepsilon$

$\overline{011}$ $\overline{010}$ $\overline{011}$ $\overline{000}$ $\overline{110}$ $\overline{101}$ $\overline{111}$ $\overline{100}$

$\sum_i n_i = 0$ $\sum_i n_i = 1$ $\sum_i n_i = 2$ $\sum_i n_i = 3$

where for simplicity we considered an "Einstein phonon" model in which $\omega_q = \omega_E$ is q-independent. Otherwise, the phonon excitation should become a continuum as each mode (labeled by q) can have a different excitation energy.

Now, consider the effect of $\hat{H}_{e-ph}$, which we may treat as a perturbation to the level diagram above. A key simplifying assumption in our model (which enabled exact solutions) is that $[\hat{H}, \hat{n}_i] = 0$. In other words, even with the $e-ph$ coupling, we can think about each of the "sub-block" above individually.

But this looks deceivingly simple! The phonon state $|\{m_q\}\rangle$ actually depends on the electronic occupation in a concealed manner. To see this more explicitly, let us write the Hamiltonian as

$$\hat{H} = \bigoplus_{\{n_i\}} \hat{H}\Big|_{\{n_i\}}$$

$$= \bigoplus_{\{n_i\}} \left(\sum_q \hat{D}_q^\dagger \left(\frac{1}{\omega_q} \sum_i n_i M_{iq} \right) \omega_q \hat{a}_q^\dagger \hat{a}_q \hat{D}_q \left(\frac{1}{\omega_q} \sum_i n_i M_{iq} \right) + \Delta\left(\{n_i\}\right) \right)$$
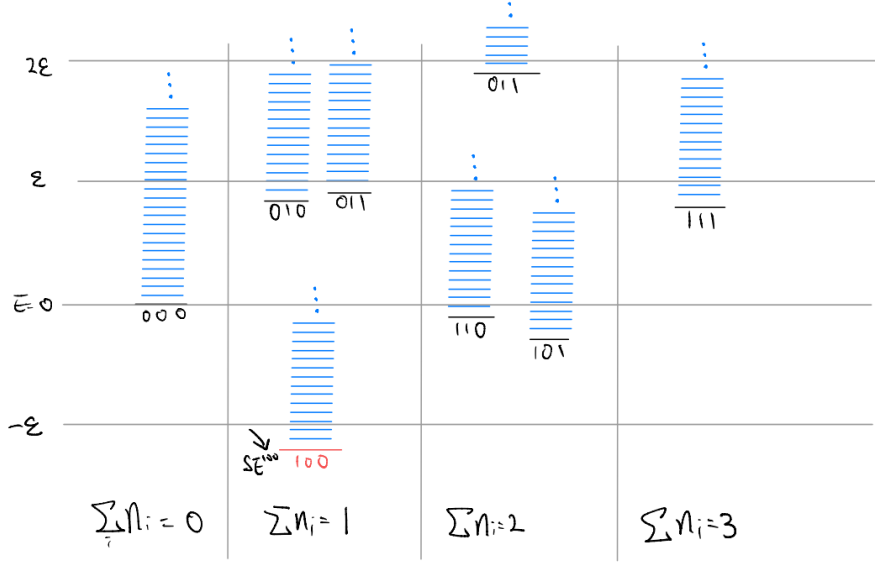
where $\oplus$ is the direct sum over the 2^N independent sectors. It's still the "same" phonon Hamiltonian, but in different basis!

E.g., let $|\{m_q\}\rangle$ be the "bare" phonon eigenstates with phonon occupancy

$$\hat{a}_q^\dagger \hat{a}_q \to m_q$$

Then the eigenstates of the Hamiltonian can be written as

$$|\{n_i\}, \{m_q\}\rangle = |\{n_i\}\rangle \otimes \left[\prod_q \hat{D}_q^\dagger \left(\frac{1}{\omega_q} \sum_i n_i M_{iq} \right) |\{m_q\}\rangle_0 \right]$$

Does this "i-dependent basis rotation" of the phonon matter? After all, the phonon energies are independent on the electronic configuration! The short answer is yes. To see why, we look into the electron's one-particle Green's function.

6.2 Electron (impurity) Greens' function

Let's look at a real-time one-particle Greens' function of the form

$$G_{ii}(t) = -i\langle\Omega|\hat{c}_i^\dagger(t)\,\hat{c}_i(0)\,|\Omega\rangle$$

where $|\Omega\rangle$ is the ground state. We will compute $G_{ii}(t)$ in two ways

1. Using the energy eigenstates we have derived. This is perhaps more transparent, but at the same time somewhat "brute force" and the solution approach looks a bit *ad hoc*, since we cannot expect to solve the many-body Hamiltonian in general

2. Solving the Heisenberg picture time evolution of the operator. This is probably the more systematic approach, and we will see that it allows for greater flexibility on the ground state

Let us start with the "brute force" approach. For concreteness, we suppose the level scheme is the one drawn before, and so the ground state is

$$|\Omega\rangle = |\{1,0,0\}\rangle \otimes \prod_q \hat{D}_q^\dagger\left(\frac{M_{1q}}{\omega_q}\right)|\{0_q\}\rangle_0$$

$$\hat{H}|\Omega\rangle = \Delta_{100}|\Omega\rangle$$

$$\Delta_{100} = \varepsilon_1 - \sum_q \frac{M_{1q}^2}{\omega_q}$$

Chapter 7

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Topics

   1. Impurity spectral function: Einstein model and numerical experiment

   Goals

   1. First example of a physically interesting spectral function

   2. Appreciating how to "extract" physical info from spectral function

Consider the state with one electron removed:

$$\hat{c}_1|\Omega\rangle = |\{0,0,0\}\rangle \otimes \prod_q \hat{D}_q^\dagger \left(\frac{M_{1q}}{\omega_q}\right) |\{0_q\}\rangle_0$$

This is *not* an eigenstate of $\hat{H}$! The eigenstates should have been

$$|\{0,0,0\}\rangle \otimes |\{m_q\}\rangle$$

Non-eigenstates means states with dynamics. So now we consider

$$
\begin{aligned}
G_{11}(t) &= (-i)\,\langle\Omega|\hat{c}_1^\dagger(t)\,\hat{c}_1(0)\,|\Omega\rangle \\
&= (-i)\,\langle\Omega|e^{i\hat{H}t}\hat{c}_1^\dagger e^{-i\hat{H}t}\hat{c}_1|\Omega\rangle \\
&= (-i)\,e^{i\Delta_{100}t}\langle\Omega|\hat{c}_1^\dagger e^{-i\hat{H}t}\hat{c}_1|\Omega\rangle \\
&= (-i)\,e^{i\Delta_{100}t}\left[\langle 0_q|_0 \prod_q \hat{D}_q\left(\frac{M_{1q}}{\omega_q}\right)\right] \otimes \langle\{100\}\,|\hat{c}_1^\dagger e^{-i\hat{H}t}\hat{c}_1 \\
&\qquad |\{100\}\rangle \otimes \prod_q \hat{D}_q^\dagger\left(\frac{M_{1q}}{\omega_q}\right)|\{0_q\}\rangle_0 \\
&= (-i)\,e^{i\Delta_{100}t}\left[\langle 0_q|_0 \prod_q \hat{D}_q\left(\frac{M_{1q}}{\omega_q}\right)\right] \exp\left\{-i\,\hat{H}\Big|_{\{000\}}t\right\} \prod_q \hat{D}_q^\dagger\left(\frac{M_{1q}}{\omega_q}\right)|\{0_q\}\rangle_0
\end{aligned}
$$

But

$$\hat{H}\Big|_{\{000\}} == \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q + \Delta_{000}$$

$$\Delta_{000} = 0$$

We have

$$G_{11}(t) = (-i)\, e^{i\Delta_{100}t} \prod_q \left(\langle -\frac{M_{1q}}{\omega_q} | e^{-i\omega_q \hat{a}_q^\dagger \hat{a}_q t} | \frac{M_{1q}}{\omega_q} \rangle_0 \right)$$

where the state in the bra and ket is the coherent state. This is just the "prop-agator" in the coherent-state basis!

$$G_{11}(t) = (-i)\, e^{i\Delta_{100}t} \prod_q \left(\langle -\frac{M_{1q}}{\omega_q} | \frac{M_{1q}}{\omega_q} e^{-i\omega_q t} \rangle_0 \right)$$

$$= (-i)\, e^{i\Delta_{100}t} \prod_q \exp\left(\frac{M_{1q}^2}{\omega_q^2} e^{-i\omega_q t} \right) \exp\left(-\frac{M_{1q}^2}{\omega_q^2} \right)$$

Let's define $g_q = \left(\frac{M_{1q}}{\omega_q} \right)^2$, then

$$G_{11}(t) = (-i)\, e^{i\Delta_{100}t} \exp\left(\sum_q g_q \left(e^{-i\omega_q t} - 1 \right) \right)$$

To make further progress, consider again the Einstein model with

$$\omega_q = \omega_E, \quad \forall q$$

Let $g = \sum_q g_q$, then

$$G_{11}(t) = (-i)\, e^{i\Delta_{100}t} \exp\left(g e^{-i\omega_E t} - g \right)$$

We can now consider the Fourier transform

$$G_{11}(\omega) = (-i)\, e^{-g} \lim_{\eta \to 0^+} \int_0^\infty dt\, e^{i\Delta_{100}t} e^{i\omega t} e^{-\eta t} \exp\left(g e^{-i\omega_E t} \right)$$

$$= (-i)\, e^{-g} \sum_{l=0}^\infty \lim_{\eta \to 0^+} \int_0^\infty dt\, \frac{g^l}{l!} e^{i(\omega + \Delta_{100} - l\omega_E + i\eta)t}$$

$$= e^{-g} \sum_{l=0}^\infty \lim_{\eta \to 0^+} \frac{g^l}{l!} \frac{1}{\omega + \Delta_{100} - l\omega_E + i\eta}$$

and same as before we find the spectral function

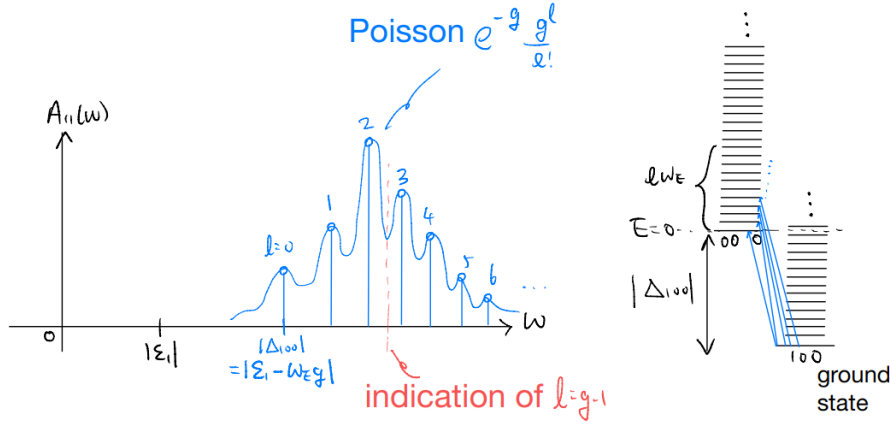$$A_{11}(\omega) = \frac{-1}{\pi} \mathrm{Im} G_{11}(\omega)$$

$$= \sum_{l=0}^\infty e^{-g} \frac{g^l}{l!} \delta\left(\omega - (-\Delta_{100} + l\omega_E) \right)$$

$$\Delta_{100} = \varepsilon_1 - \sum_q \frac{M_{1q}^2}{\omega_q} = \varepsilon_1 - \omega_E g < 0$$

The spectral function is the sum of delta functions. For which l do we get the highest weight?

$$\frac{g^{l+1}}{(l+1)!} = \left(\frac{g}{l+1}\right)\left(\frac{g^l}{l!}\right)$$

increasing for $l < g - 1$, decreasing for $l > g - 1$

Interpretation: when we try to remove an electron, we discover that in the ground state the "electron" is actually dressed by the phonons. With strong coupling ($g \gg 1$), the dominant spectral peak is far from the bare electronic orbital contribution of $|\Delta_{100}|$.

Notes:

1. The Einstein model is simple by design, and enables very explicit computation of the frequency-space Green's function (and hence spectral function). Our real-time solution, however, holds for more general phonon dispersion. When we deviate from the Einstein model we should start seeing deviation from the "sum of delta function" form of the spectral function

2. More interestingly, one should ask what happens for acoustic phonons which have $\omega_q \to 0$ as $q \to 0$. Recall the strength of the $e - ph$ coupling was parameterized by $g_q = \left(\frac{M_{iq}}{\omega_q}\right)^2$. If M_{iq} stays finite and $\omega_q \to 0$, we have diverging coupling and hence energies etc.!

This is a rather general feature: low-energy modes are "dangerous" because they are easy to excite. In finding the ground state, one should, generally speaking, check how the "fluctuations" (lowest excitations) could destabilize the ground state. This amounts to a kind of self-consistency check. If the assumed ground state implies strong fluctuations which kills itself, the ground state does

not actually "form". This is the key physical picture behind the Merlin-Wagner theorem on the absence of spontaneous continuous symmetry breaking in low dimensions.

Now, back to our impurity-phonon problem: physically, the acoustic phonons have vanishing frequency in the long-wavelength limit because they are Goldstone modes. The Goldstones exist because of symmetries, and are correspondingly constrained by symmetries. In our context, the catastrophe is avoided by having a "derivative coupling", such that the $e - ph$ coupling has a momentum dependence of $M_{iq} \propto q$ as $q \to 0$. This gives a finite coupling strength as both M_{iq} and ω_q vanish linearly in q.

Note: play with the uploaded Python code if you want to explore what happens beyond the Einstein model.

Chapter 8

lec08 20220302

Topics

1. Impurity spectral function: solving again with Heisenberg

2. Dyson series, time ordering, and time-ordered exponential

Goals

1. Learning how to deal with time-dependent perturbations

8.1 Solving again: Heisenberg picture

Our solution for the impurity (one-electron) spectral function was satisfactory (I think), in the sense that we have found a concrete expression which does encode a lot of interesting physics (e.g., enable numerical simulation, and analytical solution with the simplified Einstein phonons). Yet, it is also clear that our calculation approach worked because we have an exactly solved model. This is a luxury to have, and oftentimes people take "exactly solubility" to equate to "boring". (Of course, this is subjected to personal taste)

The bottom line is, our problem was exactly solvable because it ultimately decouples into independent QHO (shifted phonon Hamiltonian) and fermions (individually conserved particle number). We only have a minimal degree of interactions in our model, namely, the phonon-mediated density-density interactions between the electrons.

Our course is called "Quantum many-body theory", and apparently I cannot avoid introducing techniques for solving more general interacting many-body problems! This motivates to go through a more complicated approach of solving the same problem again, through the Heisenberg picture.

Recall in the Heisenberg picture the states are stationary, and the operators evolve according to

$$\hat{O}_H\left(t\right) = e^{i\hat{H}t}\hat{O}_S e^{-i\hat{H}t}$$

their time evolution is governed by the equation of motion

$$i\partial_t \hat{O}_H(t) = \left[\hat{O}_H(t), \hat{H}\right]_H$$

everything below will be in the Heisenberg picture, and we drop the subscript. Here we want to compute the real-time Green's function

$$G_{ii}(t) = \langle\Omega|\hat{c}_i^\dagger(t)\,\hat{c}_i(0)\,|\Omega\rangle$$

and so we would want to compute the time evolution of $\hat{c}_i^\dagger(t)$ under the Hamiltonian

$$\hat{H} = \sum_{i=1}^N \varepsilon_i \hat{n}_i + \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q + \sum_{i,q} \hat{n}_i M_{iq}\left(\hat{a}_q + \hat{a}_q^\dagger\right)$$

So we first find the equation of motion for $\hat{c}_i(t)$. Notice

$$\begin{aligned}
\left[\hat{c}_i^\dagger(t), \hat{n}_j(t)\right] &= \left[\hat{c}_i^\dagger(t), \hat{c}_j^\dagger(t)\,\hat{c}_j(t)\right] \\
&= \delta_{ij}\left(\hat{c}_i^\dagger(t)\left[\hat{c}_i^\dagger(t), \hat{c}_i(t)\right]\right) \\
&= \delta_{ij}\hat{c}_i^\dagger(t)\left(2\hat{c}_i^\dagger(t)\,\hat{c}_i(t) - 1\right) \\
&= -\delta_{ij}\hat{c}_i^\dagger(t)
\end{aligned}$$

we then have

$$\begin{aligned}
i\partial_t \hat{c}_i^\dagger(t) &= \left[\hat{c}_i^\dagger(t), \hat{H}\right] \\
&= \sum_j \left[\hat{c}_i^\dagger(t), \varepsilon_j \hat{n}_j(t) + \hat{n}_j(t)\sum_q M_{jq}\left(\hat{a}_q(t) + \hat{a}_q^\dagger(t)\right)\right] \\
&= -\left(\varepsilon_i + \sum_q M_{iq}\left(\hat{a}_q(t) + \hat{a}_q^\dagger(t)\right)\right)\hat{c}_i^\dagger(t) \\
&= \hat{O}(t)\,\hat{c}_i^\dagger(t)
\end{aligned}$$

$$\hat{O}(t) = -\varepsilon_i - \sum_q M_{iq}\left(\hat{a}_q(t) + \hat{a}_q^\dagger(t)\right)$$

compared to our earlier "single-site" electronic model (c.f. Lecture-4), the difference is that the orbital energy ε_i is now promoted to a time-dependent operator. The "operators" act on the phonon Fock space, and reflects the electron-phonon coupling. The time-dependence comes from the time evolution of the phonon operators, which reflects their dynamics.

This, therefore, implies that we have to also solve for the time-evolution of the phonon operators, Again, we first notice

$$\left[\hat{a}_q(t), \hat{a}_{q'}^\dagger(t)\right] = \delta_{qq'}$$

$$\Rightarrow \quad \left[\hat{a}_q(t), \hat{a}_{q'}^\dagger(t)\hat{a}_{q'}(t)\right] = \delta_{qq'}\hat{a}_q(t)$$

and so the equation of motion is

$$i\partial_t\hat{a}_q(t) = \left[\hat{a}_q(t), \sum_{q'}\left(\omega_{q'}\hat{a}_{q'}^\dagger\hat{a}_{q'} + \sum_i \hat{n}_i M_{iq'}\left(\hat{a}_{q'} + \hat{a}_{q'}^\dagger\right)\right)\right]$$

$$= \omega_q\hat{a}_q(t) + \sum_i \hat{n}_i M_{iq}$$

the $e - ph$ coupling again leads to a new piece, which requires us to consider

$$i\partial_t\hat{n}_i(t) = \left[\hat{n}_i(t), \hat{H}\right] = 0$$

which means $\hat{n}_i(t)$ is an "integral of motion" and stays constant $\hat{n}_i(t) = \hat{n}_i$.

Note: We have basically set up a hierarchy of equation of motions (EOM): when we try to solve for the evolution of an operator, we see that its EOM contains some other operators, and we have to proceed with finding the EOM of these other operators etc. Such hierarchy is not closed in general, which makes it impossible to write down a closed set of equations (and let alone finding the exact solution). From this lens, our model is exactly solved in that the hierarchy terminates, and we only need to consider the coupled equations for $\hat{c}_i^\dagger(t)$ and $\hat{a}_q(t)$. We may first solve

$$i\partial_t\hat{a}_q(t) = \omega_q\hat{a}_q(t) + \sum_i \hat{n}_i M_{iq}$$

Let

$$\hat{a}_q(t) = \hat{A} + \hat{B}e^{-i\omega_q t}$$

$$i\partial_t\hat{a}_q(t) = \omega_q\hat{B}e^{-i\omega t} = \omega_q\left(\hat{a}_q(t) - \hat{A}\right)$$

comparing the equations above,

$$-\omega_q\hat{A} = \sum_i \hat{n}_i M_{iq}$$

$$\Rightarrow \quad \hat{a}_q(t) = -\sum_i \hat{n}_i \frac{M_{iq}}{\omega_q} + \hat{B}e^{-i\omega_q t}$$

$$\hat{a}_q(0) = -\sum_i \hat{n}_i \frac{M_{iq}}{\omega_q} + \hat{B}$$

$$\Rightarrow \quad \hat{B} = \hat{a}_q(0) + \sum_i \hat{n}_i \frac{M_{iq}}{\omega_q}$$

$$\Rightarrow \quad \hat{a}_q(t) + \sum_i \hat{n}_i \frac{M_{iq}}{\omega_q} = \left(\hat{a}_q(0) + \sum_i \hat{n}_i \frac{M_{iq}}{\omega_q}\right)e^{-i\omega_q t}$$

Looks familiar? This simply reflects our earlier observation that, the "eigen" phonon operators in the $\{n_i\}$ sector is related to the bare one (i.e., in the absence of $e - ph$ coupling) by a shift using the displacement operator.

To simplify notation, let us define

$$\hat{a}_q^{\{n_i\}}(t) = \hat{a}_q(t) + \sum_i \hat{n}_i \frac{M_{iq}}{\omega_q}$$

Then we simply have

$$\hat{a}_q^{\{n_i\}}(t) = \hat{a}_q^{\{n_i\}}(0) e^{-i\omega_q t}$$

With this preparation we can go back to study the time-evolution of the fermion operator

$$i\partial_t \hat{c}_i^\dagger(t) = \hat{O}(t)\, \hat{c}_i^\dagger(t)$$

$$\hat{O}(t) = -\varepsilon_i - \sum_q M_{iq}\left(\hat{a}_q(t) + \hat{a}_q^\dagger(t)\right)$$

$$= -\varepsilon_i - \sum_q M_{iq}\left(\hat{a}_q^{\{n_i\}}(t) + \hat{a}_q^{\{n_i\}\dagger}(t) - 2\sum_j \hat{n}_j \frac{M_{jq}}{\omega_q}\right)$$

How do we solve this? Recall, if we have a simple function

$$i\partial_t f(t) = g(t)\, f(t)$$

$$\Rightarrow\ f(t) = f(0) \exp\left(-i \int_0^t g(t')\, dt'\right)$$

$$i\partial_t f(t) = f(0)\left(i\partial_t \exp\left(-i \int_0^t g(t')\, dt'\right)\right)$$

$$= f(0)\left(\partial_t \int_0^t g(t')\, dt'\right) \exp\left(-i \int_0^t g(t')\, dt'\right)$$

$$= g(t)\, f(t)$$

It is then tempting to declare our formal solution is simply

$$\hat{c}_i^\dagger(t) \stackrel{?}{=} \exp\left(-i \int_0^t \hat{O}(t')\, dt'\right) \hat{c}_i^\dagger(0)$$

But we should Remember the meaning of the exponential here is that it is a formal power series!

$$\hat{c}_i^\dagger \stackrel{?}{=} \sum_{n=0}^\infty \frac{(-i)^n}{n!} \left[\int_0^t dt' \hat{O}(t')\right]^n \hat{c}_i^\dagger(0)$$

$$= \left(1 - i \int_0^t dt_1 \hat{O}(t_1) + \frac{(-i)^2}{2} \int_0^t dt_1 \int_0^t dt_2 \hat{O}(t_1)\hat{O}(t_2) + \cdots\right) \hat{c}_i^\dagger(0)$$

$$i\partial_t \hat{c}_i^\dagger (t) \stackrel{?}{=} \left\{ \hat{O}(t) - \frac{i}{2} \left[\hat{O}(t) \left(\int_0^t dt_2 \hat{O}(t_2) \right) + \left(\int_0^t dt_1 \hat{O}(t_1) \right) \hat{O}(t) \right] + \cdots \right\} \hat{c}_i^\dagger (0)$$

versus

$$\hat{O}(t)\, \hat{c}_i^\dagger (t) = \hat{O}(t) \left(1 - i \int_0^t dt_1 \hat{O}(t_1) + \cdots \right) \hat{c}_i^\dagger (0)$$

the two expression agree to this order only if

$$\frac{1}{2} \left[\hat{O}(t) \left(\int_0^t dt_2 \hat{O}(t_2) \right) + \left(\int_0^t dt_1 \hat{O}(t_1) \right) \hat{O}(t) \right] = \hat{O}(t) \int_0^t dt_1 \hat{O}(t_1)$$

$$\Rightarrow \quad \left[\int_0^t dt_1 \hat{O}(t_1), \hat{O}(t) \right] = 0$$

But the "same" operator at different times may not commute with "itself"! E.g., consider a single QHO, let

$$\hat{O}(t) = \hat{a}(t) + \hat{a}^\dagger (t) = \hat{a}(0)\, e^{-i\omega t} + \hat{a}^\dagger (0)\, e^{i\omega t}$$

$$\left[\hat{O}(t_1), \hat{O}(t_2) \right] = \left[\hat{a}(0)\, e^{-i\omega t_1} + \hat{a}^\dagger (0)\, e^{i\omega t_1}, \hat{a}(0)\, e^{-i\omega t_2} + \hat{a}^\dagger (0)\, e^{i\omega t_2} \right]$$

$$= \left[\hat{a}^\dagger (0), \hat{a}(0) \right] e^{i\omega(t_1 - t_2)} + \left[\hat{a}(0), \hat{a}^\dagger (0) \right] e^{-i\omega(t_1 - t_2)}$$

$$= -2i \sin \omega (t_1 - t_2)$$

In other words, the "solution" we proposed is problematic when such non-commutation arises. To solve the problem, we have two (equivalent) pictures:

(1) Discretize then limit

Consider a small time interval δ_t. To leading order in δ_t, we may pretend $\hat{O}(t) \approx \hat{O}(t + \delta_t)$ is constant. Then we have

$$\hat{c}_i^\dagger (t + \delta_t) \approx e^{-i\hat{O}\delta_t} \hat{c}_i^\dagger (t)$$

Doing this successively, we can approximate a long-time evolution

and we claim this becomes exact in the limit

$$\hat{c}_i^\dagger (t) = \lim_{N \to \infty} e^{-i\hat{O}(t_{N-1})t/N} \cdots e^{-i\hat{O}(t_n)t/N} \cdots e^{-i\hat{O}(t_1)t/N} e^{-i\hat{O}(0)t/N} \hat{c}_i^\dagger (0)$$

$$t_n = \frac{nt}{N}$$

Remarks:

1. This is quite intuitive, but at the same time we did not justify its validity (e.g., error estimate, convergence of limit etc.). We will not worry about these problems, and just declare it's okay.

2. How might one even try to evaluate this? In the case when the operators are more general (complicated), it may not be feasible to work out everything explicitly and exactly using only the abstract operator algebra.

One natural way forward is to go back to some explicit "basis", e.g., in a coordinate-space basis we may replace $\hat{x} \to x$. Yet, in the same basis momentum $\hat{p} \to -i\partial_x$ is still an operator. Rather, it becomes a number only if we go to a momentum basis. Such dichotomy of "what is easy" is the defining feature (trouble) of quantum mechanics.

But we are considering small time intervals! Their failure to commute enters in $O(\delta_t^2)$. In other words, we can insert resolutions of identity for both x and p at each time-slice, and then treat them as commuting variables (since they are now only real numbers) in the limit $\delta_t \to 0$! This is the path integral picture.

(2) Fix the ordering up

Alternatively, we can also try to "repair" our good old solution

$$\hat{c}_i^\dagger (t) \sim \exp\left(-i \int_0^t dt' \hat{O}(t')\right) \hat{c}_i^\dagger (0)$$

after all, we know it is perfectly fine when $\hat{O}(t)$ at different times commute. (In particular, when it is time-independent.)

To this end, we first notice if we write

$$\hat{c}_i^\dagger (t) = \hat{U}(t) \, \hat{c}_i^\dagger (0)$$

with the "initial condition" $\hat{U}(0) = 1$, and demand it to be a solution to

$$i\partial_t \hat{c}_i^\dagger (t) = \hat{O}(t) \, \hat{c}_i^\dagger (t)$$

$$\Rightarrow \quad \left(i\partial_t \hat{U}(t)\right) \hat{c}_i^\dagger (0) = \hat{O}(t) \, \hat{U}(t) \, \hat{c}_i^\dagger (0)$$

$$\Rightarrow \quad i\partial_t \hat{U}(t) = \hat{O}(t) \, \hat{U}(t)$$

We can as well go from the "differential" equation to an "integral" equation

$$\hat{U}(t) = \hat{U}(0) - i \int_0^t dt_1 \hat{O}(t_1) \, \hat{U}(t_1)$$

This isn't quite "solving" $\hat{U}(t)$ yet, as it still appears on both left- and right-hand

sides. But we may now iterate

$$\hat{U}(t) = 1 - i \int_0^t dt_1 \hat{O}(t_1) \hat{U}(t_1)$$

$$= 1 - i \int_0^t dt_1 \hat{O}(t_1) \left[1 - i \int_0^{t_1} dt_2 \hat{O}(t_2) \hat{U}(t_2) \right]$$

$$= 1 - i \int_0^t dt_1 \hat{O}(t_1) + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1) \hat{O}(t_2) \hat{U}(t_2)$$

$$= 1 - i \int_0^t dt_1 \hat{O}(t_1) + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1) \hat{O}(t_2)$$

$$+ (-i)^3 \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \hat{O}(t_1) \hat{O}(t_2) \hat{O}(t_3) \hat{U}(t_3)$$

$$\vdots$$

we thus also get a formal power series solution to $\hat{U}(t)$, with the general form of the n-th term given by

$$\hat{U}(t) = \sum_{n=0}^{\infty} (-1)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \hat{O}(t_1) \hat{O}(t_2) \cdots \hat{O}(t_n)$$

This is called the "Dyson series". We see that it is quite "close" to the expansion of the exponential. But with two important differences:

1. we are missing a factor of $n!$ in the factorial.

2. the multiple time variables are ordered since each is bounded by the preceding one under the integral:

$$t_n < t_{n-1} < \cdots < t_2 < t_1 < t$$

   such ordering is the key to repairing our "exponential solution" with regards to the non-commuting nature $\left[\hat{O}(t), \hat{O}(t') \right] \neq 0$.

Observation (1) invites us to "over count" the terms by treating the different $\hat{O}(t_n)$ more equally, and in doing so we have to replace

$$\int_0^{t_{n-1}} dt_n \mapsto \int_0^t dt_n$$

At the same time, observation (2) instructs us to be disciplined when we perform such over-counting, since otherwise we screw up with the ordering of the operators demanded by the non-commuting nature of $\hat{O}(t)$ at different times. Combined, we claim

$$\hat{U}(t) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \mathcal{T} \left[\int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n \hat{O}(t_1) \hat{O}(t_2) \cdots \hat{O}(t_n) \right]$$

$$= \mathcal{T} \left[\exp \left\{ -i \int_0^t dt' \hat{O}(t') \right\} \right]$$

called the "time-ordered exponential". Here $\mathcal{T}$ is the "time-ordering" operator

$$\mathcal{T}\left[\hat{A}\hat{B}\hat{C}\hat{D}\right] = \hat{D}\hat{B}\hat{A}\hat{C}$$

for

Chapter 9

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Topics

1. Impurity spectral function from the Heisenberg picture: Dyson series and time-ordered exponential

2. "Sub-problem" driven QHO

3. introduction to Normal order and Wick's theorem

Goals

1. Getting familiar with time-ordering

2. Starting to appreciate how to evaluate time-ordered exponential

3. A primer to many-body perturbation theory

Last lecture, we spend most of our time on the following equation of motion

$$i\partial_t \hat{c}_i^\dagger(t) = \hat{O}(t)\,\hat{c}_i^\dagger(t)$$

and we arrived at the formal solution

$$\hat{c}_i^\dagger(t) = \hat{U}(t)\,\hat{c}_i^\dagger(0)$$

$$\hat{U}(t) = \mathcal{T}\left[\exp\left(-i\int_0^t dt'\hat{O}(t')\right)\right]$$

$$= \sum_{n=0} \frac{(-i)^n}{n!}\mathcal{T}\left[\int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n \hat{O}(t_1)\hat{O}(t_2)\cdots\hat{O}(t_n)\right]$$

we claimed this is simply the consequence of a "disciplined over-counting" of the Dyson series

$$\hat{U}(t) = \sum_{n=0}(-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \hat{O}(t_1)\hat{O}(t_2)\cdots\hat{O}(t_n)$$

To see why this "disciplined over-counting" makes sense, let us first consider the second-order term in the power series

$$\frac{(-i)^2}{2!}\mathcal{T}\left[\int_0^t dt_1 \int_0^t dt_2 \hat{O}(t_1)\hat{O}(t_2)\right]$$

$$=\frac{(-i)^2}{2!}\mathcal{T}\left[\int_0^t dt_1 \int_0^{t_1} dt_2 \underbrace{\hat{O}(t_1)\hat{O}(t_2)}_{t_1>t_2} + \int_0^t dt_1 \int_{t_1}^t dt_2 \underbrace{\hat{O}(t_1)\hat{O}(t_2)}_{t_2>t_1}\right]$$

$$=\frac{(-i)^2}{2!}\left\{\int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1)\hat{O}(t_2) + \int_0^t dt_1 \int_{t_1}^t dt_2 \hat{O}(t_2)\hat{O}(t_1)\right\}$$

Graphically, the domain of integration for the second term is

$$\int_0^t dt_1 \int_{t_1}^t dt_2 = \int_0^t dt_2 \int_0^{t_2} dt_1$$
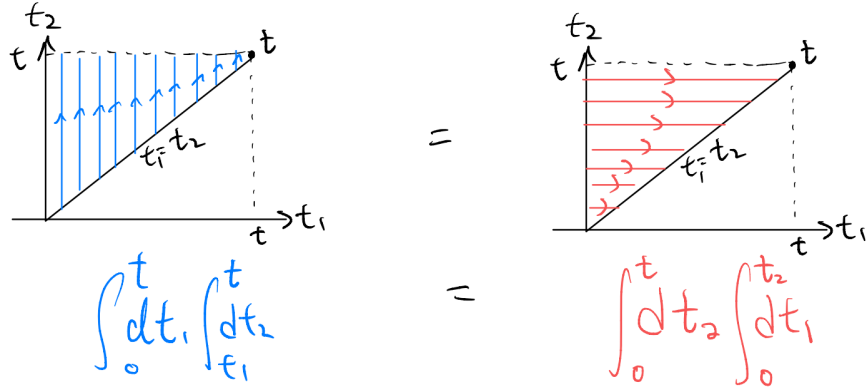
So we have

$$\frac{(-i)^2}{2!}\mathcal{T}\left[\int_0^t dt_1 \int_0^t dt_2 \hat{O}(t_1)\hat{O}(t_2)\right]$$

$$=\frac{(-i)^2}{2!}\left\{\int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1)\hat{O}(t_2) + \int_0^t dt_2 \int_0^{t_2} dt_1 \hat{O}(t_2)\hat{O}(t_1)\right\}$$

$$=\frac{(-i)^2}{2!}\left\{\int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1)\hat{O}(t_2) + \underbrace{\int_0^t dt_1 \int_0^{t_2} dt_2 \hat{O}(t_1)\hat{O}(t_2)}_{\text{relabel } t_1 \leftrightarrow t_2}\right\}$$

$$=(-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1)\hat{O}(t_2)$$

this justifies our over-counting claim (to the second order).

The argument generalizes to higher orders. For instance consider
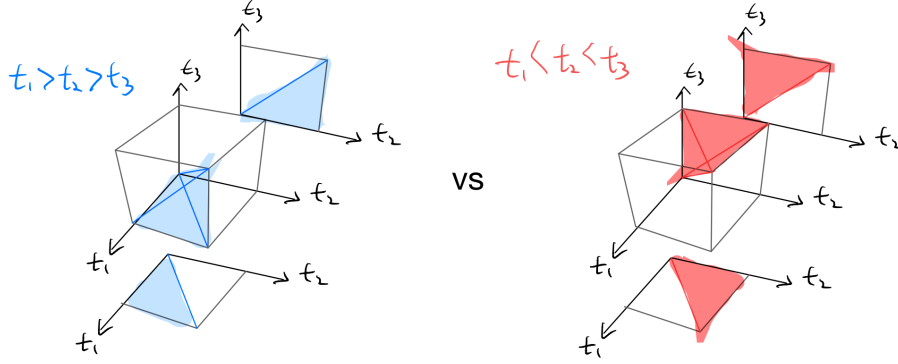
all these regions give the same term upon time-ordering and relabeling. All we need to do is to determine how many such regions are there. One way to see it is that each of the 3! permutation of t_1, t_2, t_3 corresponds to one region. E.g.,

$$(t_1, t_2, t_3) \Rightarrow t_1 < t_2 < t_3$$
$$(t_2, t_3, t_1) \Rightarrow t_2 < t_3 < t_1$$
$$(t_1, t_3, t_2) \Rightarrow t_1 < t_3 < t_2$$

$$\vdots \Rightarrow \vdots$$

More explicitly, we can also evaluate the volume of one region

$$\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_2 \, (1) = \int_0^t dt_1 \int_0^{t_1} dt_2 \, (t_2) = \int_0^t dt_1 \left(\frac{t_1^2}{2} \right) = \frac{t^3}{3 \cdot 2}$$

and so the number of regions is $t^3 / \left(\frac{t^3}{3 \cdot 2} \right) = 3!$.

Either of these arguments generalizes to the n-th order term. This establishes the equivalence of the Dyson series expansion and the time-ordered exponential.

Okay, great! With such a complicated preparation we can finally return to re-calculating the impurity Green's function (?)

$$G_{11}(t) = -i \langle \Omega | \hat{c}_1^\dagger(t) \, \hat{c}_1(0) | \Omega \rangle$$

$$= -i \langle \Omega | \underbrace{\mathcal{T} \left[\exp\left(-i \int_0^t dt' \hat{O}(t') \right) \right]}_{\text{phonon only}} \hat{c}_1^\dagger(0) \, \hat{c}_1(0) | \Omega \rangle$$

$$= (-i)_{100} \, \langle \{0_q\} | \mathcal{T} \left[\exp\left(-i \int_0^t dt' \hat{O}(t') \right) \right] | \{0_q\} \rangle_{100}$$

where

$$\hat{O}_{100}\left(t\right) = -\varepsilon_1 - \sum_q M_{1q}\left(\hat{a}_q^{\{100\}}\left(t\right) + \hat{a}_q^{\{100\}\dagger}\left(t\right) - 2\frac{M_{1q}}{\omega_q}\right)$$

$$= -\varepsilon_1 + 2\sum_q \frac{M_{1q}^2}{\omega_q} - \sum_q M_{1q}\left(\hat{a}_q^{\{100\}}\left(t\right) + \hat{a}_q^{\{100\}\dagger}\left(t\right)\right)$$

and the phonon ground state in the {100} sector is defined by (verify!)

$$\hat{a}_q^{\{100\}}\left(t\right)|\left\{0\right\}_q\rangle_{100} = 0, \quad \forall q$$

To proceed, we make two observations:

1. the constant piece in $\hat{O}(t)$ does not cause trouble, and we can just deal with it directly to get a phase;

2. The different phonon modes labeled by q do not interfere with each other, and so we can evaluate them "in parallel"

This gives

$$G_{11}\left(t\right) = \left(-i\right)\exp\left[-i\left(-\varepsilon_1 + 2\sum_q \frac{M_{1q}^2}{\omega_q}\right)\right]$$

$$\times \prod_q {}_{100}\langle 0_q|\mathcal{T}\left[\exp\left(iM_{1q}\int_0^t dt'\left(\hat{a}_q^{\{100\}}\left(t\right) + \hat{a}_q^{\{100\}\dagger}\left(t\right)\right)\right)\right]|0_q\rangle_{100}$$

Neat, but how do we evaluate this???

9.1   Sub-problem: single QHO

After massaging, we are down to evaluating the expression

$$\sim \langle 0|\mathcal{T}\left[e^{-i\int_0^t dt'\left(\zeta(t)\hat{a}^\dagger(t) + \bar{\zeta}(t)\hat{a}(t)\right)}\right]|0\rangle$$

once for each mode labeled by q, with both the phonon operators and the ground state defined by the electronic configuration {100}. We have also generalized the constant M_{iq} to a time-dependent function $\zeta(t)$. For simplicity, we consider here the equivalent problem of our good old single QHO. (Note: we mostly follow notations in Coleman Chapter-5 here)

how do we evaluate this? As we alluded to in the last lecture, we could employ path integral methods if we understand the time-ordered exponential as the time evolution of many small intervals; alternatively, we can try to evaluate it order-by-order if we take the Dyson-series like expansion.

Here, let us take the second route. (Check out Coleman 5.1.1 for an evaluation along the first route.)

Expanding up to first few terms,

$$\langle 0|\mathcal{T}\left[e^{-i\int_0^t dt'\left(\zeta(t)\hat{a}^\dagger(t)+\bar{\zeta}(t)\hat{a}(t)\right)}\right]|0\rangle$$

$$=\langle 0|0\rangle - i\langle 0|\int_0^t dt'\left(\zeta(t)\hat{a}^\dagger(t)+\bar{\zeta}(t)\hat{a}(t)\right)|0\rangle$$

$$+\frac{(-i)^2}{2}\langle 0|\mathcal{T}\left[\left(\int_0^t dt'\left(\zeta(t)\hat{a}^\dagger(t)+\bar{\zeta}(t)\hat{a}(t)\right)\right)^2\right]|0\rangle+\cdots$$

where

$$\langle 0|0\rangle = 1$$

$$\langle 0|\hat{a}^\dagger(t)|0\rangle = \langle 0|\hat{a}(t)|0\rangle = 0$$

$$\Rightarrow \quad \langle 0|\int_0^t dt'\left(\zeta(t)\hat{a}^\dagger(t)+\bar{\zeta}(t)\hat{a}(t)\right)|0\rangle = 0$$

and so our first nontrivial term to evaluate is

$$\frac{(-i)^2}{2}\langle 0|\mathcal{T}\left[\left(\int_0^t dt'\left(\zeta(t)\hat{a}^\dagger(t)+\bar{\zeta}(t)\hat{a}(t)\right)\right)^2\right]|0\rangle$$

$$=\frac{(-i)^2}{2}\langle 0|\mathcal{T}\Big[\int_0^t dt_1\int_0^t dt_2\zeta(t_1)\zeta(t_2)\hat{a}^\dagger(t_1)\hat{a}^\dagger(t_2)+\zeta(t_1)\bar{\zeta}(t_2)\hat{a}^\dagger(t_1)\hat{a}(t_2)$$

$$+\bar{\zeta}(t_1)\zeta(t_2)\hat{a}(t_1)\hat{a}^\dagger(t_2)+\bar{\zeta}(t_1)\bar{\zeta}(t_2)\hat{a}(t_1)\hat{a}(t_2)\Big]|0\rangle$$

Noticing

$$\hat{a}(t)|0\rangle = 0, \quad \langle 0|\hat{a}^\dagger(t) = 0$$

one may want to claim the only surviving term is

$$\sim \langle 0|\mathcal{T}\left[\int_0^t dt_1\int_0^t dt_2\bar{\zeta}(t_1)\zeta(t_2)\hat{a}(t_1)\hat{a}^\dagger(t_2)\right]|0\rangle$$

But this is wrong! Remember, the time-ordering operator upfront implies the actual order may not be what we have written down. Instead, let us impose the time-ordering explicitly the, we do have

$$\frac{(-i)^2}{2}\langle 0|\mathcal{T}\left[\left(\int_0^t dt'\left(\zeta(t)\hat{a}^\dagger(t)+\bar{\zeta}(t)\hat{a}(t)\right)\right)^2\right]|0\rangle$$

$$=(-i)^2\langle 0|\left[\int_0^t dt_1\int_0^{t_1} dt_2\bar{\zeta}(t_1)\zeta(t_2)\hat{a}(t_1)\hat{a}^\dagger(t_2)\right]|0\rangle$$

$$=(-i)^2\langle 0|\left[\int_0^t dt_1\int_0^{t_1} dt_2\bar{\zeta}(t_1)\zeta(t_2)e^{-i\omega(t_1-t_2)}\hat{a}(0)\hat{a}^\dagger(0)\right]|0\rangle$$

$$=(-i)^2\int_0^t dt_1\int_0^{t_1} dt_2\bar{\zeta}(t_1)\zeta(t_2)e^{-i\omega(t_1-t_2)}\langle 0|\left(\hat{a}^\dagger(0)\hat{a}(0)+1\right)|0\rangle$$

$$=(-i)^2\int_0^t dt_1\int_0^t dt_2\Theta(t_1-t_2)e^{-i\omega(t_1-t_2)}\bar{\zeta}(t_1)\zeta(t_2)$$

where we have used the Heaviside step-function to restore the full integration domain for t_2. Let us define

$$\mathscr{G}\left(t - t'\right) = \left(-i\right)\Theta\left(t - t'\right)e^{-i\omega\left(t - t'\right)}$$

then we see that

$$\langle 0|\mathcal{T}\left[e^{-i\int_0^t dt'\left(\zeta(t)\hat{a}^\dagger(t) + \bar{\zeta}(t)\hat{a}(t)\right)}\right]|0\rangle = 1 - i\int_0^t dt_1\int_0^t dt_2\bar{\zeta}\left(t_1\right)\mathscr{G}\left(t_1 - t_2\right)\zeta\left(t_2\right) + \cdots$$

where the second term is "number", and no "ordering"! With a leap of faith, let us announce the answer

$$\langle 0|\mathcal{T}\left[e^{-i\int_0^t dt'\left(\zeta(t)\hat{a}^\dagger(t) + \bar{\zeta}(t)\hat{a}(t)\right)}\right]|0\rangle = e^{-i\int_0^t dt_1\int_0^t dt_2\bar{\zeta}(t_1)\mathscr{G}(t_1 - t_2)\zeta(t_2)}$$

this is kind of natural: starting with the QHO in the ground state, we perturb it by a time-dependent linear term. So if at time t_2 we create a quanta, let it time evolve for time $t_1 - t_2$ and at time t_1 we annihilate it to go back to the ground state. We need to allow for all such processes happening at different times t_1, t_2. This "explains" the expression.

Of course, we haven't really proved the validity of our answer. More later.

9.2   Back to the main thread

As an indirect check of the expression we claimed, let us use it for the impurity-phonon problem:

$$\zeta\left(t\right) = \bar{\zeta}\left(t\right) = -M_{1q}$$

$$G_{11}\left(t\right) = \left(-i\right)e^{-i\left(-\varepsilon_1 + 2\sum_q \frac{M_{1q}^2}{\omega_q}\right)}\prod_q {}_{100}\langle 0_q|\mathcal{T}\left[e^{iM_{1q}\int_0^t dt'\left(\hat{a}_q^{\{100\}}(t) + \hat{a}_q^{\{100\}\dagger}(t)\right)}\right]|0_q\rangle_{100}$$

$$= \left(-i\right)e^{-i\left(-\varepsilon_1 + 2\sum_q \frac{M_{1q}^2}{\omega_q}\right)}\prod_q e^{-iM_{1q}^2\int_0^t dt_1\int_0^t dt_2\mathscr{G}_q(t_1 - t_2)}$$

Evaluating the double integral

$$\int_0^t dt_1\int_0^t dt_2\mathscr{G}_q\left(t_1 - t_2\right) = -i\int_0^t dt_1\int_0^t dt_2\Theta\left(t_1 - t_2\right)e^{-i\omega_q(t_1 - t_2)}$$

$$= -i\int_0^t dt_1\int_0^{t_1} dt_2 e^{-i\omega_q(t_1 - t_2)}$$

$$= -i\int_0^t dt_1\frac{1 - e^{-i\omega_q t_1}}{i\omega_q}$$

$$= -\frac{t}{\omega_q} + \frac{e^{-i\omega_q t} - 1}{-i\omega_q^2}$$

with this we conclude (recalling $g_q = \frac{M_{1q}^2}{\omega_q^2}$)

$$G_{11}(t) = (-i)\, e^{-i\left(-\varepsilon_1 + 2\sum_q \frac{M_{1q}^2}{\omega_q}\right)} \prod_q e^{i\frac{M_{1q}^2}{\omega_q}t}\, e^{\frac{M_{1q}^2}{\omega_q^2}\left(e^{-i\omega_q t}-1\right)}$$

$$= (-i)\, \underbrace{e^{-i\left(-\varepsilon_1 + \sum_q \frac{M_{1q}^2}{\omega_q}\right)t}}_{e^{i\Delta_{100}t}}\, e^{\sum_q g_q\left(e^{-i\omega_q t}-1\right)}$$

This checks out! Whether this Heisenberg picture is clearer than the exact solution or not is a matter of taste: they do have a slightly different flavor nevertheless. In the exact solution, we relied heavily on the properties of the displacement operator which we discussed way back. In contrast, in the Heisenberg picture discussion, we see that we are implicitly attacking a much more general problem, namely, how to evaluate the time-evolution operator of a more general time-dependent Hamiltonian.

Chapter 10

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Topics

1. Normal order

2. (Static) Wick's theorem

   Goals

1. Learning how to compute ground state expectation values

2. Appreciating the what it means to be "free", "Gaussian", "non-interacting"

   Remark: we will spend this week on a fairly technical (general) discussion.

10.1 Normal order

As discussed last time, we announced the answer

$$\langle 0|\mathcal{T}\left[e^{-i\int_0^t dt'\left(\zeta(t')\hat{a}^\dagger(t')+\zeta^*(t')\hat{a}(t')\right)}\right]|0\rangle = e^{-i\int_0^t dt_1\int_0^t dt_2\zeta^*(t_1)\mathscr{G}(t_1-t_2)\zeta(t_2)}$$

$$\mathscr{G}(t_1-t_2) = (-i)\Theta(t_1-t_2)e^{-i\omega(t_1-t_2)}$$

simply by "checking" the lowest nontrivial term! It will make sense to demand that we do a more honest check by considering the general terms.

Let us expand the LHS

$$\text{LHS} = \sum_{n=0}^\infty \frac{(-i)^n}{n!}\langle 0|\mathcal{T}\left[\left(\int_0^t dt'\hat{\phi}(t')\right)^n\right]|0\rangle$$

$$\hat{\phi}(t) = \zeta(t)\hat{a}^\dagger(t) + \zeta^*(t)\hat{a}(t)$$

First, we notice that the only non-vanishing terms have to come with the same number of $\hat{a}$ & $\hat{a}^\dagger$: otherwise we leave the ground state and will have zero overlap.

In particular, the odd-order terms vanish identically since there is no way to "balance" $\hat{a} \& \hat{a}^\dagger$ there. In other words,

$$\text{LHS} = \sum_{n=0} \frac{(-i)^{2n}}{(2n)!} \langle 0| \mathcal{T} \left[\left(\int_0^t dt' \hat{\phi}\left(t'\right) \right)^{2n} \right] |0\rangle$$

Let us inspect the second nontrivial term now:

$$\frac{(-i)^4}{4!} \langle 0| \mathcal{T} \left[\int_0^t dt_1 \int_0^t dt_2 \int_0^t dt_3 \int_0^t dt_4 \hat{\phi}\left(t_1\right) \hat{\phi}\left(t_2\right) \hat{\phi}\left(t_3\right) \hat{\phi}\left(t_4\right) \right] |0\rangle$$

$$= \frac{(-i)^4}{4!} \langle 0| \mathcal{T} \left[\int_0^t dt_1 \int_0^t dt_2 \int_0^t dt_3 \int_0^t dt_4 \left(\zeta\left(t_1\right) \zeta\left(t_2\right) \zeta^*\left(t_3\right) \zeta^*\left(t_4\right) \hat{a}^\dagger\left(t_1\right) \hat{a}^\dagger\left(t_2\right) \hat{a}\left(t_3\right) \hat{a}\left(t_4\right) \right. \right.$$

$$\left. \left. + \zeta\left(t_1\right) \zeta^*\left(t_2\right) \zeta^*\left(t_3\right) \zeta\left(t_4\right) \hat{a}^\dagger\left(t_1\right) \hat{a}\left(t_2\right) \hat{a}\left(t_3\right) \hat{a}^\dagger\left(t_4\right) + \cdots \right) \right] |0\rangle$$

Ideally, we want to simplify our problem using

$$\hat{a}\left(t\right) |0\rangle = 0$$

$$\langle 0| \hat{a}^\dagger\left(0\right) = 0$$

but, as we mentioned earlier, the precise ordering of the operators is to be determined by the time-ordering, which is "changing" as we perform the integrals! It is then not so obvious which terms survive and which do not.

Nevertheless, it is indeed correct that we could greatly simplify the calculation if we can bring the $\hat{a}^\dagger$ to the left and $\hat{a}$ to the right. This is called the "normal order". The normal ordering of a time-ordered operator is the key to our evaluation, facilitated by what is usually called the Wick's theorem / lemma.

Note: "the" normal order is defined with respect to the ground state. When we say we bring, e.g., $\hat{a}^\dagger$ to the left and $\hat{a}$ to the right, it is implicitly assumed that our goal is to evaluate some expectation values with respect to the vacuum. Generally speaking, a different ground state calls for a different "normal" order.

10.2   Wick's theorem

Imagine taking the product of a string of creation and annihilation operators, e.g.,

$$\hat{a}_1 \hat{a}_2^\dagger \hat{a}_3^\dagger \hat{a}_4 \hat{a}_5 \hat{a}_6^\dagger$$

here, the subscripts are quite general, in that they may not only be referring to the "modes", but could also be, e.g., indicating the time as in $\hat{a}_i^\dagger = \hat{a}^\dagger\left(t_i\right)$. We have defined the normal order to be

$$: \hat{a}_1 \hat{a}_2^\dagger \hat{a}_3^\dagger \hat{a}_4 \hat{a}_5 \hat{a}_6^\dagger := \hat{a}_2^\dagger \hat{a}_3^\dagger \hat{a}_6^\dagger \hat{a}_1 \hat{a}_4 \hat{a}_5 \quad \text{[bosonic]}$$

where the notation $::$ denotes normal ordering. A natural question here is, how different is an operator $\hat{O}$ compared to its normal order $:\hat{O}:$? Relatedly, what is the ground state expectation value

$$\langle 0|\hat{a}_1\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4\hat{a}_5\hat{a}_6^\dagger|0\rangle$$

provided that it is not obviously 0?

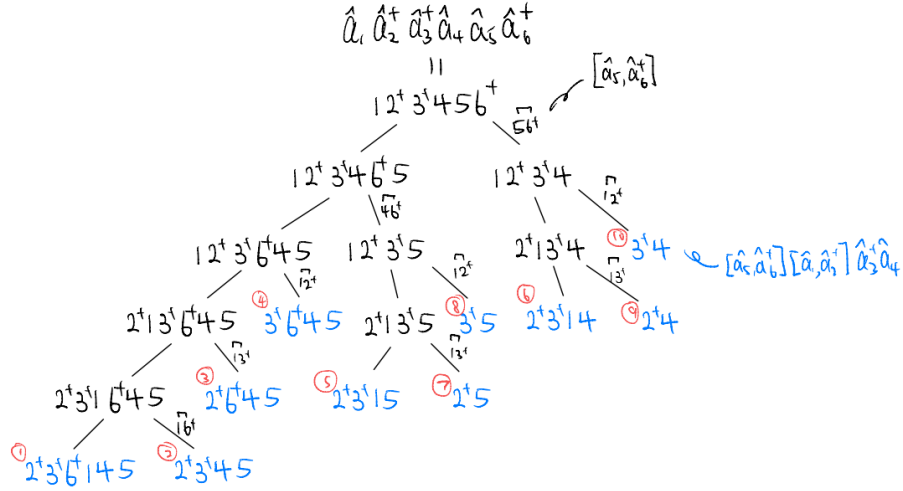To develop some feeling for the problem, let's try to bring our example to the normal order

$$\hat{a}_1\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4\hat{a}_5\hat{a}_6^\dagger$$

$$=\hat{a}_1\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4\left(\hat{a}_6^\dagger\hat{a}_5 + \underbrace{\left[\hat{a}_5,\hat{a}_6^\dagger\right]}_{c-\text{number}}\right)$$

$$=\hat{a}_1\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4\hat{a}_6^\dagger\hat{a}_5 + \left[\hat{a}_5,\hat{a}_6^\dagger\right]\hat{a}_1\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4$$

$$=\cdots$$

where the operators to be exchanged are in red color.

Some observations:

1. whenever we move an $\hat{a}$ pass an $\hat{a}^\dagger$, we generate two terms. One now has the "right" order for the two operators involved, and the other leads to a commutator multiplied to a "shorter term" with fewer operators involved.

2. We can now imagine iterating the procedure. There will be a "long string" remaining which contains the same number of operators inside (6 in our example). But each of the "short strings" would also need to be brought to a normal order, and in doing so generate even shorter strings.

3. Importantly, the process terminates when everything is normal ordered!

Let's now proceed with our example in a visually more suggestive manner

$$\hat{a}_1\,\hat{a}_2^\dagger\,\hat{a}_3^\dagger\,\hat{a}_4\,\hat{a}_5\,\hat{a}_6^\dagger$$

$$\|$$

$$1\,2^\dagger\,3^\dagger\,4\,5\,6^\dagger \qquad [\hat{a}_5,\hat{a}_6^\dagger]$$

(hand-drawn contraction tree)

we may rewrite this tree in a more conventional form

$$
\hat{a}_1\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4\hat{a}_5\hat{a}_6^\dagger = {}^{①}\!: \hat{a}_1\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4\hat{a}_5\hat{a}_6^\dagger :
$$

$$
+{}^{②}\!: \hat{a}_1^\bullet\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4\hat{a}_5\hat{a}_6^{\dagger\bullet} : +{}^{③}\!: \hat{a}_1^\bullet\hat{a}_2^\dagger\hat{a}_3^{\dagger\bullet}\hat{a}_4\hat{a}_5\hat{a}_6^\dagger :
$$

$$
+{}^{④}\!: \hat{a}_1^\bullet\hat{a}_2^{\dagger\bullet}\hat{a}_3^\dagger\hat{a}_4\hat{a}_5\hat{a}_6^\dagger : +{}^{⑤}\!: \hat{a}_1\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4^\bullet\hat{a}_5\hat{a}_6^{\dagger\bullet} :
$$

$$
+{}^{⑥}\!: \hat{a}_1\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4\hat{a}_5^\bullet\hat{a}_6^{\dagger\bullet} :
$$

$$
+{}^{⑦}\!: \hat{a}_1^\bullet\hat{a}_2^\dagger\hat{a}_3^{\dagger\bullet}\hat{a}_4^{\bullet\bullet}\hat{a}_5\hat{a}_6^{\dagger\bullet\bullet} : +{}^{⑧}\!: \hat{a}_1^\bullet\hat{a}_2^{\dagger\bullet}\hat{a}_3^\dagger\hat{a}_4^{\bullet\bullet}\hat{a}_5\hat{a}_6^{\dagger\bullet\bullet} :
$$

$$
+{}^{⑨}\!: \hat{a}_1^\bullet\hat{a}_2^\dagger\hat{a}_3^{\dagger\bullet}\hat{a}_4\hat{a}_b^{\bullet\bullet}\hat{a}_6^{\dagger\bullet\bullet} : +{}^{⑩}\!: \hat{a}_1^\bullet\hat{a}_2^{\dagger\bullet}\hat{a}_3^\dagger\hat{a}_4\hat{a}_b^{\bullet\bullet}\hat{a}_6^{\dagger\bullet\bullet} :
$$

Notes from website builder: Since the notation for the Wick contraction used in class is hard to type in LaTeXor HTML, here I use a different notation which is also widely used, like in Wikipedia wiki/Wick's theorem. Their mapping relations are

$$
\overbrace{a_1 a_2 a_3 a_4}^{\rule{20pt}{0.4pt}} \Leftrightarrow a_1^\bullet a_2 a_3 a_4^\bullet
$$

$$
\overbrace{a_1 a_2 a_3 a_4} \Leftrightarrow a_1^\bullet a_2^{\bullet\bullet} a_3^{\bullet\bullet} a_4^\bullet
$$

In particular, by bringing it to normal order we may now conclude

$$
\langle 0|\hat{a}_1\hat{a}_2^\dagger\hat{a}_3^\dagger\hat{a}_4\hat{a}_5\hat{a}_6^\dagger|0\rangle = 0
$$

since no "constants" emerge in the ordered expansion, i.e., all terms contain an $\hat{a}_i$ at the right-most end. This is not entirely obvious without calculating! Especially, given the generality of the statement: these could be acting on the same (different) modes at the same (different) times.

Suggested sanity check: try the simple case when all operators act on the same mode at the same times, i.e., evaluate $\langle 0|\hat{a}\hat{a}^{\dagger 2}\hat{a}^2\hat{a}^\dagger|0\rangle$

From this exercise we can distill out a few rules:

1. we can "expand" the original product into sum of sub-products, all of them in the normal order

2. the coefficients of the sub-products are determined by what gets removed (pairwise) when we move the operators around, these are indicated by the symbol $a_i^\bullet a_j^\bullet$. We call them "contractions"

3. we only contract $\hat{a}_i^\bullet \hat{a}_j^{\dagger\bullet}$, Terms like $\hat{a}_i^\bullet \hat{a}_j^\bullet, \hat{a}_i^{\dagger\bullet}\hat{a}_j^{\dagger\bullet}, \hat{a}_i^{\dagger\bullet}\hat{a}_j^\bullet$ do not show up because we don't need to commute them to reach normal order

In particular, points (2) and (3) above suggest a sharper definition of what a "contraction" is: it involves a pair of annihilation and creation operators, and it measures its mismatch from the normal-ordered form, i.e.,

$$\hat{\phi}_1^\bullet \hat{\phi}_2^\bullet = \hat{\phi}_1\hat{\phi}_2 - :\hat{\phi}_1\hat{\phi}_2:$$

check that, e.g.,

$$\hat{a}_i^\bullet \hat{a}_j^{\dagger\bullet} = \hat{a}_i\hat{a}_j^\dagger - \hat{a}_j^\dagger\hat{a}_i = \left[\hat{a}_i, \hat{a}_j^\dagger\right]$$

$$\hat{a}_i^{\dagger\bullet}\hat{a}_j^\bullet = \hat{a}_i^\dagger\hat{a}_j - \hat{a}_i^\dagger\hat{a}_j = 0$$

Importantly, our definition extends to the case when $\hat{phi}_i$ is a linear superposition of $\hat{a}_i$ and $\hat{a}_i^\dagger$, i.e., let

$$\hat{\phi}_i = u_i\hat{a}_i + v_i\hat{a}_i^\dagger$$

then,

$$\hat{\phi}_i^\bullet \hat{\phi}_j^\bullet = \left(u_i\hat{a}_i + v_i\hat{a}_i^\dagger\right)\left(u_j\hat{a}_j + v_j\hat{a}_j^\dagger\right) - :\left(u_i\hat{a}_i + v_i\hat{a}_i^\dagger\right)\left(u_j\hat{a}_j + v_j\hat{a}_j^\dagger\right):$$
$$= u_iv_j\hat{a}_i\hat{a}_j^\dagger - u_iv_j\hat{a}_j^\dagger\hat{a}_i$$
$$= u_iv_j\left[\hat{a}_i, \hat{a}_j^\dagger\right]$$

We may now state Wick's theorem more generally:

$$\hat{\phi}_1\hat{\phi}_2\cdots\hat{\phi}_n = \sum : \text{all possible contractions} :$$

here, by "all" we mean everything from no contraction at all, to the case of everything grouped pairwise (if n is even) and contracted. As stated, it could be that many of the included terms are 0 identically. But that's okay because it gives us a simple way to state the theorem!

Remarks:

1. Contraction is not symmetric, i.e., $\hat{\phi}_1^\bullet \hat{\phi}_2^\bullet \neq \hat{\phi}_2^\bullet \hat{\phi}_1^\bullet$. E.g., $\hat{a}_1^{\dagger\bullet}\hat{a}_2^\bullet = 0$ but $\hat{a}_2^\bullet \hat{a}_1^{\dagger\bullet} = \left[\hat{a}_2, \hat{a}_1^\dagger\right]$. The order is fixed by that in the original operator we are "expanding"

2. Wick's theorem as stated is an operator identity.

Evaluating vacuum expectation value is a special application. E.g., take four operators

$$\hat{\phi}_1\hat{\phi}_2\hat{\phi}_3\hat{\phi}_4 =: \hat{\phi}_1\hat{\phi}_2\hat{\phi}_3\hat{\phi}_4 :$$
$$+ \hat{\phi}_1^\bullet\hat{\phi}_2^\bullet : \hat{\phi}_3\hat{\phi}_4 : +\hat{\phi}_1^\bullet\hat{\phi}_3^\bullet : \hat{\phi}_2\hat{\phi}_4 : +\hat{\phi}_1^\bullet\hat{\phi}_4^\bullet : \hat{\phi}_2\hat{\phi}_3 :$$
$$+ \hat{\phi}_2^\bullet\hat{\phi}_2^\bullet : \hat{\phi}_1\hat{\phi}_4 : +\hat{\phi}_2^\bullet\hat{\phi}_4^\bullet : \hat{\phi}_1\hat{\phi}_3 : +\hat{\phi}_3^\bullet\hat{\phi}_4^\bullet : \hat{\phi}_1\hat{\phi}_2 :$$
$$+ \hat{\phi}_1^\bullet\hat{\phi}_2^\bullet\hat{\phi}_3^{\bullet\bullet}\hat{\phi}_4^{\bullet\bullet} + \hat{\phi}_1^\bullet\hat{\phi}_3^\bullet\hat{\phi}_2^{\bullet\bullet}\hat{\phi}_4^{\bullet\bullet} + \hat{\phi}_1^\bullet\hat{\phi}_4^\bullet\hat{\phi}_2^{\bullet\bullet}\hat{\phi}_2^{\bullet\bullet}$$

which contains $C_0^4 + C_2^4 + \frac{1}{2}C_2^4C_2^2$ terms. If we take the expectation value

$$\langle\Phi|\hat{\phi}_1\hat{\phi}_2\hat{\phi}_3\hat{\phi}_4|\Psi\rangle = \langle\Phi| : \hat{\phi}_1\hat{\phi}_2\hat{\phi}_3\hat{\phi}_4 : |\Psi\rangle + \hat{\phi}_1^\bullet\hat{\phi}_2^\bullet\langle\Phi| : \hat{\phi}_3\hat{\phi}_4 : |\Psi\rangle + \cdots$$

there isn't much of a simplification as all the terms will contribute in general. Yet if we take the vacuum expectation value (VEV)

$$\langle 0|\hat{\phi}_1\hat{\phi}_2\hat{\phi}_3\hat{\phi}_4|0\rangle = \hat{\phi}_1^\bullet\hat{\phi}_2^\bullet\hat{\phi}_3^{\bullet\bullet}\hat{\phi}_4^{\bullet\bullet} + \hat{\phi}_1^\bullet\hat{\phi}_3^\bullet\hat{\phi}_2^{\bullet\bullet}\hat{\phi}_4^{\bullet\bullet} + \hat{\phi}_1^\bullet\hat{\phi}_4^\bullet\hat{\phi}_2^{\bullet\bullet}\hat{\phi}_2^{\bullet\bullet}$$

as all the other normal-ordered operators will annihilate the vacuum.

How many terms are there in this VEV? Consider the VEV of a string of $2n$ operators. We are asking how many ways are there to group them in pairs, noticing that

1. the order within the pair is "unimportant", since that has to be fixed by the order in which they appeared in the original string, and

2. once contracted, we get a c-number and it doesn't matter how we order these c-numbers.

So, the number of terms is successively choosing two out of the remaining

$$\frac{1}{n!}C_2^{2n}C_2^{2n-2}\cdots C_2^4C_2^2$$
$$=\frac{1}{n!}\frac{(2n)\,(2n-1)}{2}\frac{(2n-2)\,(2n-3)}{2}\cdots\frac{4\cdot 3}{2}\frac{2\cdot 1}{2}$$
$$=(2n-1)\,(2n-3)\cdots 3\cdot 1$$
$$=(2n-1)!!$$

where $\frac{1}{n!}$ is the permutation of the contracted pairs.

Fun fact: you might think of the $2n$ operators as the vertices of 2 $2n$-vertex complete graph, then a term in the VEV corresponds to a perfect matching on this graph. The number of such perfecting matching is, as argued, $(2n-1)!!$.

How fast does this grow? For the first few,

For large n we may estimate using Stirling's approximation

$$(2n-1)!! \sim \left(\frac{2n}{e}\right)^n$$

# operators	2	4	6	8	10	12
# of terms	$1!! = 1$	$3!! = 3$	$5!! = 15$	$7!! = 105$	$9!! = 945$	$11!! = 10395$

i.e., it grows super-exponentially! Combinatorial is hard... Yet, if many terms are the same then it maybe manageable

Note that the "normal order" is not uniquely defined. In the above, we defined it with respect to the vacuum, which instructs us to pull all the $\hat{a}_i$ to the left and $\hat{a}_i^\dagger$ to the right, as they annihilate the ket and bra correspondingly.

One could have *alternative* states which are annihilated by some transformed operators, e.g., we have saw that the "phonon vacuum" depends on the electronic configuration in the impurity-phonon problem. One can think of it simply as a "basis transformation", and we can define "alternative" normal order with respect to such basis. The computation of expectation values then simplify in a similar manner.

These alternative normal orders correspond to alternative contractions, defined still as the the (c-number) mismatch between the operator and its normal ordered form. In fact, such contractions encode the pairwise correlation functions for the annihilation (creation) operators in the "alternative state". (see below) Wick's theorem then implies that, for such states for which a normal order could be defined,

general correlation functions = combinatorial product and sum of up to pairwise (two-point) correlation functions.

This is clearly very special, as generally speaking "higher order" correlation functions contain new data compared to the ones at "2nd order". The absence of such "new data" is the defining feature of a Gaussian distribution. Such states admitting a normal order are "Gaussian" in this sense.

A powerful observation about such Gaussian state $|GS\rangle$ is that we do not actually need to know how to perform the normal ordering! We just need to suppose a normal order exist such that

$$\langle GS| : \hat{\phi}_1 \hat{\phi}_2 \cdots \hat{\phi}_n : |GS\rangle = 0$$

It then follows that

$$\begin{aligned}\langle \hat{\phi}_1 \hat{\phi}_2 \rangle &= \langle GS|\hat{\phi}_1 \hat{\phi}_2|GS\rangle, \quad \text{computable in any basis} \\ &= \langle GS| : \hat{\phi}_1 \hat{\phi}_2 : + \hat{\phi}_1^\bullet \hat{\phi}_2^\bullet |GS\rangle \\ &= \hat{\phi}_1^\bullet \hat{\phi}_2^\bullet \end{aligned}$$

In the above, the second derivation requires rotating to the right basis to literally perform the normal order. In particular, the general correlation functions can now be expressed as, e.g., for four operators

$$\begin{aligned}\langle \hat{\phi}_1 \hat{\phi}_2 \hat{\phi}_3 \hat{\phi}_4 \rangle &= \hat{\phi}_1^\bullet \hat{\phi}_2^\bullet \hat{\phi}_3^{\bullet\bullet} \hat{\phi}_4^{\bullet\bullet} + \hat{\phi}_1^\bullet \hat{\phi}_3^\bullet \hat{\phi}_2^{\bullet\bullet} \hat{\phi}_4^{\bullet\bullet} + \hat{\phi}_1^\bullet \hat{\phi}_4^\bullet \hat{\phi}_2^{\bullet\bullet} \hat{\phi}_2^{\bullet\bullet} \\ &= \langle \hat{\phi}_1 \hat{\phi}_2 \rangle \langle \hat{\phi}_3 \hat{\phi}_4 \rangle + \langle \hat{\phi}_1 \hat{\phi}_3 \rangle \langle \hat{\phi}_2 \hat{\phi}_4 \rangle + \langle \hat{\phi}_1 \hat{\phi}_4 \rangle \langle \hat{\phi}_2 \hat{\phi}_3 \rangle \end{aligned}$$

Looks familiar? Jumping ahead slightly, with *fermionic* operators, the corresponding expression is

$$\langle \hat{c}_1^\dagger \hat{c}_2^\dagger \hat{c}_3 \hat{c}_4 \rangle = \langle \hat{c}_1^\dagger \hat{c}_2^\dagger \rangle \langle \hat{c}_3 \hat{c}_4 \rangle + \langle \hat{c}_1^\dagger \hat{c}_4 \rangle \langle \hat{c}_2^\dagger \hat{c}_3 \rangle - \langle \hat{c}_1^\dagger \hat{c}_3 \rangle \langle \hat{c}_2^\dagger \hat{c}_4 \rangle$$

The first term is "condensation" which will vanish unless superconducting mean field (BdG), the second term is the direct "Hartree", and the third term is the exchange "Fock" (recalling that fermions is anti-commuting). This is the famous Hartree-Fock approximation, namely, when we approximate the actual ground state with a Gaussian state, the interaction energy consists simply of the Hartree and Fock terms. (Assuming no superconductivity)

Lastly, we note that we did not actually prove Wick's theorem. We just "motivated" and then "stated" it. For our purpose, it's probably more important to understand what it means and how to use it, than to really prove it.

Instead, let us just sketch how it could be proved

1. In a "brute force" approach, we can establish Wick's theorem by induction. The key step is to notice what happens when we "squeeze" a new operator into a normal-ordered one. Supposing

$$\hat{\phi}_1 : \hat{\phi}_2 \cdots \hat{\phi}_n := \, : \hat{\phi}_1 \hat{\phi}_2 \cdots \hat{\phi}_n : + \hat{\phi}_1^\bullet \hat{\phi}_2^\bullet : \hat{\phi}_3 \hat{\phi}_4 \cdots \hat{\phi}_n :$$
$$+ \, \hat{\phi}_1^\bullet \hat{\phi}_3^\bullet : \hat{\phi}_2 \hat{\phi}_4 \cdots \hat{\phi}_n : + \cdots + + \hat{\phi}_1^\bullet \hat{\phi}_n^\bullet : \hat{\phi}_2 \hat{\phi}_3 \cdots \hat{\phi}_{n-1} :$$

   is true for n operators, then we can show that it's also true for $n + 1$ operators. With this established, the Wick's theorem can again be proved by induction: supposing it holds for products of up to n operators, then we insert a new one from the left and all the "new contractions" are generated by the proposition above.

2. Another way to prove it is to first perform a path integral with sources inserted, and then take functional derivatives. This is perhaps the more popular "physicist" proof. See Coleman Chapter-5 for a discussion.

3. More interestingly still, in the "serious QFT" literature, there's some known connection of the Wick's theorem to what is called the "homological perturbation lemma". Let me know if you think you could explain that to me.

Chapter 11

lec11 20220311

Topics

1. Wick's theorem and Gaussian states

2. Wicks' theorem, time-ordering and time-ordered exponential

 Goals

1. Appreciating what is means to be "free", "Gaussian", "non-interacting" (mean-field)

2. Completing our explicit evaluation of the time-ordered exponential

11.1   Gaussian states

In introducing the normal ordering, we tried to emphasize that its definition is implicitly dependent on a reference state, and so, correspondingly, the value of the contraction also depends on the reference state. We had already argued that the contraction simply equals to the "two-point" correlation function of the reference state. Let us show this more explicitly in a single QHO example.

To this end, let us introducing the notion of a "squeezed state" (quantum optics terminology)

$$|\zeta\rangle = \underbrace{e^{i\left(\zeta\hat{a}^{\dagger 2}+\zeta^*\hat{a}^2\right)/2}}_{\hat{S}(\zeta)}|0\rangle$$

We see that the squeezed state is "rotated" from the vacuum by a unitary, called the "squeezed operator"

$$\hat{S}(\zeta) = e^{i\left(\zeta\hat{a}^{\dagger 2}+\zeta^*\hat{a}^2\right)/2}$$

Note: our notation here differs from the usual quantum optics discussion by a factor of i. This is done for our convenience in what follows.

We claim the squeezed state is "Gaussian", and that the Wick's theorem can be applied to facilitate the evaluation of expectation values. To that end, let us first consider how the squeeze operator transform the annihilation and creation operators:

$$\hat{S}\left(\zeta\right)\hat{a}^{\dagger}\hat{S}^{\dagger}\left(\zeta\right) = \left. e^{i\left(\zeta\hat{a}^{\dagger 2}+\zeta^{*}\hat{a}^{2}\right)t/2}\hat{a}^{\dagger}e^{i\left(\zeta\hat{a}^{\dagger 2}+\zeta^{*}\hat{a}^{2}\right)t/2}\right|_{t=1}$$

where instead of computing it directly (with BCH type formulas), we use a trick that the transformation can be interpreted as a kind of Heisenberg picture evolution with a "squeezing Hamiltonian"

$$i\partial_{t}\hat{a}^{\dagger} = \left[\hat{a}^{\dagger}, \frac{1}{2}\left(\zeta\hat{a}^{\dagger 2}+\zeta^{*}\hat{a}^{2}\right)\right] = -\zeta^{*}\hat{a}$$

$$\Rightarrow \quad \partial_{t}\begin{pmatrix} \hat{a} \\ \hat{a}^{\dagger} \end{pmatrix} = i\begin{pmatrix} 0 & -\zeta \\ \zeta^{*} & 0 \end{pmatrix}\begin{pmatrix} \hat{a} \\ \hat{a}^{\dagger} \end{pmatrix}$$

$$\Rightarrow \quad \begin{pmatrix} \hat{a}\left(t\right) \\ \hat{a}^{\dagger}\left(t\right) \end{pmatrix} = \exp\left(i\begin{pmatrix} 0 & -\zeta \\ \zeta^{*} & 0 \end{pmatrix}t\right)\begin{pmatrix} \hat{a}\left(0\right) \\ \hat{a}^{\dagger}\left(0\right) \end{pmatrix}$$

For simplicity, let us further assume $\zeta = i\theta$ is purely imaginary. Then

$$\exp\left(it\begin{pmatrix} 0 & -i\theta \\ -i\theta & 0 \end{pmatrix}\right) = \exp\left(\theta t\sigma_{x}\right)$$

$$= \sum_{n:\text{even}}\frac{1}{n!}\left(\theta t\right)^{n} + \sigma_{x}\sum_{n:\text{odd}}\frac{1}{n!}\left(\theta t\right)^{n}$$

$$= \cosh\left(\theta t\right) + \sigma_{x}\sinh\left(\theta t\right)$$

$$\Rightarrow \quad \begin{pmatrix} \hat{a}\left(t\right) \\ \hat{a}^{\dagger}\left(t\right) \end{pmatrix} = \begin{pmatrix} \cosh\left(\theta t\right) & \sinh\left(\theta t\right) \\ \sinh\left(\theta t\right) & \cosh\left(\theta t\right) \end{pmatrix}\begin{pmatrix} \hat{a}\left(0\right) \\ \hat{a}^{\dagger}\left(0\right) \end{pmatrix}$$

Setting $t = 1$, we get

$$\hat{S}\left(i\theta\right)\hat{a}\hat{S}^{\dagger}\left(i\theta\right) = \cosh\theta\hat{a} + \sinh\theta\hat{a}^{\dagger}$$

Note: you might recognize this as a "Bogoliubov transformation", usually discussed by asking what linear transformations of the bosonic operators will preserve the canonical commutation relations. We have, in fact, shown explicitly how the transformation can be achieved by the conjugate action of a unitary generated by a boson-bilinear.

With such preparation, let us verify that $|\zeta = i\theta\rangle$ is indeed a Gaussian state. For simplicity, we define

$$\hat{b} = \hat{S}\left(i\theta\right)\hat{a}\hat{S}^{\dagger}\left(i\theta\right)$$

$$= \cosh\theta\hat{a} + \sinh\theta\hat{a}^{\dagger}$$

and the canonical commutation relation is preserved:

$$\left[\hat{b}, \hat{b}^{\dagger}\right] = \hat{S}\left(i\theta\right)\left[\hat{a}, \hat{a}^{\dagger}\right]\hat{S}^{\dagger}\left(i\theta\right) = 1$$

These are annihilation and creation operators, in that

$$\hat{b}|i\theta\rangle = \hat{S}\left(i\theta\right)\hat{a}\hat{S}^\dagger\left(i\theta\right)\hat{S}\left(i\theta\right)|0\rangle = \hat{S}\left(i\theta\right)\hat{a}|0\rangle = 0$$

With respect to $|i\theta\rangle$, therefore, it will be natural to define the normal order to be one in which $\hat{b}^\dagger$ is always brought to the left of $\hat{b}$.

The "new" normal order is then, for instance,

$$: \hat{a}^\dagger\hat{a} : =: \left(-\sinh\theta\hat{b} + \cosh\theta\hat{b}^\dagger\right)\left(\cosh\theta\hat{b} - \sinh\theta\hat{b}^\dagger\right) :$$
$$= -\sinh\theta\cosh\theta\hat{b}^2 + \cosh^2\theta\hat{b}^\dagger\hat{b} + \sinh^2\theta : \hat{b}\hat{b}^\dagger : -\sinh\theta\cosh\theta\hat{b}^{\dagger 2}$$

correspondingly, the contraction becomes

$$\hat{a}^{\dagger\bullet}\hat{a}^\bullet = \hat{a}^\dagger\hat{a} - : \hat{a}^\dagger\hat{a} := \sinh^2\theta\left[\hat{b}, \hat{b}^\dagger\right] = \sinh^2\theta$$

Similarly,

$$\hat{a}^\bullet\hat{a}^{\dagger\bullet} = \hat{a}\hat{a}^\dagger - : \hat{a}\hat{a}^\dagger := \cosh^2\theta$$

As argued, the contractions can be evaluated simply by looking at the "two-point" correlations. Explicitly, we have, e.g.,

$$\langle i\theta|\hat{a}^\dagger\hat{a}|i\theta\rangle = \langle 0|\hat{S}^\dagger\left(i\theta\right)\hat{a}^\dagger\hat{a}\hat{S}\left(i\theta\right)|0\rangle$$
$$= \langle 0|\left(-\sinh\theta\hat{a} + \cosh\theta\hat{a}^\dagger\right)\left(\cosh\theta\hat{a} - \sinh\theta\hat{a}^\dagger\right)|0\rangle$$
$$= \sinh^2\theta$$
$$= \hat{a}^{\dagger\bullet}\hat{a}^\bullet$$

Similarly, we can evaluate

$$\hat{a}^{\dagger\bullet}\hat{a}^{\dagger\bullet} = \langle i\theta|\hat{a}^\dagger a^\dagger|i\theta\rangle$$
$$= \langle 0|\left(-\sinh\theta\hat{a} + \cosh\theta\hat{a}^\dagger\right)^2|0\rangle$$
$$= -\sinh\theta\cosh\theta$$

The power of the Wick's theorem will be more apparent when we look at a longer string of operators. For instance, consider

$$\langle i\theta|\left(\hat{a}^\dagger a\right)^2|i\theta\rangle = \langle i\theta|\left[\left(-\sinh\theta\hat{a} + \cosh\theta\hat{a}^\dagger\right)\left(\cosh\theta\hat{a} - \sinh\theta\hat{a}^\dagger\right)\right]^2|i\theta\rangle$$
$$= \langle i\theta|\left(-\sinh\theta\hat{a} + \cosh\theta\hat{a}^\dagger\right)\left(\cosh\theta\hat{a} - \sinh\theta\hat{a}^\dagger\right)$$
$$\times \left(-\sinh\theta\hat{a} + \cosh\theta\hat{a}^\dagger\right)\left(\cosh\theta\hat{a} - \sinh\theta\hat{a}^\dagger\right)|i\theta\rangle$$
$$= \sinh^2\theta\langle i\theta|\hat{a}\left(\cosh\theta\hat{a} - \sinh\theta\hat{a}^\dagger\right)\left(-\sinh\theta\hat{a} + \cosh\theta\hat{a}^\dagger\right)\hat{a}^\dagger|i\theta\rangle$$
$$= \sinh^2\theta\left(\sinh^2\theta\langle 0|\hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger|0\rangle + \cosh^2\theta\langle 0|\hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger|0\rangle\right)$$
$$= \sinh^2\theta\left(\sinh^2\theta + 2\cosh^2\theta\right)$$

Alternatively, we can write down by wick's theorem

$$
\begin{aligned}
\langle i\theta| \left(\hat{a}^\dagger a\right)^2 |i\theta\rangle &= \langle \hat{a}^\dagger a \hat{a}^\dagger a \rangle \\
&= \langle \hat{a}^\dagger a \rangle^2 + \langle \hat{a}^\dagger a \rangle \langle a \hat{a}^\dagger \rangle + \langle \hat{a}^\dagger \hat{a}^\dagger \rangle \langle aa \rangle \\
&= \sinh^4 \theta + \sinh^2 \theta \cosh^2 \theta + \left(-\sinh\theta \cosh\theta\right)^2 \\
&= \sinh^2 \theta \left(\sinh^2 \theta + 2\cosh^2 \theta\right)
\end{aligned}
$$

as promised.

11.2 Still remember the main thread?

time to add time back: T-contraction

If you still remember, our goal was to establish

$$
\langle 0| \mathcal{T} \left[e^{-i \int_0^t dt' \left(\zeta(t') \hat{a}^\dagger(t') + \zeta^*(t') \hat{a}(t')\right)} \right] |0\rangle = e^{-i \int_0^t dt_1 \int_0^t dt_2 \zeta^*(t_1) \mathscr{G}(t_1 - t_2) \zeta(t_2)}
$$

$$
\mathscr{G}\left(t_1 - t_2\right) = -i\Theta\left(t_1 - t_2\right) e^{-i\omega(t_1 - t_2)}
$$

and by noticing

$$
\text{LHS} = \sum_{n=0} \frac{(-i)^{2n}}{(2n)!} \langle 0| \mathcal{T} \left[\left(\int_0^t dt' \hat{\phi}\left(t'\right)\right)^n \right] |0\rangle
$$

we wandered into a (long) discussion of how to compute such VEV through Wick's theorem. Now, with Wick's theorem under our belt, we would just need to consider how that "interacts" with the time-ordering upfront.

To see what the new feature is, let's start with the case of two operators: $\hat{\phi}_1$ inserted at time t_1 and $\hat{\phi}_2$ inserted at time t_2

$$
\mathcal{T} \left[\hat{\phi}_1 \hat{\phi}_2\right] = \Theta\left(t_1 - t_2\right) \hat{\phi}_1 \hat{\phi}_2 + \Theta\left(t_2 - t_1\right) \hat{\phi}_2 \hat{\phi}_1
$$

where we have used the Heaviside step function to explicitly select the correct ordering of the operators. Now we might apply Wick's theorem to the operators

$$
\begin{aligned}
\mathcal{T} \left[\hat{\phi}_1 \hat{\phi}_2\right] &= \Theta\left(t_1 - t_2\right) \left(: \hat{\phi}_1 \hat{\phi}_2 : + \hat{\phi}_1^\bullet \hat{\phi}_2^\bullet\right) + \Theta\left(t_2 - t_1\right) \left(: \hat{\phi}_2 \hat{\phi}_1 : + \hat{\phi}_2^\bullet \hat{\phi}_1^\bullet\right) \\
&=: \hat{\phi}_1 \hat{\phi}_2 : + \Theta\left(t_1 - t_2\right) \hat{\phi}_1^\bullet \hat{\phi}_2^\bullet + \Theta\left(t_2 - t_1\right) \hat{\phi}_2^\bullet \hat{\phi}_1^\bullet
\end{aligned}
$$

let us define a "T-contraction" (terminology from 1710.09248):

$$
\begin{aligned}
\overbrace{\hat{\phi}_1 \hat{\phi}_2} &= \mathcal{T}\left[\hat{\phi}_1 \hat{\phi}_2\right] - : \hat{\phi}_1 \hat{\phi}_2 : \\
&= \Theta\left(t_1 - t_2\right) \hat{\phi}_1^\bullet \hat{\phi}_2^\bullet + \Theta\left(t_2 - t_1\right) \hat{\phi}_2^\bullet \hat{\phi}_1^\bullet
\end{aligned}
$$

We now claim the Wick's theorem applies in the same way for a time-ordered product simply by replacing all the contractions by T-contractions.

To illustrate this, suppose $t_2 > t_3 > t_1$, then

$$\mathcal{T}\left[\hat{\phi}_1\hat{\phi}_2\hat{\phi}_3\right] = \hat{\phi}_2\hat{\phi}_3\hat{\phi}_1$$

$$=: \hat{\phi}_1\hat{\phi}_2\hat{\phi}_3: +\hat{\phi}_2^{\bullet}\hat{\phi}_3^{\bullet}\hat{\phi}_1 + \hat{\phi}_2^{\bullet}\hat{\phi}_1^{\bullet}\hat{\phi}_3 + \hat{\phi}_3^{\bullet}\hat{\phi}_1^{\bullet}\hat{\phi}_2$$

and indeed we have

$$\overparen{\hat{\phi}_1\hat{\phi}_2} = \Theta\left(t_1 - t_2\right)\hat{\phi}_1^{\bullet}\hat{\phi}_2^{\bullet} + \Theta\left(t_2 - t_1\right)\hat{\phi}_2^{\bullet}\hat{\phi}_1^{\bullet} = \hat{\phi}_2^{\bullet}\hat{\phi}_1^{\bullet}$$

$$\overparen{\hat{\phi}_2\hat{\phi}_3} = \Theta\left(t_2 - t_3\right)\hat{\phi}_2^{\bullet}\hat{\phi}_3^{\bullet} + \Theta\left(t_3 - t_2\right)\hat{\phi}_3^{\bullet}\hat{\phi}_2^{\bullet} = \hat{\phi}_2^{\bullet}\hat{\phi}_3^{\bullet}$$

$$\overparen{\hat{\phi}_1\hat{\phi}_3} = \Theta\left(t_1 - t_3\right)\hat{\phi}_1^{\bullet}\hat{\phi}_3^{\bullet} + \Theta\left(t_3 - t_1\right)\hat{\phi}_3^{\bullet}\hat{\phi}_1^{\bullet} = \hat{\phi}_3^{\bullet}\hat{\phi}_1^{\bullet}$$

So we have, explicitly,

$$\mathcal{T}\left[\hat{\phi}_1\hat{\phi}_2\hat{\phi}_3\right] =: \hat{\phi}_1\hat{\phi}_2\hat{\phi}_3: +\overparen{\hat{\phi}_2\hat{\phi}_3}\,\hat{\phi}_1 + \overparen{\hat{\phi}_2\hat{\phi}_1}\,\hat{\phi}_3 + \overparen{\hat{\phi}_3\hat{\phi}_1}\,\hat{\phi}_2$$

as claimed.

Long story short, no matter how the times are really ordered, we can apply the original Wick's theorem to the time-ordered product. However, the order of contraction might have been reversed if the two operators are swapped under the time ordering. The T-contraction takes care of such possible swapping (or not) using the Heaviside step function to toggle between the two.

In addition, we also inherit the general conclusion that the T-contraction can be computed as a "correlation function"

$$\langle GS|\mathcal{T}\left[\hat{\phi}_1\hat{\phi}_2\right]|GS\rangle = \langle GS|:\hat{\phi}_1\hat{\phi}_2:|GS\rangle + \overparen{\hat{\phi}_1\hat{\phi}_2} = \overparen{\hat{\phi}_1\hat{\phi}_2}$$

provided that the state is Gaussian such that there exists a definition of normal ordering with respect to that. We emphasize that we do not need to perform the actual normal ordering (basis rotation etc.) to evaluate the contraction. Its value is computed through

$$\overparen{\hat{\phi}_1\hat{\phi}_2} = \langle\mathcal{T}\left[\hat{\phi}_1\hat{\phi}_2\right]\rangle = \Theta\left(t_1 - t_2\right)\langle\hat{\phi}_1\left(t_1\right)\hat{\phi}_2\left(t_2\right)\rangle + \Theta\left(t_2 - t_1\right)\langle\hat{\phi}_1\left(t_2\right)\hat{\phi}_2\left(t_1\right)\rangle$$

where the first term is the Green's function!

11.3 Time-ordered exponential meets Green's functions

After 20 pages or so we are finally ready to evaluate the time-ordered exponential

$$\hat{\phi}\left(t'\right) = \zeta\left(t'\right)\hat{a}^{\dagger}\left(t'\right) + \zeta^*\left(t'\right)\hat{a}\left(t'\right)$$

$$\langle 0|\mathcal{T}\left[e^{-i\int_0^t dt'\hat{\phi}(t')}\right]|0\rangle$$

$$=\sum_{n=0}\frac{(-i)^{2n}}{(2n)!}\langle 0|\mathcal{T}\left[\int_0^t dt_1\int_0^t dt_2\cdots\int_0^t dt_n\hat{\phi}(t_1)\,\hat{\phi}(t_2)\cdots\hat{\phi}(t_{2n})\right]|0\rangle$$

$$=\sum_{n=0}\frac{(-i)^{2n}}{(2n)!}\int_0^t dt_1\int_0^t dt_2\cdots\int_0^t dt_n\langle 0|\mathcal{T}\left[\hat{\phi}(t_1)\,\hat{\phi}(t_2)\cdots\hat{\phi}(t_{2n})\right]|0\rangle$$

$$\langle 0|\mathcal{T}\left[\hat{\phi}(t_1)\,\hat{\phi}(t_2)\cdots\hat{\phi}(t_{2n})\right]|0\rangle$$

$$=\overbrace{\hat{\phi}(t_1)\,\hat{\phi}(t_2)}\overbrace{\hat{\phi}(t_3)\,\hat{\phi}(t_4)}\cdots\overbrace{\hat{\phi}(t_{2n-1})\,\hat{\phi}(t_{2n})}$$

$$+\overbrace{\hat{\phi}(t_1)\,\hat{\phi}(t_3)}\overbrace{\hat{\phi}(t_2)\,\hat{\phi}(t_4)}\cdots\overbrace{\hat{\phi}(t_{2n-1})\,\hat{\phi}(t_{2n})}$$

$$+\cdots;\quad (2n-1)!!\text{terms}$$

Now, we evaluate

$$\overbrace{\hat{\phi}(t_1)\,\hat{\phi}(t_2)}$$

$$=\langle 0|\mathcal{T}\left[\hat{\phi}(t_1)\,\hat{\phi}(t_2)\right]|0\rangle$$

$$=\Theta(t_1-t_2)\,\langle 0|\left(\zeta(t_1)\,\hat{a}^\dagger(t_1)+\zeta^*(t_1)\,\hat{a}(t_1)\right)$$

$$\qquad\times\left(\zeta(t_2)\,\hat{a}^\dagger(t_2)+\zeta^*(t_2)\,\hat{a}(t_2)\right)|0\rangle+(t_1\leftrightarrow t_2)$$

$$=\Theta(t_1-t_2)\,\zeta^*(t_1)\,\zeta(t_2)\,\langle 0|\hat{a}e^{-i\omega t_1}\hat{a}^\dagger e^{i\omega t_2}|0\rangle+(t_1\leftrightarrow t_2)$$

$$=\Theta(t_1-t_2)\,\zeta^*(t_1)\,\zeta(t_2)\,e^{-i\omega(t_1-t_2)}+(t_1\leftrightarrow t_2)$$

We defined

$$\mathscr{G}(t_1-t_2)=(-i)\,\Theta(t_1-t_2)\,e^{-i\omega(t_1-t_2)}$$

$$\Rightarrow\quad\int_0^t dt_1\int_0^t dt_2\,\overbrace{\hat{\phi}(t_1)\,\hat{\phi}(t_2)}$$

$$=\frac{1}{(-i)}\int_0^t dt_1\int_0^t dt_2\zeta^*(t_1)\,\mathscr{G}(t_1-t_2)\,\zeta(t_2)+(t_1\leftrightarrow t_2)$$

$$=(2i)\int_0^t dt_1\int_0^t dt_2\zeta^*(t_1)\,\mathscr{G}(t_1-t_2)\,\zeta(t_2)$$

In addition, all the other full contractions generated by Wick's theorem correspond to exactly the same expression but with some relabeling of the time indices. In other words, all the $(2n-1)!!$ terms evaluate to the same answer.

We can finally write down

$$\langle 0|\mathcal{T}\left[e^{-i\int_0^t dt'\left(\zeta(t')\hat{a}^\dagger(t')+\zeta^*(t')\hat{a}(t')\right)}\right]|0\rangle$$

$$=\sum_{n=0}\frac{(-i)^{2n}}{(2n)!}(2i)^n\left[\int_0^t dt_1\int_0^t dt_2\zeta^*(t_1)\mathscr{G}(t_1-t_2)\zeta(t_2)\right]^n\times(2n-1)!!$$

$$=\sum_{n=0}(-i)^n\frac{2^n(2n-1)!!}{(2n)!}\left[\int_0^t dt_1\int_0^t dt_2\zeta^*(t_1)\mathscr{G}(t_1-t_2)\zeta(t_2)\right]^n$$

$$=\exp\left(-i\int_0^t dt_1\int_0^t dt_2\zeta^*(t_1)\mathscr{G}(t_1-t_2)\zeta(t_2)\right)$$

where we have used

$$\frac{2^n(2n-1)!!}{(2n)!}=\frac{1}{n!}$$

Finally, we've established this honestly! (Again, see Coleman 5.1.1 if you want an alternative discussion)

Notes:

1. (For the QFT gurus in the audience) You may think that our approach to Wick's theorem is unnecessarily complicated: isn't it just taking functional derivative on the free-field S-matrix? You are right, but note that our "operator" form (as an identity) is actually a bit stronger than a relation between correlation and Green's function.

2. Our calculation above actually works more generally: we simply define

$$G(x,x';t,t')=\langle\Omega|\mathcal{T}\left[\hat{\phi}_x(t)\hat{\phi}_{x'}(t')\right]|\Omega\rangle$$

where $\hat{\phi}_x(t),\hat{\phi}_{x'}(t')$ are the "field operators" creating or annihilating particles at different points in space-time, and denotes the many-body ground state which, generally speaking, is not Gaussian = free (why should it be?). We call this the "one-particle" Green's function.

The goal of a perturbation theory is to derive an expansion of the actual quantities in terms of those for an unperturbed problem. A useful unperturbed problem is one for which the same set of quantities could be computed. (Always attack a hard problem starting from an easier starting point, and work your way there!) In our context, we take the Gaussian theory as the starting point, and the perturbative expansions are then organized and computed in terms of "Feynman diagrams".

Chapter 12

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Topics

1. Propagators

2. Frequency space, contours and real-time Green functions

Goals

1. Arriving at a more systematic treatment of the various notion of Green's functions we have encountered

12.1 Bare phonon propagator

Let us revisit the free-phonon problem again from this lens of T-contractions and correlation functions. Consider again

$$\hat{H} = \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q$$

where for simplicity we have restricted ourselves to a single "branch" and so suppressed any additional indices which might be attached to the phonon operators aside from the (crystal) momentum q.

In the real space, the phonon operators are related to the actual position (deviation) operators of the atoms through

$$\hat{\phi}_r = \frac{1}{\sqrt{V}} \sum_q e^{-iqr} \left(\frac{\hat{a}_q + \hat{a}_{-q}^\dagger}{\sqrt{2m\omega_q}} \right) = \frac{1}{\sqrt{V}} \sum_q e^{-iqr} \hat{\phi}_q$$

In the Heisenberg picture, the phonon operators evolve in time according to

$$i\partial_t \hat{a}_q(t) = \left[\hat{a}_q(t), \omega_q \hat{a}_q^\dagger(t) \hat{a}_q(t) \right] = \omega_q \hat{a}_q(t)$$

$$\hat{a}_q(t) = \hat{a}_q(0) e^{-i\omega_q t}$$

And we may evaluate the one-particle Green's function with respect to the phonon vacuum (superscript t emphasize it corresponds to the time-ordered two-point function)

$$G^t (r, r'; t, t') = -i\langle \text{vac}|\mathcal{T}\left[\hat{\phi}_r (t) \, \hat{\phi}_{r'} (t')\right]|\text{vac}\rangle$$

$$= \frac{-i}{V} \sum_{qq'} \frac{e^{-iq\cdot r} e^{-iq'\cdot r'}}{2m\sqrt{\omega_q \omega_{q'}}} \langle \text{vac}|\mathcal{T}\left[\overbrace{\left(\hat{a}_q (t) + \hat{a}^\dagger_{-q} (t)\right)}^{\hat{\phi}_q(t)} \left(\hat{a}_{q'} (t') + \hat{a}^\dagger_{-q'} (t')\right)\right]|\text{vac}\rangle$$

$$(q = -q')$$

$$= \frac{-i}{V} \sum_q \frac{e^{-iq\cdot(r-r')}}{2m\omega_q} \langle \text{vac}|\mathcal{T}\left[\hat{a}_q (t) \hat{a}^\dagger_q (t') + \hat{a}^\dagger_{-q} (t) \hat{a}_{-q} (t')\right]|\text{vac}\rangle$$

$$\Rightarrow \quad \langle \text{vac}|\mathcal{T}\left[\hat{a}_q (t) \hat{a}^\dagger_q (t')\right]|\text{vac}\rangle = \Theta (t - t') \langle \text{vac}|\hat{a}_q (t) \hat{a}^\dagger_q (t')|\text{vac}\rangle$$

$$= \Theta (t - t') e^{-i\omega_q(t-t')}$$

$$\Rightarrow \quad G^t (r, r'; t, t') = \frac{-i}{V} \sum_q \frac{e^{-iq\cdot(r-r')}}{2m\omega_q} \left(\Theta (t - t') e^{-i\omega_q(t-t')} + \Theta (t' - t) e^{-i\omega_{-q}(t'-t)}\right)$$

which depends only on $r - r'$ and $t - t'$

$$G^t (r, t) = \frac{-i}{V} \sum_q \frac{e^{-iq\cdot r}}{2m\omega_q} \left(\Theta (t) e^{-i\omega_q t} + \Theta (-t) e^{i\omega_{-q} t}\right)$$

The translation invariance, exposed in the fact that the two-point function depends only on $r - r'$ implies q is a good quantum number and it is natural to Fourier transform

$$G^t (q, t) = \sum_r e^{iq\cdot r} G^t (r, t)$$

$$= \frac{-i}{2m\omega_q} \left(\Theta (t) e^{-i\omega_q t} + \Theta (-t) e^{i\omega_{-q} t}\right)$$

We may further Fourier transform to the frequency space, using our "exponential

damping trick"

$$
\begin{aligned}
G^t(q,\omega) &= \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} dt\, G^t(q,t)\, e^{i\omega t - \eta|t|} \\
&= \frac{-i}{2m\omega_q} \lim_{\eta \to 0^+} \left(\int_0^{\infty} dt\, e^{i(\omega - \omega_q + i\eta)t} + \int_{-\infty}^0 dt\, e^{i(\omega + \omega_q + i\eta)t} \right) \\
&= \frac{-i}{2m\omega_q} \lim_{\eta \to 0^+} \left(\frac{0-1}{i(\omega - \omega_q + i\eta)} + \frac{1-0}{i(\omega + \omega_q + i\eta)} \right) \\
&= \frac{1}{2m\omega_q} \lim_{\eta \to 0^+} \left(\frac{1}{\omega - \omega_q + i\eta} - \frac{1}{\omega + \omega_q + i\eta} \right) \\
&= \frac{1}{2m\omega_q} \lim_{\eta \to 0^+} \frac{2\omega_q}{\omega^2 - (\omega_q - i\eta)^2}
\end{aligned}
$$

This is called the free/bare phonon "propagator". It is customary to denote it by D (instead of G), since in an electron-phonon problem one might want to reserve G for the electrons.

12.2 Contours, Green's function, Feynman's $i\epsilon$ prescription

Going from the real-time to frequency space, we have used an exponential damping term to regulate the oscillatory integral extending to $t \to \pm\infty$. In particular, the sign of the damping depends on the sign of t. We first introduced such tricks by alluding to the physical reality that our system cannot possibly exist all the way up to $t \to \pm\infty$ anyway, and so it is natural to regulate the integral by damping it off. Here, we provide an alternative way to make sense of such treatment.

We first notice that the (bare) phonon Green's function $D^t(q,\omega)$, viewed as a complex function, contains two poles

$$
D^+(q,\omega) = \frac{1}{2m\omega_q} \lim_{\eta \to 0^+} \left(\frac{1}{\omega - \omega_q + i\eta} - \frac{1}{\omega + \omega_q + i\eta} \right)
$$

which are infinitesimally displaced from the real line.
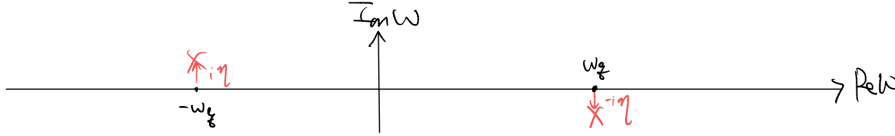
Now, imagine Fourier transforming back to the real time, which calls for an integral along the real line, with the two poles approaching our integration contour, Such integrals could alternatively be computed by trading the $\pm i\eta$ with
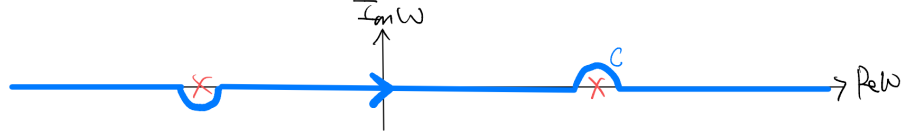
an infinitesimal deformation of the integration contour. As a sanity check, let us verify that we could indeed go back to the real-time Green's function by performing such contour integrals. Consider

$$\frac{1}{2m\omega_q} \int_C \frac{d\omega}{2\pi} \left(\frac{1}{\omega - \omega_q} - \frac{1}{\omega + \omega_q} \right) e^{-i\omega t}$$

Notice we have dropped the $\pm i\eta$, with the corresponding information encoded in how the contour C is specified.

One could evaluate this integral honestly, by splitting the contour C into 5 segments: three straight lines and two semi-circles. As the deformation is only infinitesimal, the "straight line" integrals return the Cauchy principal value whereas the "semi-circles" give half of the residues. In addition, for the principal part one ultimately gets the Dirichlet sinc integral, which gives $\sim e^{\pm i\omega_q t}(i\pi \operatorname{sgn}(t))$. Combined with the partial residues, one does get back the original time-ordered real-time Green's function.

Instead of going through the details of the steps sketeched above, let's use the usual "physicist's argument" to evaluate the integral. The main idea is to use the residue theorem, which states that (loosely) power series make sense except at the singularities (i.e., poles)

$$\oint \gamma d\zeta f(\zeta) = 2\pi i \sum \operatorname{Res}(f, a_k)$$

and for a meromorphic function with a simple pole, taking the form

$$\begin{aligned} f(\zeta) &= \frac{g(\zeta)}{\zeta - a_k} = \frac{\sum_{n=0} g_n (\zeta - a_k)^n}{\zeta - a_k} \\ &= \frac{g_0}{\zeta - a_k} + g_1 + g_2 (\zeta - a_k) + \cdots \end{aligned}$$

the residue is simply the coefficient g_0.

Now, back to our problem: to take advantage of the residue theorem we would want to "close" our contour. The natural choice will be to complete it with an arc which we send off to infinity, e.g., We then see that, by the residue theorem, only one of the poles contribute:

$$\begin{aligned} \int_{C+arc} \frac{d\omega}{2\pi} D(q, \omega) e^{-i\omega t} &= \frac{1}{2m\omega_q} \frac{2\pi i}{2\pi} \operatorname{Res}\left(\frac{-e^{-i\omega t}}{\omega + \omega_q}, \omega - \omega_q \right) \\ &= \frac{-i}{2m\omega_q} e^{i\omega_q t} \end{aligned}$$

power series makes sense except
at the singularities (i.e. poles)

$$\oint_\gamma dz \; f(z) = 2\pi i \sum Res(f, a_k)$$

sum over poles enclosed

closed oriented
contour
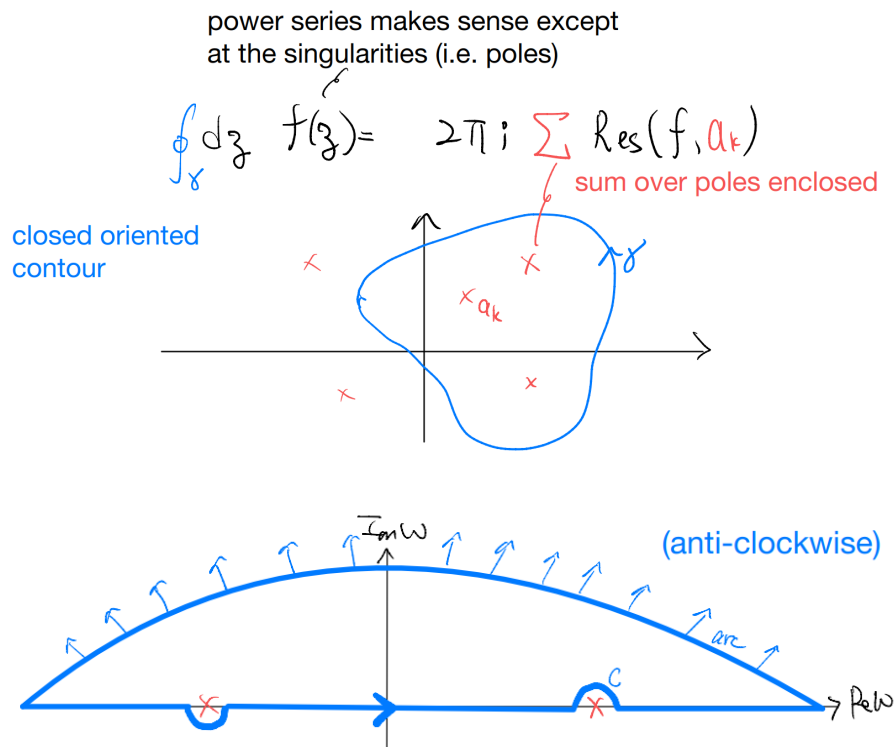
$$\Rightarrow \quad \int_C \frac{d\omega}{2\pi} D(q,\omega) e^{-i\omega t} = \frac{-i}{2m\omega_q} e^{i\omega_q t} - \int_{arc} \frac{d\omega}{2\pi} D(q,\omega) e^{-i\omega t}$$

almost! But we need to know what is the contribution from the arc. In what we
considered above, we let ω go to infinity on the upper complex plane. In other
words, we consider

$$\text{Im}(\omega) \to +\infty$$

as such, in the integrand we have

$$e^{-i\omega t} = e^{-i\text{Re}(\omega)t} e^{\text{Im}(\omega)t}$$

and it is well-behaved (and exponentially suppressed) only if we have $t < 0$ to
start with. Provided $t < 0$, the arc contribution goes to zero as the integrand is
now exponentially suppressed. This gives

$$\int_C \frac{d\omega}{2\pi} D(q,\omega) e^{-i\omega t} = \frac{-i}{2m\omega_q} e^{i\omega_q t}, \quad t < 0$$

Now, to obtain the result for $t > 0$, we should consider the alternative way of
closing off our contour (clockwise) which now encloses the other pole at $\omega = \omega_q$.
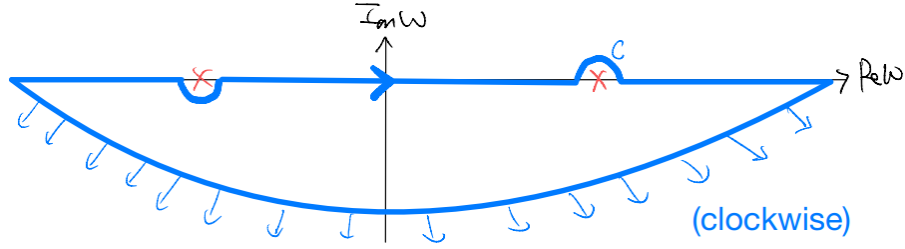
The same calculation as before then gives

$$\int_C \frac{d\omega}{2\pi} D(q,\omega) e^{-i\omega t} = \frac{-1}{2m\omega_q} \frac{2\pi i}{2\pi} \mathrm{Res}\left(\frac{e^{-i\omega t}}{\omega - \omega_q}, \omega = \omega_q\right) - \int_{arc} \frac{d\omega}{2\pi} D(q,\omega) e^{-i\omega t}$$

$$= \frac{-i}{2m\omega_q} e^{-i\omega_q t}, \quad t > 0$$

We may then combine the two cases into

$$\int_C \frac{d\omega}{2\pi} D(q,\omega) e^{-i\omega t} = \frac{-i}{2m\omega_q}\left(\Theta(t) e^{-i\omega_q t} + \Theta(-t) e^{i\omega_q t}\right) = D^t(q,t)$$

as promised. We note in passing that, this is also commonly referred to as the (Feynman) "propagator".

Such time-ordered correlation function shows up in perturbation expansion (Feynman diagrams etc.), and we will see that they can be interpreted as the free propagation of phonons, whence the name.

One may wonder what's the significance of undergoing such a lengthy discussion in order to simply Fourier transform back to the real time. The catch is that, in the calculation above, it will be natural to consider alternative contours which circumvent the two poles in some other means. For instance, consider the contour It doesn't encircle any poles if we complete it in the upper complex
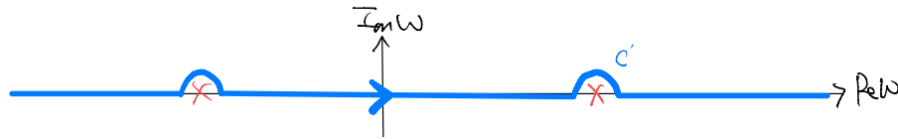
plane (Fourier transform with $t < 0$), and enclose both poles when we complete in the lower complex plane. This gives

$$\int_{C'} \frac{d\omega}{2\pi} D(q,\omega) e^{-i\omega t} = -i\Theta(t)\left(e^{-i\omega_q t} - e^{i\omega_q t}\right) = -2\Theta(t)\sin(\omega_q t)$$

What is the process corresponding to this real-time Green's function? Notice that, what we have changed is really the integration around the pole at $\omega = -\omega_q$. First consider

$$\oint \frac{d\omega}{2\pi} \frac{-e^{-i\omega t}}{\omega + \omega_q} = (-i) e^{i\omega_q t} = (-i) \left\langle \hat{a}_{-q}(0) \hat{a}^\dagger_{-q}(t) \right\rangle = (-i) \left\langle \hat{\phi}_{-q}(0) \hat{\phi}^\dagger_q(t) \right\rangle$$

Now, we can compare the two contours considered

$$(-i) \left\langle \mathcal{T} \left[\hat{\phi}_q(t) \hat{\phi}_{-q}(0) \right] \right\rangle - (-i) \left\langle \mathcal{T} \left[\hat{\phi}_{-q}(0) \hat{\phi}_q(t) \right] \right\rangle$$

$$= (-i) \Theta(t) \left\langle \hat{\phi}_q(t) \hat{\phi}_{-q}(0) \right\rangle + (-i) \Theta(-t) \left\langle \hat{\phi}_{-q}(0) \hat{\phi}_q(t) \right\rangle$$

$$\quad - (-i) \Theta(t) \left\langle \hat{\phi}_{-q}(0) \hat{\phi}_q(t) \right\rangle - (-i) \Theta(-t) \left\langle \hat{\phi}_{-q}(0) \hat{\phi}_q(t) \right\rangle$$

$$= (-i) \Theta(t) \left\langle \left[\hat{\phi}_{-q}(0), \hat{\phi}_q(t) \right] \right\rangle$$

i.e., it is the expectation value of a commutator with time $t > 0$.

By closing the contour on the lower complex plane, our real-time Green's function is non-vanishing only for $t > 0$, which suggests a kind of causality, in the sense that we only allow time to move "forward" but not backward. Indeed, this is known as the causal / retarded Green's function of the phonons, and is closely related to the response of a system when we perturb it (and the system can only respond after we perturb it, by causality). More later.

Lastly, a comment on contours vs $i\eta$: in the above, we see that the same frequency space Green's function, combined with different contour prescription (for avoiding the singularities on the real axis), gives rise to different real-time Green's functions. Yet, we also argued (heuristically) that, the contour prescription can be understood simply by the small shifts $\pm i\eta$ kicking the poles off the real axis. So, instead of specifying different contours, we can also stick with the real line (and leave the "arc" part implicit, dependent on the sign of time), and instead assign the $\pm i\eta$ as the definition for different Green's functions.

This latter perspective is perhaps more popular among physicists, and this is called "Feynman's $i\epsilon$ prescription". (Probably he used ϵ for what we denoted by η here.)

A particularly important "pole structure" for our next topic (linear response) is as follows: where the $i\eta$ displaces the poles to the lower complex plane. This
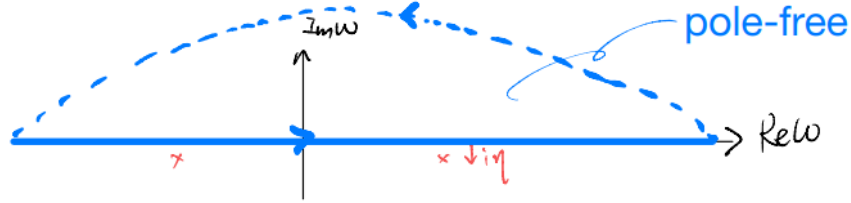
corresponds to the contours we considered just now for the phonons: When

we Fourier transform back to real time, the integral vanishes when we close the contour on the upper complex plane, i.e., the only contribution comes from $t > 0$, and the real-time Green's function is "retarded" in the sense that

$$G_{\text{ret}}\left(t, t'\right) \propto \Theta\left(t - t'\right)$$

To summarize, when we consider Fourier transform back to real time

$$f\left(t\right) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f\left(\omega\right) e^{-i\omega t}$$

$$= \int_{-\infty}^{\infty} \frac{d\text{Re}\left(\omega\right)}{2\pi} f\left(\omega\right) e^{-i\text{Re}(\omega)t} e^{\text{Im}(\omega)t}$$

$$\sim \begin{cases} \Theta\left(t\right), & t > 0 \\ \Theta\left(-t\right), & t < 0 \end{cases}$$

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega)\, e^{-i\omega t}$$

$$= \int_{-\infty}^{\infty} \frac{d(Re\omega)}{2\pi} f(\omega)\, e^{-i Re(\omega) t}\, e^{(Im\omega) t}$$

$t > 0$
$\sim \Theta(t)$

$t < 0$
$\sim \Theta(t)$

close contour in the lower complex plane

close contour in the lower complex plane

contributions from

Chapter 13

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Topics

1. Linear response

2. Susceptibility and retarded Greens' function

 Goals

1. Establishing a more precise connection between Green's function and experimental observables

13.1 Recap: reasons for thinking about Green's functions

Let us briefly recap what we have learnt about (zero-temperature) Green's functions.

1. We argued that, in real time, they could be understood simply as the matrix-element of the time-evolution operator evaluated in the ground state ("Level I")

2. We also showed that, in the frequency space, the Green's function contains important physical information about the ground state and its excitations ("Level II")

3. We then see that specific "time-ordered" combination of the real-time Green's function form the basic ingredients when we try to solve equation of motion with time-dependent operator "coefficients", which leads to the time-ordered exponential ("Level III")

4. We just saw that, in fact, all these Green's functions are really the same in the frequency space, but just with different contour prescription in going to the real time (at least for free phonons)!

In particular, we saw that when we close the contour on the lower complex plane, we get the "retarded Green's function" taking the form

$$G^{\text{ret}}(q,t) = (-i)\,\Theta(t)\left\langle\left[\hat{A}(t),\hat{B}(0)\right]\right\rangle$$

It has a sense of causality, in that it is non-vanishing only for $t > 0$. Furthermore, when $\hat{A}$ and $\hat{B}$ are Hermitian,

$$
\begin{aligned}
\left(-i\left[\hat{A}(t),\hat{B}(0)\right]\right)^{\dagger} &= \left(-i\hat{A}(t)\hat{B}(0)+i\hat{B}(0)\hat{A}(t)\right)^{\dagger}\\
&= i\hat{B}(0)\hat{A}(t)-i\hat{A}(t)\hat{B}(0)\\
&= -i\left[\hat{A}(t),\hat{B}(0)\right]
\end{aligned}
$$

this implies our retarded Green's function could be measurable! Note how things start to fall into place: the mysterious "conventional factor" $(-i)$ now makes sense too!

13.2 Linear response

Let us now consider a general problem and see how, indeed, the retarded Green's functions appear as the response of a system to perturbations.

Consider a static Hamiltonian $\hat{H}_0$ which wee disturb at some time by a perturbation $\hat{V}(t)$. The full Hamiltonian is given by

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$$

in the Schrodinger picture, i.e., the Schrodinger states evolve as

$$i\partial_t|\Psi_S(t)\rangle = \hat{H}(t)\,|\Psi_S(t)\rangle$$

Taking the perspective that "the system" is simply described by $\hat{H}_0$ and $\hat{V}(t)$ is only "a probe", it will be natural to try going into a Heisenberg picture defined using $\hat{H}_0$ (instead of $\hat{H}(t)$). Consider an operator $\hat{O}$ which is time-independent in the Schrodinger picture:

$$\langle\Psi_S(t)\,|\hat{O}_S|\Psi_S(t)\rangle = \langle\Psi_S(t)\,|e^{-i\hat{H}_0 t}\left(e^{i\hat{H}_0 t}\hat{O}_S e^{-i\hat{H}_0 t}\right)e^{i\hat{H}_0 t}|\Psi_S(t)\rangle$$

$$\hat{O}_I(t) = e^{i\hat{H}_0 t}\hat{O}_S e^{-i\hat{H}_0 t}$$

where $\hat{O}_I(t)$ is equivalently Heisenberg picture for $\hat{O}$ defined using $\hat{H}_0$. Of course, this is something like a hybrid picture, because ultimately our full Hamiltonian (and so the "true" Heisenberg picture) also contains the perturbation.

We call this the "interaction picture". The equations of motions are now

$$i\partial_t\hat{O}_I(t) = \left[\hat{O}_I(t),\hat{H}_0\right]$$

same as the Heisenberg picture for the unperturbed system.

$$
\begin{aligned}
i\partial_t |\Psi_I(t)\rangle &= i\partial_t \left(e^{i\hat{H}_0 t} |\Psi_S(t)\rangle \right) \\
&= -\hat{H}_0 \left(e^{i\hat{H}_0 t} |\Psi_S(t)\rangle \right) + e^{i\hat{H}_0 t} \left(i\partial_t |\Psi_S(t)\rangle \right) \\
&= -\hat{H}_0 |\Psi_I(t)\rangle + e^{i\hat{H}_0 t} \left(\hat{H}_0 + \hat{V}(t) \right) e^{-i\hat{H}_0 t} |\Psi_I(t)\rangle \\
&= \hat{V}_I(t) |\Psi_I(t)\rangle
\end{aligned}
$$

$$
\hat{V}_I(t) = e^{i\hat{H}_0 t} \hat{V}(t) e^{-i\hat{H}_0 t}
$$

i.e., the "effective Hamiltonian" for $|\Psi_I(t)\rangle$ is simply the perturbation, but with the operators acquiring additional time-dependence according to the Heisenberg picture of the unperturbed system. (Note: this holds even if $\hat{V}$ itself is time-independent to start with.)

We have seen already how such equation of motion could be solved: the (formal) solution is simply the time-ordered exponential:

$$
|\Psi_I(t)\rangle = \mathcal{T} \left[e^{-i \int_{t_0}^{t} dt' \hat{V}_I(t')} \right] |\Psi_I(t_0)\rangle
$$

In particular, at $t_0 \to -\infty$ we simply have the original ground state $|\Omega\rangle$ of the unperturbed system $\hat{H}_0$, so

$$
|\Psi_I(t)\rangle = \mathcal{T} \left[e^{-i \int_{-\infty}^{t} dt' \hat{V}_I(t')} \right] |\Omega\rangle
$$

We are now all set-up to consider how the system responds to the perturbations! As discussed, the expectation value of a physical observable is

$$
O(t) = \langle \Psi_I(t) | \hat{O}_I(t) | \Psi_I(t) \rangle
$$

We could evaluate it as a perturbation series in powers of $\hat{V}$. Recall, $\hat{O}_I(t)$ is simply equivalently to the unperturbed Heisenberg operator, and so the lowest order term comes from

$$
\begin{aligned}
|\Psi_I(t)\rangle &= \mathcal{T} \left[e^{-i \int_{-\infty}^{t} dt' \hat{V}_I(t')} \right] |\Omega\rangle \\
&= \left(I - i \int_{-\infty}^{t} dt' \hat{V}_I(t') + \cdots \right) |\Omega\rangle
\end{aligned}
$$

$$
\begin{aligned}
O(t) &= \langle \Omega | \left(I + i \int_{-\infty}^{t} dt' \hat{V}_I(t') + \cdots \right) \hat{O}_I(t) \left(I - i \int_{-\infty}^{t} dt' \hat{V}_I(t') + \cdots \right) |\Omega\rangle \\
&\approx \langle \Omega | \hat{O}_I(t) |\Omega\rangle - i \langle \Omega | \left[\hat{O}_I(t), \int_{-\infty}^{t} dt' \hat{V}_I(t') \right] |\Omega\rangle
\end{aligned}
$$

$$\delta O\left(t\right) = O\left(t\right) - \langle\Omega|\hat{O}_S|\Omega\rangle$$
$$= O\left(t\right) - \langle\Omega|\hat{O}_I\left(t\right)|\Omega\rangle$$
$$= -i\langle\Omega|\left[\hat{O}_I\left(t\right), \int_{-\infty}^{t} dt'\hat{V}_I\left(t'\right)\right]|\Omega\rangle$$

This relates the change in the observable to the lowest (linear) order in the perturbation $\hat{V}$. Let us further assume the perturbation takes the form

$$\hat{V}_S\left(t\right) = \hat{O}'_S f\left(t\right)$$

$$\Rightarrow \hat{V}_I\left(t\right) = \hat{O}'_I f\left(t\right)$$

i.e., its only time-dependence in the Schrodinger picture comes solely from a time-dependent "driving force" $f(t)$.

Our discussions simplify further in the frequency space. Consider the Fourier transform of the force

$$f\left(t\right) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f\left(\omega\right) e^{-i\omega t}$$

$$\Rightarrow \delta O\left(t\right) = \left(-i\right) \int_{-\infty}^{t} dt' \langle\Omega|\left[\hat{O}_I\left(t\right), \hat{O}'_I\left(t'\right)\right]|\Omega\rangle \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f\left(\omega\right) e^{-i\omega t'}$$
$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f\left(\omega\right)\left(-i\right) \int_{-\infty}^{t} dt' \langle\Omega|\left[\hat{O}_I\left(t\right), \hat{O}'_I\left(t'\right)\right]|\Omega\rangle e^{-i\omega t'}$$

$$\langle\Omega|\left[\hat{O}_I\left(t\right), \hat{O}'_I\left(t'\right)\right]|\Omega\rangle = \langle\Omega|\left[\hat{O}_I\left(t-t'\right), \hat{O}'_I\left(0\right)\right]|\Omega\rangle$$

where the time-translation invariance follows from a static non-perturbed $\hat{H}_0$, and that our interaction picture operators are simply the Heisenberg picture operators with respect to $\hat{H}_0$. Let $\delta_t = t - t' > 0$, then

$$\int_{-\infty}^{t} dt' \left(-i\right) \langle\Omega|\left[\hat{O}_I\left(t-t'\right), \hat{O}'_I\left(0\right)\right]|\Omega\rangle e^{-i\omega t'}$$
$$= \left(\int_{0}^{\infty} d\delta_t \left(-i\right) \langle\Omega|\left[\hat{O}_I\left(\delta_t\right), \hat{O}'_I\left(0\right)\right]|\Omega\rangle e^{i\omega\delta_t}\right) e^{-i\omega t}$$

Let us define the susceptibility

$$\chi\left(\omega\right) = \int_{-\infty}^{\infty} d\delta_t \left(-i\right) \Theta\left(\delta_t\right) \langle\Omega|\left[\hat{O}_I\left(\delta_t\right), \hat{O}'_I\left(0\right)\right]|\Omega\rangle e^{i\omega\delta_t}$$

where we have again traded the integration bound with the Heaviside step function.

Importantly, notice that $\chi(\omega)$ is simply the frequency-space version of some retarded Green's function!

When the dust settles, we arrive at

$$\delta O\left(t\right) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \chi\left(\omega\right) f\left(\omega\right) e^{-i\omega t}$$

and so, when we Fourier transform the observable, we get

$$\delta O\left(\omega\right) = \chi\left(\omega\right) f\left(\omega\right)$$

$$\Rightarrow \quad \chi\left(\omega\right) = \frac{\delta O\left(\omega\right)}{f\left(\omega\right)}$$

i.e., the susceptibility is measurable simply as the ratio of the Fourier component of the (change in the) observable and the driving force we used to perturb the system, and it is given by

$$\chi\left(\omega\right) = \int_{-\infty}^{\infty} dt \chi_R\left(t\right) e^{i\omega t}$$

$$\chi_R\left(t\right) = \left(-i\right) \Theta\left(t\right) \langle\Omega| \left[\hat{O}_I\left(t\right), \hat{O}_I^{'}\left(0\right)\right] |\Omega\rangle, \quad \text{retarded}$$

Such relationships (linear-response susceptibilities to retarded Green's functions) are called "Kubo formulas". It is customary to split it into real and imaginary parts:

$$\chi\left(\omega\right) = \Re\left[\chi\left(\omega\right)\right] + i\Im\left[\chi\left(\omega\right)\right]$$

$$\Re\left[\chi\left(\omega\right)\right] = \int_{-\infty}^{\infty} \chi_R\left(t\right) \cos\left(\omega t\right)$$

$$\Im\left[\chi\left(\omega\right)\right] = \int_{-\infty}^{\infty} \chi_R\left(t\right) \sin\left(\omega t\right)$$

From which we see that the real part is an even function of ω, whereas the imaginary part is odd. Therefore, we may also simply write

$$\Re\left[\chi\left(\omega\right)\right] = \frac{\chi\left(\omega\right) + \chi\left(-\omega\right)}{2}$$

$$\Im\left[\chi\left(\omega\right)\right] = \frac{\chi\left(\omega\right) - \chi\left(-\omega\right)}{2i}$$

You might recall that, the imaginary susceptibility corresponds to energy dissipation / absorption. To see why, let us consider a "monochromatic" drive

$$f\left(t\right) = f_0 \cos\left(\Omega t\right)$$

$$f\left(\omega\right) = \pi f_0 \delta\left(\omega + \Omega\right) + \pi f_0 \delta\left(\omega - \Omega\right)$$

Correspondingly, the change in the physical observable is

$$
\begin{aligned}
\delta O\left(t\right) &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \chi\left(\omega\right) f\left(\omega\right) e^{-i\omega t} \\
&= \int_{-\infty}^{\infty} \frac{d\omega}{2} f_0 \chi\left(\omega\right) \left(\delta\left(\omega+\Omega\right)+\delta\left(\omega-\Omega\right)\right) e^{-i\omega t} \\
&= \frac{f_0}{2} \chi\left(\Omega\right) e^{-i\Omega t} + \frac{f_0}{2} \chi\left(-\Omega\right) e^{i\Omega t} \\
&= f_0 \cos\left(\Omega t\right) \Re\left[\chi\left(\Omega\right)\right] + f_0 \sin\left(\Omega t\right) \Im\left[\chi\left(\Omega\right)\right]
\end{aligned}
$$

In other words, the real part $\Re[\chi(\omega)]$ corresponds to the in-phase (also known as reactive) response, whereas the imaginary part $\Im[\chi(\omega)]$ corresponds to the out-of-phase response. As you might recall, the out-of-phase response corresponds to energy dissipation / absorption. To see that, let us consider a generalized power

$$
\begin{aligned}
P\left(t\right) &= f\left(t\right) \frac{d}{dt} \delta O\left(t\right), \quad \left(\text{c.f.} P = Fv = F\frac{dx}{dt}\right) \\
&= f_0^2 \cos\left(\Omega t\right) \frac{d}{dt} \left(\Re\left[\chi\left(\Omega\right)\right] \cos\left(\Omega t\right) + \Im\left[\chi\left(\Omega\right)\right] \sin\left(\Omega t\right)\right) \\
&= f_0^2 \Omega \left(-\Re\left[\chi\left(\Omega\right)\right] \cos\left(\Omega t\right) \sin\left(\Omega t\right) + \Im\left[\chi\left(\Omega\right)\right] \cos^2\left(\Omega t\right)\right) \\
&= \frac{f_0^2 \Omega}{2} \left(-\Re\left[\chi\left(\Omega\right)\right] \sin\left(2\Omega t\right) + \Im\left[\chi\left(\Omega\right)\right] \cos\left(2\Omega t\right) + \Im\left[\chi\left(\Omega\right)\right]\right)
\end{aligned}
$$

When we average the power over one period of the drive, the only survive piece is

$$
\langle P\left(t\right)\rangle = \pi f_0^2 \Im\left[\chi\left(\Omega\right)\right]
$$

this shows explicitly the imaginary (the odd-in-frequency) part of the susceptibility captures the dissipation / absorption of the system.

These are very general conclusions, and, in fact, apply similarly even to systems at finite temperature. In particular, it provides a general platform for understanding the response, fluctuation, and dissipation in a system.

Let us now unpack these formal calculations by considering a "canonical" example.

13.3   Driven QHO

As our first example, let us consider again our old friend now perturbed by a driving term

$$
\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega_0^2 \hat{x}^2 - \frac{1}{2}\omega_0 = \omega_0 \hat{a}^\dagger \hat{a}
$$

$$
\hat{a} = \frac{1}{\sqrt{2}} \left(\sqrt{m\omega_0}\hat{x} + i\frac{\hat{p}}{\sqrt{m\omega_0}}\right)
$$

$$
\hat{V}_s = f\left(t\right)\hat{x}
$$

Let us consider how the position of the particle responds to the drive, i.e., we look at the susceptibility

$$
\begin{aligned}
\chi\left(t\right) &= \left(-i\right)\Theta\left(t\right)\langle 0|\left[\hat{x}\left(t\right),\hat{x}\left(0\right)\right]|0\rangle \\
&= \frac{\left(-i\right)\Theta\left(t\right)}{2m\omega_0}\langle 0|\left[\hat{a}\left(t\right)+\hat{a}^{\dagger}\left(t\right),\hat{a}\left(0\right)+\hat{a}^{\dagger}\left(0\right)\right]|0\rangle \\
&= \frac{\left(-i\right)\Theta\left(t\right)}{2m\omega_0}\left(e^{-i\omega_0 t}-e^{i\omega_0 t}\right) \\
&= -\frac{\Theta\left(t\right)}{m\omega_0}\sin\left(\omega_0 t\right)
\end{aligned}
$$

Hopefully this looks familiar. We already saw that it corresponds to the frequency-space pole structure
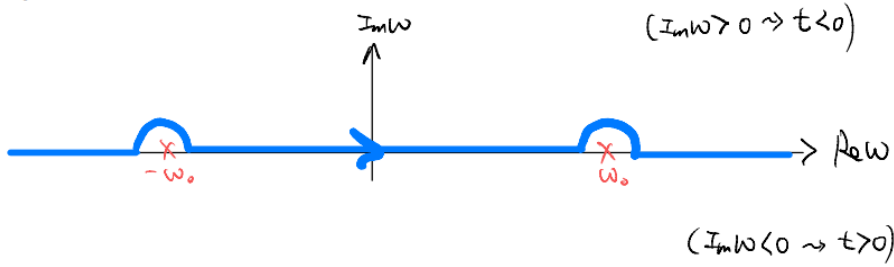
In the $i\eta$ prescription, we have

$$
\begin{aligned}
\chi\left(\omega\right) &= \frac{1}{2m\omega_0}\lim_{\eta\to 0^+}\left(\frac{1}{\omega-\omega_0+i\eta}-\frac{1}{\omega+\omega_0+i\eta}\right) \\
&= \frac{1}{2m\omega_0}\lim_{\eta\to 0^+}\frac{2\omega_0}{\left(\omega+i\eta\right)^2-\omega_0^2} \\
&= \frac{1}{m}\lim_{\eta\to 0^+}\frac{1}{\omega^2-\omega_0^2+2i\omega\eta}
\end{aligned}
$$

This may look familiar to you: the response has a strong peak at the natural frequency, with the peak width controlled by $i\eta$.

Furthermore, we can extract the imaginary part. Recall the Sokhotski-Plemelj theorem

$$
\lim_{\eta\to 0^+}\frac{1}{x\pm i\eta}=P\frac{1}{x}\mp i\pi\delta\left(x\right)
$$

$$
\begin{aligned}
\Rightarrow\quad \Im\left[\chi\left(\omega\right)\right] &= \frac{1}{2m\omega_0}\Im\left[\lim_{\eta\to 0^+}\left(\frac{1}{\omega-\omega_0+i\eta}-\frac{1}{\omega+\omega_0+i\eta}\right)\right] \\
&= \frac{\pi}{2m\omega_0}\left(-\delta\left(\omega-\omega_0\right)+\delta\left(\omega+\omega_0\right)\right)
\end{aligned}
$$

Earlier, we introduced this as the "spectral" function, obtained by the spectral decomposition for a general many-body Hamiltonian, which could be understood

as the matrix-element-weighed density of states. Here, we see that, indeed, it corresponds to experimental observables.

Chapter 14

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Topics

1. Recap of what we have learnt

2. Adiabatic turning on, Gell-Mann-Low theorem

3. Primer into interacting electrons

 Goals

1. Introducing many-body perturbation theory

2. Setting up methods for treating interacting electrons

14.1   Recap: what have we learnt so far?

Today happens to be the mid-way point of our course: let's quickly recap what we've covered
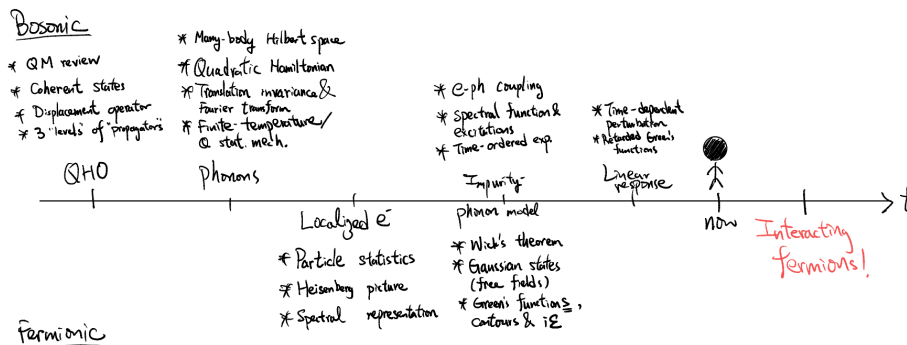
14.2   Adiabatic turning on & Gell-Mann-Low Theorem

Suppose we have a Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V}$$

where we view $\hat{V}$ as a perturbation and $\hat{H}_0$ defines the "unperturbed" problem. As the name suggests, we consider the scenario in which the unperturbed problem is solvable, such that we can attempt to systematically add the corrections from $\hat{V}$ to our physical observables. The typical setup is that $\hat{H}_0$ is a free theory (with Gaussian ground states), and $\hat{V}$ is an interaction. We will refer to $\hat{V}$ as the "interaction" as such.

One clever trick for developing such a perturbation theory is to imagine turning on the perturbation $\hat{V}$ "slowly". Imagine modifying our Hamiltonian into (in Schrodinger picture)

$$\hat{H}\,(t) = \hat{H}_0 + e^{-|t|/\tau}\hat{V}$$

such that it interpolates from $\hat{H}_0$ to $\hat{H} = \hat{H}_0 + \hat{V}$ as go from $t = -\infty$ to $t = 0$, and interpolates back to $\hat{H}_0$ as we further send $t \to +\infty$
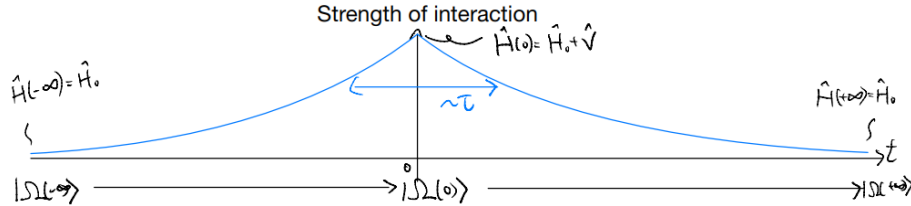
Now, let us suppose we start with the ground state $|\Omega_0\rangle$ of $\hat{H}_0$ at $t \to -\infty$. In the Schrodinger's picture, the state evolve according to

$$i\partial_t|\Omega\,(t)\rangle = \hat{H}\,(t)\,|\Omega\,(t)\rangle$$

with the initial value

$$|\Omega\,(-\infty)\rangle = |\Omega_0\rangle$$

We (probably) don't know how to solve the time-evolution of the state exactly. If we knew, we could have solved $\hat{H}$ directly! Instead, let us imagine plotting the many-body eigen-energies as a function of t:

Suppose the excitation gap remains finite for all values of t. This sets a timescale

$$\tau_A \sim \frac{1}{\min\left(\Delta E\,(t)\right)}$$

The adiabatic theorem then states that, so long as the dynamics in $\hat{H}(t)$ is slow compared to τ_A, i.e., $\tau \gg \tau_A$, then our "black dot" stays in the lowest branch to good approximation.
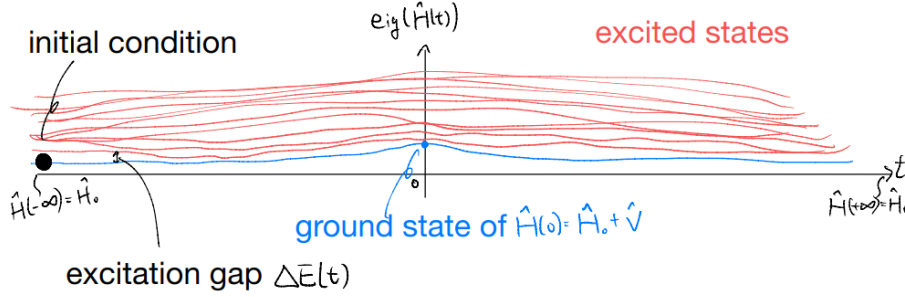
Heuristically, this could be understood from energy considerations: to transit from the ground state to the excited state, we need to supply energy, In our setup, the only possible energy source is the dynamics in $\hat{H}(t)$, with scale set by $1/\tau$. If we keep that arbitrarily slow, i.e., take $\tau \to \inf \infty$, then we are not giving energy to the system to make a transition to the excited states. In other words, we stay in the instantaneous ground state.

We caution that the adiabatic limit is tricky for two reasons

1. For a many-body system in the thermodynamic limit, there may be gapless excitations directly above the ground state. As such there is no reason to expect the adiabatic theorem to hold at all. However, one might imagine circumventing the difficulty by considering a finite system and taking the adiabatic limit first, before taking the thermodynamic limit. In practice, of course, these are subtle problems, and we will not address them carefully here.

2. More importantly, the interaction may be strong enough that a quantum phase transition occurs as we crank the interaction strength up to its full value. Such quantum phase transitions are characterized by a crossing of the energy levels as a function of the interpolation time t. In that case, the adiabatic theorem also fails. And, indeed, one should not hope to get a satisfactory perturbation theory starting from a "wrong" $\hat{H}_0$!

Setting the subtleties aside, let us now consider taking expectation values (with a goal of finally computing some physical observables). We can choose to work in the Heisenberg picture of $\hat{H}(t)$, and consider the time-ordered Green's functions, i.e., quantities of the form

$$\langle \Omega_H(-\infty)| \mathcal{T} \left[\hat{O}_H^{(1)}(t_1) \hat{O}_H^{(2)}(t_2) \cdots \hat{O}_H^{(n)}(t_n) \right] |\Omega_H(-\infty)\rangle$$

The motivation for specializing to time-ordered operators will be clear in a moment, and we consider times t_i which remain finite even as $\tau \to \infty$, i.e., we stay near $t = 0$ in the adiabatic limit.

In the above, we take advantage of the fact that, in the Heisenberg picture, the state is stationary and all the time-dependence is assigned to the operators. One may for a moment revert back to the Schrodinger picture, supposing for

simplicity that $t_1 > t_2 > \cdots > t_n$ such that the time-ordering does nothing. The quantity we wrote down can be understood as

$$\langle \Omega_S(t_1) | \mathcal{T} \left[\hat{O}_S^{(1)}(t_1) \hat{U}_S(t_1, t_2) \hat{O}_S^{(2)}(t_2) \cdots \hat{U}_S(t_{n-1}, t_n) \hat{O}_S^{(n)}(t_n) \right] | \Omega_S(t_n) \rangle$$

where $\hat{U}_S$ is the time-evolution operator in the Schrodinger picture

$$\hat{U}_S(t_i, t_j) = \mathcal{T} \left[\exp \left(-i \int_{t_i}^{t_j} dt' \hat{H}_S(t') \right) \right]$$

In the adiabatic limit, for finite times t_i, we have

$$\hat{H}_S(t_i) \to \hat{H}$$

$$|\Omega_S(t_i)\rangle \to |\Omega\rangle$$

where $|\Omega\rangle$ denotes the many-body ground state of full Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$. As such, we see that, in the adiabatic limit, we are simply computing some sort of correlation functions for the interacting ground state.

At the same time, we know that the "initial state"

$$|\Omega_H(-\infty)\rangle = |\Omega_S(-\infty)\rangle = |\Omega_0\rangle$$

is simply the ground state of the unperturbed Hamiltonian $\hat{H}_0$. This connects the "hard problems" of interest (concerning the interacting system) to those in our "simple starting point".

To show this more explicitly, we recall the interaction picture introduced in the last lecture. For our problem, it is natural to use $\hat{H}_0$ to define the dynamics of the operators, such that the interaction-picture operators (for the full problem with adiabatic turning on) evolve in time according to the Heisenberg picture defined with respect to $\hat{H}_0$. Starting from the reference time of $t \to -\infty$, the quantum states evolve in the interaction picture according

$$|\Omega_I(t)\rangle = \hat{S}(t, -\infty) |\Omega_0\rangle$$

$$\hat{S}(t, -\infty) = \mathcal{T} \left[\exp \left(-i \int_{-\infty}^{t} dt' \hat{V}_I(t') \right) \right]$$

where $\hat{V}_I(t)$ is the interaction Hamiltonian (perturbation) in the interaction picture. The "S-matrix" is unitary and could be related to backward time evolution

$$\hat{S}^\dagger(t_1, t_2) \hat{S}(t_1, t_2) = I$$

$$\hat{S}^\dagger(t_1, t_2) = \hat{S}(t_2, t_1)$$

Now, in computing observables we know that

$$\langle \Omega_0 | \hat{O}_H(t) | \Omega_0 \rangle = \langle \Omega_I(t) | \hat{S}(t, -\infty) \hat{O}_H(t) \hat{S}^\dagger(t, -\infty) | \Omega_I(t) \rangle$$

$$\hat{O}_I(t) = \hat{S}(t, -\infty) \hat{O}_H(t) \hat{S}^\dagger(t, -\infty)$$

where the state $|\Omega_0\rangle$ doesn't evolve in the Heisenberg picture. i.e., we have

$$\hat{O}_H(t) = \hat{S}^\dagger(t, -\infty)\,\hat{O}_I(t)\,\hat{S}(t, -\infty) = \hat{S}(-\infty, t)\,\hat{O}_I(t)\,\hat{S}(t, -\infty)$$

Supposing for the moment that $t_1 > t_2 > \cdots > t_n$, in the interaction picture we have

$$\langle\Omega_0|\mathcal{T}\left[\hat{O}_H^{(1)}(t_1)\,\hat{O}_H^{(2)}(t_2)\cdots\hat{O}_H^{(n)}(t_n)\right]|\Omega_0\rangle$$

$$=\langle\Omega_0|\hat{O}_H^{(1)}(t_1)\,\hat{O}_H^{(2)}(t_2)\cdots\hat{O}_H^{(n)}(t_n)|\Omega_0\rangle$$

$$=\langle\Omega_0|\hat{S}(-\infty, t_1)\,\hat{O}_I^{(1)}(t_1)\,\hat{S}(t_1, -\infty)\,\hat{S}(-\infty, t_2)\,\hat{O}_I^{(2)}(t_2)\,\hat{S}(t_2, -\infty)$$

$$\cdots\hat{S}(t_{n-1}, -\infty)\,\hat{S}(-\infty, t_n)\,\hat{O}_I^{(n)}(t_n)\,\hat{S}(t_n, -\infty)|\Omega_0\rangle$$

$$=\langle\Omega_0|\hat{S}(-\infty, t_1)\,\hat{O}_I^{(1)}(t_1)\,\hat{S}(t_1, t_2)\,\hat{O}_I^{(2)}(t_2)\cdots\hat{O}_I^{(n)}(t_n)\,\hat{S}(t_n, -\infty)|\Omega_0\rangle$$

$$=\langle\Omega_0|\hat{S}(-\infty, +\infty)\,\mathcal{T}\left[\hat{S}(+\infty, t_1)\,\hat{O}_I^{(1)}(t_1)\,\hat{S}(t_1, t_2)\,\hat{O}_I^{(2)}(t_2)\cdots\hat{O}_I^{(n)}(t_n)\,\hat{S}(t_n, -\infty)\right]|\Omega_0\rangle$$

$$=\langle\Omega_I(+\infty)|\mathcal{T}\left[\hat{S}(+\infty, -\infty)\,\hat{O}_I^{(1)}(t_1)\,\hat{O}_I^{(2)}(t_2)\cdots\hat{O}_I^{(n)}(t_n)\right]|\Omega_I(-\infty)\rangle$$

when the dust settles, we see that the final expression is independent on the initial time-ordering. In other words, even if the times were ordered differently in the beginning, we still get the same expression at the end. Importantly, all the insertion of the S-matrix can be lumped into a single one going $-\infty$ to $+\infty$. The time-ordering ensures that we break it down into pieces in the actual expression.

The only problem left is that what we have is not an "expectation value" with respect to a given state. This can be fixed by noticing that, in the adiabatic limit, the state $|\Omega_0\rangle$ is both the initial and final state. Yet, in the interaction picture the states have to evolve, and so we can only reconcile the initial and final states up to a phase in the interaction picture:

$$|\Omega_I(-\infty)\rangle = |\Omega_0\rangle$$

$$|\Omega_I(+\infty)\rangle = \hat{S}(+\infty, -\infty)\,|\Omega_I(-\infty)\rangle = e^{2i\delta}|\Omega_0\rangle$$

In particular, the phase can be understood as the overlap

$$\langle\Omega_0|\Omega_I(+\infty)\rangle = \langle\Omega_0|\hat{S}(+\infty, -\infty)\,|\Omega_0\rangle = e^{2i\delta}$$

$$\langle\Omega_I(+\infty)| = e^{-2i\delta}\langle\Omega_0| = \frac{\langle\Omega_0|}{\langle\Omega_0|\hat{S}(+\infty, -\infty)\,|\Omega_0\rangle}$$

Altogether, we conclude

$$\langle\Omega_H(-\infty)|\mathcal{T}\left[\hat{O}_H^{(1)}(t_1)\,\hat{O}_H^{(2)}(t_2)\cdots\hat{O}_H^{(n)}(t_n)\right]|\Omega_H(-\infty)\rangle$$

$$=\frac{\langle\Omega_0|\mathcal{T}\left[\hat{O}_I^{(1)}(t_1)\,\hat{O}_I^{(2)}(t_2)\cdots\hat{O}_I^{(n)}(t_n)\,\hat{S}(+\infty, -\infty)\right]|\Omega_0\rangle}{\langle\Omega_0|\hat{S}(+\infty, -\infty)\,|\Omega_0\rangle}$$

where

$$\hat{S}\left(+\infty, -\infty\right) = \mathcal{T}\left[\exp\left(-i\int_{-\infty}^{+\infty} dt' \hat{V}_I\left(t'\right)\right)\right]$$

and the interaction-picture operators evolve according to the Heisenberg picture with respect to $\hat{H}_0$. Furthermore, we end up with an expression involving only the ground-state expectation value of the unperturbed problem. This fulfills our promise of relating the interacting problem to the unperturbed one. The remaining task is "simply" to expand in powers $\hat{V}_I$ and we would get a perturbation series!

Remark: the final expression obtained above is highly reminiscent of what we have learnt in statistics mechanics. Recall, for instance, that the average energy

$$\left\langle\hat{H}\right\rangle = \frac{\text{Tr}\left(\hat{H} e^{-\beta\hat{H}}\right)}{\mathcal{Z}\left(\beta\right)} = -\partial_\beta \ln \mathcal{Z}\left(\beta\right)$$

This suggests that we can define

$$\mathcal{Z}\left[J^\alpha\left(t\right)\right] = \langle\Omega_0|\mathcal{T}\left[\exp\left(-i\int_{-\infty}^{+\infty} dt' \left(\hat{V}_I\left(t'\right) + J^\alpha\left(t\right)\hat{O}^\alpha\left(t\right)\right)\right)\right]|\Omega_0\rangle$$

such that our expression can be simplified further into something like

$$\frac{\langle\Omega_0|\mathcal{T}\left[\hat{O}_I^{(1)}\left(t_1\right)\hat{O}_I^{(2)}\left(t_2\right)\cdots\hat{O}_I^{(n)}\left(t_n\right)\hat{S}\left(+\infty, -\infty\right)\right]|\Omega_0\rangle}{\langle\Omega_0|\hat{S}\left(+\infty, -\infty\right)|\Omega_0\rangle} \sim \left.\partial_{J_1}\partial_{J_2}\cdots\partial_{J_n} \ln \mathcal{Z}\left[J^\alpha\left(t\right)\right]\right|_{J=0}$$

this is the spirit of a generating functional (c.f. PS3). In any case, we see that a close parallel with statistics mechanics emerges.

14.3 Interacting electrons

Let us be brave and go straight now to a problem of interacting electrons. Consider a fermionic problem with the full Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V}$$

$$\hat{H}_0 = \sum_{x,y,\sigma,\sigma'} \hat{c}_{x\sigma}^\dagger h_{xy}^{\sigma\sigma'} \hat{c}_{y\sigma'}$$

$$\hat{V} = \sum_{x,y} V\left(|x-y|\right) : \hat{n}_x\hat{n}_y :$$

where $\hat{n}_x = \sum_\sigma \hat{c}_{x\sigma}^\dagger \hat{c}_{x\sigma}$ denotes the on-site density of the electrons. Notice that the interaction term is normal-ordered, such that

$$: \hat{n}_x\hat{n}_y := \sum_{\sigma\sigma'} : \hat{c}_{x\sigma}^\dagger \hat{c}_{x\sigma}\hat{c}_{y\sigma'}^\dagger \hat{c}_{y\sigma'} :$$

$$= \sum_{\sigma\sigma'} \hat{c}_{x\sigma}^\dagger \hat{c}_{y\sigma'}^\dagger \hat{c}_{y\sigma'}\hat{c}_{x\sigma}$$

and the last line holds even if $x = y$ & $\sigma = \sigma'$, in which case the term vanishes. This ensures

$$\hat{V}|0\rangle = 0$$

$$\hat{V}\left(\hat{c}_{x\sigma}^\dagger|0\rangle\right) = 0$$

i.e., there is no interaction when we have zero or one electron.

Of course, it's quite meaningless if we just state the Hamiltonian and leave it there. Let us attempt to evaluate some physical quantities, say the dielectric function. (The full problem is more complicated, with distinctions between longitudinal vs transverse response and DC versus AC etc. In the following, we only sketch a simplified version of the key points.)

Recall, in a medium the EM scalar potential is modified into

$$\phi_0\left(r\right) = \frac{\rho_{\text{ext}}}{4\pi\varepsilon_0 r} \quad \rightarrow \quad \phi\left(r\right) = \frac{\rho_{\text{ext}}}{4\pi\varepsilon r}$$

In momentum space, we have

$$\phi\left(q\right) \sim \frac{\rho_{\text{ext}}\left(q\right)}{q^2\varepsilon\left(q\right)}$$

The modification to the dielectric "constant" (which is q dependent here) can also be understood as a modification of the "true" charge density in the medium, due to the screening from the system. I.e., we can consider

$$\phi\left(q\right) \sim \frac{\rho_{\text{tot}}\left(q\right)}{q^2\varepsilon_0}$$

$$\rho_{\text{tot}}\left(q\right) = \rho_{\text{ext}}\left(q\right) + \rho_{\text{sc}}\left(q\right)$$

Comparing the two, we find

$$\frac{\rho_{\text{ext}}\left(q\right) + \rho_{\text{sc}}\left(q\right)}{\varepsilon_0} = \frac{\rho_{\text{tot}}\left(q\right)}{\varepsilon_0}$$

$$\Rightarrow \quad \frac{\varepsilon_0}{\varepsilon\left(q\right)} = 1 + \frac{\rho_{\text{sc}}\left(q\right)}{\rho_{\text{ext}}\left(q\right)}$$

Now, within linear response, the screening charges appear as a response to the external potential

$$\rho_{\text{sc}}\left(q\right) \sim -\chi\left(q, \omega = 0\right)\frac{\rho_{\text{ext}}\left(q\right)}{4\pi\varepsilon_0 q^2}$$

where

$$\chi\left(q, \omega\right) = i\int_{-\infty}^{\infty} dt\,\Theta\left(t\right)\left\langle\left[\hat{\rho}\left(q, t\right), \hat{\rho}\left(-q, 0\right)\right]\right\rangle e^{i\omega t}$$

is the density-density response function (maybe up to the sign). This gives

$$\frac{\varepsilon_0}{\varepsilon\left(q\right)} = 1 - \frac{\chi\left(q\right)}{4\pi\varepsilon_0 q^2}$$

So we could determine the dielectric function by evaluating the density-density response function! But, how do we relate that to the Gell-Mann-Low formula (and hence perturbation theory)?

Chapter 15

Lec15 20220325

Topics

1. What's so hard about interaction?

2. Bare electron propagator

3. Full electron propagator

Goals

1. Appreciating the steps it takes to develop perturbation theory

2. Familiarizing with the one-particle Green's function

15.1   Interacting, so what?

Let's first recall where we were last time. We considered an interacting problem of electrons, given schematically by

$$\hat{H} = \hat{H}_0 + \hat{V}$$

$$\hat{H}_0 \sim t\hat{c}^\dagger \hat{c}$$

$$\hat{V} \sim V\hat{c}^\dagger \hat{c}^\dagger \hat{c}\hat{c}$$

and we asked what is, for instance, the dielectric function of the system. They key point to note is that

$$\phi(r) \sim \frac{\rho_{\text{ext}}}{\varepsilon r} \sim \frac{\rho_{\text{tot}}}{\varepsilon_0 r}$$

$$\rho_{\text{tot}} = \rho_{\text{ext}} + \rho_{sc}$$

where ρ_{sc} encodes how the system responds to the external potential, and in linear response is given by

$$\delta\rho(t) \sim -\chi^{\text{ret}}(t)\rho_{\text{ext}}$$

$$\chi^{\text{ret}}(t) = i\Theta(t)\langle[\hat{\rho}(t),\hat{\rho}(0)]\rangle$$

is the retarded density-density response function of the interacting problem. (Note: we have deliberately kept the discussion schematic above, and ignored all the spatial / momentum dependence etc.)

In principle, we can go ahead and compute the expectation value. Before attempting that, however, let us make a clarification remark about the interaction pictures involved:

1. Linear response: Full, interacting Hamiltonian as the unperturbed problem and the external "probe" as the perturbation. The susceptibility are understood to be in the Heisenberg picture with respect to the full interacting Hamiltonian

2. Adiabatic turning on: "Bare", solvable (non-interacting / free / Gaussian) Hamiltonian as the unperturbed problem and "adiabatic turning on of interactions" as the perturbation.

These two are really quite different. In particular, we bear in mind that the susceptibility (is equal to retarded density-density response function) is a Heisenberg picture quantity with respect to the full Hamiltonian

$$\chi^{\text{ret}}(t) = i\Theta(t)\langle\Omega_H|\left[\hat{\rho}_H(t),\hat{\rho}_H(0)\right]|\Omega_H\rangle$$

We also call this a retarded two-particle Green's function. "Two-particle" because each density operator $\hat{\rho} \sim \hat{c}^\dagger\hat{c}$.

Here, the ground state $|\Omega_H\rangle$ is that of the interacting problem $\hat{H} = \hat{H}_0 + \hat{V}$.

Furthermore, we do not immediately know how to evaluate this expression! Recall, to take advantage of the magic of the S-matrix, time-ordering, and adiabatic turning on, we focused on the time-ordered Green's function, so the closest analog we have is

$$\chi^{\mathcal{T}}(t) = \langle\Omega_H|\mathcal{T}\left[\hat{\rho}_H(t)\,\hat{\rho}_H(0)\right]|\Omega_H\rangle$$

which can now be rewritten, though the adiabatic turning on, into a formal expression

$$\chi^{\mathcal{T}}(t) = \frac{\langle\Omega_0|\mathcal{T}\left[\hat{\rho}_I(t)\,\hat{\rho}_I(0)\exp\left(-i\int_{-\infty}^{\infty}dt'\hat{V}_I(t')\right)\right]|\Omega_0\rangle}{\langle\Omega_0|\mathcal{T}\left[\exp\left(-i\int_{-\infty}^{\infty}dt'\hat{V}_I(t')\right)\right]|\Omega_0\rangle}$$

The numerator can be expanded in a Dyson's series

$$\langle\Omega_0|\mathcal{T}\left[\hat{\rho}_I(t)\,\hat{\rho}_I(0)\exp\left(-i\int_{-\infty}^{\infty}dt'\hat{V}_I(t')\right)\right]|\Omega_0\rangle$$

$$=\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1 dt_2\cdots dt_n\langle\Omega_0|\mathcal{T}\left[\hat{\rho}_I(t)\,\hat{\rho}_I(0)\,\hat{V}_I(t_1)\,\hat{V}_I(t_2)\cdots\hat{V}_I(t_n)\right]|\Omega_0\rangle$$

where the expectation value to take is, schematically,

$$V^n \langle \Omega_0 | \mathcal{T} \left[\hat{c}_t^\dagger \hat{c}_t \hat{c}_0^\dagger \hat{c}_0 \ \hat{c}_{t_1}^\dagger \hat{c}_{t_1}^\dagger \hat{c}_{t_1} \hat{c}_{t_1} \ \hat{c}_{t_2}^\dagger \hat{c}_{t_2}^\dagger \hat{c}_{t_2} \hat{c}_{t_2} \cdots \ \hat{c}_{t_n}^\dagger \hat{c}_{t_n}^\dagger \hat{c}_{t_n} \hat{c}_{t_n} \right] | \Omega_0 \rangle$$

where, for sanity's sake, we have dropped all labels and instead used the subscript to denote the time. Bear in mind that, here, t and 0 are "external" and $t_1, t_2, \cdots, t_n$ are all integrated over.

We know how to evaluate such an expression. It's "just" Wick's theorem and contractions! We know that the answer will be some combinatorial product of our basic building block

$$G_0 \left(q, t \right) = \langle \Omega_0 | \mathcal{T} \left[\hat{c}_q \left(t \right) \hat{c}_q^\dagger \left(0 \right) \right] | \Omega_0 \rangle$$

known as the (bare) Feynman propagator.

A brute force evaluation for the lowest orders, say up to V^2, may seem perhaps tedious but possibly doable. But, it is wrong to think that such a calculation will suffice for finding the lowest order interaction corrections: we have to remember there is also a denominator, which is essentially the same power series but without the "density-density" part! Fortunately, as we have seen from the statistics mechanics correspondence, there is a way to handle both the numerator and the denominator in one-shot: by taking log!

In the following, we address these challenges, one at a time. Before we lose sight of the picture and get buried in the technical details, it may be good to first summarize how we will attack the problem

1. Evaluate the "bare" (Feynman) propagator

2. Attempt to evaluate the Dyson's series by "brute force", through Wick's theorem to Feynman diagrams as a mnemonic

3. Take care of the denominator: linked cluster theorem

4. Dyson's equation and dressed propagators: resummation of series and 1PI

5. Partial resummation and approximations

6. Analytic continuation and going back to real time

15.2   Bare (Feynman) propagator

The starting point of our perturbation theory is, of course, the unperturbed problem. Here, we consider the "free" part of the problem, with the Hamiltonian

$$\hat{H}_0 = \sum_{x,y,\sigma,\sigma'} \hat{c}_{x\sigma}^\dagger h_{xy}^{\sigma\sigma'} \hat{c}_{y\sigma'}$$

As discussed briefly (c.f. lecture on localized electrons), we can define "eigenmodes" such that

$$\hat{H}_0 = \sum_i \varepsilon_i \hat{\tilde{c}}_i^\dagger \hat{\tilde{c}}_i = \sum_i \varepsilon_i \hat{\tilde{n}}_i$$

is readily diagonalized, with all the eigenstates built by specifying the values $\hat{\tilde{n}}_i = 0, 1$ for the full set of mutually commuting number operators.

The ground state, i.e., the lowest energy state, is constructed by setting

$$\tilde{n}_i = \begin{cases} 1, & \text{if} \varepsilon_i < 0 \\ 0, & \text{if} \varepsilon_i > 0 \end{cases}$$

and occupation of modes with exactly $\varepsilon_i = 0$ does not affect the energy of the state. Such zero modes, if exist, lead to ground-state degeneracy.

Furthermore, these are eigenmodes, in the sense that their equations of motion are simply

$$i\partial_t \hat{\tilde{c}}_i^\dagger (t) = \left[\hat{\tilde{c}}_i^\dagger (t), \hat{H}_0 \right] = -\varepsilon_i \hat{\tilde{c}}_i^\dagger (t)$$

$$\Rightarrow \quad \hat{\tilde{c}}_i^\dagger (t) = e^{i\varepsilon_i t} \hat{\tilde{c}}_i^\dagger (0)$$

Let us now assume the system has translation invariance, such that we can further Fourier transform

$$\hat{\tilde{c}}_{k\sigma}^\dagger = \frac{1}{\sqrt{V}} \sum_x \hat{\tilde{c}}_{x\sigma}^\dagger e^{ik \cdot x}$$

$$\Rightarrow \quad \hat{H}_0 = \sum_k \hat{\tilde{c}}_{k\sigma}^\dagger h^{\sigma\sigma'} (k) \hat{\tilde{c}}_{k\sigma'}$$

The momentum-space singular particle Hamiltonian is customary called the Bloch Hamiltonian. Its eigenvalues eig($h(k)$) form energy bands which, for local Hamiltonian, are continuous in the (quasi-)momentum k. The number of bands equals to the dimension of the Bloch Hamiltonian, which in turns is given by the number of fermion modes we retain in each unit cell. For simplicity, let us take that we only have one orbital per cell, such that $h(k)$ is 2×2 because of the spin-$\frac{1}{2}$ nature of electrons.

For spin-rotation invariant systems, $h(k) = \varepsilon_k \sigma^0$ and we have a single band (which is doubly degenerate). Our earlier discussion applies equally well, but now the energy is labeled by the momentum k (instead of a generic index).

For a simple dispersion, say a "consine band", there is a single Fermi surface defined by $\varepsilon_k = 0$. The ground state is then the filled Fermi sea

$$|\Omega_0\rangle = \prod_{|k| < |k_F|} \hat{c}_k^\dagger |0\rangle$$

With this setup we can now evaluate the "bare propagator". Remember, the building block of our perturbation theory is the "basic T-contraction".

$$iG_0^F (k, t) = \left\langle \mathcal{T} \left[\hat{c}_k (t) \hat{c}_k^\dagger (0) \right] \right\rangle_0$$

where we have used the fact that our ground state is translation invariant in both space and time (in particular, we used $\left\langle \hat{c}_k \hat{c}_{k'}^\dagger \right\rangle \propto \delta_{kk'}$ to focus on a single
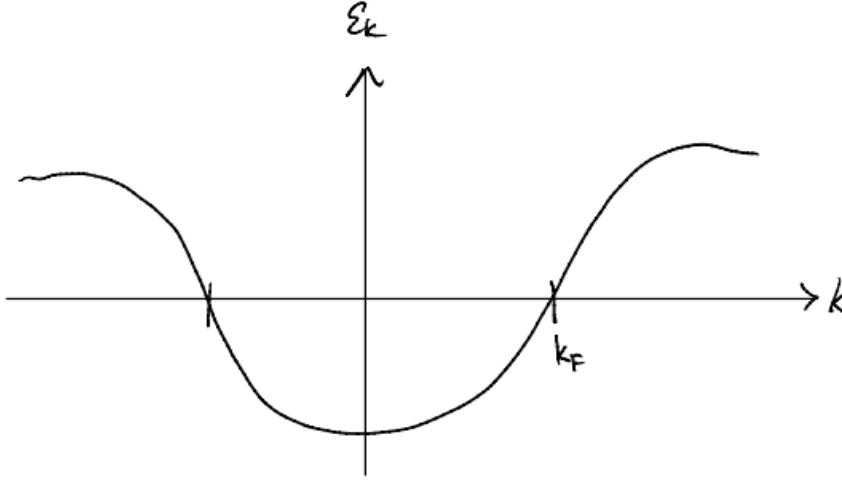
momentum). Evaluating

$$iG_0^F (k,t) = \Theta (t) \left\langle \hat{c}_k (t) \hat{c}_k^\dagger (0) \right\rangle - \Theta (-t) \left\langle \hat{c}_k^\dagger (0) \hat{c}_k (t) \right\rangle$$

$$= \Theta (t) \Theta (|k| - |k_F|) e^{-i\varepsilon_k t} - \Theta (-t) \Theta (|k_F| - |k|) e^{-i\varepsilon_k t}$$

where the first term is the electron-excitation above the Fermi sea and the second term is the hole-excitation within the Fermi sea. Going to frequency space, we have

$$iG_0^F (k,\omega) = \int_{-\infty}^{\infty} dt G_0^F (k,t) e^{i\omega t}$$

$$= \Theta (|k| - |k_F|) \lim_{\eta \to 0^+} \frac{(e^{-\infty} - 1)}{i (\omega - \varepsilon_k + i\eta)} - \Theta (|k_F| - |k|) \lim_{\eta \to 0^+} \frac{(1 - e^{-\infty})}{i (\omega - \varepsilon_k - i\eta)}$$

$$G_0^F (k,\omega) = \lim_{\eta \to 0^+} \left(\frac{\Theta (|k| - |k_F|)}{\omega - \varepsilon_k + i\eta} + \frac{\Theta (|k_F| - |k|)}{\omega - \varepsilon_k - i\eta} \right)$$

Noticing that the Heaviside step function is simply an "on-off switch", it will be natural to further define

$$\eta_k = \text{sign} (|k| - |k_F|) \, \eta$$

and we might write

$$G_0^F (k,\omega) = \lim_{\eta_k \to 0^\pm} \frac{1}{\omega - \varepsilon_k + i\eta_k}$$

we call this the (Feynman) propagator.

Notice that, in our single band problem, we have a single pole at each momentum k. (Contrast with the phonon propagator, which have two poles for
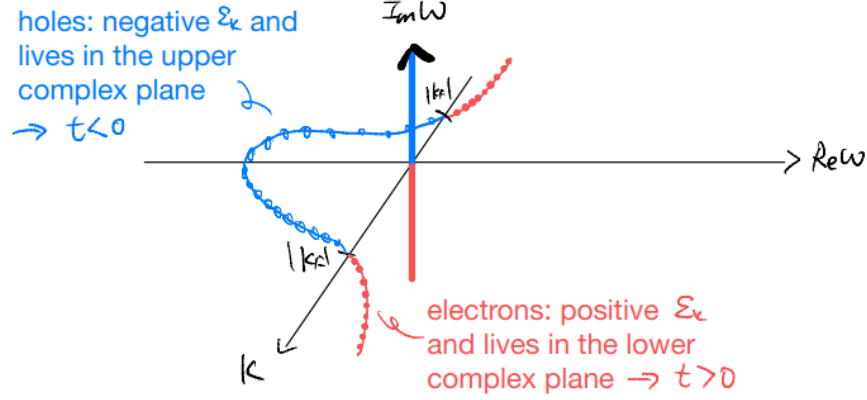
each momentum k.) In particular, we see that a single Green's function capture both the electron and hole excitations. The union of the two comes about in an interesting way, with the nature of the excitation (electron versus hole) encoded in the location of the pole (lower versus upper complex plane). In fact, going back to the real-time expression, we see that:

1. Electron piece $\Theta\left(t\right)\left\langle \hat{c}_k\left(0\right)\hat{c}_k^\dagger\left(t\right)\right\rangle$: $t>0$, forward in time

2. Hole piece $\Theta\left(-t\right)\left\langle \hat{c}_k^\dagger\left(0\right)\hat{c}_k\left(t\right)\right\rangle$: $t<0$, backward in time

Remarks: The problem of QED electron is completely analogous. The only changes are

1. the Fermi "wave vector" happens to be $k_F=0$

2. the "filled Fermi sea" is the whole set of negative energy solutions to Dirac equation

3. we call the "holes" positrons

What we mentioned above is a paraphrasing of Feynman's famous interpretation that positron (electron traveling backward in time). (There is a second part of the interpretation: there is only one electron in the universe and it keeps traveling forward and backward. This "one-electron universe" is attributed to Wheeler, Feynman's PhD advisor.)

Let us clarify two points before moving on:

1. What happened to the spin index? In principle, the one-particle propagator (two-point Green's function) should be a matrix, since each of the two fermions carries an index. (E.g., we simplify the momentum part using $\left\langle \hat{c}_k\hat{c}_{k'}^\dagger\right\rangle \sim \delta_{kk'}$) Correspondingly, when we restore spin indices, we simply have

$$G_{\sigma\sigma'}^F(k,t) = -i\left\langle \mathcal{T}\left[\hat{c}_{k\sigma}\left(t\right)\hat{c}_{k\sigma'}^\dagger\left(t\right)\right]\right\rangle$$

for spin-rotation-invariant system, we also have $\left\langle \hat{c}_\sigma \hat{c}_{\sigma'}^\dagger \right\rangle \sim \delta_{\sigma\sigma'}$

$$G_{\sigma\sigma'}^F (k, t) = G^F (k, t) \delta_{\sigma\sigma'}$$

and so we could focus on the "single band" discussion as if the spin did not exist. The spin, however, will actually still be important in giving "overall factors" for the different terms in the perturbation expansion.

2. Some of you might notice that the way we defined the propagator is actually ad hoc in a sense. Let us consider, instead, the contraction

$$(-i) \left\langle \mathcal{T} \left[\hat{c}_k^\dagger (t) \hat{c}_k (0) \right] \right\rangle$$
$$= (-i) \left[\Theta (t) \left\langle \hat{c}_k^\dagger (t) \hat{c}_k (0) \right\rangle - \Theta (-t) \left\langle \hat{c}_k (0) \hat{c}_k^\dagger (t) \right\rangle \right]$$
$$= -i e^{i\varepsilon_k t} \left[\Theta (t) \Theta (|k_F| - |k|) - \Theta (-t) \Theta (|k| - |k_F|) \right]$$
$$= -G_0^F (k, -t)$$

and, as such, we see that this alternative contraction does not provide us with additional data. (But, as a corollary, it also suggest that the "arrow of time" we assigned to electrons versus holes is not entirely unambiguous.) Similarly, we may go to frequency space and get

$$(-i) \int_{-\infty}^{\infty} dt \left\langle \mathcal{T} \left[\hat{c}_k^\dagger (t) \hat{c}_k (0) \right] \right\rangle e^{i\omega t} = - \int_{-\infty}^{\infty} dt G_0^F (k, -t) e^{i\omega t} = -G_0^F (k, -\omega)$$

Chapter 16

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Topics

1. Interacting electron propagator: qualitative picture

2. Spectral function (again) and Landau Fermi liquid

3. Full propagator and Feynman diagrams

Goals

1. Appreciating the qualitative features of the interacting propagator and their relation to Fermi liquids

2. Connecting perturbative expansion to Feynman diagrams

16.1 Spectral function yet again: let's go interacting!

Having evaluated the bare propagator, let us consider the actual one-particle propagator in the interacting problem. It is defined in exactly the same way (suppressing the spin index):

$$G^F(k,t) = -i\langle\Omega|\mathcal{T}\left[\hat{c}_k(t)\,\hat{c}_k^\dagger(0)\right]|\Omega\rangle$$

where we emphasize that the expectation value is taken with respect to the interacting ground state. Note that this is *not* a "contraction": the interacting ground state is not Gaussian in general. Instead, we should think of this propagator as a two-point correlation function (in space-time, and Fourier-transformed).

Before we dwell into the technical calculation (through Gell-Mann-Low, perturbative expansion etc.), it may be good to highlight how interaction modifies

the propagator. To this end we revisit the "spectral decomposition".

$$
\begin{aligned}
& iG^F(k,t) \\
=& \langle\Omega|\mathcal{T}\left[\hat{c}_k(t)\,\hat{c}_k^\dagger(0)\right]|\Omega\rangle \\
=& \Theta(t)\sum_n \langle\Omega|e^{i\hat{H}t}\hat{c}_k e^{-i\hat{H}t}|n\rangle\langle n|\hat{c}_k^\dagger|\Omega\rangle - \Theta(-t)\sum_n \langle\Omega|\hat{c}_k^\dagger|n\rangle\langle n|e^{i\hat{H}t}\hat{c}_k e^{-i\hat{H}t}|\Omega\rangle \\
=& \Theta(t)\sum_n \left|\langle n|\hat{c}_k^\dagger|\Omega\rangle\right|^2 e^{-i(E_n-E_\Omega)t} - \Theta(-t)\sum_n |\langle n|\hat{c}_k|\Omega\rangle|^2\, e^{i(E_n-E_\Omega)t}
\end{aligned}
$$

$$
G^F(k,\omega) = \lim_{\eta\to0^+}\sum_n\left(\frac{\left|\langle n|\hat{c}_k^\dagger|\Omega\rangle\right|^2}{\omega-(E_n-E_\Omega)+i\eta} + \frac{|\langle n|\hat{c}_k|\Omega\rangle|^2}{\omega+(E_n-E_\Omega)-i\eta}\right)
$$

Let us simplify the expression by making a few definitions.

1. if $\langle n|\hat{c}_k^\dagger|\Omega\rangle \neq 0$,
$$
\begin{cases}
M_n(k) = \langle n|\hat{c}_k^\dagger|\Omega\rangle \\
\varepsilon_n = E_n - E_\Omega > 0 \\
\eta_n = \eta \to 0^+
\end{cases}
$$

2. else if $\langle n|\hat{c}_k|\Omega\rangle \neq 0$,
$$
\begin{cases}
M_n(k) = \langle n|\hat{c}_k|\Omega\rangle \\
\varepsilon_n = -(E_n - E_\Omega) < 0 \\
\eta_n = -\eta \to 0^-
\end{cases}
$$

3. else,
$$
M_n(k) = 0
$$

$$
\Rightarrow \quad G^F(k,\omega) = \lim_{\eta_n\to0^\pm}\sum_n \frac{|M_n(k)|^2}{\omega-\varepsilon_n+i\eta_n}
$$

We might connect to physical observables by looking at the spectral function. However, the propagator, being the a T-ordered two-point function, is not an observable directly. Instead, we could look at its retarded version, the trick, as usual, is to shift the poles to the lower complex plane. Consider

$$
G^F(k,\omega+i\delta) = \lim_{\eta_n\to0^\pm}\sum_n \frac{|M_n(k)|^2}{\omega-\varepsilon_n+i(\delta+\eta_n)}
$$

and we take the limit in which δ overrides η_n such that all the poles are now in the lower complex plane. We may now consider the spectral function again by

looking at the imaginary part

$$A(k,\omega) = -\frac{1}{\pi}\Im\left[\lim_{\delta\to 0^+} G^F(k,\omega+i\delta)\right]$$
$$= \sum_n |M_n(k)|^2\,\delta(\omega-\varepsilon_n)$$

(Note: Coleman 5.3.3 considers shifting the poles to the upper complex plane instead, and so a sign difference from the above.)

Importantly, the spectral function enjoys a "normalization":

$$\int_{-\infty}^{\infty} d\omega\, A(k,\omega) = \sum_n |M_n(k)|^2$$
$$= \sum_n \left(\left|\langle n|\hat{c}_k^\dagger|\Omega\rangle\right|^2 + |\langle n|\hat{c}_k|\Omega\rangle|^2 + 0\right)$$

one term per n, among these three possibilities

$$= \sum_n \left(\langle\Omega|\hat{c}_k|n\rangle\langle n|\hat{c}_k^\dagger|\Omega\rangle + \langle\Omega|\hat{c}_k^\dagger|n\rangle\langle n|\hat{c}_k|\Omega\rangle\right)$$
$$= \langle\Omega|\hat{c}_k\hat{c}_k^\dagger + \hat{c}_k^\dagger\hat{c}_k|\Omega\rangle$$
$$= 1$$

Therefore, it is common to talk about the "transfer of spectral weight": the area under the spectral function a conserved quantity, and so it is meaningful to talk about its "transfer".

From the spectral function, we can already picture what should happen when interaction kicks in. Let's start with the non-interacting limit (i.e., the spectral function corresponding to the bare propagator)

$$A_0(k,\omega) = \frac{-1}{\pi}\Im\left[\lim_{\delta\to 0^+} G_0(k,\omega+i\delta)\right]$$
$$= \frac{-1}{\pi}\Im\left[\lim_{\delta\to 0^+}\frac{1}{\omega-\varepsilon_k+i\delta}\right]$$
$$= \delta(\omega-\varepsilon_k)$$

In particular, the delta function has weight 1, as all the "area under the curve" has been hidden under the delta function. From the spectral decomposition itself, we see that this happens because there is exactly one eigenstate of $\hat{H}_0$ which is reached by one electron addition / removal with the right momentum.

One may wonder what happens beyond the simple single-band picture. Generally speaking, even in the non-interacting limit one can get a few delta functions, with their respective weight corresponding to the overlap of the "test" electron compared to the eigenbasis. This is essentially the idea of a projected density-of-states in, e.g., DFT calculations.
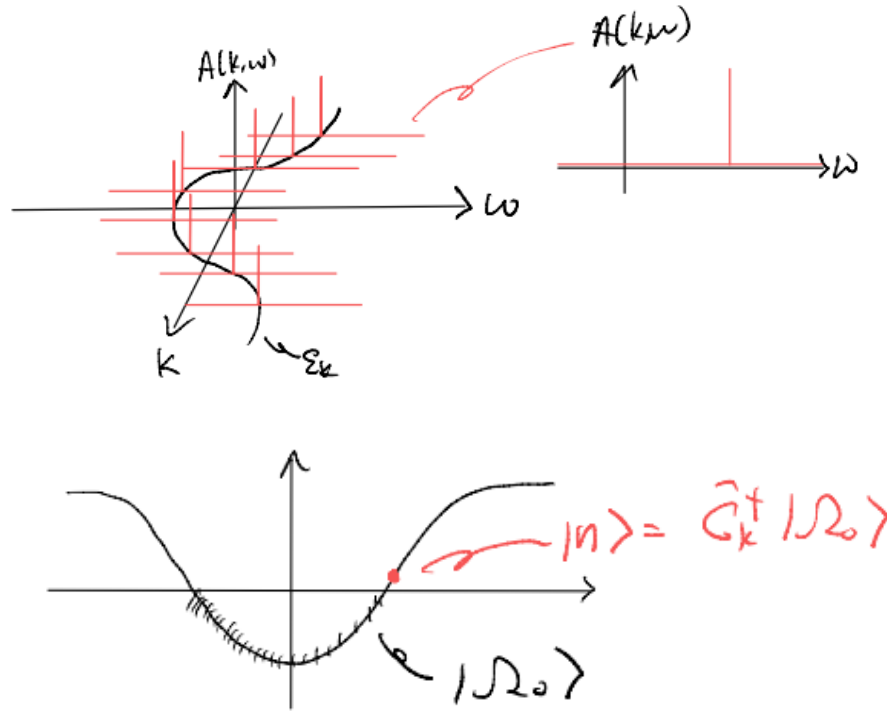
Now, let's ask what happens when we add interaction. As we have seen from the impurity-phonon problem already (beyond the Einstein model), we expect the delta functions to be smeared out into a continuous background:

What is the physical meaning of Γ_k? From the uncertainty principle, we know that ΔE & Δt form a canonical pair. In other words, an infinitely sharp peak (i.e., a delta function), with an infinite precision in energy, corresponds to an infinite lifetime (indeed, that happens when one can construct an eigenstate of the Hamiltonian with exact that energy on top of the ground state). Alternatively, with a finite Γ_k, there is a finite uncertainty in E, and so we also expect a finite uncertainty in Δt. This suggests $\frac{1}{\Gamma_k}$ corresponds to the lifetime of the quasi-particle.

How does interaction lead to a finite lifetime? Imagine creating an excitation on top of the Fermi sea:

In other words, as interaction mixes the states with the same number of electrons (one extra compared to the ground state), the state with "one electron added" becomes superposed with configuration like (1 hole + 2 electrons), (2 holes + 3 electrons) etc.

Now imagine an excitation with an infinitesimal energy compared to the ground state, and so infinitesimally close to the Fermi surface. In our cartoon above, such an excitation has "no where to go" since the particle-hole pair created accompanying its scattering will have to be even closer to the Fermi
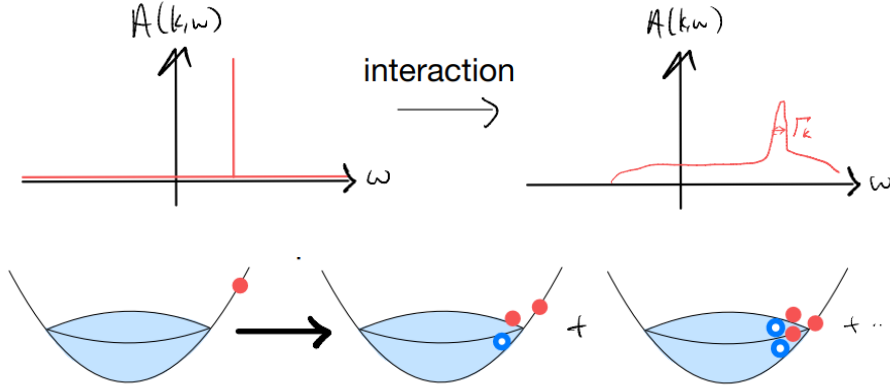
surface.

   Heuristically, one expects the quasi-particle decay to be suppressed for excitations close to the Fermi surface. In 3D, the lifetime is given by

$$\tau_k \sim \frac{1}{\Gamma_k} \sim \frac{1}{\varepsilon_k^2}$$

where ε_k is the excitation energy. (A more accurate description requires a phase-space analysis, and in fact our hand-waving arguments fails in 1D.)

   This observation implies that, in fact, our picture for the spectral function is qualitatively different when we consider momenta lying on the Fermi surface: in that case, we recover a delta function on top of a broad background:
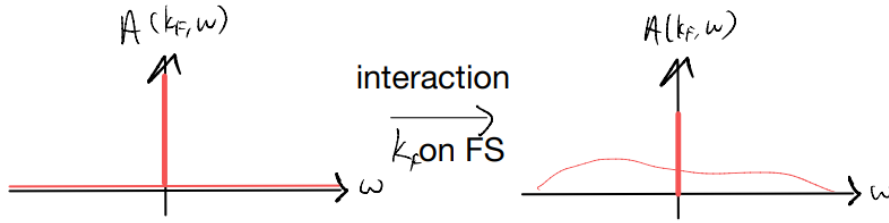
   Furthermore, by our "spectral weight conservation" argument, the area under the broad "incoherent" background consumes the weight of the delta function. This is usually denoted by the quasi-particle weight

$$\begin{cases} A(k_F, \omega) = Z_k \delta(\omega - \varepsilon_k) + A_{int} \\ Z_k \leq 1 \end{cases}$$

Physically, such a delta function manifests as a jump when the quantity is integrated. As it turns out, this quantity is simply the electron occupation

number (momentum distribution function). Consider

$$n_k = \langle\Omega|\hat{c}_k^\dagger\hat{c}_k|\Omega\rangle = \sum_n |\langle n|\hat{c}_k|\Omega\rangle|^2 = \sum_n |M_n(k)|^2$$

for the "1 hole" states. Comparing with the spectral function

$$A(k,\omega) = \sum_n |M_n(k)|^2 \, \delta a(\omega - \varepsilon_n)$$

where ε_n is positive (negative) for "1 electron (1 hole)" states

$$\Rightarrow \quad n_k = \int_{-\infty}^0 d\omega A(k,\omega)$$
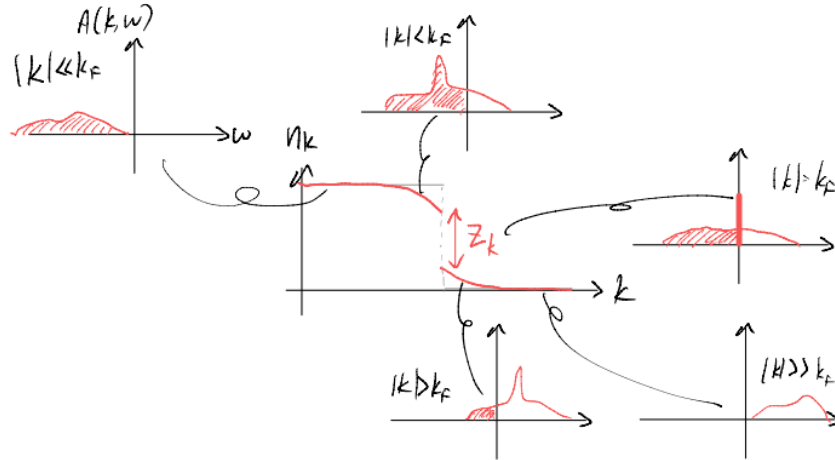
Such jump indicates the presence of infinitely long-lived electron-like quasi particle on the Fermi surface. This is the hallmark of a Landau Fermi liquid.

16.2   Interacting propagator: attempting a perturbative expansion

Having explored the qualitative features of the propagator, let us attempt to evaluate it. Recall

$$G_{\sigma\sigma}^F(k,t) = (-i)\langle\Omega|\mathcal{T}\left[\hat{c}_{k\sigma}(t)\,\hat{c}_{k\sigma}^\dagger(0)\right]|\Omega\rangle_H$$

$$= (-i)\frac{\langle\Omega_0|\mathcal{T}\left[\hat{c}_{k\sigma}(t)\,\hat{c}_{k\sigma}^\dagger(0)\,\hat{S}(\infty,-\infty)\right]|\Omega_0\rangle_I}{\langle\Omega_0|\hat{S}(\infty,-\infty)|\Omega_0\rangle_I}$$

where the interaction-picture operator evolution is determined by that of the unperturbed, non-interacting problem $\hat{H}_0$ (and so it is solvable). The interaction is all "hidden" in the S-matrix

$$\hat{S}\left(\infty, -\infty\right) = \mathcal{T}\left[\exp\left(-i\int_{-\infty}^{\infty} dt'\hat{V}_I\left(t'\right)\right)\right]$$

Assuming translation invariance, consider interaction of the form (c.f. PS4)

$$\hat{V} = \frac{1}{2}\sum_{pp'q}V\left(q\right)\sum_{\sigma\sigma'}\hat{c}_{p+q,\sigma}^{\dagger}\hat{c}_{p'-q,\sigma'}^{\dagger}\hat{c}_{p',\sigma'}\hat{c}_{p,\sigma}$$

here, q has the interpretation of a momentum transfer. Note also that, since the term is normal-ordered, it vanishes automatically if $p = p\prime$ or $2q = p\prime - p$.

Let us now attempt to expand the numerator directly in a power series of V (through the Dyson's series for the S-matrix):

0th:

$$\left(-i\right)\langle\Omega_0|\mathcal{T}\left[\hat{c}_{k\sigma}\left(t\right)\hat{c}_{k\sigma}^{\dagger}\left(0\right)\right]|\Omega_0\rangle = G_0^F\left(k, t\right)$$

1st:

$$\frac{\left(-i\right)^2}{2}\sum_{pp'q}V\left(q\right)\sum_{\mu\mu'}\int_{-\infty}^{\infty}dt_1\langle\Omega_0|\mathcal{T}\left[\hat{c}_{k\sigma}\left(t\right)\hat{c}_{k\sigma}^{\dagger}\left(0\right)\hat{c}_{p+q,\mu}^{\dagger}\left(t_1\right)\hat{c}_{p'-q,\mu'}^{\dagger}\left(t_1\right)\hat{c}_{p',\mu'}\left(t_1\right)\hat{c}_{p,\mu}\left(t_1\right)\right]|\Omega_0\rangle$$

The core part of the evaluation is the time-ordered expectation value for the product of three fermion creation and three annihilation operators. Since our unperturbed ground state is a Gaussian state, we can use Wick's theorem

$$\langle\cdots\rangle_{\mathcal{T}} \;\mapsto\; \langle\Omega_0|\mathcal{T}\left[\cdots\right]|\Omega_0\rangle$$

$$\left\langle\hat{c}_{k\sigma}\left(t\right)\hat{c}_{k\sigma}^{\dagger}\left(0\right)\hat{c}_{p+q,\mu}^{\dagger}\left(t_1\right)\hat{c}_{p'-q,\mu'}^{\dagger}\left(t_1\right)\hat{c}_{p',\mu'}\left(t_1\right)\hat{c}_{p,\mu}\left(t_1\right)\right\rangle_{\mathcal{T}}$$

$$\sim\left(123\right) - \left(132\right) + \left(312\right) - \left(321\right) + \left(231\right) - \left(213\right)$$

$$= \left\langle\hat{c}_{k\sigma}\left(t\right)\hat{c}_{k\sigma}^{\dagger}\left(0\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{p'-q,\mu'}^{\dagger}\left(t_1\right)\hat{c}_{p',\mu'}\left(t_1\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{p+q,\mu}^{\dagger}\left(t_1\right)\hat{c}_{p,\mu}\left(t_1\right)\right\rangle_{\mathcal{T}}$$

$$-\left\langle\hat{c}_{k\sigma}\left(t\right)\hat{c}_{k\sigma}^{\dagger}\left(0\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{p+q,\mu}^{\dagger}\left(t_1\right)\hat{c}_{p',\mu'}\left(t_1\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{p'-q,\mu'}^{\dagger}\left(t_1\right)\hat{c}_{p,\mu}\left(t_1\right)\right\rangle_{\mathcal{T}}$$

$$+\left\langle\hat{c}_{k\sigma}\left(t\right)\hat{c}_{p+q,\mu}^{\dagger}\left(t_1\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{k\sigma}^{\dagger}\left(0\right)\hat{c}_{p',\mu'}\left(t_1\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{p'-q,\mu'}^{\dagger}\left(t_1\right)\hat{c}_{p,\mu}\left(t_1\right)\right\rangle_{\mathcal{T}}$$

$$-\left\langle\hat{c}_{k\sigma}\left(t\right)\hat{c}_{p+q,\mu}^{\dagger}\left(t_1\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{p'-q,\mu'}^{\dagger}\left(t_1\right)\hat{c}_{p',\mu'}\left(t_1\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{k\sigma}^{\dagger}\left(0\right)\hat{c}_{p,\mu}\left(t_1\right)\right\rangle_{\mathcal{T}}$$

$$+\left\langle\hat{c}_{k\sigma}\left(t\right)\hat{c}_{p'-q,\mu'}^{\dagger}\left(t_1\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{p+q,\mu}^{\dagger}\left(t_1\right)\hat{c}_{p',\mu'}\left(t_1\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{k\sigma}^{\dagger}\left(0\right)\hat{c}_{p,\mu}\left(t_1\right)\right\rangle_{\mathcal{T}}$$

$$-\left\langle\hat{c}_{k\sigma}\left(t\right)\hat{c}_{p'-q,\mu'}^{\dagger}\left(t_1\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{k\sigma}^{\dagger}\left(0\right)\hat{c}_{p',\mu'}\left(t_1\right)\right\rangle_{\mathcal{T}}\left\langle\hat{c}_{p+q,\mu}^{\dagger}\left(t_1\right)\hat{c}_{p,\mu}\left(t_1\right)\right\rangle_{\mathcal{T}}$$

Imagine writing down all these without copy-and-pasting! Certainly it calls for a more paper-saving representation. If you still remember, performing the "full contraction" is closely related to problem of "matching" on a graph.

$$\hat{C}_{k\sigma}(t) \qquad\qquad \hat{C}_{P,\mu}(t_i) \qquad\qquad \hat{C}_{p',\mu'}(t_i)$$

$$\hat{C}^{+}_{k,\sigma}(0) \qquad\qquad \hat{C}^{+}_{p+q,\mu}(t_i) \qquad\qquad \hat{C}^{+}_{p'-q,\mu'}(t_i)$$

Along the same line, let us use six vertices to represent the six operators we need to contract

For instance, the first of the six terms above becomes

$$\left\langle \hat{C}_{k\sigma}(t)\, \hat{C}^{+}_{k,\sigma}(0) \right\rangle_{T} \left\langle \hat{C}^{+}_{p'-q,\mu'}(t_i)\hat{C}_{p',\mu}(t_i) \right\rangle_{T} \left\langle \hat{C}^{+}_{p+q,\mu}(t_i)\, \hat{C}_{P,\mu}(t_i) \right\rangle_{T}$$

By the same token, the second term becomes

$$-\left\langle \hat{C}_{k\sigma}(t)\, \hat{C}^{+}_{k,\sigma}(0) \right\rangle_{T} \left\langle \hat{C}^{+}_{p+q,\mu}(t_i)\hat{C}_{p',\mu}(t_i) \right\rangle_{T} \left\langle \hat{C}^{+}_{p'-q,\mu'}(t_i)\, \hat{C}_{P,\mu}(t_i) \right\rangle_{T}$$

The reset follow similarly:

Note that some relative sign changes appear in the diagrams above, Here, essentially one sign change accompanies every crossing off the lines: starting from one crossing-free diagram, every crossing corresponds to an exchange of two fermion positions, which leads to a sign change. Furthermore, recall that

$$+ \langle \hat{C}_{k\sigma}(t) \hat{C}^\dagger_{p+q,\mu}(t_1) \rangle_\eta \langle \hat{C}^\dagger_{k,\sigma}(0) \hat{C}_{p',\mu'}(t_1) \rangle_\tilde{p} \langle \hat{C}^\dagger_{p'-q,\mu'}(t_1) \hat{C}_{p,\mu}(t_1) \rangle_T$$
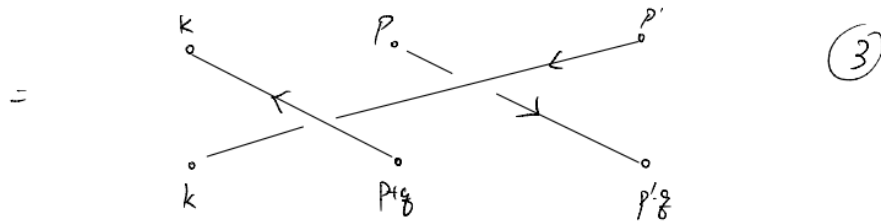
$$- \langle \hat{C}_{k\sigma}(t) \hat{C}^\dagger_{p+q,\mu}(t_1) \rangle_\eta \langle \hat{C}^\dagger_{k,\sigma}(0) \hat{C}_{p,\mu}(t_1) \rangle_\tilde{p} \langle \hat{C}^\dagger_{p'-q,\mu'}(t_1) \hat{C}_{p',\mu'}(t_1) \rangle_T$$
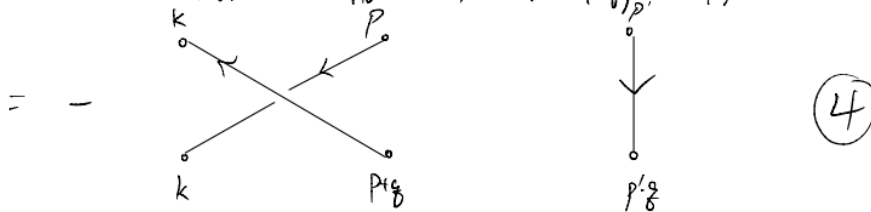
when we reverse the arrow of the propagator, we also acquire sign changes. At this stage it seems quite annoying to keep track of the overall sign. We will later see that, fortunately, there is a simple way to keep track.

$$+ \langle \hat{C}_{k\sigma}(t)\, \hat{C}^{\dagger}_{p'-q,\mu'}(t_1)\rangle_{T} \langle \hat{C}^{\dagger}_{p+q,\mu}(t_1)\, \hat{C}_{p',\mu'}(t_1)\rangle_{T} \langle \hat{C}^{\dagger}_{k,\sigma}(0)\, \hat{C}_{p,\mu}(t_1)\rangle_{T}$$

$=$

$\;$ (5)
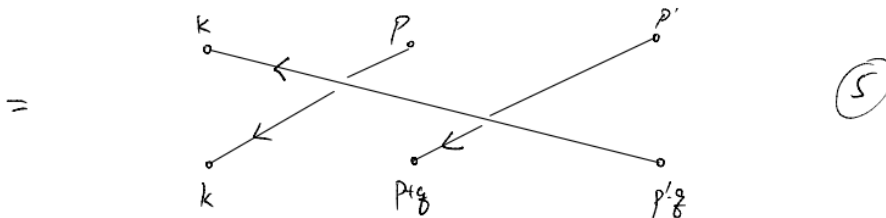
$$- \langle \hat{C}_{k\sigma}(t)\, \hat{C}^{\dagger}_{p'-q,\mu'}(t_1)\rangle_{T} \langle \hat{C}^{\dagger}_{p+q,\mu}(t_1)\, \hat{C}_{p,\mu}(t_1)\rangle_{T} \langle \hat{C}^{\dagger}_{k,\sigma}(0)\, \hat{C}_{p',\mu'}(t_1)\rangle_{T}$$

$=$ $-$
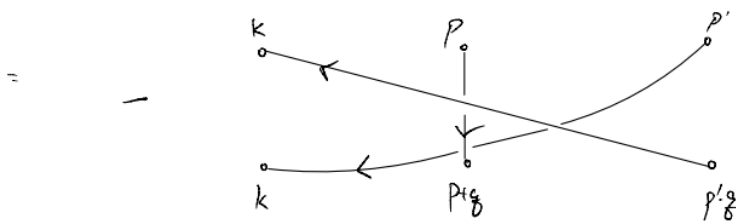
Chapter 17

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Topics

1. Feynman diagrams

2. Linked cluster theorem

Goals

1. Understanding the relation between diagrams and Green's functions

2. Introducing common techniques in diagrammatic

Last time, we discussed how one might use diagrams to organize the (many) contractions one obtains when evaluating a Dyson's series expansion of the full propagator. Recall, to the first order in V, we have six possible contraction patterns, which can be conveniently indicated by "matching" vertices in a pair wise manner.

However, we should not forget that our terms come with "coefficients" and integrals. E.g., focusing

$$
\frac{(-i)^2}{2} \sum_{pp'q} V(q) \sum_{\mu\mu'} \int_{-\infty}^{\infty} dt_1 \left\langle \hat{c}_{k\sigma}(t) \hat{c}_{k\sigma}^\dagger(0) \right\rangle_{\mathcal{T}} \left\langle \hat{c}_{p'-q,\mu'}^\dagger(t_1) \hat{c}_{p',\mu'}(t_1) \right\rangle_{\mathcal{T}} \left\langle \hat{c}_{p+q,\mu}^\dagger(t_1) \hat{c}_{p,\mu}(t_1) \right\rangle_{\mathcal{T}}
$$

$$
= (-i) \left\langle \hat{c}_{k\sigma}(t) \hat{c}_{k\sigma}^\dagger(0) \right\rangle_{\mathcal{T}} \int_{-\infty}^{\infty} dt_1 \sum_q \frac{(-i) V(q)}{2} \sum_{p'\mu'} \left\langle \hat{c}_{p'-q,\mu'}^\dagger(t_1) \hat{c}_{p',\mu'}(t_1) \right\rangle_{\mathcal{T}} \sum_{p\mu} \left\langle \hat{c}_{p+q,\mu}^\dagger(t_1) \hat{c}_{p,\mu}(t_1) \right\rangle_{\mathcal{T}}
$$

$$
= G_{\sigma\sigma}^F(k,t) \int_{-\infty}^{\infty} dt_1 \frac{(-i) V(q=0)}{2} \left(\sum_p \operatorname{Tr}\left((-i) G_0^F(p,0^-) \right) \right)^2
$$
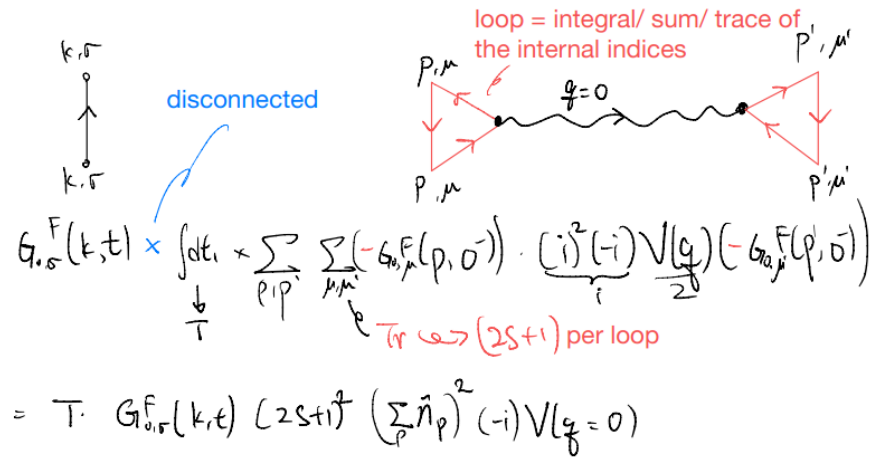
where the internal and summed / integrated over variables are colored in red and external variables in blue. note that

$$
\left\langle \hat{c}_{p+q,\mu}^\dagger(t_1) \hat{c}_{p,\mu}(t_1) \right\rangle_{\mathcal{T}} = -\delta(q) \lim_{t\to 0^-} G_{0\mu}^F(p,t) = \delta(q) \hat{n}_p
$$

and that the integral $\int_{-\infty}^{\infty} dt_1$ has nothing to integrate!

Instead of interpreting that as infinity, which is not very helpful, we can instead "regularize" it by claiming $\int dt_1 = T$, the duration of time in which we turn on the interaction.

Staring at the expression above, we see that the three propagators in the expression actually do rather different things. In particular, one of them is completely external (and has nothing to do with the interaction), whereas the other two effectively "caps" the interaction and gives us some integrals to do. In the same spirit as the diagrams we have drawn above, it will be natural to "complete" the diagram by indicating more clearly which of the propagators are related to the interaction:
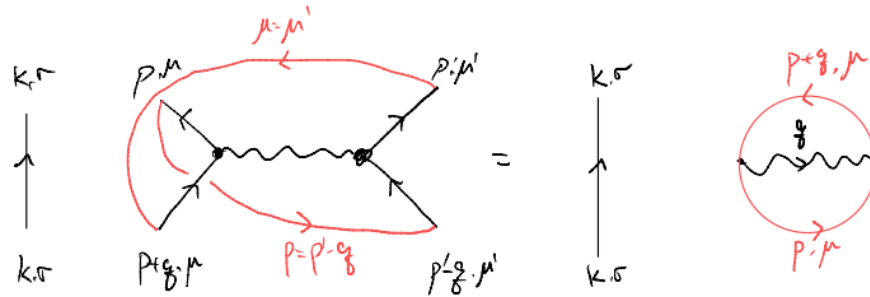
Similarly, we may now draw / write down the second term

notice that we have traded the crossing with a loop, this suggests the sign

is now given by a loop counting (not proven here), and the term is

$$G_{0\sigma}^F (k,t) \times \int dt_1 \sum_{pq} G_{0\mu}^F (p,0^-) \frac{iV(q)}{2} G_{0\mu}^F (p+q,0^-) \times (-2S-1)$$

$$= -(2S+1) T G_{0\sigma}^F (k,t) \sum_{pq} \frac{-iV(q)}{2} n_{p+q} n_p$$

Indeed, let us verify

$$-(-i)^2 \sum_{pp'q} \frac{V(q)}{2} \sum_{\mu\mu'} \int_{-\infty}^{\infty} dt_1 \underbrace{\left\langle \hat{c}_{k\sigma}(t)\, \hat{c}_{k\sigma}^\dagger(0) \right\rangle_{\mathcal{T}}}_{iG_{0\sigma}^F(k,t)} \underbrace{\left\langle \hat{c}_{p+q,\mu}^\dagger(t_1)\, \hat{c}_{p',\mu'}(t_1) \right\rangle_{\mathcal{T}}}_{\delta_{\mu\mu'}\hat{n}_{p+q}\delta(p+q-p')} \underbrace{\left\langle \hat{c}_{p'-q,\mu'}^\dagger(t_1)\, \hat{c}_{p,\mu}(t_1) \right\rangle_{\mathcal{T}}}_{\hat{n}_p}$$

$$= -\sum_{pq} \frac{-iV(q)}{2} T (2S+1) G_{0\sigma}^F (k,t)\, \hat{n}_{p+q} \hat{n}_p$$

Hopefully, the idea is now clear: starting with the operator to be contracted, which we represent diagrammatically as
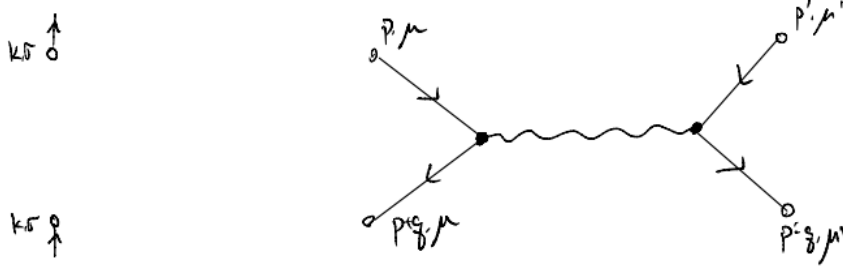
we "connect the dots" in all possible ways, as instructed by the Wick's theorem. All terms here will lead to, schematically, $\sim G \cdot G \cdot V \cdot G$, but the contraction can pair various internal indices and so some parts may get combined. Furthermore, we have to keep track of the sign and multiplicity factors (in our context, one sign change and one factor of $(2S+1)$ per fermion loop).

For instance, the rest of our terms become
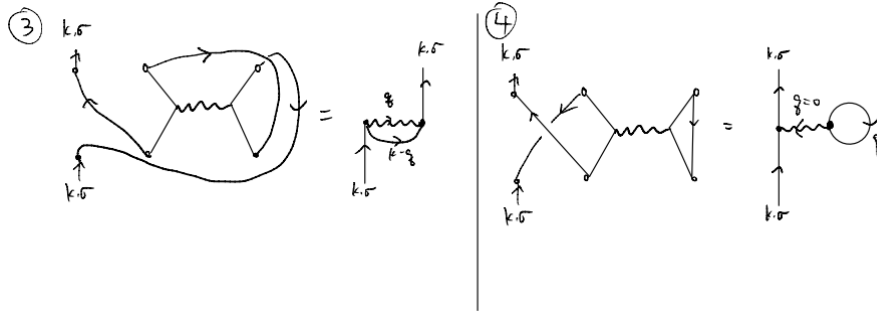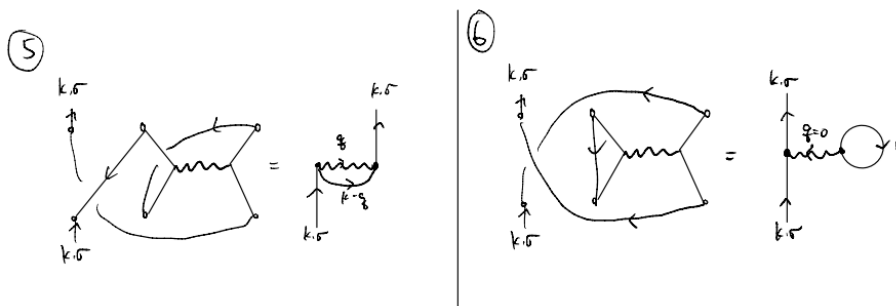
Combined, we see that these four diagrams, correspondingly initially to four distinct contraction patterns, actually give only two distinct terms. One could, and should, check that the prefactors and signs all agree, and as such we may write schematically that

$$(-i)\langle \Omega_0 | T[\hat{C}_{k,\sigma}(t)\, \hat{C}^{+}_{k,\sigma}(0)\, e^{-i\int dt_1\, \hat{V}(t_1)}] | \Omega_0 \rangle$$

Now we may start to guess how the higher order terms look like. For instance, suppose we consider a V^2 term. We will begin by drawing what we ought to connect
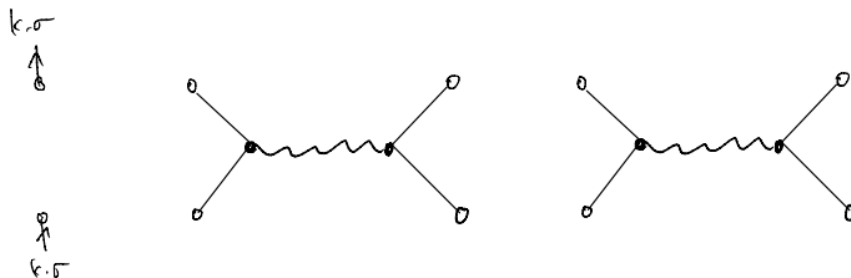
where we leave the internal variables implicit. For our current problem, we have 10 "vertices" (5 for $\hat{c}$ and 5 for $\hat{c}^\dagger$) to connect. For instance, one can have (skipping the directions)
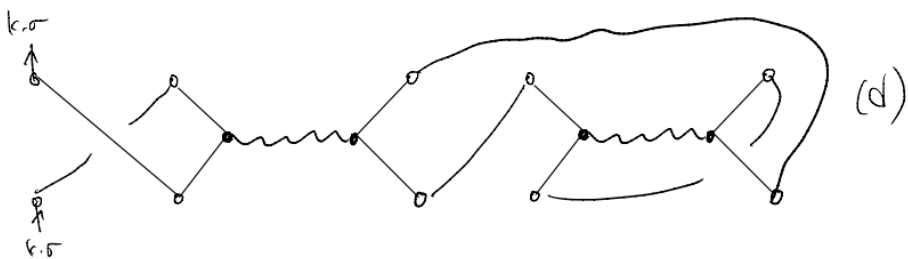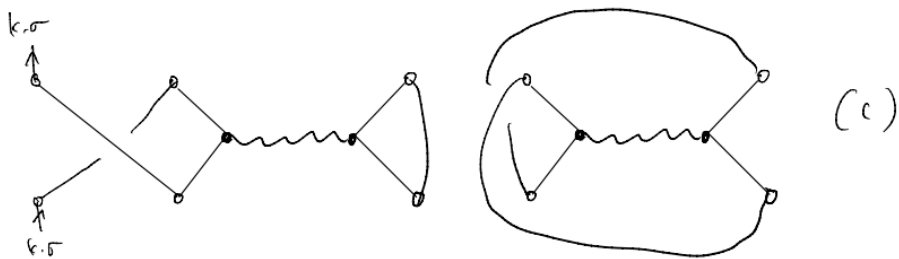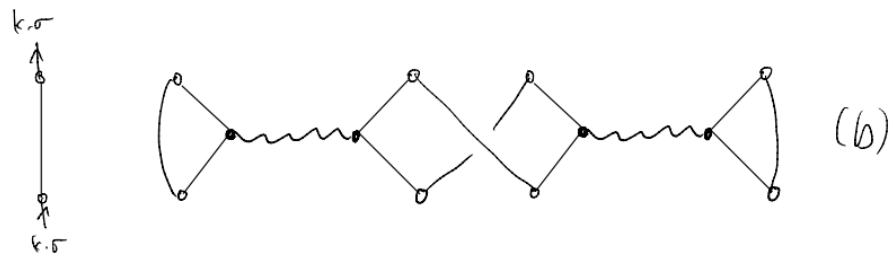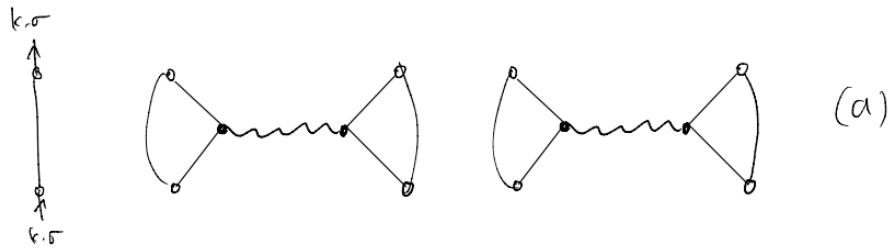
We may clean up the drawings and arrive at a more compact form
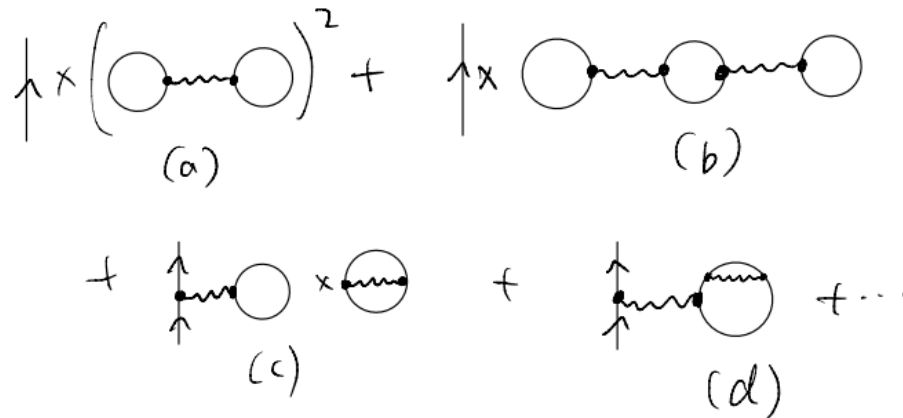
Now, instead of what we have been doing, namely, first consider all the possible contractions, one could as well start directly with the "compact" diagrams and ask the reverse question of what the corresponding contraction is, and how many contractions are there which will give the same diagram. This "reversed" approach is essentially called "Feynman diagrams", and the rules for converting the diagrams back to some integrals (corresponding to an actual term in the perturbative expansion) are called Feynman rules.

17.1   Linked-cluster theorem

In this process, a question naturally arises: how do we organize the diagrams? So far, we have only considered the order-by-order expansion in powers of V. That, however, is not necessarily the best organization principle. Instead, we could notice that,

$$\left\langle T\left[\hat{c}_k(\tau)\hat{c}_k^\dagger(0)\, e^{-i\int dt_1\,\hat{V}(t_1)}\right]\right\rangle_T$$

In other words, in our brute-force expansion, many of the diagrams actually consist of disconnected pieces. Out of these disconnected pieces, exactly one depends on the external variables. The rest are all "(linked) loops" and so whatever variables they carry are dummy and eventually integrated / summed over. As such, we see that it is natural to factor out the "linked-cluster" terms,

which get multiplied to all possible ways of forming "disconnected clusters of loops" which do not depend on our external variables.

What are these "purely internal" diagrams? Remember, form Gell-Mann-Low, we see that the full propagator takes the form of

$$\langle\Omega|\mathcal{T}\left[\hat{c}_k\left(t\right)\hat{c}_k^\dagger\left(0\right)\right]|\Omega\rangle = \frac{\langle\Omega_0|\mathcal{T}\left[\hat{c}_k\left(t\right)\hat{c}_k^\dagger\left(0\right)\exp\left(-i\int_{-\infty}^\infty dt\hat{V}_I\left(t\right)\right)\right]|\Omega_0\rangle}{\langle\Omega_0|\mathcal{T}\left[\exp\left(-i\int_{-\infty}^\infty dt\hat{V}_I\left(t\right)\right)\right]|\Omega_0\rangle}$$

So far, we only focused on the numerator. Let us imagine performing the same kind of perturbative expansion for the denominator.

Diagrammatically, we see that we necessarily get what we have factored out above! This is almost a consequence of tautology: in the numerator, we factor out everything that is "purely internal", and the denominator is, indeed, "purely internal". On top of that, they follow the same set of contraction / diagram-drawing rules, and so they must look the same.

The only question, therefore, is whether or not all the details like signs and coefficients will exactly agree with each other. The answer is a reassuring yes, and we conclude

the linked clusters!

i.e., although we worried about how to properly count powers of V given the cancellation from the denominator, this can be fixed by simply focusing on the diagrams which do not contain any disconnected pieces! This is called the linked-cluster theorem. Of course we only motivated why the linked-cluster theorem makes sense, and didn't actually prove it. There are usually two approaches to prove it:

1. Show that, indeed, these terms in the numerator and denominator cancel out with all the signs and factors agreeing with each other;

2. Go back to the statistics mechanics correspondence, in which the linked-cluster diagrams emerge naturally upon taking the log (and in the statistics mechanics context this is called the cumulant expansion)

In the interest of time, we will not prove it here (we are not in a position to do so anyway: the heuristic discussion above doesn't contain enough details to really establish the theorem). If you are interested, you can consult Coleman-7.2 for a cool argument along route(2), through introducing the generating functional and a replica trick for $\ln(S)$

Chapter 18

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Topics

1. Frequency space Feynman diagrams

2. Self-energy

3. Jellium Hamiltonian

Goals

1. Getting familiarized with how to translate Feynman diagrams to expressions / integrals in the frequency-momentum space

2. Appreciating how the interaction correction to the propagator can be grouped into one single quantity, the self-energy

18.1   Going to frequency space

So far, we have used a "hybrid" discussion with momentum and real time. We have seen that momentum is conserved at each vertex, e.g.,
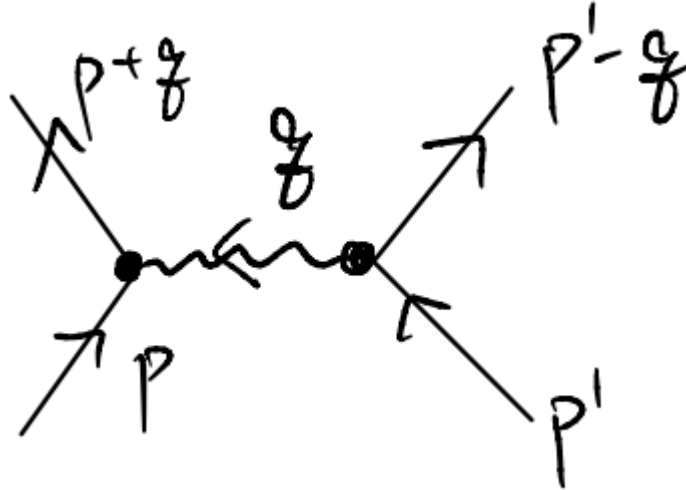
which is a consequence of the translation invariance of the full interacting Hamiltonian.

It will be natural to ask if a similar conservation holds for frequency (energy). We expect the answer to be yes, since we are considering a time-independent Hamiltonian. Let us just go through an example in some details to see how that comes about, which hopefully also helps us build up our technical muscle in translating diagrams into expressions.

Recall, the Fourier transform for the (bare) propagator is

$$G^F(k, \omega) = \int_{-\infty}^{\infty} dt G^F(k, t) e^{i\omega t} e^{-\eta|t|}$$

Consider a slightly more complicated diagram in $G^F(k, \omega)$
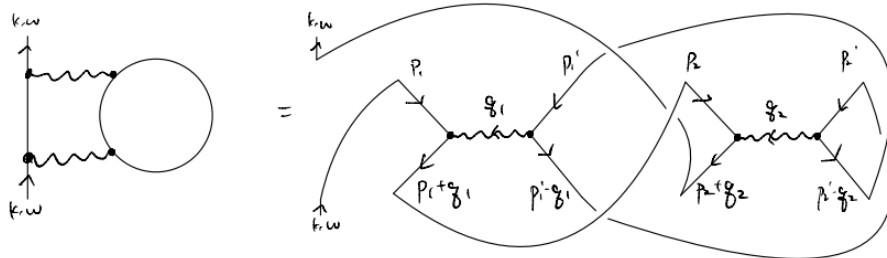
The contraction imposes delta-functions in the momenta, and it will be con-

venient to first consider the effects of that

$$
\begin{cases}
p_1 = k \\
p_2 = p_1 + q_1 \\
p_2 + q_2 = k \\
p_2' - q_2 = p_1' \\
p_1' - q_1 = p_2'
\end{cases}
\qquad \Rightarrow \qquad
\begin{cases}
p_1 = k \\
p_2 = k + q_1 \\
q_2 = -q_1 \\
p_2' = p_1' - q_1
\end{cases}
$$

$$
\Rightarrow \quad \sum_{p_1 p_1' q_1 p_2 p_2' q_2} = \sum_{p_1' q_1}
$$

i.e., there are only two independent internal momenta. In fact, it will be convenient (and more conventional) to label the diagram using these two momenta
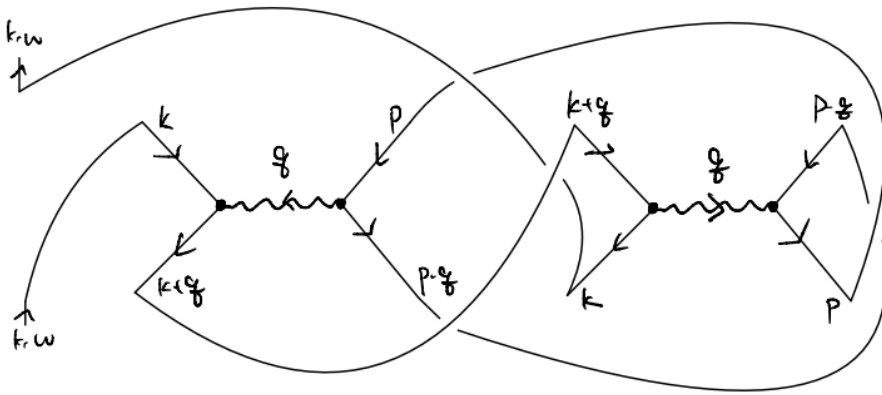
This corresponds to the expression (suppressing spin)

$$
\# \int dt dt_1 dt_2 e^{i\omega t} \sum_{pq} V(q) V(-q)
$$

$$
\times \left\langle \hat{c}_k(t) \hat{c}_k^{\dagger\cdots}(0) \; \hat{c}_{k+q}^{\dagger\cdots}\hat{c}_{p-q}^{\dagger\cdots}\hat{c}_p^{\cdots}\hat{c}_k^{\cdots} \; \hat{c}_k^{\dagger\cdot}\hat{c}_p^{\dagger\cdots}\hat{c}_{p-q}^{\cdots}\hat{c}_{k+q}^{\cdots} \right\rangle_{\mathcal{T}}
$$

$$
=\# \int dt dt_1 dt_2 e^{i\omega t} \sum_{pq} V(q) V(-q)
$$

$$
\times \left\langle \hat{c}_k(t) \hat{c}_k^{\dagger} \right\rangle_{\mathcal{T}} \left\langle \hat{c}_k^{\dagger}(0) \hat{c}_k \right\rangle_{\mathcal{T}} \left\langle \hat{c}_{k+q}^{\dagger}\hat{c}_{k+q} \right\rangle_{\mathcal{T}} \left\langle \hat{c}_{p-q}^{\dagger}\hat{c}_{p-q} \right\rangle_{\mathcal{T}} \left\langle \hat{c}_p^{\dagger}\hat{c}_p \right\rangle_{\mathcal{T}}
$$

$$
\sim \# \int dt dt_1 dt_2 e^{i\omega t} \sum_{pq} V(q) V(-q)
$$

$$
\times G_0^F(k, t-t_2) \left(-G_0^F(k, t_1)\right) \left(-G_0^F(k+q, t_2-t_1)\right) \left(-G_0^F(p-q, t_2-t_1)\right) G_0^F(p, t_1-t_2)
$$

$$
\Downarrow G_0^F(k, t) = \int \frac{d\omega}{2\pi} G_0^F(k, \omega) e^{-i\omega t}
$$

$$
=\# \int dt dt_1 dt_2 \sum_{pq} e^{i\omega t} e^{-i\omega_1(t-t_2)} e^{-i\omega_2 t_1} e^{-i\omega_3(t_2-t_1)} e^{-i\omega_4(t_2-t_1)} e^{-i\omega_5(t_1-t_2)}
$$

$$
\times V(q) V(-q) G_0^F(k, \omega_1) G_0^F(k, \omega_2) G_0^F(k+q, \omega_3) G_0^F(p-q, \omega_4) G_0^F(p, \omega_5)
$$

Let's focus on the phases

$$
\int dt dt_1 dt_2 e^{i(\omega-\omega_1)t} e^{i(-\omega_2+\omega_3+\omega_4-\omega_5)t_1} e^{i(\omega_1-\omega_3-\omega_4+\omega_5)t_2}
$$

$$
\Rightarrow \begin{cases} \omega_1 = \omega \\ \omega_2 = \omega_3 + \omega_4 - \omega_5 \\ \omega_5 = \omega_3 + \omega_4 - \omega_1 \end{cases} \qquad \Rightarrow \begin{cases} \omega_1 = \omega \\ \omega_2 = \omega \\ \omega_3 = \omega + \omega_5 - \omega_4 \end{cases}
$$

i.e., there are only two independent internal frequencies, which we may choose to parameterize as

$$
\# \int \frac{d\tilde{\omega} d\tilde{\omega}}{'} (2\pi)^2 \sum_{pq} V(q) V(-q)
$$

$$
V(q) V(-q) G_0^F(k, \omega) G_0^F(k, \omega) G_0^F(k+q, \omega+\tilde{\omega}) G_0^F(p-q, \tilde{\omega}') G_0^F(p, \tilde{\omega}+\tilde{\omega}')
$$

Of course, it would have been much easier to label the frequency in the original diagram, simply by imposing a "frequency (i.e., energy) conservation at every vertex":
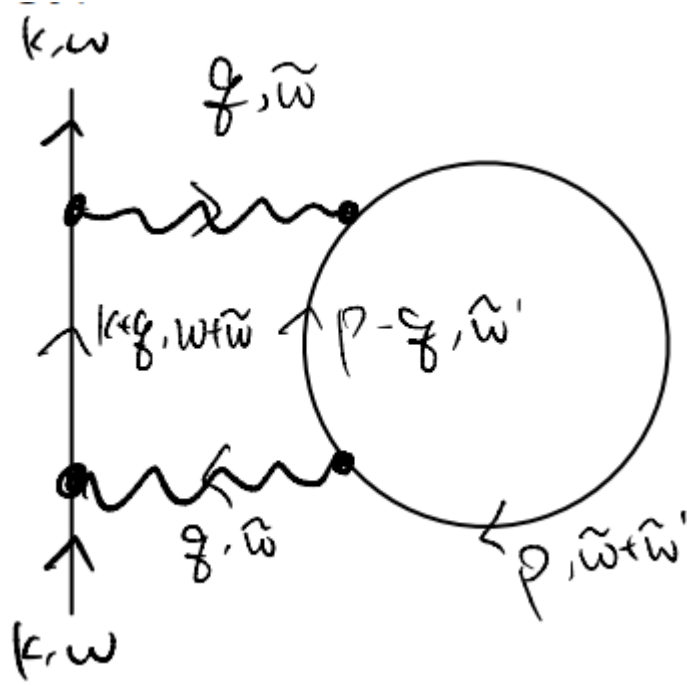
(Note: the wavy lines do not actually depend on the frequency we attached to them, since we considered instantaneous interactions)

Now it should be clearer how to translate the diagram into an expression: we first label all the lines with momentum and frequencies (i.e., 4-momentum in the relativistic case), with the understanding that any internal variables are integrated / summed over. Then each fermion line corresponds to a bare fermion propagator $G_0^F(k, \omega)$, whereas each wavy line corresponds to an interaction term $V(q)$.

The remaining question, important for actual calculations, concerns the prefactor which we did not keep track of (deliberately). It is affected by
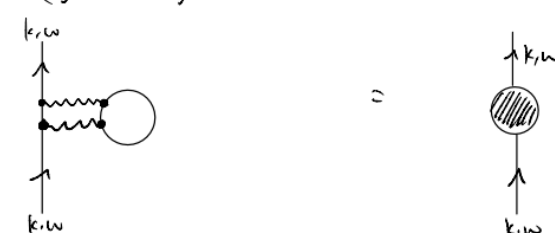
1. factors of $-i$: this can be absorbed into the "dictionary"

2. fermionic sign and spin degeneracy: each fermion loop contributes a factor of $-(2S+1)$

3. "symmetry factor": generally speaking, different contraction patterns can lead to the same diagram up to relabeling, and this cancels (partly) the combinatorial factors appearing in the expansion of the exponential. However, high-symmetry diagrams generally appear a fewer number of times than a "generic" diagram, since some "relabelings" collide. This gives a symmetry factor for the diagram.

At this stage, almost every field-theory textbook contains a box (or two) called "the Feynman rules". Let us not repeat them here beyond the sketch

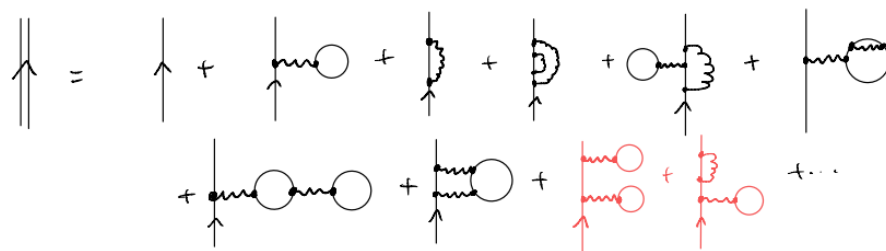above. Instead, see, e.g., Coleman 7.2.

18.2   Dyson's equation and self-energy

Clearly, it was very tedious to keep track of all these factors. It makes sense for us to abstract the expression a bit by writing / drawing

$$G_0^F(k,\omega) \left(\int \cdots \right) G_0^F(k,\omega) = G_0^F(k,\omega) \, \Sigma(k,\omega) \, G_0^F(k,\omega)$$

Furthermore, we have only considered one particular term in the perturbative expansion among the many. One can imagine having arbitrarily complicated diagrams. It will be natural to group all these possibilities into some general blob. That brings us to the notion of Dyson's equation and self-energy.

Our general goal will, again, be ensuring that redundant pieces in the perturbative analysis can be simplified as much as possible. To appreciate how, let us consider expanding the full propagator in terms of the connected diagrams:

We see that the higher-order terms are basically built around the basic first-order terms taking the form

Of course, "built" is a vague word to use here. To be more precise, we see that the last two terms are special, in that they are the only ones (among the ones drawn) for which three out of the five bare propagators are at momentum k. Indeed, let us translate one of them into explicit expressions
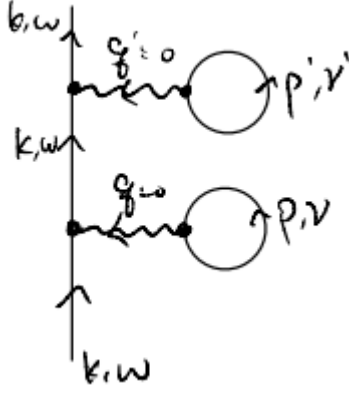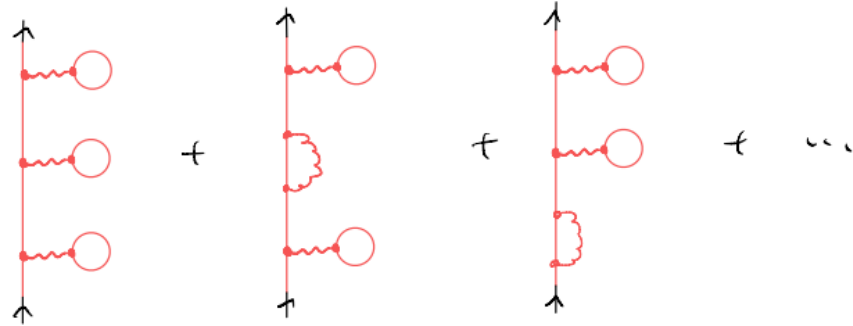

$$G_0^F(k, \omega) \left(V(q = 0) \int \frac{d\nu \, dp}{(2\pi)^{d+1}} \text{Tr}\left(G_0^F(p, 0^-)\right) \right)$$

$$\times G_0^F(k, \omega) \times \left(V(q' = 0) \int \frac{d\nu' \, dp'}{(2\pi)^{d+1}} \text{Tr}\left(G_0^F(p', 0^-)\right) \right) \times G_0^F(k, \omega)$$

$$= G_0^F(k, \omega) \, \blacksquare \, G_0^F(k, \omega) \, \blacksquare \, G_0^F(k, \omega)$$

These kind of terms exist at all orders. E.g., keeping the same form of $G_0^F(k, \omega) \, \blacksquare \, G_0^F(k, \omega) \, \blacksquare \, G_0^F(k, \omega)$ but at order V^3:
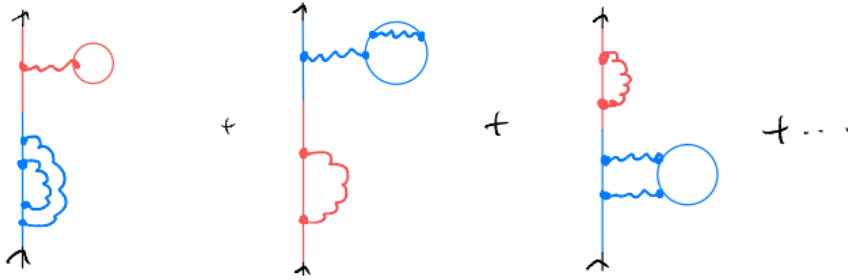
Notice how the blue parts correspond to the "non-simple" terms in our $O(V^2)$ discussion. And, Also at order V^3, we can have terms of the form $G_0^F(k, \omega) \, \blacksquare \, G_0^F(k, \omega) \, \blacksquare \, G_0^F(k, \omega) \, \blacksquare \, G_0^F(k, \omega)$

Hopefully we have grasped the pattern emerging: the expansion of the full propagator in terms of the connected diagrams can be rewritten schematically as
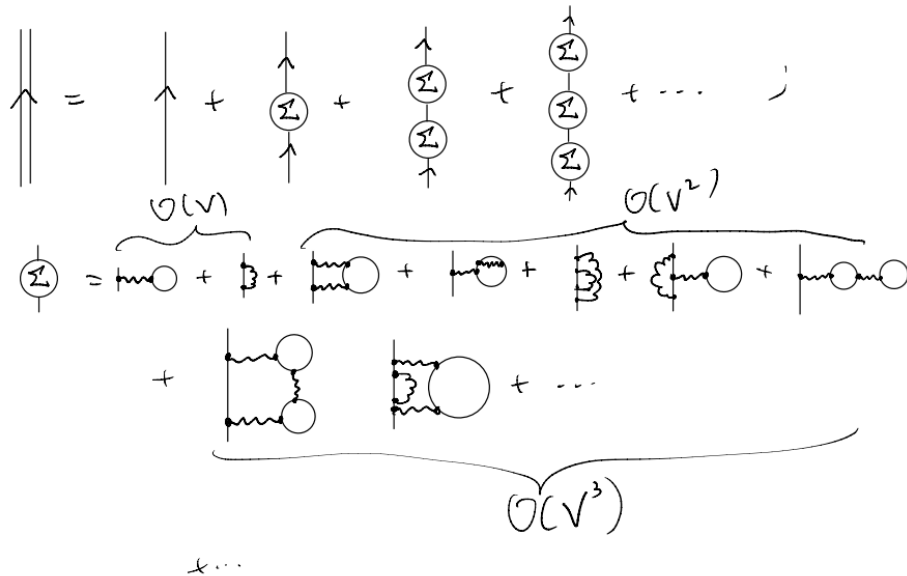

From this, we see that we can further restrict our attention to some special classes of diagrams: instead of considering all connected diagrams, it suffices to consider those diagrams which have the following property: it stays connected even if we cut one "internal" fermion line open. We call them "one-particle irreducible", abbreviated as 1PI.

As promised, we arrive at yet another great simplification of the (formal) analysis by introducing Σ. Translating the diagrams back to equations (suppressing the frequency-momentum dependence)
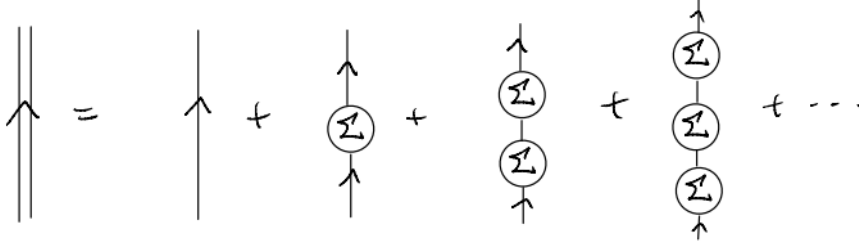
$$G^F = G_0^F + G_0^F \Sigma G_0^F + G_0^F \left(\Sigma G_0^F \right)^2 + G_0^F \left(\Sigma G_0^F \right)^3 + \cdots$$

As written, it is suggestive that we are simply summing over a geometric series. Indeed, using essentially the same old trick, we see that the expansion above can be drawn / written succinctly as
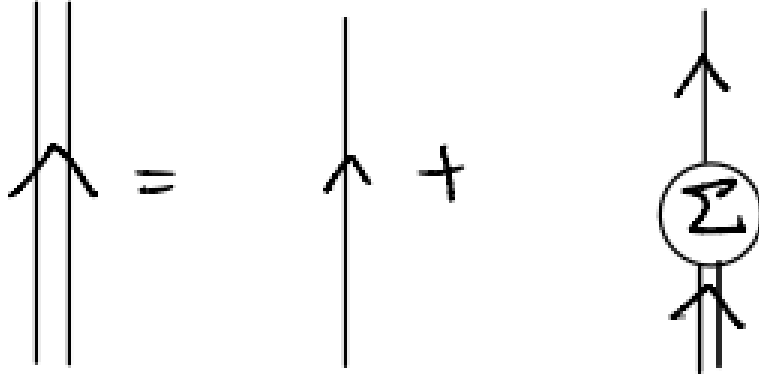
$$G^F = G_0^F + G_0^F \Sigma G^F$$

$$\Rightarrow \quad \left(1 - G_0^F \Sigma \right) G^F = G_0^F$$

$$\Rightarrow \quad G^F(k, \omega) = \frac{1}{1 - G_0^F(k, \omega) \Sigma(k, \omega)} G_0^F(k, \omega)$$

where in the last line, we reinstate the (k, ω) dependence.

To summarize, although we claimed it would be a hard task to compute the "full propagator" in an interacting problem, we can actually condense the entire calculation to that of computing the self-energy $\Sigma(k, \omega)$. Contrast this with the naive approach, in which we expand the numerator and denominator separately, order-by-order!

18.3   Jellium, or, homogeneous electron gas

Having built the machinery needed to tackle interacting quantum many-body problems (perturbatively), let us go back to our motivating example: electrons in free space interacting with each other through Coulomb interaction.

Instead of just having the electrons all by themselves at zero temperature, however, we know that, in practice, almost all "low temperature" systems are electrically neutral. Otherwise, the Coulomb energy diverges as we inter-particle spacing approaches zero. As such, let us instead imagine a homogenous system in which we have a uniform background charge distribution which cancels exactly the charge of the charge of the electron.

The modified interaction is now (passing to a continuum description)

$$\hat{V} = \frac{e^2}{2} \int d^3r d^3r' \frac{: (\hat{\rho}(r) - \rho(0))(\hat{\rho}(r') - \rho(0)) :}{|r - r'|}$$

$$\rho_0 = \langle \hat{\rho}(r) \rangle$$

where the electron density is

$$\hat{\rho}(r) = \sum_\sigma \hat{\Psi}^\dagger_{r\sigma} \hat{\Psi}_{r\sigma}$$

Chapter 19

lec19 20220408

Topics

1. Jellium: positive background charge

2. Hartree-Fock (self-)energy

3. Dielectric function, effective interaction, and RPA

Goals

1. Putting our formalism to use

2. A first taste on physics of interacting electrons

Recall the jellium model Hamiltonian

$$
\hat{H} = \int \frac{d^3 p}{(2\pi)^3} \varepsilon_p \sum_\sigma \hat{\psi}_{p\sigma}^\dagger \hat{\psi}_{p\sigma} + \frac{e^2}{2} \int d^3 r d^3 r' \frac{: (\hat{\rho}(r) - \rho(0))(\hat{\rho}(r') - \rho(0)) :}{|r - r'|}
$$

in which we assumed the presence of a positive, neutralizing background uniform charge of $e\rho_0$ such that the Coulomb energy only depends on the variation of local charge density, and equals to zero when we replace $\langle \hat{\rho}(r) \rangle \to \rho_0$. As the ground state is uniform (or, at least, we assume that is the case), it will be interesting to ask the following: is there an interaction energy in the ground state?

To answer this question, it will be helpful to first Fourier transform into the momentum space. Here we define

$$
\hat{\psi}_{r\sigma}^\dagger = \int \frac{d^3 k}{(2\pi)^3} \hat{\psi}_{k\sigma}^\dagger e^{-ikr}
$$

$$
\hat{\psi}_{k\sigma}^\dagger = \int d^3 r \hat{\psi}_{r\sigma}^\dagger e^{ikr}
$$

where we used the "plane-wave" normalization

$$\int d^3r e^{ikr} = (2\pi)^3 \, \delta(k)$$

In momentum space, the density operator reads

$$\hat{\rho}(r) = \int \frac{d^3k d^3p}{(2\pi)^6} \sum_\sigma \hat{\psi}^\dagger_{k\sigma} \hat{\psi}_{p\sigma} e^{-i(k-p)r}$$

and the number of electrons is

$$N_e = \int d^3r \hat{\rho}(r)$$

$$= \int d^3r \frac{d^3k d^3p}{(2\pi)^6} \sum_\sigma \hat{\psi}^\dagger_{k\sigma} \hat{\psi}_{p\sigma} e^{-i(k-p)r}$$

$$= \int \frac{d^3k}{(2\pi)^3} \sum_\sigma \hat{\psi}^\dagger_{k\sigma} \hat{\psi}_{k\sigma}$$

$$\hat{n}_k = \sum_\sigma \hat{\psi}^\dagger_{k\sigma} \hat{\psi}_{k\sigma}$$

The interaction term is now given by

$$\hat{V} = \frac{e^2}{2} \int d^3r d^3r' : (\hat{\rho}(r) - \rho(0)) (\hat{\rho}(r') - \rho(0)) : V(r-r')$$

$$= \frac{e^2}{2} \int d^3r d^3r' : \hat{\rho}(r) \hat{\rho}(r') : V(r-r')^{(1)}$$

$$- e^2 \rho_0 \int d^3r d^3r' \hat{\rho}(r) V(r-r')^{(2)} + \frac{e^2 \rho_0^2}{2} \int d^3r d^3r' V(r-r')^{(3)}$$

Let us look at these three terms one-by-one

$$(1) = \frac{e^2}{2} \int d^3r d^3r' \frac{d^3k d^3p d^3k' d^3p'}{(2\pi)^{12}}$$

$$\times \sum_{\sigma\sigma'} e^{-i(k-p)r} e^{-i(k'-p')r} V(r-r') : \hat{\psi}^\dagger_{k\sigma} \hat{\psi}_{p\sigma} \hat{\psi}^\dagger_{k'\sigma'} \hat{\psi}_{p'\sigma'} :$$

Let $R = r + r'$ and $\delta_r = r - r'$

$$(1) = \frac{e^2}{16} \int d^3R d^3\delta_r \frac{d^3k d^3p d^3k' d^3p'}{(2\pi)^{12}}$$

$$\times \sum_{\sigma\sigma'} e^{-i(k-p+k'-p')R/2} e^{-i(k-p-k'+p')\delta_r/2} V(\delta_r) : \hat{\psi}^\dagger_{k\sigma} \hat{\psi}_{p\sigma} \hat{\psi}^\dagger_{k'\sigma'} \hat{\psi}_{p'\sigma'} :$$

Integrating over the center of mass R gives

$$\int d^3R e^{-i(k-p+k'-p')R/2} = 8(2\pi)^3 \, \delta(k - p + k' - p')$$

$$\Rightarrow \begin{cases} k = p + q \\ k' = p' - q \end{cases}$$

$$V(q) = \int d^3\delta_r V(\delta_r) e^{-iq\delta_r}$$

$$(1) = \frac{e^2}{2} \int \frac{d^3p d^3p' d^3q}{(2\pi)^9} V(q) \sum_{\sigma\sigma'} : \hat{\psi}^\dagger_{p+q,\sigma} \hat{\psi}^\dagger_{p'-q,\sigma'} \hat{\psi}_{p'\sigma'} \hat{\psi}_{p\sigma} :$$

It will be instructive to look at the piece contributed by $q = 0$:

$$\Rightarrow \frac{e^2}{2} \int \frac{d^3p d^3p'}{(2\pi)^6} \frac{V(q=0)}{\mathcal{V}} \sum_{\sigma\sigma'} : \hat{\psi}^\dagger_{p,\sigma} \hat{\psi}_{p\sigma} \hat{\psi}^\dagger_{p',\sigma'} \hat{\psi}_{p'\sigma'} :$$

$$= \frac{e^2}{2} \frac{V(q=0)}{\mathcal{V}} : \left(\int \frac{d^3p}{(2\pi)^3} \hat{n}_p \right)^2 :$$

$$= \frac{e^2}{2} V(q=0) N_e \rho_0$$

$$(2) = -e^2 \rho_0 \int d^3r d^3r' \frac{d^3k d^3p}{(2\pi)^6} \frac{\sum_\sigma \hat{\psi}^\dagger_{k\sigma} \hat{\psi}_{p\sigma} e^{-i(k-p)r}}{|r - r'|}$$

$$= -8e^2 \rho_0 \int d^3R d^3\delta_r \frac{d^3k d^3p}{(2\pi)^6} \frac{\sum_\sigma \hat{\psi}^\dagger_{k\sigma} \hat{\psi}_{p\sigma} e^{-i(k-p)R/2} e^{-i(k-p)\delta_r/2}}{|\delta_r|}$$

$$= -e^2 \rho_0 \int \frac{d^3k}{(2\pi)^3} \sum_\sigma \hat{\psi}^\dagger_{k\sigma} \hat{\psi}_{k\sigma} \int d^3\delta_r V(\delta_r)$$

$$= -e^2 \rho_0 N_e V(q=0)$$

$$(3) = \frac{e^2 \rho_0^2}{2} \int d^3r d^3r' V(r - r')$$

$$= \frac{e^2 \rho_0^2 \mathcal{V}}{2} \int d^3\delta_r V(\delta_r)$$

$$= \frac{e^2 \rho_0 N_e}{2} V(q=0)$$

Combined, we have

$$(2) + (3) = -\frac{e^2 \rho_0 N_e}{2} V(q=0)$$

But this is, as anticipated, exactly the $q = 0$ piece in (2). This gives

$$\hat{V} = \frac{1}{2} \int \frac{d^3p d^3p' d^3q}{(2\pi)^9} V^*(q) \sum_{\sigma\sigma'} : \hat{\psi}^\dagger_{p+q,\sigma} \hat{\psi}^\dagger_{p'-q,\sigma'} \hat{\psi}_{p'\sigma'} \hat{\psi}_{p\sigma} :$$

where, using the Fourier transform of the Coulomb potential, we have

$$V^*(q) = \begin{cases} \frac{4\pi e^2}{q^2}, & \text{if } q \neq 0 \\ 0, & \text{if } q = 0 \end{cases}$$

In other words, the positive background charge precisely cancels the $q = 0$ piece of the Coulomb potential. As we will soon see this is intuitive.

For simplicity, we simply write $V(q)$ instead of $V^*(q)$ in the following, with the understanding that the $q = 0$ piece has been removed.

19.1   Hartree-Fock (self-)energy

As an application of the perturbative theory we discussed, let's look at the self-energy of the electron in the jellium model.

As mentioned, the self-energy consist of all 1PI diagram

Keeping the lowest order contributions, we have only two terms:

$$V(q = 0) \int \frac{d^3p}{(2\pi)^3} G_0^F(p, \tilde{\omega})$$

But we have $V(q = 0) = 0$! In other words, this Hartree term vanishes identically in the jellium model. One way to phrase this is that, the positive background charges contribute a potential term which precisely cancel the Hartree term in the e-e interaction. (c.f. Coleman 7.7.1)

What about the Fock term? We have (restoring vector notation for clarity)

$$= \int \frac{d^3\vec{p}d\tilde{\omega}}{(2\pi)^4} \left(iV\left(\vec{p}-\vec{k}\right) \right) G_0^F\left(\vec{p},\tilde{\omega}\right) e^{i\omega 0^+}$$

$$= \int \frac{d^3\vec{p}d\tilde{\omega}}{(2\pi)^3} \frac{4\pi e^2}{\left(\vec{p}-\vec{k}\right)^2} \int \frac{d\tilde{\omega}}{2\pi} i G_0^F\left(\vec{p},\tilde{\omega}\right) e^{i\omega 0^+}$$

$$\Downarrow i G_0^F\left(\vec{p}, t \to 0^-\right) = \lim_{t\to 0^-} \left\langle \mathcal{T}\left[\hat{c}_{\vec{p}}(t)\, \hat{c}_{\vec{p}}^\dagger(0) \right] \right\rangle_0 = -n_{\vec{p}}$$

$$= -\int \frac{d^3\vec{p}d\tilde{\omega}}{(2\pi)^3} \frac{4\pi e^2}{\left(\vec{p}-\vec{k}\right)^2} n_{\vec{p}}$$

$$= -\frac{4\pi e^2}{(2\pi)^3} \int_0^{k_F} p^2 dp \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \frac{1}{p^2+k^2-2pk\cos\theta}$$

$$\Downarrow u = \cos\theta$$

$$= -\frac{e^2}{\pi} \int_0^{k_F} p^2 dp \int_{-1}^1 \frac{du}{p^2+k^2-2pku}$$

$$= -\frac{e^2}{2\pi k} \int_0^{k_F} dp \left(p \ln \frac{(k+p)^2}{(k-p)^2} \right)$$

$$= -\frac{e^2}{\pi k} \int_0^{k_F} dp \left(p \ln \left| \frac{k+p}{k-p} \right| \right)$$

$$= -\frac{e^2 k_F}{\pi} \left(1 + \frac{k_F^2-k^2}{2kk_F} \ln \left| \frac{k_F+k}{k_F-k} \right| \right)$$

$$\left| \frac{k_F+k}{k_F-k} \right| \geq 1$$

As such, we have $\Sigma^{\mathrm{HF}}(k,\omega) < 0$, due to the Fock / exchange piece!

We might plot the self-energy as a function of k (Plot by Wolfram alpha)
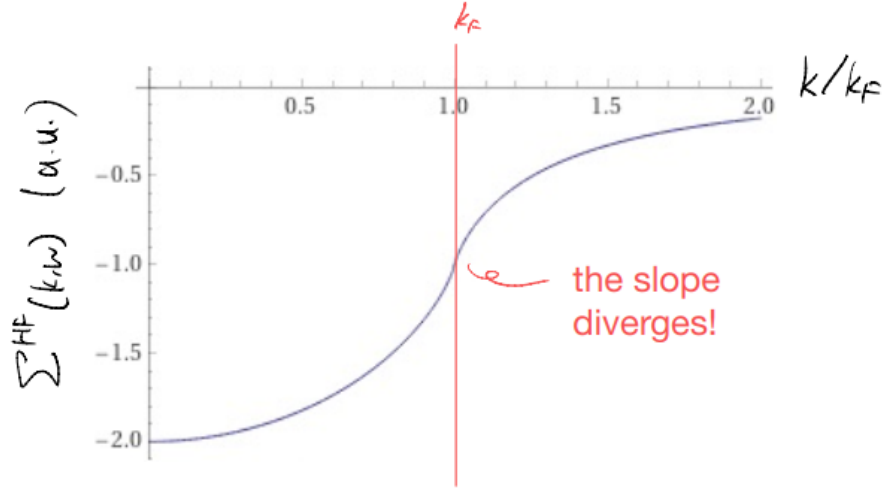
We can also compute the Hartree-Fock ground state energy. Recall, the full propagator is

$$G \simeq \frac{1}{G_0^{-1} - \Sigma_k^{\mathrm{HF}}} = \frac{1}{\omega - \varepsilon_k - \Sigma_k^{\mathrm{HF}} + i\eta}$$

and so we could simply interpret the self-energy as an interaction correction to the dispersion. The ground state energy per particle is

$$E = \frac{2 \cdot 4\pi}{N_e} \int_0^{k_F} \frac{dk}{(2\pi)^3} k^2 \left(\varepsilon_k + \Sigma_k^{\mathrm{HF}}\right)$$

Instead of computing this seriously (doable, just some integrals), let us simply compare the competition between the two terms.

First, the kinetic energy

$$E_{\mathrm{kinetic}} \sim \frac{1}{N_e} \int_0^{k_F} dk \left(\frac{k^4}{2m}\right) \sim \frac{k_F^5}{N_e}$$

The number of electrons equals to the volume inside the Fermi surface, and so

$$N_e \sim k_F^3 \quad \Rightarrow E_{\mathrm{kinetic}} \sim K_F^2$$

In contrast, the exchange energy scales as

$$E_{\mathrm{ex}} \sim -\frac{k_F}{N_e} \int_0^{k_F} k^2 dk \left(1 + \frac{k_F^2 - k^2}{2kk_F} \ln\left|\frac{k_F + k}{k_F - k}\right|\right)$$

$$= -\frac{k_F^4}{N_e} \int_0^1 dy y^2 \left(1 + \frac{1 - y^2}{2y} \ln\left|\frac{1 + y}{1 - y}\right|\right)$$

$$\sim -\frac{k_F^4}{N_e}$$

$$\sim -k_F$$

The inverse of the Fermi wave vector is a length scale characterizing the interparticle spacing (i.e., the density of the electrons), and this is typically parameterized by

$$\frac{4\pi \left(r_s a_0\right)^3}{3}\rho_0 = 1$$

$$\Rightarrow k_F \sim \frac{1}{r_s a_0}$$

where a_0 is the Bohr radius. In other words, r_s is the radius, in terms of the Bohr radius, of a sphere containing one electron. A high density electron gas has a small r_s. This implies the ground state energy of the jellium model is, within the Hartree-Fock approximation

$$E \simeq \frac{\#}{r_s^2} - \frac{\#1}{r_s} + \cdots$$

It turns out that, in the "standard" units, the energy is

$$E \simeq \frac{2.2099}{r_s^2} - \frac{0.9163}{r_s} + \cdots$$

(c.f. Mahan Eq.(5.28)).

An important observation to make is that the kinetic energy dominates for small r_s! I.e., the interaction correction is small for a high-density gas. In contrast, at low density the interaction effects become more important.

19.2   Dielectric function and RPA

After 5 lectures or so we are finally ready to tackle our "humble" motivating question: how do we compute the basic quantities of an interacting electronic system, like the dielectric function? Recall, the key insight is that the system could respond to the external perturbation and screen part of that. Such response leads to an effective dielectric function in the medium (restoring units for highlight)

$$V\left(q\right) = \frac{e^2}{\varepsilon_0 q^2} \to \frac{e^2}{\left(\varepsilon\varepsilon_0\right) q^2}$$

Equivalently, we can also think of the response of the system as modifying the effective interaction between the elctrons. In our perturbative theory, such modification comes from processes like
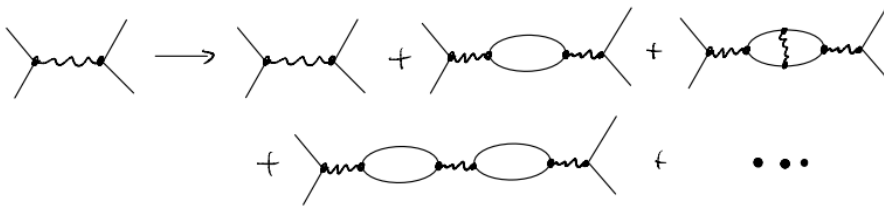
Of course more distinct terms appear as we go to higher orders in the interaction strength. In the same spirit as the 1PI discussion, it makes sense to organize the diagrams as

such terms are called the "polarization bubble". Physically, they represent (virtual) processes in which electron-hole pairs emerge, interact, and then disappear. In fact, our "wavy line" could be recognized as the photon (although we didn't keep their dynamics in the theory), and such diagrams are simply the self-energy for the photon. correspondingly, we also have a Dyson's equation

$$iV_{\text{eff}} = iV + (iV)(i\chi)(iV_{\text{eff}})$$

$$\Rightarrow V_{\text{eff}}(q,\omega) = \frac{V(q)}{1 + V(q)\chi(q,\omega)}$$

As with the earlier discussion on electron self-energy, we see that all the correction to the interaction has been encapsulated in the bubble

In the simplest approximation we simply drop all the higher order terms

this is called the "random phase approximation". Of course, in the way we introduced it, the approximation seems rather ad hoc. The name "RPA" is also quite mysterious. This can be better justified by

1. In the original treatment, the RPA was introduced by looking at the equation of motion and assuming certain terms with non-cancelling momentum average to zero. This is (?) the origin of the name "random phase" (I think??). See Mahan 5.5.2.

2. One can also ask more seriously which terms in the electronic self-energy, at every order of interaction V, diverges most significantly with the Coulomb potential. E.g., compare

   from this analysis, the key divergence comes from terms with the maximal number of interaction depending on one single momentum $q \to 0$. I.e., in the polarization bubble we ignore diagrams with wavy lines featuring internal momentum. This corresponds to the RPA (discussed in a seminal paper by Gell-Mann and Brueckner)

3. From yet another angle, the RPA can also be justified as the exact (mean-field) result in the large-N limit, if we promote the "flavor" symmetry of the electron from $SU(2) \to SU(N)$: recall each fermion loop corresponds to a trace over the spin indices. At the same order of V, diagrams with the maximum number of fermion loops dominate in the large-N limit. This again implies the RPA approximation.

In any case, within the RPA and for the Coulomb potential, we have

$$V_{\text{eff}}(q,\omega) = \frac{V(q)}{1 + V(q)\,\chi_{\text{RPA}}(q,\omega)} = \frac{4\pi e^2}{q^2\left(1 + \frac{4\pi e^2}{q^2}\chi_{\text{RPA}}(q,\omega)\right)}$$

$$\varepsilon_{\text{RPA}} = 1 + \frac{4\pi e^2}{q^2}\chi_{\text{RPA}}(q,\omega)$$

Chapter 20

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Topics

1. Jellium in RPA, Lindhard function

2. Screening

3. Plasmon

 Goals

1. Computing the dielectric function in RPA

2. Appreciating how screening and plasmons in metals arise in our formalism

20.1   RPA: recap

Let us recap what we last considered before the one-week break. We consider the electrons in 3D continuum space interacting with the "neutralized" Coulomb

$$\hat{V} = \frac{1}{2} \int \frac{d^3p \, d^3p' \, d^3q}{(2\pi)^9} V(q) : \hat{\psi}^\dagger_{p+q,\sigma} \hat{\psi}^\dagger_{p'-q,\sigma'} \hat{\psi}_{p'\sigma'} \hat{\psi}_{q\sigma} :$$

$$V(q) = \begin{cases} \frac{4\pi e^2}{q^2}, & \text{if } q \neq 0 \\ 0, & \text{if } q = 0 \end{cases}$$

where $V(q = 0) = 0$ follows from the cancellation from the uniform positive background, and corresponding the Hartree term

We motivated the RPA by asking how we might incorporate screening into our evaluation of the (finite-frequency) dielectric function. This could be understood by considering the Dyson's equation for the "photon"

$$V_{\text{eff}}(q, \omega) = \frac{V(q)}{1 + V(q)\chi(q, \omega)}$$

$$i\chi(q, \omega) = i\chi_{\text{RPA}}(q, \omega) + \cdots$$

Our main task for "performing the RPA" is, therefore, to evaluate

$$i\chi_{\text{RPA}}(q,\omega) = -\int \frac{d\tilde{\omega}}{2\pi} \int \frac{d^3p}{(2\pi)^3} \sum_\sigma G_\sigma(p+q,\tilde{\omega}+\omega) G_\sigma(p,\tilde{\omega})$$

$$= -(2S+1)\int \frac{d\tilde{\omega}d^3p}{(2\pi)^4} \frac{1}{\omega+\tilde{\omega}-\varepsilon_{p+q}+i\eta_{p+q}} \frac{1}{\tilde{\omega}-\varepsilon_p+i\eta_p} e^{i\tilde{\omega}0^+}$$

We could perform the frequency integral by noticing the function contains two poles, and closing the contour in the upper complex plane

In particular, we enclose the poles only if they correspond to "hole" excitations (which live in the upper complex plane), i.e., the pole contribution in proportional to n_k:

$$i\chi_{\text{RPA}}(q,\omega) = -(2S+1)\frac{2\pi i}{2\pi} \int \frac{d^3p}{(2\pi)^3} \left(\frac{n_{\vec{p}}}{\omega+\varepsilon_{\vec{p}}-\varepsilon_{\vec{p}+\vec{q}}} + \frac{n_{\vec{p}+\vec{q}}}{\varepsilon_{\vec{p}+\vec{q}}-\omega-\varepsilon_{\vec{p}}} \right)$$

$$\Rightarrow \chi_{\text{RPA}}(q,\omega) = (2S+1)\int \frac{d^3p}{(2\pi)^3} \frac{n_{\vec{p}}-n_{\vec{p}+\vec{q}}}{\varepsilon_{\vec{p}+\vec{q}}-\varepsilon_{\vec{p}}-\omega}$$

Note that we have, with a sleight of hand, dropped the $i\eta$ factors. More later.

The integral above is called Lindhard function. Its evaluation is very similar to what we have seen for the Fock / exchange self-energy:

$$\chi_{\text{RPA}}(q,\omega) = (2S+1)\int \frac{d^3p}{(2\pi)^3} \left(\frac{n_{\vec{p}}}{\varepsilon_{\vec{p}+\vec{q}}-\varepsilon_{\vec{p}}-\omega} - \frac{n_{\vec{p}}}{\varepsilon_{\vec{p}}-\varepsilon_{\vec{p}-\vec{q}}-\omega} \right)$$

$$= \frac{2S+1}{(2\pi)^3} \int_0^{k_F} dp \int_0^\pi d\theta p^2 \sin\theta \int_0^{2\pi} d\phi$$

$$\times \left(\frac{2m}{q^2+2pq\cos\theta-2m\omega} - \frac{2m}{2pq\cos\theta-q^2-2m\omega} \right)$$

$$\int_0^\pi d\theta \sin\theta \frac{1}{a+b\cos\theta} = \int_{-1}^1 du \frac{1}{a+bu} = \frac{1}{b}\ln\left(\frac{a+bu}{a-bu}\right)$$

$$\chi_{\text{RPA}}(q,\omega) = \frac{2S+1}{4\pi^2} \int_0^{k_F} dp \frac{p^2 m}{pq} \left[\ln\left(\frac{-2m\omega+q^2+2pq}{-2m\omega+q^2-2pq}\right) - \ln\left(\frac{-2m\omega-q^2+2pq}{-2m\omega-q^2-2pq}\right) \right]$$

$$= \frac{(2S+1)mk_F}{4\pi^2\tilde{q}} \int_0^1 d\tilde{p}\tilde{p} \left[\ln\left(\frac{-\tilde{\omega}/\tilde{q}+\tilde{q}+2\tilde{p}}{-\tilde{\omega}/\tilde{q}+\tilde{q}-2\tilde{p}}\right) - \ln\left(\frac{-\tilde{\omega}/\tilde{q}-\tilde{q}+2\tilde{p}}{-\tilde{\omega}/\tilde{q}-\tilde{q}-2\tilde{p}}\right) \right]$$

$$\tilde{p} = \frac{p}{k_F}, \tilde{q} = \frac{q}{k_F}, \tilde{\omega} = \frac{\omega}{k_F^2/2m}$$

$$\int_0^1 dx\, x \ln\left(\frac{a+x}{a-x}\right) = \frac{x^2}{2}\ln\left(\frac{a+x}{a-x}\right)\Big|_0^1 - \int_0^1 \frac{x^2}{2}\frac{2a}{a^2-x^2}dx$$

$$= \frac{1}{2}\ln\left(\frac{a+1}{a-1}\right) + a\int_0^1\left(1 - \frac{a^2}{a^2-x^2}\right)dx$$

$$= \frac{1}{2}\ln\left(\frac{a+1}{a-1}\right) + a - \frac{a^2}{2}\int_0^1\left(\frac{1}{a+x} + \frac{1}{a-x}\right)dx$$

$$= \frac{1}{2}\ln\left(\frac{a+1}{a-1}\right) + a - \frac{a^2}{2}\ln\left(\frac{a+x}{a-x}\right)\Big|_0^1$$

$$= \frac{1}{2}\left(1 - a^2\right)\ln\left(\frac{a+1}{a-1}\right) + a$$

$$\chi_{\text{RPA}}\left(q,\omega\right) = \frac{(2S+1)\,mk_F}{4\pi^2 \tilde{q}}\left(a_+ + \frac{1}{2}\left(1 - a_+^2\right)\ln\left(\frac{a_+ + 1}{a_+ - 1}\right) - (a_+ \leftrightarrow a_-)\right)$$

$$a_\pm = \pm\frac{\tilde{q}}{2} - \frac{\tilde{\omega}}{2\tilde{q}}$$

The prefactor could be simplified further using the 3D density of states (per spin)

$$N_0 = \frac{d}{d\varepsilon_k}\left(\frac{4\pi}{3}\frac{(2m\varepsilon_k)^{3/2}}{(2\pi)^3}\right)\Bigg|_{k=k_F}$$

$$= 2\pi\left(\frac{\sqrt{2m}}{2\pi}\right)^3 \sqrt{\varepsilon_{k_F}}$$

$$= \frac{2mk_F}{4\pi^2};\quad \varepsilon_k = \frac{k^2}{2m}$$

$$\chi_{\text{RPA}}\left(q,\omega\right) = \frac{(2S+1)\,N_0}{2\tilde{q}}\left(\frac{1}{2}\left(1 - a_+^2\right)\ln\left(\frac{a_+ + 1}{a_+ - 1}\right) - (a_+ \leftrightarrow a_-) + \tilde{q}\right)$$
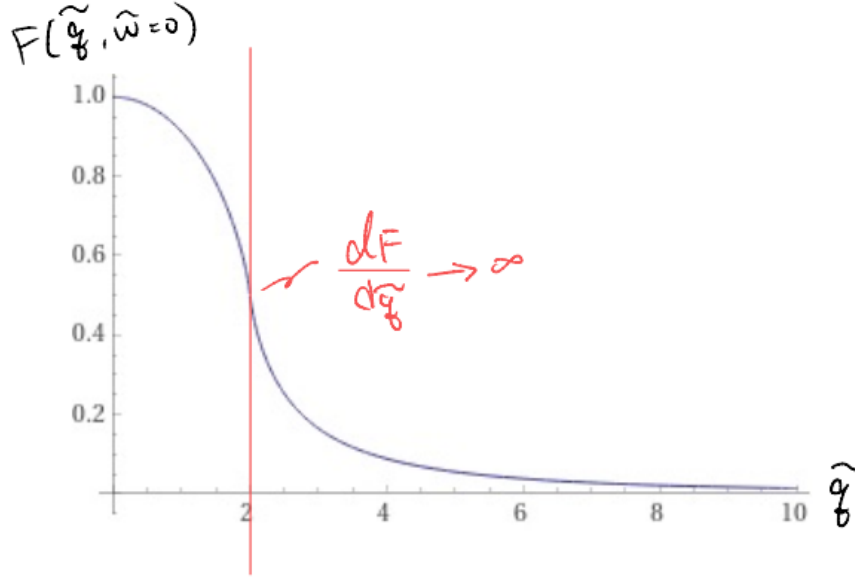
$$= (2S+1)\,N_0 F\left(\tilde{q},\tilde{\omega}\right)$$

$$F\left(\tilde{q},\tilde{\omega}\right) = \frac{1}{4\tilde{q}}\left(1 - a_+^2\right)\ln\left(\frac{a_+ + 1}{a_+ - 1}\right) - (a_+ \leftrightarrow a_-) + \frac{1}{2}$$

The function $F(\tilde{q},\tilde{\omega})$ is known as the Lindhard function. Let us first consider its static limit

$$\lim_{\omega\to 0} a_\pm = \lim_{\omega\to 0}\left(\pm\frac{\tilde{q}}{2} - \frac{\tilde{\omega}}{2\tilde{q}}\right) = \pm\frac{\tilde{q}}{2}$$

$$F\left(\tilde{q}, \tilde{\omega} = 0\right) = \frac{1}{4\tilde{q}}\left(1 - \frac{\tilde{q}^2}{4}\right)\left[\ln\left(\frac{\tilde{q}+2}{\tilde{q}-2}\right) - \ln\left(\frac{-\tilde{q}+2}{-\tilde{q}-2}\right)\right] + \frac{1}{2}$$

$$= \frac{1}{2\tilde{q}}\left(1 - \frac{\tilde{q}^2}{4}\right)\ln\left|\frac{\tilde{q}+2}{\tilde{q}-2}\right| + \frac{1}{2}$$

Notice that, this time, we have a singularity at $\tilde{q} = 2 \Rightarrow q = 2k_F$ when the absolute value inside the log changes sign. We may plot it (the following by Wolfram alpha)

More generally, we obtain the RPA result for the dielectric function

$$V_{\text{eff}}\left(q, \omega\right) = \frac{V\left(q\right)}{1 + V\left(q\right)\chi_{\text{RPA}}\left(q, \omega\right)} = \frac{1}{\varepsilon_{\text{RPA}}\left(q, \omega\right)}V\left(q\right)$$

$$\Rightarrow \varepsilon_{\text{RPA}}\left(q, \omega\right) = 1 + V\left(q\right)\chi_{\text{RPA}}\left(q, \omega\right)$$

$$= 1 + \frac{4\pi e^2}{q^2}\left(2S+1\right)N_0 F\left(\frac{q}{k_F}, \frac{\omega}{k_F^2/2m}\right)$$

20.2 Screening

One interesting observation now is that, in the static limit,

$$\lim_{q\to 0}\varepsilon_{\text{RPA}}\left(q, \omega = 0\right) = \lim_{q\to 0}\left(1 + \frac{4\pi e^2}{q^2}\left(2S+1\right)N_0 F\left(\frac{q}{k_F}, \frac{\omega}{k_F^2/2m}\right)\right) \to +\infty$$

such divergence of the dielectric constant is characteristic of a metal, in which the charges always move to shield the interior from any possible external, static

electric field. The picture may be clearer if we instead consider the effective interaction

$$V_{\text{eff}}(q, \omega = 0) \overset{\text{RPA}}{=} \frac{V(q)}{1 + V(q)(2S+1)N_0 F\left(\frac{q}{k_F}, 0\right)}$$

$$= \frac{4\pi e^2}{q^2 + 4\pi e^2 (2S+1) N_0 F\left(\frac{q}{k_F}, 0\right)}$$

$$\overset{q \to 0}{\approx} \frac{4\pi e^2}{q^2 + k^2}$$

We may Fourier transform back to the real space, which gives (c.f. PS4)

$$V_{\text{eff}}^{\text{static}} \overset{\text{RPA}}{=} \frac{e^2 e^{-kr}}{r}$$

and we could interpret $k^{-1} = \frac{1}{\sqrt{4\pi e^2 (2S+1) N_0}}$ as the length scale characterizing the screening of any stray charges in the metal. This is known as the Thomas-Fermi screening length.

20.3   Plasmon

As a second interesting observation, we consider the other order of the limits, in which we first send $q \to 0$ and keep ω finite. This order of limit might be considered by expanding the integrand directly

$$\chi^{\text{RPA}}(q,\omega) = \frac{(2S+1)N_0}{2\tilde{q}} \int_0^1 d\tilde{p}\,\tilde{p} \left[\ln\left(\frac{-\tilde{\omega}/\tilde{q} + \tilde{q} + 2\tilde{p}}{-\tilde{\omega}/\tilde{q} + \tilde{q} - 2\tilde{p}}\right) - \ln\left(\frac{-\tilde{\omega}/\tilde{q} - \tilde{q} + 2\tilde{p}}{-\tilde{\omega}/\tilde{q} - \tilde{q} - 2\tilde{p}}\right)\right]$$

$$= \frac{(2S+1)N_0}{2\tilde{q}} \int_0^1 d\tilde{p}\,\tilde{p} \ln\left(\frac{(\tilde{\omega}/\tilde{q})^2 - (\tilde{q} + 2\tilde{p})^2}{(\tilde{\omega}/\tilde{q})^2 - (\tilde{q} - 2\tilde{p})^2}\right)$$

$$\Downarrow \omega \neq 0; q \to 0$$

$$= \frac{(2S+1)N_0}{2} \int_0^1 d\tilde{p}\,\tilde{p} \left(-\frac{8\tilde{p}\tilde{q}^2}{\tilde{\omega}^2} + O\left(\tilde{q}^4\right)\right)$$

$$\approx -\frac{4(2S+1)N_0}{3} \frac{\tilde{q}^2}{\tilde{\omega}^2} + O\left(\tilde{q}^4\right)$$

$$= -\frac{4(2S+1)N_0}{3} \frac{q^2}{k_F^2 \omega^2} \frac{k_F^4}{4m^2} + O\left(\tilde{q}^4\right)$$

$$= -\frac{(2S+1)k_F^2}{3m} \frac{mk_F}{2\pi^2} \frac{q^2}{m\omega^2} + O\left(\tilde{q}^4\right)$$

$$= -n_0 \frac{q^2}{m\omega^2} + O\left(\tilde{q}^4\right)$$

$$n_0 = \frac{(2S+1)}{(2\pi)^3} \frac{4}{3}\pi k_F^3$$

where n_0 is the electron density. This gives the dielectric function

$$\lim_{q \to 0} \varepsilon_{\text{RPA}}\left(q, \omega\right) = 1 + \frac{4\pi e^2}{q^2}\left(-n_0 \frac{q^2}{m\omega^2} + O\left(\tilde{q}^4\right)\right) = 1 - \frac{\omega_p^2}{\omega^2}\left(1 + O\left(q^2\right)\right)$$

where

$$\omega_p = \sqrt{\frac{4\pi e^2 n_0}{m}}$$

is the plasma frequency. This characterizes the time it takes for the electrons to respond to an oscillating electric field: while they screen stray charges completely in the static limit, such screening is ineffective when the field is changing at frequencies $\omega > \omega_p$ such that the electron distribution is not able to follow.

To get a more physical sense, let us try to put in some numbers. First we go from the CGS-ESU units to SI:

$$\omega_p = \sqrt{\frac{4\pi e^2 n_0}{m}} \to \sqrt{\frac{e^2 n_0}{\varepsilon_0 m}}$$

As an example, consider sodium

$$\begin{cases} n_0 = 2.65 \times 10^{22} cm^{-3} = 2.65 \times 10^{28} m^{-3} \\ m = 1.06 m_e = 9.656 \times 10^{-31} kg \end{cases}$$

and putting in

$$\begin{cases} e^2/\varepsilon_0 = 0.29 \times 10^{-26} kg m^3 s^{-2} \\ \hbar = 6.58 \times 10^{-16} eV \cdot s^{-1} \end{cases}$$

We find

$$\hbar \omega_p = 5.87 eV$$

In comparison, the visible spectrum is around $\sim 1.6 - 3.3 eV$. This explains why metals are shiny: visible light is not oscillating fast enough to penetrate, and it gets reflected.