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

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

In position basis, the eigenvalues satisfy

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

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

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

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

$$\begin{aligned}\hat{H}\left(\hat{a}^\dagger|E\rangle\right)&=\hbar\omega\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\hat{a}^\dagger|E\rangle\\&=\hbar\omega\left(\hat{a}^\dagger\hat{a}\hat{a}^\dagger+\frac{1}{2}\hat{a}^\dagger\right)|E\rangle\\&=\hbar\omega\left(\hat{a}^{\dagger2}\hat{a}+\hat{a}^\dagger+\frac{1}{2}\hat{a}^\dagger\right)|E\rangle\\&=\hat{a}^\dagger\left(\hat{H}+\hbar\omega\right)|E\rangle\\&=\hat{a}^\dagger\left(E+\hbar\omega\right)|E\rangle\\&=\left(E+\hbar\omega\right)\left(\hat{a}^\dagger|E\rangle\right)\end{aligned}$$

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,

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\phi_0(x)|^2 dx = \mathcal{N}^2 \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar} dx \\ &= \mathcal{N}^2 \sqrt{\frac{\hbar}{2m\omega}} \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar} \exp\left(-\left(\sqrt{\frac{\hbar}{2m\omega}} x \right)^2 /2 \right) d\left(\sqrt{\frac{\hbar}{2m\omega}} x \right) \\ &= \mathcal{N}^2 \sqrt{\frac{\hbar}{2m\omega}} \sqrt{2\pi} \end{aligned}$$

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

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

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,

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

versus

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

we conclude

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

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

We have

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

Normalization:

$$\begin{aligned}1 = \langle\alpha|\alpha\rangle &= |C_0(\alpha)|^2 \sum_{m,n=0} \frac{(\alpha^*)^m\,\alpha^n}{\sqrt{m!}\sqrt{n!}}\langle m|n\rangle \\ &= |C_0(\alpha)|^2 \sum_{m=0}\frac{|\alpha|^{2m}}{m!} \\ &= |C_0(\alpha)|^2\, e^{|\alpha|^2}\end{aligned}$$

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

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

This looks almost like the exponential! Recall

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

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

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

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,

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

Check

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

"Displacement"? compute (also using BCH formula)

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

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

E.g., 1. Average energy

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

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

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

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.

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

Note:

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

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

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

we usually say they form an over-complete basis.

Resolution of identity

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

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

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

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

And we can define the propagator

$$\begin{aligned} K(\beta,\alpha;t) &= \langle\beta|e^{-i\hat{H}t/\hbar}|\alpha\rangle \\ &= e^{-i\omega t/2}\langle\beta|\alpha e^{-i\omega t}\rangle \\ &= e^{-i\omega t/2}e^{-\left(|\alpha|^2+|\beta|^2\right)/2}\exp\left(\alpha e^{-i\omega t}\beta^*\right) \end{aligned}$$

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

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

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

$$\begin{aligned} |\phi\rangle &= \sum_{n=0}|n\rangle\langle n|\phi\rangle = \sum_{n=0}|n\rangle\phi_n \\ e^{-i\hat{H}t/\hbar} &= \sum_{n=0}|n\rangle\langle n|e^{-in\omega t}e^{-i\omega t/2} \\ |\phi(t)\rangle &= \sum_{n=0}|n\rangle\phi_n e^{-in\omega t}e^{-i\omega t/2} \end{aligned}$$

Coherent states

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

$$\begin{aligned}|\phi(t)\rangle &= \int \frac{d^2\alpha d^2\beta}{\pi^2}|\beta\rangle\langle\beta|e^{-i\hat{H}t/\hbar}|\alpha\rangle\phi(\alpha) \\ &= \int \frac{d^2\beta}{\pi}|\beta\rangle \int \frac{d^2\alpha}{\pi}K(\beta,\alpha;t)\,\phi(\alpha) \\ &= \int \frac{d^2\beta}{\pi}|\beta\rangle\phi(\beta;t)\end{aligned}$$

position basis

$$\begin{aligned}K(x',x;t) &= \langle x'|e^{-i\hat{H}t/\hbar}|x\rangle \\ |\phi\rangle &= \int dx|x\rangle\langle x|\phi\rangle = \int dx|x\rangle\phi(x) \\ \phi(x',t) &= \langle x'|t\rangle = \int dx K(x',x;t)\,\phi(x)\end{aligned}$$

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

$$\begin{aligned}\left(i\hbar\partial_t - \hat{H}\right)e^{-i\hat{H}t/\hbar} &= 0 \\ K(x;t) &= \langle x|e^{-i\hat{H}t/\hbar}|0\rangle \\ \left(i\hbar\partial_t - \hat{H}\left(x,\partial_x,\partial_x^2\right)\right)K(x;t) &= 0\end{aligned}$$

Now let's define

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

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

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

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

Note: consider the integral with $a < b$

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

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

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

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

I.e., G solves the differential equation

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\hat{\phi}^\alpha_i D^{\alpha\beta}_{ij} \hat{\phi}^\beta_j &= \hat{\phi}^T \cdot D \cdot \hat{\phi} \\
&= \left(\hat{\phi}^T U^T\right) \cdot \left(U^* D U^\dagger\right) \cdot \left(U\hat{\phi}\right) \\
&= \sum_{\vec{q},\vec{q}'} \hat{\phi}^\alpha_{\vec{q}} D^{\alpha\beta}_{\vec{q}} \delta\left(\vec{q}+\vec{q}'\right) \hat{\phi}^\beta_{\vec{q}'} \\
&= \sum_{\vec{q}} \hat{\phi}^\alpha_{\vec{q}} D^{\alpha\beta}_{\vec{q}} \hat{\phi}^\beta_{-\vec{q}}
\end{aligned}$$

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

So $\hat{\phi}^{\alpha}_{\vec{q}}$ and $\hat{\phi}^{\alpha}_{-\vec{q}}$ 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 $\sim \Delta C^{\dagger}_{\vec{q}} C^{\dagger}_{-\vec{q}}$)

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.

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

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

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

We further diagonalize the block

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

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

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

we should now define the creation and annihilation operators

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

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

As usual, let's check

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

Anticipating the answer, let's compute

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

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

where we have used $\omega^{\alpha}_{\vec{q}} = \omega^{\alpha}_{-\vec{q}}$ as $D^{\alpha\beta}_{\vec{q}} = \left(D^{\alpha\beta}_{-\vec{q}}\right)^*$.

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

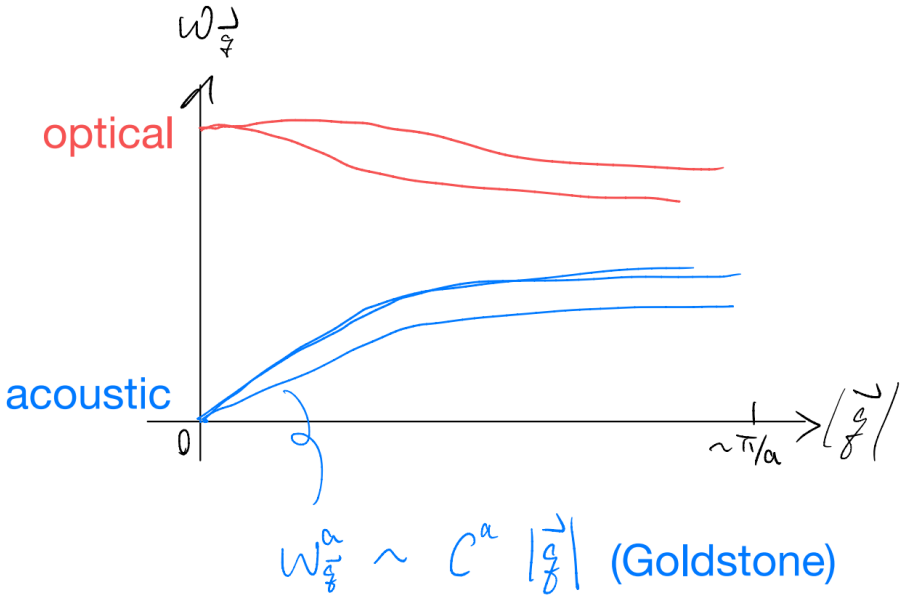
$$\begin{aligned}
\hat{H} &= \frac{1}{2}\sum_{\alpha}\left(\hat{\Pi}^{\alpha 2}_{\vec{0}} + \omega^{\alpha 2}_{\vec{0}}\hat{\Phi}^{\alpha 2}_{\vec{0}}\right) + \sum_{\alpha,\vec{q}:q>0}\left(\hat{\Pi}^{\alpha}_{\vec{q}}\hat{\Pi}^{\alpha}_{-\vec{q}} + \omega^{\alpha 2}_{\vec{q}}\hat{\Phi}^{\alpha}_{\vec{q}}\hat{\Phi}^{\alpha}_{-\vec{q}}\right) \\
&= \frac{1}{2}\sum_{\alpha}\left(\hat{\Pi}^{\alpha 2}_{\vec{0}} + \omega^{\alpha 2}_{\vec{0}}\hat{\Phi}^{\alpha 2}_{\vec{0}}\right) + \sum_{\alpha,\vec{q}:q>0}\omega^{\alpha}_{\vec{q}}\left(\hat{a}^{\alpha\dagger}_{\vec{q}}\hat{a}^{\alpha}_{\vec{q}} + \hat{a}^{\alpha\dagger}_{-\vec{q}}\hat{a}^{\alpha}_{-\vec{q}} + 1\right) \\
&= \frac{1}{2}\sum_{\alpha}\left(\hat{\Pi}^{\alpha 2}_{\vec{0}} + \omega^{\alpha 2}_{\vec{0}}\hat{\Phi}^{\alpha 2}_{\vec{0}}\right) + \sum_{\alpha,\vec{q}:q\neq 0}\omega^{\alpha}_{\vec{q}}\left(\hat{a}^{\alpha\dagger}_{\vec{q}}\hat{a}^{\alpha}_{\vec{q}} + \frac{1}{2}\right)
\end{aligned}$$

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 $D^{\alpha\beta}_{\vec{q}}$ 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".



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

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

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

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

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

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

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

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

$$\begin{aligned}
\mathcal{Z}(\beta) = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) &= \sum_{\left\{n_{\vec{q}}^{\alpha}\right\}} \langle \left\{n_{\vec{q}}^{\alpha}\right\} | e^{-\beta \hat{H}} | \left\{n_{\vec{q}}^{\alpha}\right\} \rangle \\
&= \sum_{\left\{n_{\vec{q}}^{\alpha}\right\}} \exp\left(-\beta \sum_{\vec{q},\alpha} \omega_{\vec{q}}^{\alpha} n_{\vec{q}}^{\alpha}\right) \\
&= \sum_{\left\{n_{\vec{q}}^{\alpha}\right\}} \prod_{\vec{q},\alpha} \exp\left(-\beta \omega_{\vec{q}}^{\alpha} n_{\vec{q}}^{\alpha}\right) \\
&= \prod_{\vec{q},\alpha} \sum_{n_{\vec{q}}^{\alpha}=0}^{\infty} \exp\left(-\beta \omega_{\vec{q}}^{\alpha} n_{\vec{q}}^{\alpha}\right) \\
&= \prod_{\vec{q},\alpha} \frac{1}{1 - \exp\left(-\beta \omega_{\vec{q}}^{\alpha}\right)} \\
\Rightarrow \ln \mathcal{Z}(\beta) &= -\sum_{\vec{q},\alpha} \ln\left(1 - e^{-\beta \omega_{\vec{q}}^{\alpha}}\right)
\end{aligned}$$

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

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

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

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

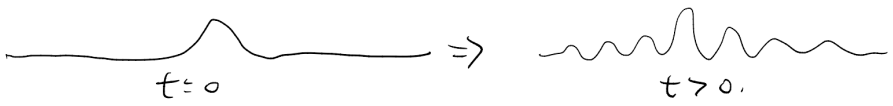
$$\partial_J \ln \mathcal{Z}\left(\beta, J\right) = \frac{\partial_J \mathrm{Tr}\left(e^{-\beta\hat{H}+J\hat{O}}\right)}{Z\left(\beta, J\right)} \stackrel{?}{=} \frac{\mathrm{Tr}\left(\hat{O}e^{-\beta\hat{H}+J\hat{O}}\right)}{Z\left(\beta, J\right)}$$

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

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.

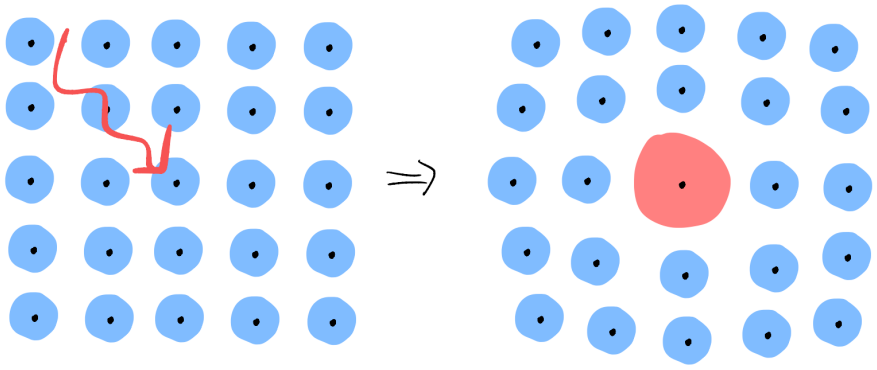
In any case, we have completely solved the free phonon problem, in the sense that for any observables we would want to compute, we have a way of doing so (by rotating to the decoupled QHO basis).

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

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

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 $\hat{b}^\dagger_x$. That's why this is called "second quantization".

3. implicitly, we have defined an object which maps space to quantum operators: $\vec{r} \to \hat{b}^\dagger_x$. Such maps are called "fields". (E.g., think about electric field $\vec{r} \to \vec{E_r}$. 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,

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

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:

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

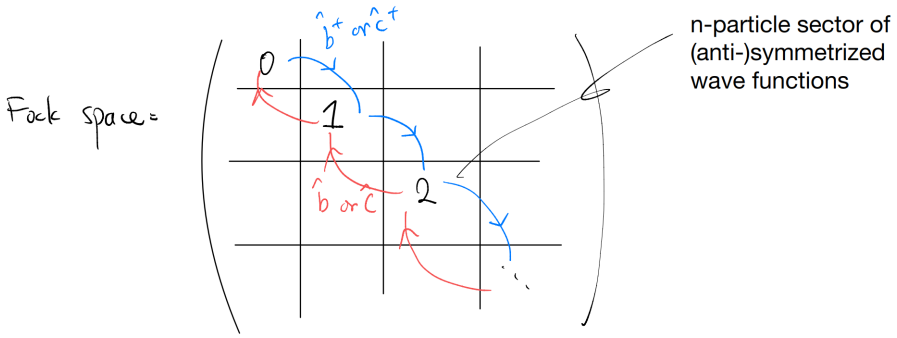
This implies the fermionic creation and annihilation operators should satisfy canonical anti-commutation relations. Let $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$. For fermions

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

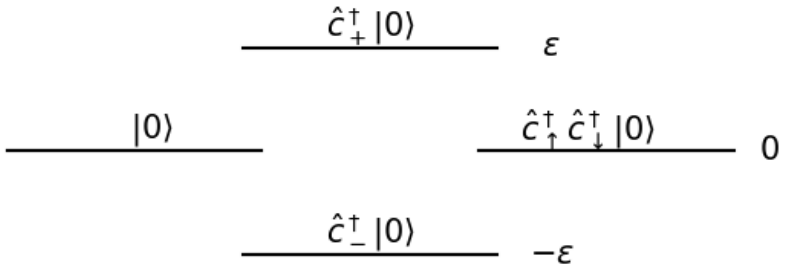
$$\begin{cases} \left\{\hat{c}_{\pm}^{\dagger}, \hat{c}_{\pm}\right\} = \frac{1}{2}\left\{\hat{c}_{\uparrow}^{\dagger} \pm \hat{c}_{\downarrow}^{\dagger}, \hat{c}_{\uparrow} \pm \hat{c}_{\downarrow}\right\} = \frac{1}{2}\left(1 \pm 0 \pm 0 + 1\right) = 1 \\ \left\{\hat{c}_{+}^{\dagger}, \hat{c}_{-}\right\}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

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

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

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

$$\begin{aligned} \hat{H} &= \sum_{i} \left(\sum_{\alpha} \hat{c}_{\alpha}^{\dagger} U_{\alpha i}\right) \varepsilon_i \left(\sum_{\beta} \left(U^{\dagger}\right)_{i\beta} \hat{c}_{\beta}\right) \\ &= \sum_{i} \varepsilon_i \hat{c}_i^{\dagger} \hat{c}_i \quad \text{canonicaltransformation} \end{aligned}$$

(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

$$\begin{aligned} G_{\uparrow\uparrow}(t) &= -i\langle\Omega|e^{i\hat{H}t}\hat{c}_{\uparrow}e^{-i\hat{H}t}\hat{c}_{\uparrow}^{\dagger}|\Omega\rangle \\ &= -i\langle\Omega|\hat{c}_{\uparrow}(t)\,\hat{c}_{\uparrow}^{\dagger}(0)\,|\Omega\rangle \end{aligned}$$

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,

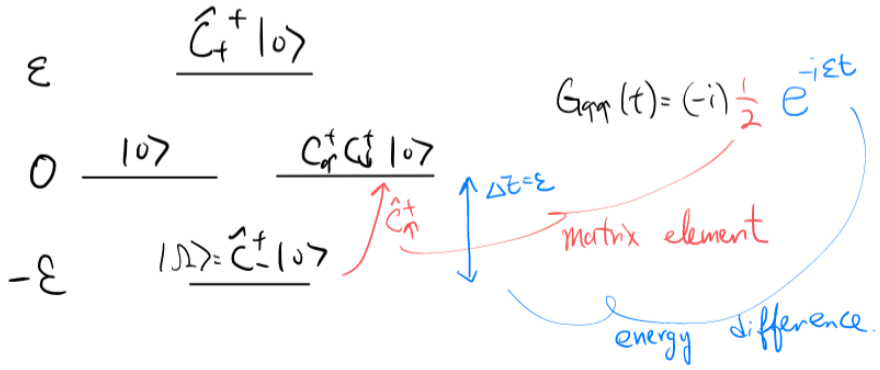
$$\begin{aligned} i\partial_t\left(\hat{c}_{\pm}^{\dagger}(t)\right) &= \left[\hat{c}_{\pm}^{\dagger}(t), \hat{H}\right] \\ &= \hat{U}^{\dagger}\left[\hat{c}_{\pm}^{\dagger}, \pm\varepsilon\hat{c}_{\pm}^{\dagger}\hat{c}_{\pm}\right]\hat{U} \\ &= \hat{U}^{\dagger}\left(\pm\varepsilon\hat{c}_{\pm}^{\dagger}\right)\left[\hat{c}_{\pm}^{\dagger}, \hat{c}_{\pm}\right]\hat{U} \\ &= \hat{U}^{\dagger}\left(\pm\varepsilon\hat{c}_{\pm}^{\dagger}\right)\left(2\hat{c}_{\pm}^{\dagger}\hat{c}_{\pm} - 1\right)\hat{U} \\ &= \mp\varepsilon\hat{c}_{\pm}^{\dagger}(t) \end{aligned}$$

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

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

$$\begin{aligned} G_{\uparrow\uparrow}(t) &= -i\langle\Omega|\hat{c}_{\uparrow}(t)\,\hat{c}_{\uparrow}^{\dagger}(0)\,|\Omega\rangle \\ &= -\frac{i}{2}\langle\Omega|\left(\hat{c}_{+}(t) + \hat{c}_{-}(t)\right)\left(\hat{c}_{+}^{\dagger}(0) + \hat{c}_{-}^{\dagger}(0)\right)|\Omega\rangle \\ &= -\frac{i}{2}\langle 0|\hat{c}_{-}\left(\hat{c}_{+}e^{-i\varepsilon t} + \hat{c}_{-}e^{i\varepsilon t}\right)\left(\hat{c}_{+}^{\dagger} + \hat{c}_{-}^{\dagger}\right)\hat{c}_{-}^{\dagger}|0\rangle \\ &= -\frac{i}{2}\langle 0|\hat{c}_{-}\hat{c}_{+}e^{-i\varepsilon t}\hat{c}_{+}^{\dagger}\hat{c}_{-}^{\dagger}|0\rangle \\ &= -\frac{i}{2}e^{-i\varepsilon t}\langle 0|\left(1 - \hat{c}_{+}^{\dagger}\hat{c}_{+}\right)\left(1 - \hat{c}_{-}^{\dagger}\hat{c}_{-}\right)|0\rangle \\ &= -\frac{i}{2}e^{-i\varepsilon t} \end{aligned}$$

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:

$$\begin{aligned} G_{\alpha\alpha}(t) &= -i\langle\Omega|\hat{c}_\alpha(t)\,\hat{c}_\alpha^\dagger(0)\,|\Omega\rangle_H \\ &= -i\langle\Omega|e^{i\hat{H}t}\hat{c}_\alpha e^{-i\hat{H}t}\hat{c}_\alpha^\dagger|\Omega\rangle_S \end{aligned}$$

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

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

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

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

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

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

$$\begin{aligned} G_{\alpha\alpha}(\omega) &\stackrel{?}{=} \int_{-\infty}^{\infty} dt G_{\alpha\alpha}(t) e^{i\omega t} \\ &= -i \sum_n \int_{-\infty}^{\infty} \left|\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle\right|^2 e^{i(\omega-\Delta E_n)t} \end{aligned}$$

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 $\eta \to 0^+$

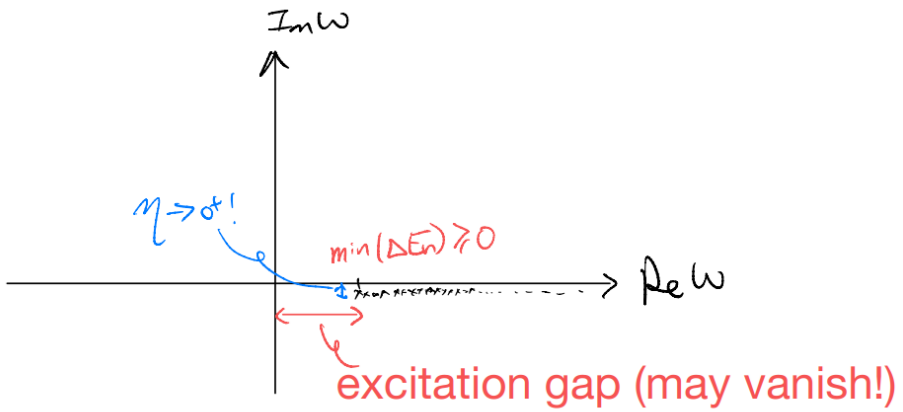
$$\begin{aligned} G_{\alpha\alpha}(\omega) &= \lim_{\eta\to 0^+} (-i) \int_0^{\infty} dt G_{\alpha\alpha}(t) e^{i\omega t} e^{-\eta t} \\ &= \lim_{\eta\to 0^+} (-i) \sum_n \left|\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle\right|^2 \int_0^{\infty} e^{i(\omega-\Delta E_n+i\eta)t} \\ &= \lim_{\eta\to 0^+} \sum_n \frac{(-i)\left|\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle\right|^2}{i(\omega-\Delta E_n+i\eta)} \left(e^{-\eta(+\infty)} - 1\right) \\ &= \lim_{\eta\to 0^+} \sum_n \frac{\left|\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle\right|^2}{\omega-\Delta E_n+i\eta} \end{aligned}$$

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:

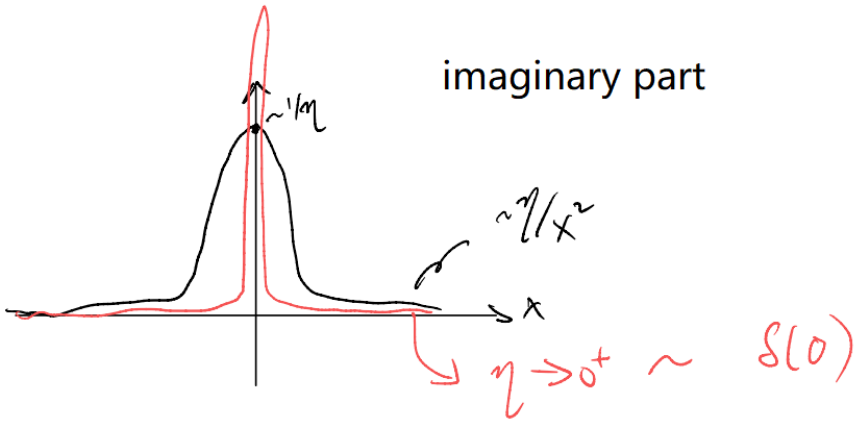
$$A_{\alpha\alpha}(\omega) = \frac{-1}{\pi}\mathrm{Im}\left[G_{\alpha\alpha}(\omega)\right] = \sum_n \left|\langle n|\hat{c}_\alpha^\dagger|\Omega\rangle\right|^2 \delta(\omega-\Delta E_n)$$



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:

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

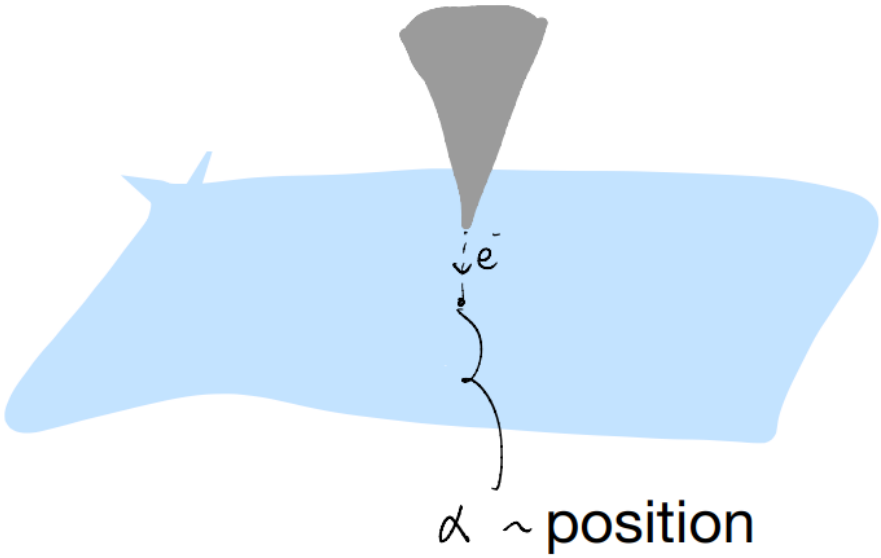
$$\Rightarrow \lim_{\eta\to 0^+} \mathrm{Im}\left[\frac{1}{x+i\eta}\right] = -\pi\delta\left(0\right)$$

This gives

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

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)



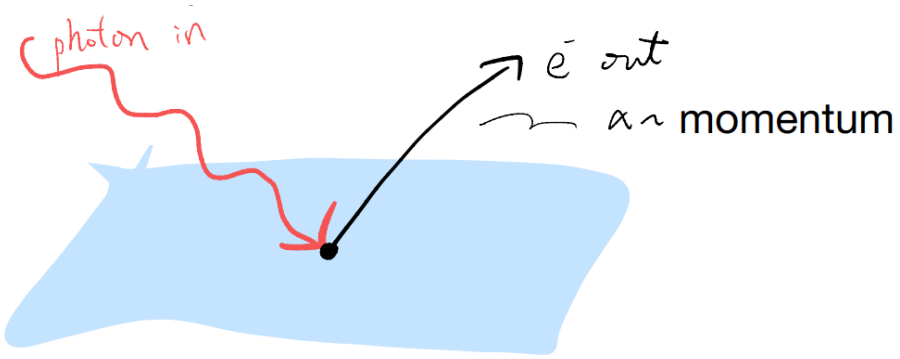
But STM doesn't only try to add electrons! The tip also tries to "pull" electrons out of the sample, i.e., remove electron from the ground state, Similarly for ARPES

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

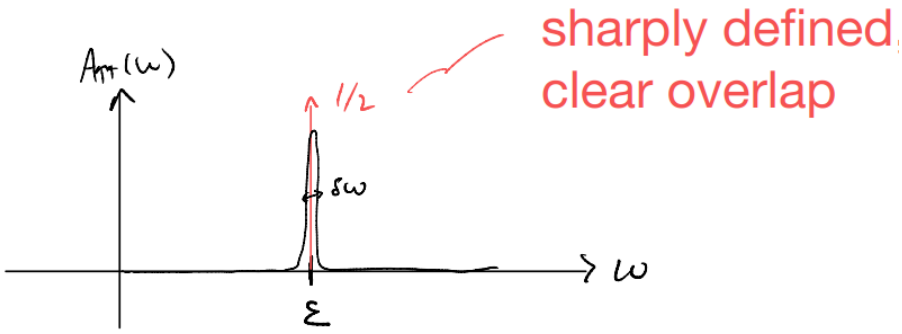
Now, let's imagine plotting this spectral function. First, let us revert to our simple "single-orbital" example

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



$$G_{\uparrow\uparrow}(t) = -i\frac{1}{2}e^{-i\varepsilon t}$$

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

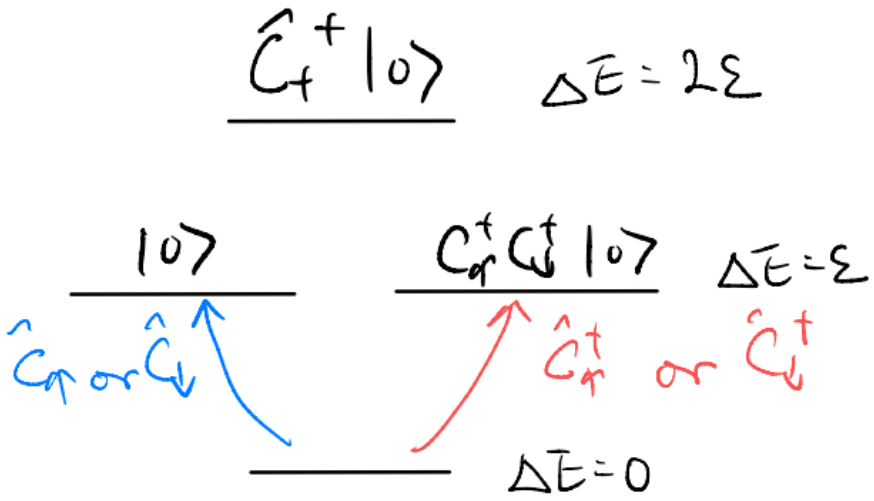


If this was an experimental result, how would we interpret it? There is a sharp "resonance" when we try to add an up electron with energy ε to the ground state. The overlap is $\frac{1}{2}$. Suppose we can do similar experiments and measure $A_{\downarrow\downarrow}(\omega)$, as well as those associated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

we will conclude:

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



(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:

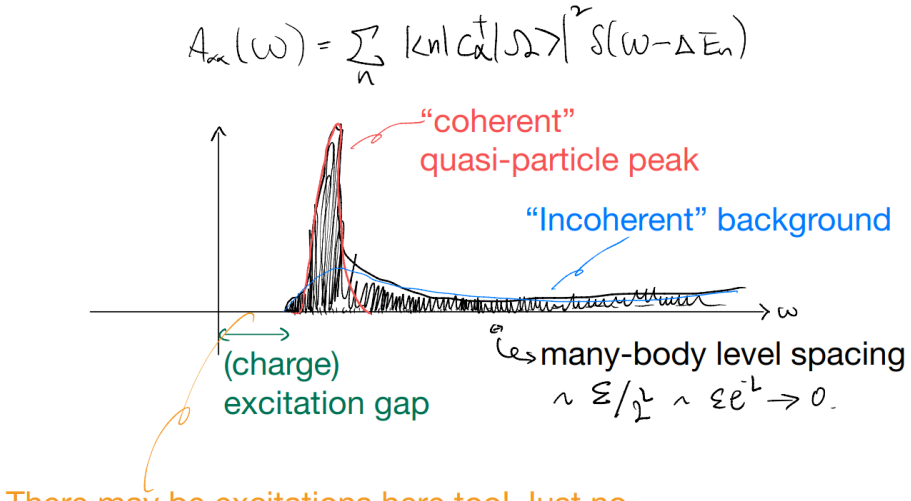
1. We assumed above that we can choose to tunnel spin up versus down electrons independently. This is a kind of "resolution", giving "spin-resolved" spectral function (e.g., spin-polarized STM tips). If we don't have such spin resolution, we can only conclude (a) but not (b). More resolved means more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

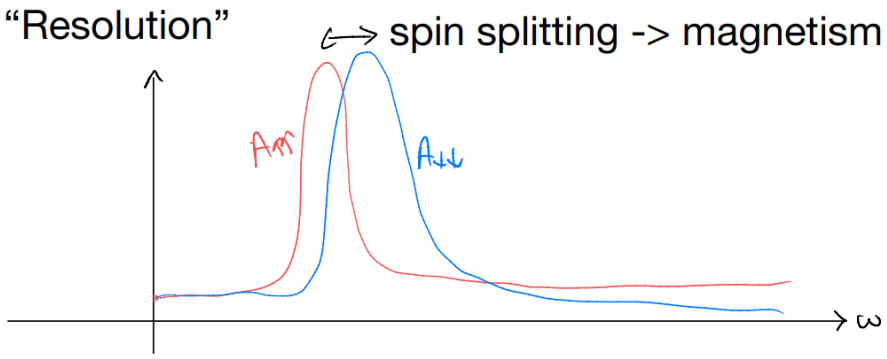
2. For such a "small" system, one can imagine cooking up fancier measurements to "better resolve" the system. That's in the spirit of quantum tomography. We don't usually have the luxury of such measurement capability in many-body quantum systems so we won't go further down there.

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





1. the excitations cannot be understood as quasi-particles

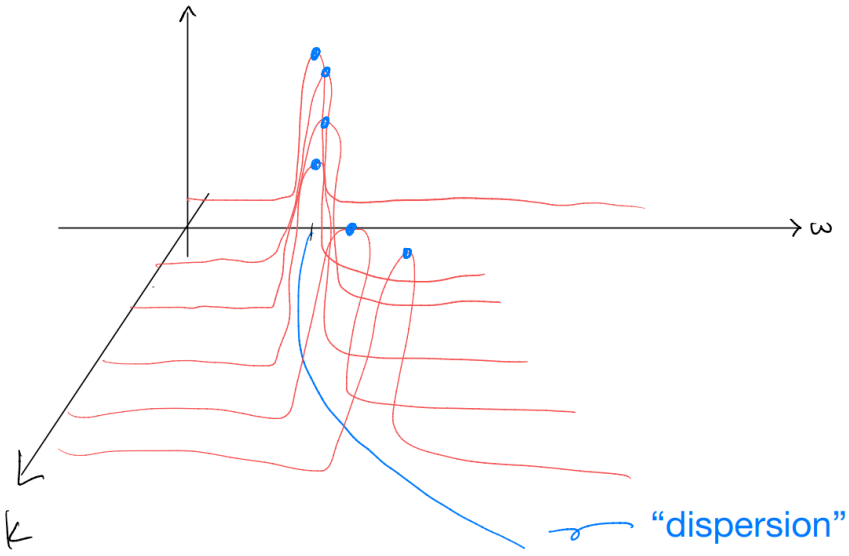
2. quasi-particles exist, but they have poor overlap with the physical electrons

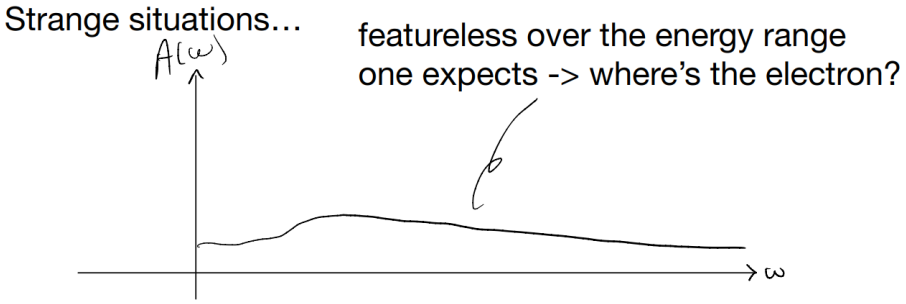
Either will be very interesting! But beyond our scope...

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

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





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.

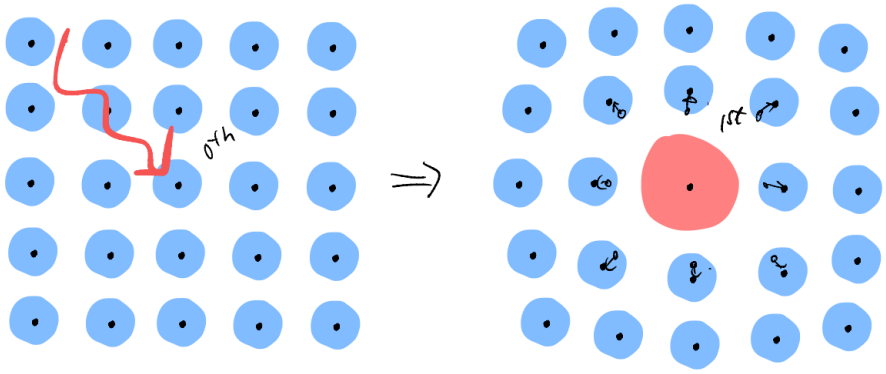
Such generalized Green's functions appear under different considerations, and we may want to give them different names, Nevertheless, they are all variations on the same tune, much like Schubert's trout quintet! More later...

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

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

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

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

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

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

$$\begin{aligned}
\delta\hat{H}^i_{ph} &= \sum_r M^i_r \hat{u}_r \\
&= \sum_r M^i_r \frac{1}{\sqrt{V}} \sum_q e^{-iq\cdot r} \frac{\hat{a}_q + \hat{a}^\dagger_{-q}}{\sqrt{2m\omega_q}} \\
&= \sum_q \underbrace{\frac{1}{\sqrt{2m\omega_q}} \left(\frac{1}{\sqrt{V}} \sum_r M^i_r e^{-iq\cdot r} \right)}_{} \left(\hat{a}_q + \hat{a}^\dagger_{-q} \right) \\
&= \sum_q M^i_q \left(\hat{a}_q + \hat{a}^\dagger_{-q} \right) \\
&= \sum_q \left(M^i_q \hat{a}_q + M^i_{-q} \hat{a}^\dagger_q \right)
\end{aligned}$$

let us further assert that $M^i_r = M^i_{-r}$ such that $M^i_q = M^i_{-q}$

$$\Rightarrow \delta\hat{H}^i_{ph} = \sum_q M^i_q \left(\hat{a}_q + \hat{a}^\dagger_q \right)$$

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

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

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 $\hat{c}^\dagger_i \hat{c}_j \left(\hat{a}_q + \hat{a}^\dagger_q \right) + h.c.$ 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^i_q 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

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

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

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.

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

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

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 $n_i n_j = n_i \delta_{ij}$.

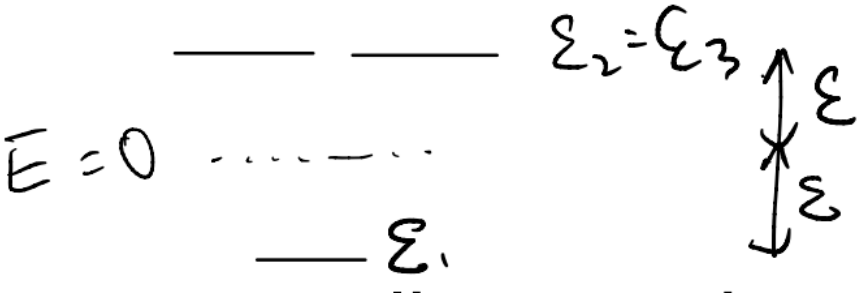
As such, we now know all the eigenstates and energy of our Hamiltonian. They can be labeled by two sets of integers

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

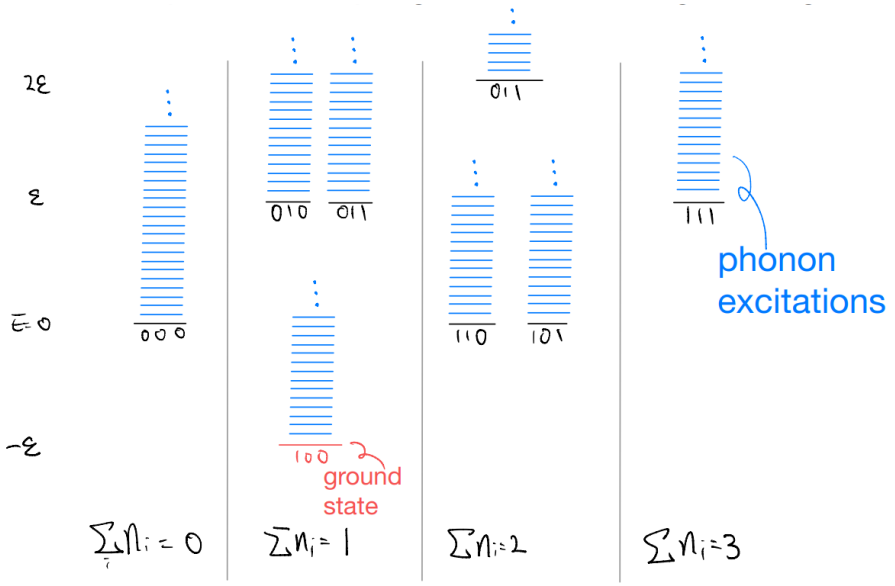
The energy is

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

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



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

$$\begin{aligned}\hat{H} &= \bigoplus_{\{n_i\}} \hat{H}\Big|_{\{n_i\}} \\ &= \bigoplus_{\{n_i\}} \left(\sum_q \hat{D}_q^\dagger \left(\frac{1}{\omega_q} \sum_i n_i M_{iq} \right) \omega_q \hat{a}_q^\dagger \hat{a}_q \hat{D}_q \left(\frac{1}{\omega_q} \sum_i n_i M_{iq} \right) + \Delta\left(\{n_i\}\right) \right)\end{aligned}$$

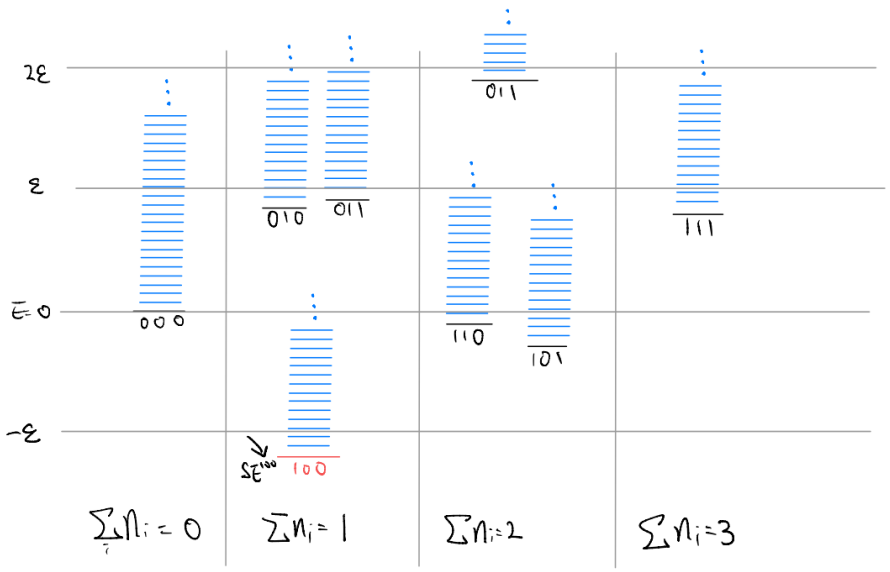
where $\oplus$ is the direct sum over the 2^N independent sectors. It's still the "same" phonon Hamiltonian, but in different basis!

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 "propagator" in the coherent-state basis!

$$\begin{aligned} G_{11}(t) &= (-i)\, e^{i\Delta_{100}t} \prod_q \left(\langle -\frac{M_{1q}}{\omega_q} | \frac{M_{1q}}{\omega_q} e^{-i\omega_q t} \rangle_0 \right) \\ &= (-i)\, e^{i\Delta_{100}t} \prod_q \exp\left(\frac{M_{1q}^2}{\omega_q^2} e^{-i\omega_q t} \right) \exp\left(-\frac{M_{1q}^2}{\omega_q^2} \right) \end{aligned}$$

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

$$\begin{aligned} G_{11}(\omega) &= (-i)\, e^{-g} \lim_{\eta \to 0^+} \int_0^\infty dt e^{i\Delta_{100}t} e^{i\omega t} e^{-\eta t} \exp\left(g e^{-i\omega_E t} \right) \\ &= (-i)\, e^{-g} \sum_{l=0}^\infty \lim_{\eta \to 0^+} \int_0^\infty dt \frac{g^l}{l!} e^{i(\omega + \Delta_{100} - l\omega_E + i\eta)t} \\ &= e^{-g} \sum_{l=0}^\infty \lim_{\eta \to 0^+} \frac{g^l}{l!} \frac{1}{\omega + \Delta_{100} - l\omega_E + i\eta} \end{aligned}$$

and same as before we find the spectral function

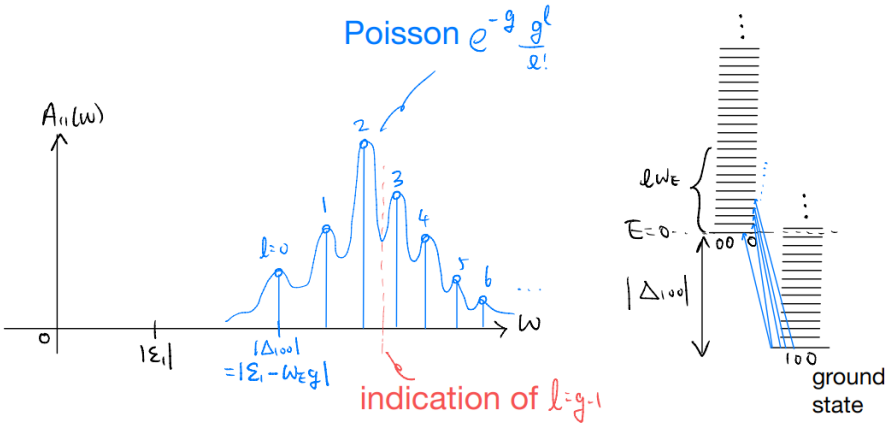
$$\begin{aligned} A_{11}(\omega) &= \frac{-1}{\pi} \mathrm{Im} G_{11}(\omega) \\ &= \sum_{l=0}^\infty e^{-g} \frac{g^l}{l!} \delta\left(\omega - (-\Delta_{100} + l\omega_E) \right) \end{aligned}$$

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

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

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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

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

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

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

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

and so the equation of motion is

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

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 $\hat{c}^\dagger_i(t)$ 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

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

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

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

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

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

$$\begin{aligned}i\partial_t f(t) &= f(0)\left(i\partial_t \exp\left(-i\int_0^t g(t')\,dt'\right)\right) \\ &= f(0)\left(\partial_t \int_0^t g(t')\,dt'\right)\exp\left(-i\int_0^t g(t')\,dt'\right) \\ &= g(t) f(t)\end{aligned}$$

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!

$$\begin{aligned}\hat{c}_i^\dagger &\stackrel{?}{=} \sum_{n=0}^\infty \frac{(-i)^n}{n!}\left[\int_0^t dt' \hat{O}(t')\right]^n \hat{c}_i^\dagger(0) \\ &= \left(1 - i\int_0^t dt_1 \hat{O}(t_1) + \frac{(-i)^2}{2}\int_0^t dt_1 \int_0^t dt_2 \hat{O}(t_1)\hat{O}(t_2) + \cdots\right)\hat{c}_i^\dagger(0)\end{aligned}$$

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

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

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

$$\begin{aligned} \left[\hat{O}(t_1), \hat{O}(t_2) \right] &= \left[\hat{a}(0)\, e^{-i\omega t_1} + \hat{a}^\dagger(0)\, e^{i\omega t_1}, \hat{a}(0)\, e^{-i\omega t_2} + \hat{a}^\dagger(0)\, e^{i\omega t_2} \right] \\ &= \left[\hat{a}^\dagger(0), \hat{a}(0) \right] e^{i\omega(t_1 - t_2)} + \left[\hat{a}(0), \hat{a}^\dagger(0) \right] e^{-i\omega(t_1 - t_2)} \\ &= -2i \sin\omega(t_1 - t_2) \end{aligned}$$

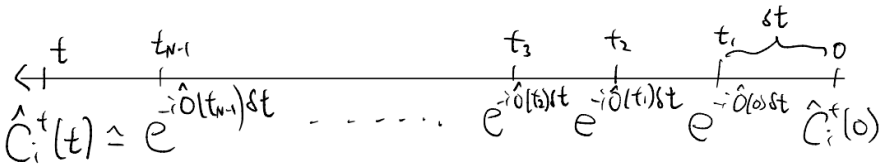
In other words, the "solution" we proposed is problematic when such non-commutation arises. To solve the problem, we have two (equivalent) pictures:

(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

$$\begin{aligned}
\hat{U}(t) &= 1 - i\int_0^t dt_1 \hat{O}(t_1)\,\hat{U}(t_1) \\
&= 1 - i\int_0^t dt_1 \hat{O}(t_1)\left[1 - i\int_0^{t_1} dt_2 \hat{O}(t_2)\,\hat{U}(t_2)\right] \\
&= 1 - i\int_0^t dt_1 \hat{O}(t_1) + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1)\,\hat{O}(t_2)\,\hat{U}(t_2) \\
&= 1 - i\int_0^t dt_1 \hat{O}(t_1) + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1)\,\hat{O}(t_2) \\
&\quad + (-i)^3 \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \hat{O}(t_1)\,\hat{O}(t_2)\,\hat{O}(t_3)\,\hat{U}(t_3) \\
&\vdots
\end{aligned}$$

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

$$\begin{aligned}
\hat{U}(t) &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \mathcal{T}\left[\int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n \hat{O}(t_1)\,\hat{O}(t_2)\cdots\hat{O}(t_n)\right] \\
&= \mathcal{T}\left[\exp\left\{-i\int_0^t dt' \hat{O}(t')\right\}\right]
\end{aligned}$$

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

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

$$\begin{aligned}\hat{U}(t) &= \mathcal{T}\left[\exp\left(-i\int_0^t dt'\hat{O}(t')\right)\right] \\ &= \sum_{n=0}\frac{(-i)^n}{n!}\mathcal{T}\left[\int_0^t dt_1\int_0^t dt_2\cdots\int_0^t dt_n \hat{O}(t_1)\,\hat{O}(t_2)\cdots\hat{O}(t_n)\right]\end{aligned}$$

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

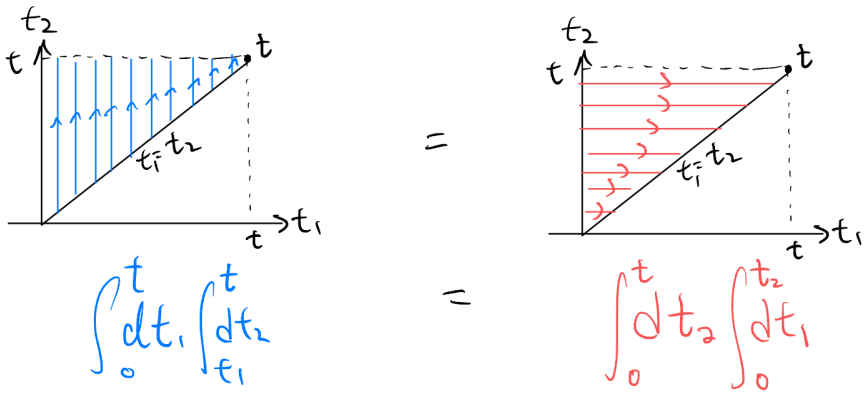
$$\hat{U}(t) = \sum_{n=0}(-i)^n\int_0^t dt_1\int_0^{t_1} dt_2\cdots\int_0^{t_{n-1}} dt_n \hat{O}(t_1)\,\hat{O}(t_2)\cdots\hat{O}(t_n)$$

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

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

Graphically, the domain of integration for the second term is

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

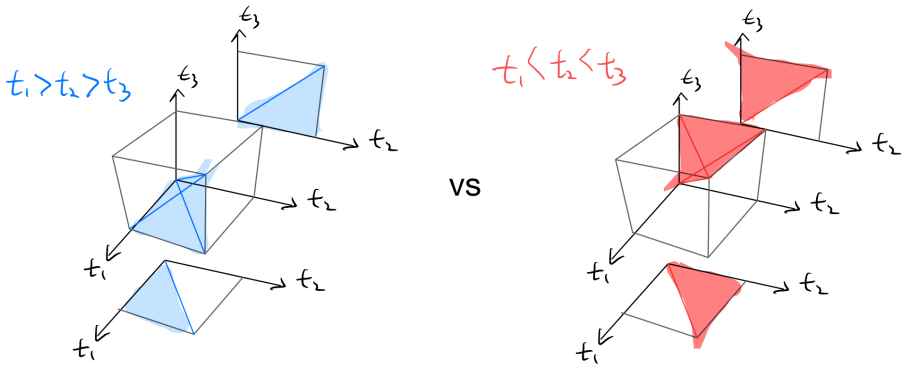


So we have

$$\begin{aligned}
&\frac{(-i)^2}{2!}\mathcal{T}\left[\int_0^t dt_1 \int_0^t dt_2 \hat{O}(t_1)\hat{O}(t_2)\right] \\
=&\frac{(-i)^2}{2!}\left\{\int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1)\hat{O}(t_2) + \int_0^t dt_2 \int_0^{t_2} dt_1 \hat{O}(t_2)\hat{O}(t_1)\right\} \\
=&\frac{(-i)^2}{2!}\left\{\int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1)\hat{O}(t_2) + \underbrace{\int_0^t dt_1 \int_0^{t_2} dt_2 \hat{O}(t_1)\hat{O}(t_2)}_{\text{relabel } t_1 \leftrightarrow t_2}\right\} \\
=&(-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \hat{O}(t_1)\hat{O}(t_2)
\end{aligned}$$

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.,

$$\begin{aligned}(t_1, t_2, t_3) &\Rightarrow t_1 < t_2 < t_3\\ (t_2, t_3, t_1) &\Rightarrow t_2 < t_3 < t_1\\ (t_1, t_3, t_2) &\Rightarrow t_1 < t_3 < t_2\\ &\vdots \Rightarrow \vdots\end{aligned}$$

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 (?)

$$\begin{aligned}G_{11}(t) &= -i\langle\Omega|\hat{c}_1^\dagger(t)\,\hat{c}_1(0)\,|\Omega\rangle\\ &= -i\langle\Omega|\underbrace{\mathcal{T}\left[\exp\left(-i\int_0^t dt'\hat{O}(t')\right)\right]}_{\text{phonon only}}\hat{c}_1^\dagger(0)\,\hat{c}_1(0)\,|\Omega\rangle\\ &= (-i)_{100}\,\langle\{0_q\}\,|\mathcal{T}\left[\exp\left(-i\int_0^t dt'\hat{O}(t')\right)\right]|\,\{0_q\}\rangle_{100}\end{aligned}$$

where

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

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

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

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

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

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,

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

where

$$\begin{aligned}
\langle 0|0\rangle &= 1 \\
\langle 0|\hat{a}^\dagger\left(t\right)|0\rangle &= \langle 0|\hat{a}\left(t\right)|0\rangle = 0 \\
\Rightarrow \quad \langle 0|\int_0^t dt'\left(\zeta\left(t\right)\hat{a}^\dagger\left(t\right)+\bar{\zeta}\left(t\right)\hat{a}\left(t\right)\right)|0\rangle &= 0
\end{aligned}$$

and so our first nontrivial term to evaluate is

$$\begin{aligned}
&\frac{(-i)^2}{2}\langle 0|\mathcal{T}\left[\left(\int_0^t dt'\left(\zeta\left(t\right)\hat{a}^\dagger\left(t\right)+\bar{\zeta}\left(t\right)\hat{a}\left(t\right)\right)\right)^2\right]|0\rangle \\
=&\frac{(-i)^2}{2}\langle 0|\mathcal{T}\Big[\int_0^t dt_1\int_0^t dt_2\zeta\left(t_1\right)\zeta\left(t_2\right)\hat{a}^\dagger\left(t_1\right)\hat{a}^\dagger\left(t_2\right)+\zeta\left(t_1\right)\bar{\zeta}\left(t_2\right)\hat{a}^\dagger\left(t_1\right)\hat{a}\left(t_2\right) \\
&+\bar{\zeta}\left(t_1\right)\zeta\left(t_2\right)\hat{a}\left(t_1\right)\hat{a}^\dagger\left(t_2\right)+\bar{\zeta}\left(t_1\right)\bar{\zeta}\left(t_2\right)\hat{a}\left(t_1\right)\hat{a}\left(t_2\right)\Big]|0\rangle
\end{aligned}$$

Noticing

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

one may want to claim the only surviving term is

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

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

$$\begin{aligned}
&\frac{(-i)^2}{2}\langle 0|\mathcal{T}\left[\left(\int_0^t dt'\left(\zeta\left(t\right)\hat{a}^\dagger\left(t\right)+\bar{\zeta}\left(t\right)\hat{a}\left(t\right)\right)\right)^2\right]|0\rangle \\
=&\left(-i\right)^2\langle 0|\left[\int_0^t dt_1\int_0^{t_1} dt_2\bar{\zeta}\left(t_1\right)\zeta\left(t_2\right)\hat{a}\left(t_1\right)\hat{a}^\dagger\left(t_2\right)\right]|0\rangle \\
=&\left(-i\right)^2\langle 0|\left[\int_0^t dt_1\int_0^{t_1} dt_2\bar{\zeta}\left(t_1\right)\zeta\left(t_2\right)e^{-i\omega(t_1-t_2)}\hat{a}\left(0\right)\hat{a}^\dagger\left(0\right)\right]|0\rangle \\
=&\left(-i\right)^2\int_0^t dt_1\int_0^{t_1} dt_2\bar{\zeta}\left(t_1\right)\zeta\left(t_2\right)e^{-i\omega(t_1-t_2)}\langle 0|\left(\hat{a}^\dagger\left(0\right)\hat{a}\left(0\right)+1\right)|0\rangle \\
=&\left(-i\right)^2\int_0^t dt_1\int_0^t dt_2\Theta\left(t_1-t_2\right)e^{-i\omega(t_1-t_2)}\bar{\zeta}\left(t_1\right)\zeta\left(t_2\right)
\end{aligned}$$

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

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

then we see that

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

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:

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

$$\begin{aligned}
G_{11}(t) &= (-i)\,e^{-i\left(-\varepsilon_1+2\sum_q\frac{M_{1q}^2}{\omega_q}\right)}\prod_q {}_{100}\langle 0_q|\mathcal{T}\left[e^{iM_{1q}\int_0^t dt'\left(\hat{a}_q^{\{100\}}(t)+\hat{a}_q^{\{100\}\dagger}(t)\right)}\right]|0_q\rangle_{100} \\
&= (-i)\,e^{-i\left(-\varepsilon_1+2\sum_q\frac{M_{1q}^2}{\omega_q}\right)}\prod_q e^{-iM_{1q}^2\int_0^t dt_1\int_0^t dt_2\mathscr{G}_q(t_1-t_2)}
\end{aligned}$$

Evaluating the double integral

$$\begin{aligned}
\int_0^t dt_1\int_0^t dt_2\mathscr{G}_q(t_1-t_2) &= -i\int_0^t dt_1\int_0^t dt_2\Theta(t_1-t_2)\,e^{-i\omega_q(t_1-t_2)} \\
&= -i\int_0^t dt_1\int_0^{t_1} dt_2 e^{-i\omega_q(t_1-t_2)} \\
&= -i\int_0^t dt_1\frac{1-e^{-i\omega_q t_1}}{i\omega_q} \\
&= -\frac{t}{\omega_q}+\frac{e^{-i\omega_q t}-1}{-i\omega_q^2}
\end{aligned}$$

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

$$\begin{aligned} G_{11}(t) &= (-i)\, e^{-i\left(-\varepsilon_1 + 2\sum_q \frac{M_{1q}^2}{\omega_q}\right)} \prod_q e^{i\frac{M_{1q}^2}{\omega_q}t} e^{\frac{M_{1q}^2}{\omega_q^2}\left(e^{-i\omega_q t}-1\right)} \\ &= (-i)\, \underbrace{e^{-i\left(-\varepsilon_1 + \sum_q \frac{M_{1q}^2}{\omega_q}\right)t}}_{e^{i\Delta_{100}t}} e^{\sum_q g_q\left(e^{-i\omega_q t}-1\right)} \end{aligned}$$

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.