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

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

Let's now define

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

which gives

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

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

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

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

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

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

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

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

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

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

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

To get the normalization,

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

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

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

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 operatos 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

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

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

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

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

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

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

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

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

Check

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

"Displacement"? compute (also using BCH formula)

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

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

E.g., 1. Average energy

$$\begin{aligned}
\langle\alpha|\hat{H}|\alpha\rangle&=\langle0|\hat{D}^{\dagger}\left(\alpha\right)\hbar\omega\left(\hat{a}^{\dagger}\hat{a}+\frac{1}{2}\right)\hat{D}\left(\alpha\right)\left|0\right\rangle\\
&=\langle0|\hbar\omega\left(\left(\hat{a}^{\dagger}+\alpha^{*}\right)\left(\hat{a}+\alpha\right)+\frac{1}{2}\right)\left|0\right\rangle\\
&=\frac{\hbar\omega}{2}+\hbar\omega\langle0|\left(\hat{a}^{\dagger}\hat{a}+\hat{a}^{\dagger}\alpha+\alpha^{*}\hat{a}+\left|\alpha\right|^{2}\right)\left|0\right\rangle\\
&=\hbar\omega\left(\left|\alpha\right|^{2}+\frac{1}{2}\right)
\end{aligned}$$

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 betwween 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

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

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

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

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

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

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

Note: consider the integral with $a<b$

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

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

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

Now let's compute

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

I.e., G solves the differential equation

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

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

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

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

Notes:

1. This is *THE* mathematical meaning of a "Green function"
2. In physics, the meaning and usage of "Green functions" and "propagator" are kind of messed up
3. As discussed in "level 2", when we say "Green function" in our context we really refer to some correlation function

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

$$\hat{H} = \hat{H}_0 + \hat{V}$$
$$\left(i\hbar\partial_t - \hat{H}\right)|\Psi\rangle = 0$$
$$\left(i\hbar\partial_t - \hat{H}_0\right)|\Psi\rangle = \hat{V}|\Psi\rangle$$

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

Of course, the true story is (much) more complicated than that. Anyway this suggests the bare Green functions from the starting point for solving the perturbed system. This is the general theme of pertubative 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 statatics 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 cannonical 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 hense unitary). I.e., there exists an orthogonal matrix O

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

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

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

where repeated indices are summed.

Chapter 3

lec03 202200211

topics:

1. free phonons: solving with (without) and with (without) invariance
2. acoustic versus optical phonons
3. finite temperature: density matrix

goals

1. getting used to fourier transformation and cannonical 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 clain is diagonalized by

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

This basis rotation induces one on the the operators

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

we can verify

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

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 cannonical 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 swith notation slightly $D_{ij}^{\alpha\beta} \to D_{\vec{R}\vec{R}'}^{\alpha\beta}$.

Here, we let $\vec{R}, \vec{R}'$ denote unit cell coordinattes. 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 trnasform. 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. $\hat{\phi}_{\vec{q}}^{\alpha\dagger} = \frac{1}{\sqrt{V}}\sum_{\vec{R}} e^{-i\vec{q}\cdot\vec{R}}\hat{\phi}_{\vec{R}}^{\alpha} = \hat{\phi}_{-\vec{q}}^{\alpha}$
2. $\hat{t}_{\vec{a}}\hat{\phi}_{\vec{q}}^{\alpha}\hat{t}_{\vec{a}}^{-1} = \frac{1}{\sqrt{V}}\sum_{\vec{R}} e^{i\vec{q}\cdot\vec{R}}\hat{\phi}_{\vec{R}+\vec{a}}^{\alpha} = e^{-i\vec{q}\cdot\vec{a}}\hat{\phi}_{\vec{q}}^{\alpha}$, where $\hat{t}_{\vec{a}}$ is lattice translation by $\vec{a}$

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

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

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

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

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

We further diagonalize the block

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

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

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

we should now define the creation and annihilation operators

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

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

As usual, let's check

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

Anticipating the answer, let's compute

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

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

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

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

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

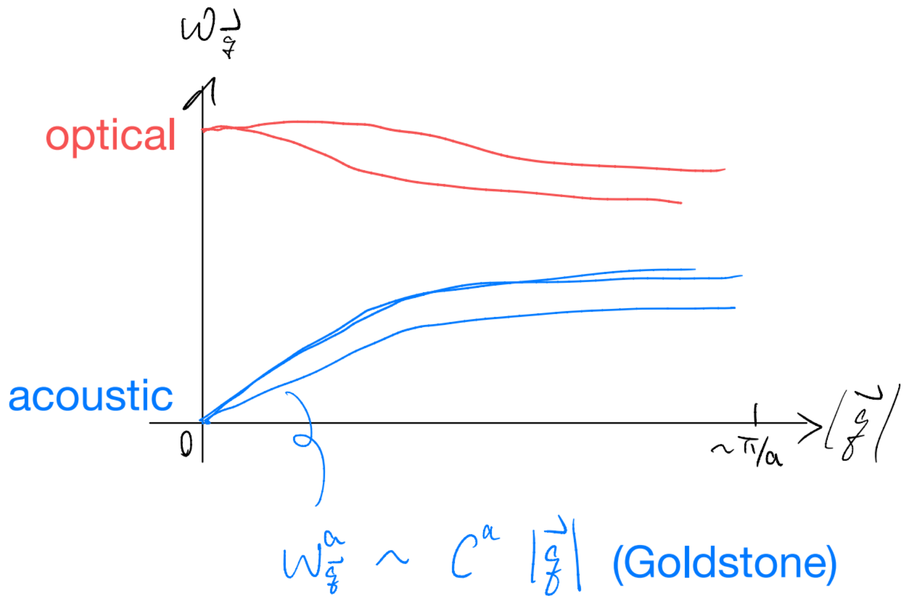
Notice that we have treated $\vec{q} = 0$ differently. This is more than a formality (e.g. we would have double counted if we simply group the sums for $\vec{q}$ and $-\vec{q}$). Physically, having crystal momentum of $\vec{q} = \vec{0}$ implies

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 constranit 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 abbretiate for Classical Mechanics)

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

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.

$$\begin{aligned}
\hat{\rho} &= \frac{e^{-\beta\hat{H}}}{\mathcal{Z}} \\
\mathcal{Z} &= \mathrm{Tr}\left(e^{-\beta\hat{H}}\right) \\
\beta &= \frac{1}{k_B T} \\
\mathrm{Tr}\left(\hat{\rho}\right) &= 1
\end{aligned}$$

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

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

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

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

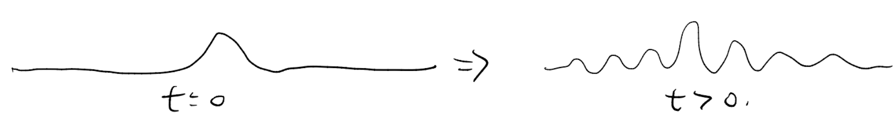
$$\partial_J \ln \mathcal{Z}\left(\beta, J\right) = \frac{\partial_J \mathrm{Tr}\left(e^{-\beta\hat{H}+J\hat{O}}\right)}{Z\left(\beta, J\right)} \stackrel{?}{=} \frac{\mathrm{Tr}\left(\hat{O}e^{-\beta\hat{H}+J\hat{O}}\right)}{Z\left(\beta, J\right)}$$

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

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.

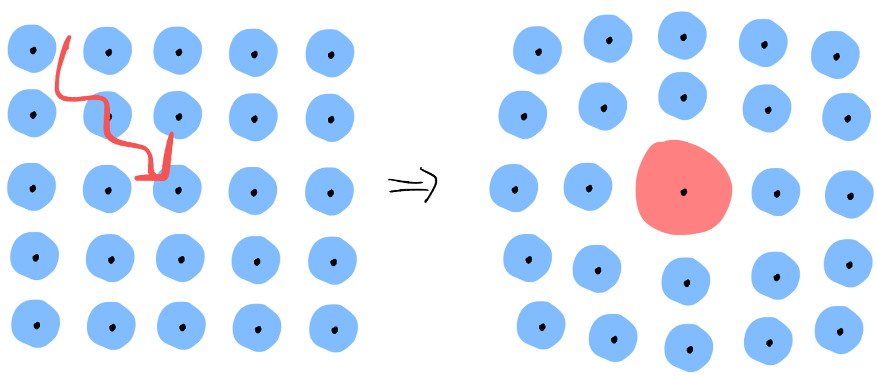
In any case, we have completely solved the free phonon problem, in the sense that for any observables we would want to compute, we have a way of doing so (by rotating to the decoupled QHO basis).

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

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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 iis 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 dependss on two coordinate variables

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

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

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

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 cannonical commutation). Whence the name "QFT"

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

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

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:

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

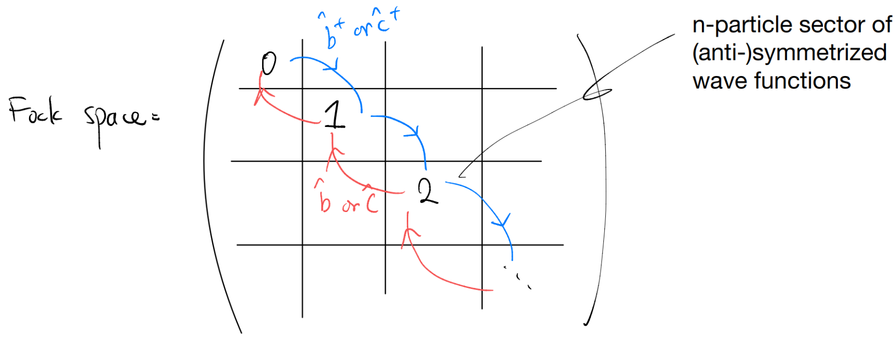
This implies the fermionic creation and annihilation operators should satisfy cannonical anti-commutation relations. Let $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$. For fermions

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

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

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

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 cannonical 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 hense no statistics. If you have multple 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

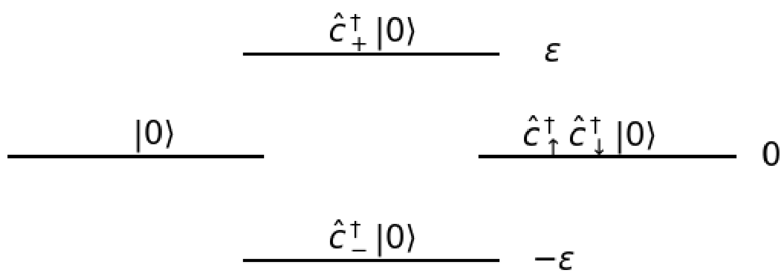
$$\begin{cases} \left\{ \hat{c}_{\pm}^{\dagger}, \hat{c}_{\pm} \right\} = \frac{1}{2} \left\{ \hat{c}_{\uparrow}^{\dagger} \pm \hat{c}_{\downarrow}^{\dagger}, \hat{c}_{\uparrow} \pm \hat{c}_{\downarrow} \right\} = \frac{1}{2} \left(1 \pm 0 \pm 0 + 1 \right) = 1 \\ \left\{ \hat{c}_{+}^{\dagger}, \hat{c}_{-}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

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

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

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

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

(c.f. the phonon discusion)

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

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 resepct to a fixed state $|\Psi\rangle(0)$. This perspective is called the "Heisenberg picture".

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

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

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:

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

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 a noperator, it is understood that we are in the Heisenberg picture.

Back to our example. Recall we were compairing

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

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 measureing correlation across time. Yet, this is *NOT* by itself a physical observable! We cannot understand it as the expectation vlue 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,

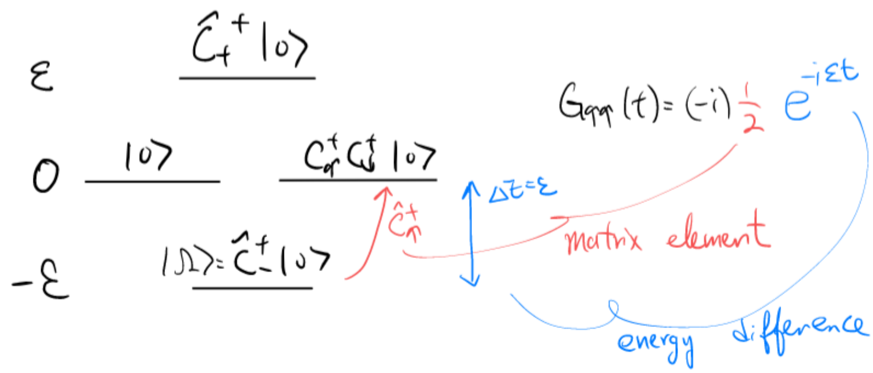
$$
\begin{aligned}
i\partial_t\left(\hat{c}_{\pm}^{\dagger}(t)\right) &= \left[\hat{c}_{\pm}^{\dagger}(t), \hat{H}\right] \\
&= \hat{U}^{\dagger}\left[\hat{c}_{\pm}^{\dagger}, \pm\varepsilon\hat{c}_{\pm}^{\dagger}\hat{c}_{\pm}\right]\hat{U} \\
&= \hat{U}^{\dagger}\left(\pm\varepsilon\hat{c}_{\pm}^{\dagger}\right)\left[\hat{c}_{\pm}^{\dagger},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

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

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 $\dim(\mathcal{H}) \sim 2^V$.