# Fourier Transform of Operators

$$a^{+}(\varphi)\,|0\rangle = |\varphi\rangle = \int_x \langle x|\varphi\rangle\, |x\rangle$$

$$= \int_x \langle x|\varphi\rangle\, a^{+}(x)\,|0\rangle$$

$$\Rightarrow \quad a^{+}(\varphi) = \int_x a^{+}(x)\, \langle x|\varphi\rangle$$

e.g. if $\varphi$ corresponds to the ground state of simple harmonic oscillator, then

$$a^{+}(\varphi) = \left(\frac{m\omega}{\pi}\right)^{1/4} \int_x a^{+}(x)\, e^{-m\omega x^2/2}$$

This provides another way to think about the commutation relations. e.g.

$$a(x_1)\, a^{+}(x_2) - s\, a^{+}(x_2)\, a(x_1) = \delta(x_1 - x_2)$$

is the most common way to write the commutation | anti-commutation relations. But Fourier transforming it gives.

$$a(\varphi_1)\, a^{+}(\varphi_2) - s\, a^{+}(\varphi_2)\, a(\varphi_1)$$

$$= \langle \varphi_1|\varphi_2\rangle \quad \text{as expected.}$$

Intuition for

$$a(\varphi)\, |u_1 \cdots u_n\rangle \qquad - (1)$$

$$= \sum_j (s)^{j-1} \langle \varphi | u_j \rangle\, |u_1 \cdots (\text{no } u_j) \cdots u_n\rangle$$

Let's work in the real space basis.

$$a(x)\, |x_1 \cdots x_n\rangle$$

$$= a(x) \quad a^\dagger(x_1)\, a^\dagger(x_2) \cdots a^\dagger(x_n)\, |0\rangle$$

if $x$ does not belong to the set $\{x_1, x_2, \cdots x_n\}$ then this is identically zero. So let's assume that $x = x_j$.

Passing $x$ through $x_1$ to $x_{j-1}$ yields a sign of $s^{j-1}$ $\Rightarrow$ $a(x)|x_1 \cdots x_n\rangle$

$$= s^{j-1} \quad a^\dagger(x_1) \cdots a^\dagger(x_{j-1})\, a(x_j) a^\dagger(x_j) \cdots a^\dagger(x_n)\, |0\rangle$$

$$= s^{j-1} \quad a^\dagger(x_1) \cdots a^\dagger(x_{j-1}) [1 + s\, a^\dagger(x_j) a(x_j)] \cdots a^\dagger(x_n)\, |0\rangle$$

$$= s^{j-1}\, |x_1 \cdots (\text{no } x_j) \cdots x_n\rangle$$

Fourier transforming yields (1) above.

# General operators using Creation / Annihilation operators.

The best part about operators $a^\dagger(u_i)$, $a(u_i)$ is that instead of asking "what is i'th particle doing?" (which is a badly framed question since we are dealing with identical particles), we can ask "which processes is the single particle level $|u_i\rangle$ is participating in?" (which is a well posed question for identical particles because it focusses on levels rather than particles — single-particle levels $|u_i\rangle$ are ofcourse distinguished from each other by the level '$i$').

To quote Weinberg: "As far as we know, every electron in the universe is identical to every other electron, except for the values taken by their positions (or momenta) and spin components.

Following Feynman's chapter-6, consider an operator $A^{(1)}$ that acts <u>only</u> on single-particle states.

For the action of an operator to respect the identical nature of the particles, we would like to find a <u>many-body</u> counterpart of $A^{(1)}$ that acts as:

$$A\,|\psi\rangle = A\,|u_1, \ldots\ldots, u_n\rangle$$

$$= A \sum_P S^P\, |u_{P(1)}\rangle |u_{P(2)}\rangle \ldots |u_{P(n)}\rangle$$

$$= \sum_P S^P \Big[ \big(A^{(1)} |u_{P(1)}\rangle\big) |u_{P(2)}\rangle \ldots |u_{P(n)}\rangle$$

$$+ |u_{P(1)}\rangle \big[A^{(1)} |u_{P(2)}\rangle\big] \ldots |u_{P(n)}\rangle$$

$$+ |u_{P(1)}\rangle |u_{P(2)}\rangle \ldots A^{(1)} |u_{P(n)}\rangle$$

i.e. A represents the "sum of $A^{(1)}$" over all particles, and thus respect their identical nature. For example if $|u_i\rangle$ is an eigenvector of $A^{(1)}$ with the eigenvalue $u_i$, then

$$A|\psi\rangle = \sum_P S^P \left(u_{p(1)} + u_{p(2)} + \cdots + u_{p(n)}\right) |u_{p(1)}\rangle |u_{p(2)}\rangle \cdots |u_{p(n)}\rangle$$

$$= (u_1 + u_2 + \cdots u_n)|\psi\rangle.$$

Next consider a more interesting operator $A^{(1)} = |\alpha\rangle\langle\beta|$. Using definition of A above

$$A|\psi\rangle = \sum_P S^P \Big[ \langle\beta|u_{p(1)}\rangle |\alpha\rangle |u_{p(2)}\rangle \cdots |u_{p(n)}\rangle$$

$$+ |u_{p(1)}\rangle \langle\beta|u_{p(2)}\rangle |\alpha\rangle |u_{p(3)}\rangle \cdots |u_{p(n)}\rangle$$

$$+ |u_{p(1)}\rangle |u_{p(2)}\rangle \cdots \langle\beta|u_{p(n)}\rangle |\alpha\rangle \Big]$$

$$= \langle \beta | u_1 \rangle \, | \alpha, u_2, \ldots u_n \rangle$$

$$+ \langle \beta | u_2 \rangle \, | u_1, \alpha, \ldots u_n \rangle$$

$$\ldots\ldots$$

$$+ \langle \beta | u_n \rangle \, | u_1, u_2, \ldots \alpha \rangle$$

$$= \sum_{k=1}^{n} \langle \beta | u_k \rangle \, | u_1 \, u_2 \ldots u_{k-1} \, \alpha \, u_{k+1} \ldots u_n \rangle$$

This looks like as if we are destroying state $|\beta\rangle$ and creating $|\alpha\rangle$. So it makes sense to compare with the the action of $a^+(\alpha)\, a(\beta)$.

$$a^+(\alpha) \, a(\beta) \, | u_1 \, u_2 \ldots u_n \rangle$$

$$= a^+(\alpha) \sum_{k=1}^{n} S^{k-1} \langle \beta | u_k \rangle \, | u_1 \, u_2 \ldots (\text{no } u_k) \ldots u_n \rangle$$

$$= \sum_{k=1}^{n} S^{k-1} \langle \beta | u_k \rangle \, | \alpha \, u_1 \, u_2 \ldots (\text{no } u_k) \ldots u_n \rangle$$

$$= \sum_{k=1}^{n} \langle \beta | u_k \rangle \, | u_1 \, u_2 \ldots u_{k-1} \, \alpha \, u_{k+1} \ldots u_n \rangle$$

$$\Rightarrow \quad \boxed{A = a^{+}(\alpha)\ a(\beta)}$$

Next consider a more general operator that acts on single particle states : $A^{(1)} = \sum_{\alpha\beta} A^{(1)}_{\alpha\beta} |\alpha\rangle\langle\beta|$

where $A^{(1)}_{\alpha\beta} = \langle\beta| A^{(1)} |\alpha\rangle$

Using linearity,

$$A = \sum_{\alpha\beta} a^{+}(\alpha)\ a(\beta)\ A^{(1)}_{\alpha\beta}$$

Examples :

(i) $A^{(1)} = \mathbb{1}^{(1)}$ = identity operator acting on a single particle state.

$$\Rightarrow \quad A = \sum_{\alpha} a^{+}(\alpha)\ a(\beta) \langle\alpha|\mathbb{1}|\beta\rangle$$

$$= \sum_{\alpha} a^{+}(\alpha)\, a(\alpha)$$

$$= \sum_{\alpha} \hat{n}_{\alpha} = \text{total particle number.}$$

One can write this in any basis one wishes to:

$$\sum_{\alpha} a^{\dagger}_{\alpha} a_{\alpha} = \int d^d x \; a^{\dagger}(x) a(x)$$

$$= \int \frac{d^d p}{(2\pi)^d} \; a^{\dagger}(p) a(p)$$

(ii) Hamiltonian of non-interacting particles

Now we return to the problem we started from at the beginning of lecture-1:

$$H^{(1)} = \frac{p^2}{2m} + V(x)$$

$$\langle x | H^{(1)} | x' \rangle = -\frac{\nabla^2}{2m} \delta^d (x - x') + V(x) \delta^d (x - x')$$

$$\Rightarrow \quad H = \int d^d x \, d^d x' \langle x | H^{(1)} | x' \rangle \; a^{\dagger}(x) a(x')$$

$$= \int d^d x \, d^d x' \left[ -\frac{\nabla^2}{2m} \delta^d (x - x') + V(x) \delta^d (x - x') \right] a^{\dagger}(x) a(x')$$

$$= \int d^d x \quad a^\dagger(x) \left[ -\frac{\nabla^2}{2m} + V(x) \right] a(x)$$

Since $a(x) = \int a(p)\, e^{ip\cdot x} \frac{d^d p}{(2\pi)^d}$

H also equals

$$\int \frac{d^d p}{(2\pi)^d} \quad \frac{p^2}{2m} a^\dagger(p)\, a(p)$$

$$+ \int \frac{d^d p\, d^d q}{(2\pi)^d} \quad a^\dagger(p+q)\, a(p)\, V(q)$$

where $V(q) = \int d^d x\, V(x)\, e^{-iq\cdot x}$

Finally consider writing H in the eigenbasis of $H^{(1)}$ (recall the two-particle problem we solved), which we denote by $|u_\alpha\rangle$

$$\langle u_\alpha | H^{(1)} | u_\beta \rangle = E_{u_\alpha} \delta_{\alpha\beta}$$

$$\Rightarrow \boxed{H = \sum_{\alpha} E_{u_\alpha} \, a^{+}(u_\alpha)\, a(u_\alpha)}$$

It is crucial to note that H is the Hamiltonian of the system irrespective of how many particles there are in a given problem. This is because the operators $a, a^{+}$ act in multi-particle space. This is the essence of working in this notation.

In the old notation,

$H = \sum_n H^{(n)}$ where $H^{(n)}$ is the Hamiltonian for n-particles:

$$H^{(n)} = \sum_{u_1 \cdots u_n} E_{u_1 \cdots u_n} |u_1 \cdots u_n\rangle\langle u_1 \cdots u_n|$$

and $E_{u_1 \cdots u_n} = E_{u_1} + E_{u_2} + \cdots + E_{u_n}$

(see defn. of $E_{u_\alpha}$ at the top of this page).

Working in terms of creation / annihilation operators enormously simplify the expressions (and actual calculations, as we will soon see).

## Hamiltonian of interacting particles using creation / annihilation operators.

Consider a two-body Hamiltonian $H^{(2)}(x_i, x_j)$ e.g. a Coulomb potential between charged particles

$$\sim \frac{e^2}{|x_i - x_j|}.$$

To simplify the calculation, let's work in the real-space basis where the operator is already diagonal.

Thus, the action of $H(2)$ on two-particle state is

$$H^{(2)} = \frac{1}{2} \int d^3x \, d^3y \, |x,y\rangle H^{(2)}(x,y) \langle x,y|$$

and therefore action of $H$ on many-body state is thus:

$$H \underbrace{|x_1, x_2 \cdots x_N\rangle}_{\text{recall this is sym / anti sym already,}}$$

$$= \frac{1}{2} \sum_{i \neq j} H^{(2)}(x_i, x_j) |x_1, \cdots x_n\rangle$$

The form of $H^{(2)}$ suggests that in terms of the creation-annihilation operators:

$$H = \frac{1}{2} \int d^3x \, d^3y \, a^\dagger(x) a^\dagger(y) H^{(2)} a(y) a(x)$$

Lets verify that this is indeed correct:

$$a(y)\, a(x)\, |x_1 \cdots x_n\rangle$$

$$= a(y) \sum_{k=1}^{n} s^{k-1} \langle x | x_k\rangle\, |x_1 \cdots (\text{no } x_k) \cdots x_n\rangle$$

$$= a(y) \sum_{k=1}^{n} s^{k-1} \delta^d(x - x_k)\, |x_1 \cdots (\text{no } x_k) \cdots x_n\rangle$$

$$= \sum_{k=1}^{n} s^{k-1} \delta^d(x - x_k) \sum_{\substack{j=1 \\ j \neq k}}^{n} \eta_{jk}\, |x_1 \cdots (\text{no } x_k, x_j) \cdots x_n\rangle\, \delta^d(y - x_j)$$

$$\eta_{jk} = \begin{cases} s^{j-1} & \text{if } j < k \\ s^{j} & \text{if } j > k \end{cases}$$

(easy to see this)

$$\Rightarrow a^+(x)\, a^+(y)\, a(y)\, a(x)\, |x_1 \ldots x_n\rangle$$

$$= \sum_{j \neq k} s^{k-1}\, \eta_{jk}\, \delta^d(x - x_k)\, \delta^d(y - x_j)\, |x, y, x_1 \ldots (\text{no } x_k, x_j) \ldots x_n\rangle$$

double summation

$$= \sum_{j \neq k} s^{k-1}\, \eta_{jk}\, \delta^d(x - x_k)\, \delta^d(y - x_j)\, |x_k, x_j, \ldots (\text{no } x_k, x_j) \ldots x_n\rangle$$

if $j < k$

$$x_1 x_2 \ldots x_j \ldots x_k \ldots x_n$$

The phase factor picked up in going from $|x_k, x_j \ldots (\text{no } x_k, x_j) \ldots x_n\rangle$ to $|x_1 \ldots x_j \ldots x_k \ldots x_n\rangle$ is

$s^{j-1}\, s^{k-1}$ which cancels out $s^{k-1}\, \eta_{jk}$ factor.

The other case also works out similarly.

$$\Rightarrow \quad a^+(x)\, a^+(y)\, a(y)\, a(x) \, |x_1 \cdots x_n\rangle$$

$$= \sum_{j \neq k} \delta^d(x - x_k)\, \delta^d(y - x_j)\, |x_1 \cdots x_n\rangle$$

$$\Rightarrow \quad \frac{1}{2} \int d^d x \, d^d y \; a^+(x)\, a^+(y)\, H^{(2)}(x,y)\, a(y)\, a(x)$$

$$= \frac{1}{2} \sum_{i \neq j} H^{(2)}(x_i, x_j)\, |x_1 \cdots x_n\rangle$$

Thus,

$$\boxed{H = \frac{1}{2} \int d^d x \, d^d y \; a^+(x)\, a^+(y)\, H^{(2)}(x,y)\, a(y)\, a(x)}$$

Example #1 Coulomb Hamiltonian

$$H^{(2)}(x,y) = \frac{e^2}{|x-y|}$$

$$\Rightarrow H = \frac{1}{2}\int d^dx\, d^dy\; a^\dagger(x)\, a^\dagger(y)\, \frac{e^2}{|x-y|}\, a(y)\, a(x)$$

Fourier transforming in $d=3$

$$H = \frac{1}{2}\int \frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3}\frac{d^3p'}{(2\pi)^3}\; \frac{e^2}{q^2}\; a^\dagger(p+q)\, a^\dagger(p'-q)\, a(p')\, a(p)$$

Example #2 Contact Interaction

$$H^{(2)}(x,y) = \delta^d(x-y)$$

$$\Rightarrow H = \frac{1}{2}\int d^dx\, d^dy\; a^\dagger(x)\, a^\dagger(y)\, a(y)\, a(x)\, \delta^d(x-y)$$

$$= \frac{1}{2}\int d^dx\, [a^\dagger(x)]^2\, a^2(x)$$

(~ non-zero only for bosons)

## Summary so far :

**One-body Hamiltonians using creation-annihilation operators :**

Old notation :

$$\hat{H}^{old} = \sum_{i=1}^{n} \hat{H}^{(1)}(x_i)$$

New notation :

$$\hat{H}^{new} = \sum_{x,x'} \langle x | \hat{H}^{(1)} | x' \rangle \; a^{+}(x)\, a(x')$$

Important note: $n$ (= no. of particles) does not enter into $\hat{H}$ in the new notation at all. This is because $\hat{H}$ now acts in the multi-particle Hilbert space. Therefore, the precise relation is :

$$\hat{H}^{old} = P^{(n)} \; \hat{H}^{new} \; P^{(n)}$$

where $P^{(n)}$ is the projection operator onto $n$-particle Hilbert space.

## Two body Hamiltonians using creation-annihilation operators

Old notation:

$$\hat{H}^{old} = \sum_{i,j=1}^{n} \hat{H}^{(2)}(x_i, x_j)$$

New notation:

$$\hat{H}^{new} = \frac{1}{2} \sum_{\substack{x x' \\ y y'}} \langle x, y | \hat{H}^{(2)} | x', y' \rangle \, a^{+}(x)\, a^{+}(y)\, a(y')\, a(x')$$

Once again,

$$\hat{H}^{old} = P^{(n)} \hat{H}^{new} P^{(n)}$$

The fact that the particles are bosons or fermions is captured solely by the commutation-anticommutation relations. Recall:

$$\boxed{\begin{aligned} a^+(x)\, a^+(y) &= s\, a^+(y)\, a^+(x) \\ a(x)\, a(y) &= s\, a(y)\, a(x) \\ a(x)\, a^+(y) - s\, a^+(y)\, a(x) &= \delta^d(x-y) \end{aligned}}$$

## Recovering Schrodinger's Equation in the New Notation

First consider one-body Hamiltonian

$$H = \int d^d x \; a^+(x) \left[ -\frac{\nabla^2}{2m} + V(x) \right] a(x)$$

lets consider a $\underline{\text{single}}$ particle whose motion is described by the above $H$

$$\Rightarrow \int d^d x \; a^+(x) \left[ -\frac{\nabla^2}{2m} + V(x) \right] a(x) \, |\psi\rangle$$

$$= E\, |\psi\rangle$$

The main idea is that one can expand $|\psi\rangle$ as:

$$|\psi\rangle = \int d^dx \, u(x) \, a^+(x) \, |0\rangle$$

where $|0\rangle$ is a state with no particles.

$$\Rightarrow \int d^dx \; a^+(x) \left[ -\frac{\nabla^2}{2m} + V(x) \right] a(x) \int d^dx' \; u(x') \; a^+(x') \; |0\rangle$$

$$= E \int d^dx \, u(x) \; a^+(x) \; |0\rangle$$

Now one can use commutation / anti-commutation relations to simplify this

$$\Rightarrow \int d^dx' \int d^dx \quad a^+(x) \left[ -\frac{\nabla^2}{2m} + V(x) \right] u(x') \; \left[ \delta^d(x-x') + S \; a^+(x') \, a(x) \right] |0\rangle$$

$$= E \int d^dx \; u(x) \; a^+(x) |0\rangle$$

$$\Rightarrow \int d^dx \quad a^+(x) \left[ \frac{-1}{2m} \frac{d^2 u(x)}{dx^2} + V(x) u(x) \right] |0\rangle$$

$$= E \int d^dx \quad u(x) \; a^+(x) |0\rangle$$

Now we take dot product with $a^\dagger(x')|0\rangle$

$$\Rightarrow \int d^dx \langle 0| a(x') \, a^\dagger(x) \left[ -\frac{1}{2m}\frac{d^2 u(x)}{dx^2} + V(x)\, u(x) \right] |0\rangle$$

$$= E \int d^dx \, \langle 0| a(x') \, a^\dagger(x) |0\rangle \, u(x)$$

Once more using the commun/anti-com. relations.

$$\Rightarrow \boxed{-\frac{1}{2m}\frac{d^2 u(x)}{dx^2} + V(x)\, u(x) = E\, u(x)}$$

Thus, the wave-$f^n$ in the older notation is just the expansion coefficient of $a^\dagger(x)$ in the wave-$f^n$ in newer notation.

Next consider two particles in the same potential:

Now expand

$$\psi(x, y) = \int_{x,y} a^+(x)\, a^+(y)\, \psi(x, y) \, |0\rangle$$

$\Rightarrow$

$$\int d^d x \; a^+(x) \left[ -\frac{\nabla_x^2}{2m} + V(x) \right] a(x) \int d^d x' \, d^d y' \; \psi(x', y') \, a^+(x') \, a^+(y') \, |0\rangle$$

$$= E \int d^d x \, d^d y \; \psi(x, y) \, a^+(x) \, a^+(y) \, |0\rangle$$

Let's focus on the L.H.S. first;

$$\int d^d x \, d^d x' \, d^d y' \; a^+(x) \left[ -\frac{\nabla_x^2}{2m} + V(x) \right] \psi(x', y') \; a(x) \, a^+(x') \, a^+(y') \, |0\rangle$$

$$= \int d^d x\, d^d x'\, d^d y'\, a^+(x) \left[ -\frac{\nabla_x^2}{2m} + V(x) \right] \psi(x', y')\, a(x)\, a^+(x')\, a^+(y') |0\rangle$$

$$= \int d^d x\, d^d x'\, d^d y'\, a^+(x) \left[ -\frac{\nabla^2_x}{2m} + V(x) \right] \psi(x', y') \left[ \delta^d(x-x') + s\, a^+(x')\, a(x) \right] a^+(y') |0\rangle$$

$$= \int d^d x\, d^d x'\, d^d y'\, a^+(x) \left( -\frac{\nabla^2_x}{2m} + V(x) \right) \psi(x', y') \left[ \delta^d(x-x')\, a^+(y') + s\, a^+(x')\, \delta^d(x-y') \right] |0\rangle$$

$$= \int d^d x\, d^d y'\, a^+(x) \left( -\frac{\nabla^2_x}{2m} + V(x) \right) \psi(x, y')\, a^+(y') |0\rangle$$

$$+ s \int d^d x\, d^d x'\, a^+(x) \left[ -\frac{\nabla^2_x}{2m} + V(x) \right] \psi(x', x)\, a^+(x') |0\rangle$$

$$= \int d^d x\, d^d x'\, a^+(x)\, a^+(x') \left[ -\frac{\nabla^2_x}{2m} + V(x) \right] \psi(x, x')$$

$$+ s \int d^d x\, d^d x'\, a^+(x')\, a^+(x) \left[ -\frac{\nabla^2_{x'}}{2m} + V(x') \right] \psi(x, x')$$

Taking dot product with $a^+(x) a^+(x') |0\rangle$

$$\Rightarrow \left[ -\frac{\nabla^2_x}{2m} + V(x) \right] \psi(x, x')$$

$$+ \left[ -\frac{\nabla^2_{x'}}{2m} + V(x') \right] \psi(x, x')$$

$$= E \, \psi(x, x')$$

Clearly, $\psi(x, x') = u_\alpha(x) \, u_{\alpha'}(x')$ is a solution, and now

$$|\psi\rangle = \int_{x, x'} u_\alpha(x) \, u_{\alpha'}(x') \, a^+(x) \, a^+(x') |0\rangle$$

is automatically symmetrized / anti-symmetrized.

Indeed, $|\psi\rangle = |u_\alpha \, u_{\alpha'}\rangle$

since $|u_\alpha\rangle = \int_x a^+(x) \, u_\alpha(x) |0\rangle$