QFT by Lancaster and Blundell
Sec. 3.5 and Ch. 4.1 and 4.2

Wayne Dam

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3.5 The Continuum Limit

- From the uncoupled QSHO model we have $\hat{a}_k^\dagger|0\rangle \propto |...,1_k,....\rangle$. A single quanta is produced in the k'th oscillator.

- From 3.3 we are asserting there are creation operators that create particles in particular momentum states.

- So that from the vacuum state $|0\rangle$,

$$\hat{a}_p^\dagger|0\rangle = |p\rangle. \tag{1}$$

  A single particle is created with momentum, p.

- Using the *occupation number representation* we can create multiple particles as,

$$\hat{a}_{p_1}^\dagger \hat{a}_{p_1}^\dagger \hat{a}_{p_2}^\dagger|0\rangle = |21\rangle. \tag{2}$$

  Two particles with momentum p_1 and on with momentum p_2.

- In general we convert from the regular state representation to the number occupation representation as,

$$|\underbrace{p_1,...,p_1}_{n(p_1)},\underbrace{p_2,...,p_2}_{n(p_2)},\underbrace{p_3,...,p_3}_{n(p_3)},\ldots\rangle = |n(p_1),n(p_2),n(p_3),\ldots\rangle \tag{3}$$

- Recall from 3.1 we are treating the particles as they are in a box of size L with periodic boundary conditions and so the eigenstates are of the form $\psi(x) = \frac{1}{\sqrt{L}} e^{ipx}$ and the momentum taking discrete values,

$$p_k = \frac{2\pi k}{L}. \tag{4}$$

- So we have momentum p_1, p_2, etc.

- Letting L go to infinity the discrete values of p get closer and closer together so we can consider them a continuum.

- So instead of

$$\left[\hat{a}_{p_i}, \hat{a}^\dagger_{p_j}\right] = \delta_{ij}, \tag{5}$$

we have

$$\left[\hat{a}_p, \hat{a}^\dagger_q\right] = \delta(p - q). \tag{6}$$

Example (1. Hamiltonian operator giving the total energy.)

- Work out and explain (3.34) ... $\hat{H} = \int_p d^3p\ E_p \hat{a}_p{}^\dagger \hat{a}_p$

Consistency Check (pg. 35):

Example 3.6

1. Expect this to be a delta function since momentum basis vectors are orthogonal.

For single-particle states, we have

$$\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \langle 0|\hat{a}_{\boldsymbol{p}}\hat{a}^\dagger_{\boldsymbol{p}'}|0\rangle. \tag{3.35}$$

We use the commutation relations to get

$$\begin{aligned} \langle \boldsymbol{p}|\boldsymbol{p}'\rangle &= \langle 0|\left[\delta^{(3)}(\boldsymbol{p}-\boldsymbol{p}') \pm \hat{a}^\dagger_{\boldsymbol{p}'}\hat{a}_{\boldsymbol{p}}\right]|0\rangle \\ &= \delta^{(3)}(\boldsymbol{p}-\boldsymbol{p}'), \end{aligned} \tag{3.36}$$

which is the right answer. We can check this by working out a position space wave function. We'll start by making a change of basis[8] $|\boldsymbol{x}\rangle = \int \mathrm{d}^3q\, \phi^*_{\boldsymbol{q}}(\boldsymbol{x})|\boldsymbol{q}\rangle$, which involves expanding a position state in terms of momentum states. Using this expansion, we obtain

2. Expect the projection of the momentum basis onto the position basis to be the momentum function as a function of x.

$$\langle \boldsymbol{x}|\boldsymbol{p}\rangle = \int \mathrm{d}^3q\, \phi_{\boldsymbol{q}}(\boldsymbol{x})\langle \boldsymbol{q}|\boldsymbol{p}\rangle = \phi_{\boldsymbol{p}}(\boldsymbol{x}). \tag{3.37}$$

This is clearly okay, but rather trivial. More interesting is the case of a two-particle state

3. More complicated identity verified for two-particle states.

$$\langle \boldsymbol{p}'\boldsymbol{q}'|\boldsymbol{q}\boldsymbol{p}\rangle = \langle 0|\hat{a}_{\boldsymbol{p}'}\hat{a}_{\boldsymbol{q}'}\hat{a}^\dagger_{\boldsymbol{q}}\hat{a}^\dagger_{\boldsymbol{p}}|0\rangle. \tag{3.38}$$

Commuting, we obtain

$$\langle \boldsymbol{p}'\boldsymbol{q}'|\boldsymbol{q}\boldsymbol{p}\rangle = \delta^{(3)}(\boldsymbol{p}'-\boldsymbol{p})\delta^{(3)}(\boldsymbol{q}'-\boldsymbol{q}) \pm \delta^{(3)}(\boldsymbol{p}'-\boldsymbol{q})\delta^{(3)}(\boldsymbol{q}'-\boldsymbol{p}), \tag{3.39}$$

where we take the plus sign for bosons and minus sign for fermions. Again we can work out the position space wave function by making a change of basis $|\boldsymbol{x}\boldsymbol{y}\rangle = \frac{1}{\sqrt{2!}}\int \mathrm{d}^3p'\mathrm{d}^3q'\, \phi^*_{\boldsymbol{p}'}(\boldsymbol{x})\phi^*_{\boldsymbol{q}'}(\boldsymbol{y})|\boldsymbol{p}'\boldsymbol{q}'\rangle$ (where the factor of $\frac{1}{\sqrt{2!}}$ is needed to prevent the double counting that results from the unrestricted sums). This gives us

$$\frac{1}{\sqrt{2!}}\int \mathrm{d}^3p'\mathrm{d}^3q'\,\phi_{\boldsymbol{p}'}(\boldsymbol{x})\phi_{\boldsymbol{q}'}(\boldsymbol{y})\langle \boldsymbol{p}'\boldsymbol{q}'|\boldsymbol{p}\boldsymbol{q}\rangle = \frac{1}{\sqrt{2}}\left[\phi_{\boldsymbol{p}}(\boldsymbol{x})\phi_{\boldsymbol{q}}(\boldsymbol{y}) \pm \phi_{\boldsymbol{q}}(\boldsymbol{x})\phi_{\boldsymbol{p}}(\boldsymbol{y})\right], \tag{3.40}$$

which is the well-known expression for two-particle states.

Ch. 4. Making Second Quantization Work

Definition (What this means)

- **First quantization**: Particles behave like waves (Schrodinger's equation)
- **Second quantization**: Waves behave like particles (Creation/Annihilation Operators)

- Not clearly stated in the text but what we want to do for now is this:

Goal

Rewrite our current formalism using **states and transformation of states** into equivalent statements involving **creation and annihilation operators**.

$\Rightarrow$ Take operators and rewrite them to act on states in the **occupation number representation**.

- For example, the Hamiltonian from the previous slide.

$$\hat{H} = \int_p d^3p \; E_p \hat{a}_p{}^\dagger \hat{a}_p \tag{7}$$

- How do we do this conversion in general for an *arbitrary operator?*

4.1 Field Operators

- We have creation and annihilation operators $\hat{a}_p^\dagger$ and $\hat{a}_p$ which create and annihilate particles into particular momentum states.
- This creates particles that have a specific momentum but they will be extended in space. Why?

Proof that $\langle x | p \rangle = e^{ipx}$.

- A particle in a specific momentum state is a solution of the eigen-equation,

$$\hat{P}|p\rangle = p|p\rangle \tag{8}$$

where $\hat{P}$ is the momentum operator, p is the momentum and $|p\rangle$ is the particle state labelled by the momentum.

- Recall that:
  1. The momentum operator in position space is given by $\hat{P} = -i\frac{\partial}{\partial x}$.
  2. The wave function of the particle in position space is just the projection of its state onto an $\langle x|$ basis vector, $\psi(x) \equiv \langle x | \psi \rangle$.

- So from (8) by multiplying from the left by $\langle x|$,

$$\langle x | \hat{P} | p \rangle = p\langle x | p \rangle \tag{9}$$

$$-i\frac{\partial}{\partial x}\psi_p(x) = p\psi_p(x). \tag{10}$$

- This is a standard d.e. we've seen many times and has the solution,

$$\psi_p(x) = \langle x | p \rangle = e^{ipx}. \tag{11}$$

□

Fourier transform relation between position and momentum.

- By taking the Hermitian we get the dual formula for the wave function of a particle at a single position represented in momentum space,

$$\psi_x(p) = \langle p|x\rangle = e^{-ipx}. \tag{12}$$

- Using these two equations we find a remarkable relationship between the space and momentum representations of a general state $\Longrightarrow$ They are Fourier transforms of each other!

- Suppose we have a general state $|\alpha\rangle$. Then it's wave function in position space is give by,

$$\psi_\alpha(x) = \langle x|\alpha\rangle = \langle x|I|\alpha\rangle \tag{13}$$

$$= \langle x|\left(\sum_p |p\rangle\langle p|\right)|\alpha\rangle \tag{14}$$

$$= \sum_p \langle x|p\rangle\langle p|\alpha\rangle \tag{15}$$

$$\Rightarrow \boxed{\psi_\alpha(x) = \sum_p e^{ipx}\psi_\alpha(p)}. \tag{16}$$

- Now do the same but taking the wave function of $|\alpha\rangle$ in momentum space.

$$\psi_\alpha(p) = \langle p|\alpha\rangle = \langle p|I|\alpha\rangle \tag{17}$$

$$= \langle p| \left(\sum_x |x\rangle\langle x| \right) |\alpha\rangle \tag{18}$$

$$= \sum_x \langle p|x\rangle\langle x|\alpha\rangle \tag{19}$$

$$\Rightarrow \boxed{\psi_\alpha(p) = \sum_p e^{-ipx}\psi_\alpha(x)}. \tag{20}$$

- Comparing the two boxed equations we see the position and momentum wave functions of a general state are just Fourier transforms of each other as promised.

- This gives us a nice interpretation of Heisenberg's inequality for Gaussian wave packets (without proof here).

$$\Delta x \Delta p = 1. \tag{21}$$

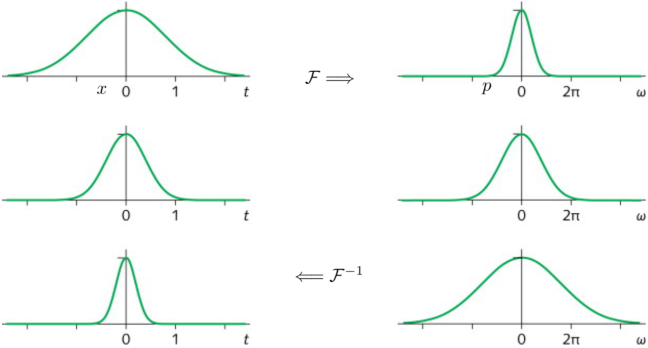


Figure: Example of the inverse relationship of the width of a Gaussian waveform under Fourier transforms.

Derivation of delta function.

- In addition to the completion of the identity and Fourier transform another formulaic trick that is often used is the delta function identities,

$$\int_{x=-\infty}^{\infty} dx \ e^{i(k-k')x} = \delta_{kk'} \tag{22}$$

and its dual

$$\sum_{k=-\infty}^{\infty} e^{ik(x-x')} = \delta(x-x'). \tag{23}$$

- The proof of these is standard undergrad but for our purposes it's better to simply see why they're true and just apply them.

- Take the sum over k version.
It says if $x \neq x'$ then the sum is zero and if $x = x'$ the sum is infinity (we're going to ignore normalization constants here and the fact its "area" is one).

- Note. The following argument will give a mathematician kittens. Always stress you are using it as a visual aid, not a proof. As physicists, though, we don't care.

Derivation of delta function.

- Now look at the argument in exponential $\sum_{k=-\infty}^{\infty} e^{ik(x-x')}$.
- Suppose $x - x' = 0$. The argument then becomes 0 and we end up with the infinite sum

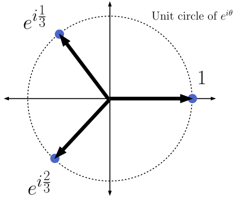
$$\sum_{k=-\infty}^{\infty} e^{0} = \sum_{k=-\infty}^{\infty} 1 = \infty \tag{24}$$

  and we get infinity.
- Take $x - x'$ to be non-zero now. The basic idea is that the sum is essentially an average of points around the unit circle and they all cancel each other to give zero.
- Suppose $x - x' = \frac{1}{3}$ for definiteness. Then as k ranges from minus infinity to infinity the summand takes on only three unique values.

$$e^{i\ 0\cdot\frac{1}{3}},\ e^{i\ 1\cdot\frac{1}{3}},\ e^{i\ 2\cdot\frac{1}{3}} \tag{25}$$

$$1,\ e^{i\frac{1}{3}},\ e^{i\ \frac{2}{3}} \tag{26}$$

- These points are shown on the unit circle in the figure below.



- Note that the (complex) sum of these three points is zero. Either take the vector sum of the three black arrows, or just consider that the origin is the centroid of the three points.

- As k in the sum of exponentials ranges over infinity only these three points are actually summed and so the entire infinite sum is zero, as expected.

- Setting $x - x'$ to any other rational number just repeats the argument. If the value is irrational then as you range over k the entire unit circle fills up and the average is still zero.

- This gives some geometric intuition to the delta function formulation. A similar argument can be made for the integral where we are now continuously summing.

Summary - Three important tools

Summary

1. Resolution of the identity.

Given a set of complete orthonormal basis vectors in dimension n (which could be infinite), $\{|i\rangle\}_{i=1}^{n}$, we have

$$I = \sum_{i=1}^{n} |i\rangle\langle i|. \tag{27}$$

We proved this last fall in the linear algebra talks for finite dimensional vector spaces,

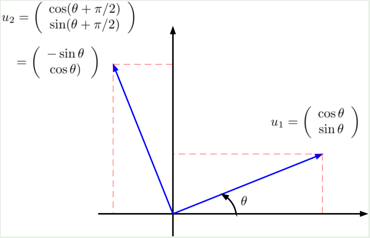
$$I = \sum_{i} u_i u_i^{\dagger}. \tag{28}$$

It holds in the infinite dimensional case of orthonormal basis functions, $\{\phi_i(x)\}_{i=1}^{\infty}$.

$$\delta(y - x) = \sum_{i} \phi_i(x)\phi_i(y)^{*}. \tag{29}$$

Example (Example Resolution of Identity - Two Dimensional Case)

- A general two-dimensional basis is shown in the figure.



- Using the basis $u_1 = (\cos\theta, \sin\theta)^T$, $u_2 = (-\sin\theta, \cos\theta)^T$, we can expand the identity as,

$$\sum_{i=1}^{2} u_i u_i^\dagger = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \end{pmatrix} + \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix} \begin{pmatrix} -\sin\theta & \cos\theta \end{pmatrix} \tag{30}$$

$$= \begin{pmatrix} c^2 & cs \\ sc & s^2 \end{pmatrix} + \begin{pmatrix} s^2 & -sc \\ -cs & c^2 \end{pmatrix} \tag{31}$$

$$= \begin{pmatrix} c^2+s^2 & cs-sc \\ sc-cs & s^2+c^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \checkmark \tag{32}$$

Example (Example Resolution of Identity - Infinite dimensional case.)

- In the infinite dimensional case of orthonormal basis functions, $\{\phi_i(x)\}_{i=1}^{\infty}$, the equivalent identity function is the Dirac delta function,

$$\delta(y-x) = \sum_{i=1}^{\infty} \phi_i(x)\phi_i(y)^*. \tag{33}$$

- We've seen two examples of an infinite set of basis functions from the eigenfunction solutions for the Hamiltonian of the infinite square well (Mike) and the quantum SHO (Matt).

- For the infinite quantum well of width $[-L/2, L/2]$ the normalized eigenfunctions are,

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin(k_n x), \text{ for n even} \tag{34}$$

$$= \sqrt{\frac{2}{L}}\cos(k_n x), \text{ for n odd} \tag{35}$$

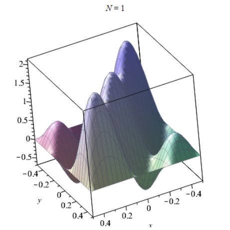
where $k_n = \frac{n\pi}{L}$.

- So we have the explicit resolution of the identity (function),

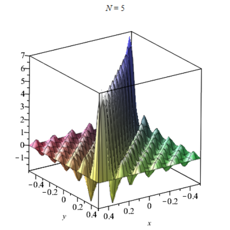
$$\delta(x-y) = \frac{2}{L}\sum_{n=2,4,\dots} \sin(\frac{n\pi}{L}x)\cdot\sin(\frac{n\pi}{L}y) + \frac{2}{L}\sum_{n=1,3,\dots} \cos(\frac{n\pi}{L}x)\cdot\cos(\frac{n\pi}{L}y). \tag{36}$$

Example (Example Resolution of Identity - Infinite dimensional case, cont'd.)

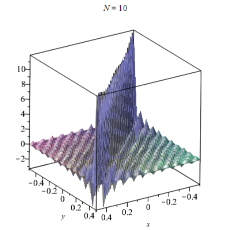
- It's interesting to plot this sum for finite terms to see how it approaches the delta function in the limit of the number of terms going to infinity.



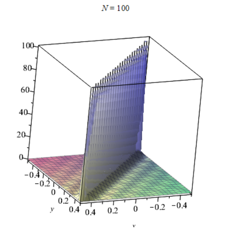
(a) $N = 1$



(b) $N = 5$



(c) $N = 10$



(d) $N = 100$

Summary, cont'd

2. Fourier dual relationship between position and momentum.

$$\psi_p(x) = \boxed{\langle x | p \rangle = e^{ipx}} \tag{37}$$

$$\psi_x(p) = \boxed{\langle p | x \rangle = e^{-ipx}}. \tag{38}$$

For a general state $|\alpha\rangle$,

$$\psi_\alpha(x) = \sum_p e^{ipx} \psi_\alpha(p) \tag{39}$$

$$\psi_\alpha(p) = \sum_x e^{-ipx} \psi_\alpha(x). \tag{40}$$

Summary, cont'd

3. **Dual Fourier/exponential decompositions of the identity.** We have the dual continuous in position and discrete in momentum exponential decompositions of the identity,

$$\int_{x=-\infty}^{\infty} dx\ e^{i(k-k')x} = \delta_{kk'} \tag{41}$$

$$\sum_{k=-\infty}^{\infty} e^{ik(x-x')} = \delta(x-x'). \tag{42}$$

Derivation of field operators.

- We can now use this to write a creation operator that creates a particle at a single *position*.
  This particle will be in a state $|x\rangle$ for some particular position x.
- We start with the expression for a particle in a momentum state $|p\rangle$ written using the creation operator on the vacuum state, $|p\rangle = \hat{a}_p^\dagger|0\rangle$.
- Then use the resolution of the identity in terms of momentum states, $I = \sum_p |p\rangle\langle p|$.
- So we can write the position state as,

$$|x\rangle = I|x\rangle = \sum_p |p\rangle \underbrace{\langle p| \cdot |x\rangle} \tag{43}$$

$$= \sum_p \langle p|x\rangle|p\rangle \tag{44}$$

$$= \sum_p \langle p|x\rangle \hat{a}_p^\dagger|0\rangle \tag{45}$$

$$= \underbrace{\sum_p e^{-ipx}\hat{a}_p^\dagger}|0\rangle \tag{46}$$

$$\equiv \hat{\psi}^\dagger(x)|0\rangle \tag{47}$$

- We have defined the creation operator,

$$\hat{\psi}^\dagger(x) = \sum_p e^{-ipx} \hat{a}_p^\dagger, \tag{48}$$

that creates a particle at position x and the corresponding annihilation operator,

$$\hat{\psi}(x) = \sum_p e^{ipx} \hat{a}_p. \tag{49}$$

that annihilates a particle at position x.

- Note the position and momentum creation/annihilation operators are essentially Fourier transforms of each other.

- Let's do some consistency checks.

- If the state $|\psi\rangle = \hat{\psi}^\dagger(x)|0\rangle$ is a particle at a particular location, then
  1. There should only be one particle (use the number operator).
  2. It should be at x (use projection).

Observation 1: There should only be one particle

- For the first, expand out the created state as

$$|\psi\rangle = \hat{\psi}^\dagger(x)|0\rangle = \sum_p e^{-ipx}\hat{a}_p^\dagger|0\rangle. \tag{50}$$

- For the total number of particles in this state we can use the number operator $\hat{n}_q = \hat{a}_q^\dagger \hat{a}_q$ (which measures the number of particles in state p) and then sum over all momentum states. Consider

$$\sum_q \hat{n}_q|\psi\rangle = \sum_{qp} \hat{a}_q^\dagger \hat{a}_q \hat{a}_p^\dagger|0\rangle e^{-ipx}. \tag{51}$$

- Now use the fact that $\hat{a}_q\hat{a}_p^\dagger|0\rangle = \delta_{pq}|0\rangle$. Why?

- Substituting this in gives us

$$\sum_q \hat{n}_q|\psi\rangle = \sum_{qp} e^{-ipx}\hat{a}_q^\dagger\delta_{pq}|0\rangle = \sum_p e^{-ipx}\hat{a}_p^\dagger|0\rangle, \tag{52}$$

which is just $|\psi\rangle$ from (50).

- So $\sum_q \hat{n}_q|\psi\rangle = |\psi\rangle$ and there is just a single particle. ✔.

Observation 2: The particle should be localized at a single position.

- Let's take our created state, $|\psi\rangle = \hat{\psi}^\dagger(x)|0\rangle$, and find its overlap with a position state $|y\rangle$, i.e., we project state $|\psi\rangle$ onto $|y\rangle$.
  $\Rightarrow$ We expect this to be zero unless $y = x$. Why?

- We calculate the overlap as follows,

$$\langle y|\psi\rangle = \langle y|\hat{\psi}^\dagger(x)|0\rangle \tag{53}$$

$$= \langle y|\sum_p e^{-ipx}\hat{a}_p^\dagger|0\rangle \tag{54}$$

$$= \sum_p e^{-ipx}\langle y|p\rangle \tag{55}$$

$$= \sum_p e^{-ipx}e^{ipy} \tag{56}$$

$$= \sum_p e^{ip(y-x)} \tag{57}$$

$$= \delta(y-x) \tag{58}$$

- So we correctly have zero overlap of the created state with $|y\rangle$ unless $y = x$. ✓

- We can similarly work out the commutation relations between the creation and annihilation operators.

Check: What are the commutation relations between the position creation and annihilation operators?

Example 4.2

The field operators satisfy commutation relations. For example

$$\left[\hat{\psi}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{y})\right] = \frac{1}{\mathcal{V}} \sum_{\boldsymbol{pq}} \mathrm{e}^{\mathrm{i}(\boldsymbol{p}\cdot\boldsymbol{x} - \boldsymbol{q}\cdot\boldsymbol{y})} [\hat{a}_{\boldsymbol{p}}, \hat{a}^{\dagger}_{\boldsymbol{q}}], \tag{4.13}$$

and using $[\hat{a}_{\boldsymbol{p}}, \hat{a}^{\dagger}_{\boldsymbol{q}}] = \delta_{\boldsymbol{pq}}$ we have that

$$\left[\hat{\psi}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{y})\right] = \frac{1}{\mathcal{V}} \sum_{\boldsymbol{pq}} \mathrm{e}^{\mathrm{i}(\boldsymbol{p}\cdot\boldsymbol{x} - \boldsymbol{q}\cdot\boldsymbol{y})} \delta_{\boldsymbol{pq}} = \frac{1}{\mathcal{V}} \sum_{\boldsymbol{p}} \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})} = \delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}), \tag{4.14}$$

where the last equality follows from eqn 4.6. By the same method you can show

$$\left[\hat{\psi}^{\dagger}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{y})\right] = \left[\hat{\psi}(\boldsymbol{x}), \hat{\psi}(\boldsymbol{y})\right] = 0. \tag{4.15}$$

These results are for boson operators, but we can derive analogous results for fermion operators:

$$\begin{aligned} \left\{\hat{\psi}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{y})\right\} &= \delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}), \\ \left\{\hat{\psi}^{\dagger}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{y})\right\} &= \left\{\hat{\psi}(\boldsymbol{x}), \hat{\psi}(\boldsymbol{y})\right\} = 0. \end{aligned} \tag{4.16}$$

4.2 How to Second Quantize an Operator

- We have second quantized states into expressions involving creation and annihilation operators.

- We also need to do the same for *operators*.
  They allow us to calculate:
  i.) Time evolution of states, $|\psi(t)\rangle \sim |\psi(0)\rangle \cdot e^{i\hat{H}t}$.
  ii.) Values (and probabilities) of physical measurements, $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$.

- Note we've already seen the number operator in this second quantized form, $\hat{n}_p = \hat{a}_p^\dagger \hat{a}_p$.
  We want to be able to do this in general.

- Given some operator $\hat{A}$ and a basis $\{|i\rangle\}$, we can use (again!) the resolution of the identity, $I = \sum_i |i\rangle\langle i|$, twice to write,

$$\hat{A} = \sum_{ij} |i\rangle\langle i| \cdot \hat{A} \cdot |j\rangle\langle j| \tag{59}$$

$$= \sum_{ij} |i\rangle \cdot \underbrace{\langle i|\hat{A}|j\rangle}_{\text{scalar } A_{ij}} \cdot \langle j| \tag{60}$$

$$= \sum_{ij} A_{ij} |i\rangle\langle j| \tag{61}$$

- And we have the standard expansion of an operator in terms of its matrix components in a particular basis, $A_{ij} = \langle i|\hat{A}|j\rangle$
- Example 4.3 on pages 39–41 give a derivation for the corresponding expansion in terms of creation and annihilation operators,

$$\boxed{\hat{A} = \sum_{ij} A_{ij}\hat{a}_i^\dagger \hat{a}_j.} \tag{62}$$

- It uses the *same* matrix elements A_{ij} as the basis expansion in (61).
- The creation operator $\hat{a}_i^\dagger$ creates a particle in the state $|i\rangle$ while the annihilation operator $\hat{a}_j$ destroys a particle in the state $|j\rangle$.
- This naturally handles multiple particles.

This is remarkable!

Given a standard first quantized operator in terms of a basis we can immediately write down it's second quantized version in terms of creation and annihilation operators. No work is required!

$$\sum_{ij} A_{ij}|i\rangle\langle j| \Longrightarrow \sum_{ij} A_{ij}\hat{a}_i^\dagger \hat{a}_j \tag{63}$$

The interpretation of (62) is “beautifully simple.”

$$\boxed{\hat{A} = \sum_{ij} A_{ij} \hat{a}_i^\dagger \hat{a}_j.}$$

The operator $\hat{A}$ is a sum over all processes in which you use $\hat{a}_j$ to remove a single particle in state $|j\rangle$, multiply it by the matrix element A_{ij} , and then use $\hat{a}_i^\dagger$ to place that particle into a final state $|i\rangle$. This operator A thus describes all possible single-particle processes that can occur and operates on a many-particle state. See figure below.

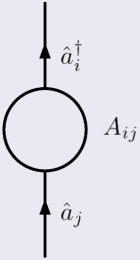


Figure: A process represented by the operator $\hat{A}$.

We can now do some very cool things.

Example (4.4 (i) Second Quantized Resolution of the Identity)

- The most simple and trivial example of an operator on states is the identity operator, I.
  It simply leaves the state in its current form, $I|\psi\rangle = |\psi\rangle$.
- What is it's second quantized version in terms of creation and annihilation operators?
- We can (yet again!) use the resolution of the identity in some basis,

$$I = \sum_i |i\rangle\langle i|. \tag{64}$$

- This is a special case of the form $\sum_{ij} A_{ij}|i\rangle\langle j|$ with $A_{ij} = \delta_{ij}$.
- This results in the second quantized upgrade,

$$\sum_i \hat{a}_i^\dagger \hat{a}_i = \hat{n}, \tag{65}$$

  which is just our number operator that counts one for every particle in the state it operates on. So, $I \overset{\text{2nd quantization}}{\Longrightarrow} \hat{n}$.

Example (4.4 (ii) Second Quantized Momentum Operator)

- The usual momentum operator can be written $\hat{A} = \hat{p} = \sum_p p|p\rangle\langle p|$ which immediately upgrades to,

$$\hat{p} = \sum_p p\hat{a}_p^\dagger \hat{a}_p = \sum_p p\hat{n}_p \tag{66}$$

  So, $\hat{p} \overset{\text{2nd quantization}}{\Longrightarrow} \sum_p p\hat{n}_p$.

- In general we can second quantize a *function* of the momentum operator $\hat{A} = f(\hat{p})$ as,

$$\hat{A} = \sum_p f(p)\hat{a}_p^\dagger \hat{a}_p = \sum_p f(p)\hat{n}_p. \tag{67}$$

  Remember the talk I gave on eigen-decompositions last fall and how you can take a function of a matrix (i.e., a linear operator) by just taking the function on its eigenvalues? That is what is happening here.

- For a free particle its Hamiltonian is given by $\hat{H} = \hat{p}^2/2m$. Its corresponding second quantized form is then,

$$\hat{H} = \sum_p \frac{p^2}{2m}\hat{n}_p. \tag{68}$$

What's going on? Why are we doing this?

- The "big idea" here is that we are rewriting our notation:
  $\Rightarrow$ Instead of working with states and their labels we are replacing them with operators acting on the vacuum state.

- It's completely equivalent to what we've been doing up until now. It's just a reformulation, but ...

  It opens the door to dealing with problems involving non-constant number of particles and particles changing into other particles when they interact.

- Plus, the occupancy number notation has the property of particles being indistinguishable *built in*.

- We don't have to use the symmetric and anti-symmetric forms of wave functions any longer. The commutation relations of the creation and annihilation operators enforce the particular symmetry (bosons vs. fermions) we are using. (*I think. Matt?)*

Example (Example of equivalence of notations.)

- Let's check their equivalence using the identity operator using a basis $\{|i\rangle\}$.
- We have $I = \sum_i |i\rangle\langle i| \xrightarrow{\text{2nd quantization}} \sum_i \hat{a}_i^\dagger \hat{a}_i \equiv \hat{n}$.
- And $|\psi\rangle = \sum_i \psi_i |i\rangle \xrightarrow{\text{2nd quantization}} \sum_i \psi_i \hat{a}_i^\dagger |0\rangle$.

Old State Formulation

$$\begin{aligned} I \cdot |\psi\rangle &= \sum_i |i\rangle\langle i| \cdot |\psi\rangle \\ &= \sum_i |i\rangle \cdot \psi_i \\ &= |\psi\rangle \end{aligned}$$

New Operator Formulation

$$\begin{aligned} I \cdot |\psi\rangle &= \sum_i \hat{a}_i^\dagger \hat{a}_i \cdot \sum_j \psi_j \hat{a}_j^\dagger |0\rangle \\ &= \sum_{ij} \psi_j \hat{a}_i^\dagger \underbrace{\hat{a}_i \hat{a}_j^\dagger |0\rangle} \\ &= \sum_{ij} \psi_j \hat{a}_i^\dagger \delta_{ij} |0\rangle \\ &= \sum_i \psi_i \hat{a}_i^\dagger |0\rangle \\ &= \sum_i \psi_i |i\rangle = |\psi\rangle \end{aligned}$$

They are completely equivalent formalisms.

Homework: Do the same for a general operator $B = \sum_i b_i |i\rangle\langle i|$ where the b_i are the operator's eigenvalues.

Example (4.4 (iii) Second Quantized Functions of *Position*)

- What happens if our operator is a function of $\hat{x}$, rather than $\hat{p}$?
  For example a potential, $V(x)$.
- The equation $\hat{A} = \sum_{ij} A_{ij} \hat{a}_i^\dagger \hat{a}_j$ is valid even if our states $|i\rangle$ and $|j\rangle$ are position states.
- The creation and annihilation operators are now just the field operators $\hat{\psi}^\dagger_(x)$ and $\hat{\psi}_(x)$, and the sum over momentum values becomes an integral over space.
- We then can write down our second-quantized operator $\hat{V}$ as,

$$\hat{A} = f(\hat{p}) = \sum_p f(p) \hat{a}_p^\dagger \hat{a}_p \tag{69}$$

$$\Downarrow$$

$$\hat{V} = f(\hat{x}) = \int_x d^3x \; V(x) \hat{\psi}^\dagger(x) \hat{\psi}(x). \tag{70}$$

Example (4.4 (iii) Second Quantized Functions of *Position*, cont'd)

- Recall the Fourier transform relation between position and momentum creation operators we derived earlier,

$$\hat{\psi}^{\dagger}(x) = \sum_{p} e^{-ipx}\hat{a}_{p}^{\dagger}, \quad \hat{\psi}(x) = \sum_{p} e^{ipx}\hat{a}_{p} \tag{71}$$

.

- Substituting into $\hat{V} = \int_x d^3x \; V(x)\hat{\psi}^{\dagger}(x)\hat{\psi}(x)$ we get,

$$\hat{V} = \int_x d^3x \; V(x) \cdot \sum_{p_1} e^{-ip_1x}\hat{a}_{p_1}^{\dagger} \cdot \sum_{p_2} e^{ip_2x}\hat{a}_{p_2} \tag{72}$$

$$= \sum_{p_1 p_2} \hat{a}_{p_1}^{\dagger}\hat{a}_{p_2} \int_x d^3x \; V(x) e^{-i(p_1-p_2)x} \tag{73}$$

$$\boxed{\hat{V} = \sum_{p_1 p_2} \tilde{V}_{p_1-p_2}\hat{a}_{p_1}^{\dagger}\hat{a}_{p_2}} \tag{74}$$

where $\tilde{V}_p = \int_x d^3x \; V(x)e^{-ipx}$ is the standard Fourier transform of $V(x)$.

- Note that the operator $\hat{V}$ is no longer diagonal in terms of momentum. The $\hat{a}$ operators create and annihilate particles with different momenta.

Example (4.4 (iii) Second Quantized Functions of *Position*, cont'd)

- We can think of this term as representing a process of an incoming particle with momentum p_2 which interacts with a potential field (represented by $V_{p_1-p_2}$ and then leaves again with momentum p_1.

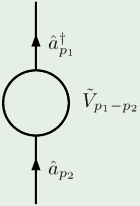


Figure: A process represented by eqn (74). The sequence of events is: annihilate a particle with momentum p_2, count the potential energy $\tilde{V}_{p_1-p_2}$, create a particle with momentum p_1.

Summing over all momentum states involves repeating this counting process which can be imagined as counting sheep crossing through a gate (annihilate a sheep on the left-hand side of the gate, count the scalar potential term in the sum, create a sheep again on the right-hand side of the gate, now move on to the next sheep ...).

Example (4.5 A concrete toy example — influence of a potential.)

- Look at the influence of the potential on a simple system described by a Hamiltonian,

$$\hat{H} = \underbrace{E_0 \sum_p \hat{d}_p^\dagger \hat{d}_p}_{\hat{H}_0} \underbrace{- \frac{V}{2} \sum_{p_1 p_2} \hat{d}_{p_1}^\dagger \hat{d}_{p_2}}_{\hat{V}} \tag{75}$$

  Here $\hat{H}_0$ is the standard non-interacting baseline Hamiltonian.
  $\hat{V}$ is a kind of interaction term whose influence is modulated by the value V.

- We put two constaints on this system to start with,
  1. There are only three momentum allowed, so states are given in a basis $|n_{p_1}, n_{p_2}, n_{p_3}\rangle$.
  2. There is only a single particle in the system, so the basis is given by $|100\rangle, |010\rangle, |001\rangle$.

- Question: What would the basis be for two particles?
  The dimension of the space we would be operating in?

- Equation (75) looks rather messy.
  How do we work with it? How do we interpret it? What does it mean?

Example (4.5 A concrete toy example — influence of a potential, cont'd)

- Remember this is an operator acting in a vector space spanned by $|100\rangle, |010\rangle, |001\rangle$.

- We can represent this operator as a matrix H by calculating its matrix elements, $H_{IJ} = \langle I\,|\,\hat{H}\,|\,J\rangle$, where I, J runs over the basis vectors.

- Taking the basis in the order given we have $H_{11} = \langle 100\,|\,\hat{H}\,|\,100\rangle$, $H_{23} = \langle 010\,|\,\hat{H}\,|\,001\rangle$, etc.

$$H = \begin{array}{c|ccc} & |100\rangle & |010\rangle & |001\rangle \\ \hline \langle 100| & \langle 100\,|\,\hat{H}\,|\,100\rangle & \cdots & \\ \langle 010| & \langle 010\,|\,\hat{H}\,|\,100\rangle & \cdots & \\ \langle 001| & \vdots & & \end{array} \tag{76}$$

- How do we calculate these inner products that make up the matrix elements?

- Look at a particular term from the potential operator operating on a basis ket,

$$\hat{V}|001\rangle = \sum_{p_1 p_2} \hat{d}^\dagger_{p_1} \hat{d}_{p_2} \cdot |001\rangle \tag{77}$$

- Note this sum comprises $3 \times 3 = 9$ terms. And this has to be done for each inner product.

Example (4.5 A concrete toy example — influence of a potential, cont'd)

- Letting the two p indices range over their values we get,

$$\begin{aligned} \hat{d}_1^\dagger \hat{d}_1 |100\rangle &= |100\rangle & \hat{d}_2^\dagger \hat{d}_1 |100\rangle &= |010\rangle & \hat{d}_3^\dagger \hat{d}_1 |100\rangle &= |001\rangle \\ \hat{d}_1^\dagger \hat{d}_2 |100\rangle &= 0 & \hat{d}_2^\dagger \hat{d}_2 |100\rangle &= 0 & \hat{d}_3^\dagger \hat{d}_2 |100\rangle &= 0 \\ \hat{d}_1^\dagger \hat{d}_3 |100\rangle &= 0 & \hat{d}_2^\dagger \hat{d}_3 |100\rangle &= 0 & \hat{d}_3^\dagger \hat{d}_3 |100\rangle &= 0 \end{aligned} \tag{78}$$

- This gives us,

$$\sum_{p_1 p_2} \hat{d}_{p_1}^\dagger \hat{d}_{p_2} \cdot |001\rangle = |100\rangle + |010\rangle + |001\rangle, \tag{79}$$

  which we can now use to fill in the first column of the matrix elements for $\hat{V}$.

- Hitting this sequentially on the left by the basis bra's we get

$$\langle 100 | \Sigma | 100\rangle = \langle 100| \cdot \Big(\underbrace{|100\rangle}_{=1} + \underbrace{|010\rangle}_{=0} + \underbrace{|001\rangle}_{=0} \Big) = 1 \tag{80}$$

$$\langle 010 | \Sigma | 100\rangle = \langle 010| \cdot \Big(|100\rangle + \underbrace{|010\rangle}_{=1} + |001\rangle \Big) = 1 \tag{81}$$

$$\langle 001 | \Sigma | 100\rangle = \langle 001| \cdot \Big(|100\rangle + |010\rangle + \underbrace{|001\rangle}_{=1} \Big) = 1 \tag{82}$$

Example (4.5 A concrete toy example — influence of a potential, cont'd)

- So the first column of the matrix elements of $\hat{V}$ are all ones.
- Working similarly you can show the remaining elements of the V matrix are also all ones.
- And the matrix H_0 is just the diagonal identity matrix.
- Putting this all together we find that,

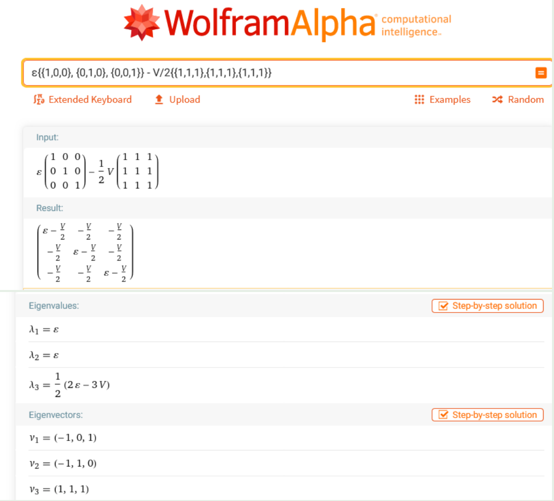
$$H = E_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{V}{2} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \tag{83}$$

- Given this Hamiltonian we can now calculate the values of energy we would measure from this systems. The corresponding eigenvectors are the states the system would fall into after the measurement.
- Note that H depends on the two parameters, E_0 and V. So we have to do the calculation algebraically.

Example (4.5 A concrete toy example — influence of a potential, cont'd)

- For even such a simple small system this is tedious and error prone.
  $\Longrightarrow$ Use a computer algebra system, e.g., Maple, Mathematica, Maxima.

- Also available for free is Wolfram Alpha, an online CAS useful for small problems.



Example (4.5 A concrete toy example — influence of a potential, cont'd)

- So we have the eigenvalues, or energy levels, and corresponding eigenvecotrs,

$$\begin{array}{lcl} E_0 - \frac{3V}{2} & \to & (1,1,1) \\ E_0 & \to & (-1,1,0) \\ E_0 & \to & (-1,0,1) \end{array} \tag{84}$$

- The ground or lowest level state is just an equal superposition of all three basis vectors, i.e., a superposition of a particle in each of the three possible momenta. $\Longrightarrow \frac{1}{\sqrt{3}}\left(|100\rangle + |010\rangle + |001\rangle\right)$

- The other two eigen-states are a superposition of a state in two momenta.

- Question: What changes if we allow two particles now? Or more? Or more momenta, p_i?
  $\Longrightarrow$ Do demo.

Example (4.5 A concrete toy example — influence of a potential, cont'd)

- Finally, given that our potential is,

$$\hat{V} = -\frac{V}{2} \sum_{p_1 p_2} \hat{d}^\dagger_{p_1} \hat{d_{p_2}}, \tag{85}$$

we know the general formulation takes the form,

$$\hat{V} = \sum_{p_1 p_2} \tilde{V}_{p_1 - p_2} \hat{a}^\dagger_{p_1} \hat{a_{p_2}} \tag{86}$$

where $\tilde{V}_p = \int_x d^3x \; V(x) e^{-ipx}$ is the standard Fourier transform of $V(x)$.

- We can ask what does the potential look like in space, as a function of x? That is, $V(x)$. This is what we are used to seeing.

- Invert the Fourier transform to get,

$$V(x) \sim \sum_p V_p e^{ipx}. \tag{87}$$

- In our case V_p is just a constant, $-\frac{V}{2}$.

Example (4.5 A concrete toy example — influence of a potential, cont'd)

- Recall that for particles in a box they are constrained to having a momentum of $p_m = \frac{2\pi m}{L}$, where L is the length of the box and m and integer.
- For the three momenta here let's take the values of $m = -1, 0, 1$, giving $p_m = -\frac{2\pi}{L}, 0, \frac{2\pi}{L}$.
- Substituting into the exponential sum for $V(x)$ and simplifying we get,

$$V(x) \sim -\frac{V}{2}\left(e^{-2\pi ix/L} + 1 + e^{2\pi ix/L}\right) = -\frac{V}{2}\left(1 + 2\cos\frac{2\pi x}{L}\right). \tag{88}$$

Setting $V = 1$ and $L = 1$ we can plot $V(x)$ to get,

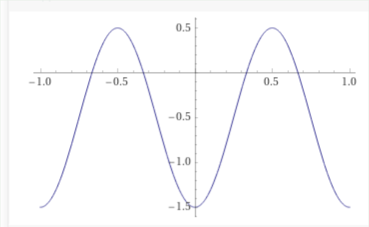


Figure: $V(x)$

Example (4.6 Second quantization of wave function.)

- What is the equivalent of the probability density of the wave function in second-quantized language?

Example 4.6

1.) What is the equivalent of the probability density of the wave function in second-quantized language? The answer is that the number density of particles at a point $\boldsymbol{x}$ is described by the **number density operator** $\hat{\rho}(\boldsymbol{x})$ given by

$$\begin{aligned} \hat{\rho}(\boldsymbol{x}) &= \hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}(\boldsymbol{x}) \\ &= \frac{1}{\mathcal{V}} \sum_{\boldsymbol{p}_1 \boldsymbol{p}_2} \left[\mathrm{e}^{-\mathrm{i}(\boldsymbol{p}_1 - \boldsymbol{p}_2)\cdot \boldsymbol{x}} \right] \hat{a}^\dagger_{\boldsymbol{p}_1} \hat{a}_{\boldsymbol{p}_2}. \end{aligned} \tag{4.41}$$

2.) This operator enables us to write the potential energy operator for a single particle in an external potential as

$$\hat{V} = \int \mathrm{d}^3x\, V(\boldsymbol{x})\hat{\rho}(\boldsymbol{x}). \tag{4.42}$$