Part One

Free Fields

Like a bird on a wire,
like a drunk in midnight choir,
I have tried in my way to be free.
Sung by Joe Cocker
Lyrics by Leonard Cohen

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Scalars: Spin 0 Fields

..if I look back at my life as a scientist and a teacher, I think the most important and beautiful moments were when I say, "ah-hah, now I see a little better" … this is the joy of insight which pays for all the trouble one has had in this career.

Victor F. Weisskopf
Quarks, Quasars, and Quandaries

3.0 Preliminaries

This chapter presents the most fundamental concepts in the theory of quantum fields, and contains the very essence of the theory. Master this chapter, and you are well on your way to mastering that theory.

3.0.1 Background

Seeking a relativistic quantum theory?

Early efforts to incorporate special relativity into quantum mechanics started with the non-relativistic Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\phi = H\phi \qquad \text{where } H = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\nabla^2 + V\,, \tag{3-1}$$

Try relativistic Hamiltonian in Schrödinger equation

and attempted to find a relativistic, rather than non-relativistic, form for the Hamiltonian H.[1] One might guess that approach would lead to a valid relativistic Schrödinger equation. This is, in essence, true but there is one problem, as we will see below.

In special relativity, the 4-momentum vector is Lorentz covariant, meaning its length in 4D space is invariant. For a free particle (i.e., $V = 0$),

Relativistic energy E

$$p^\mu p_\mu = m^2c^2 = g_{\mu\nu}p^\mu p^\nu = \begin{bmatrix} E/c & p^1 & p^2 & p^3 \end{bmatrix}\begin{bmatrix} E/c \\ -p^1 \\ -p^2 \\ -p^3 \end{bmatrix} \rightarrow \frac{E^2}{c^2} = \mathbf{p}^2 + m^2c^2\,. \tag{3-2}$$

Relativistic E → relativistic operator H

Changing dynamical variables over to operators (as happens in quantization), i.e.,

$$E \rightarrow H \qquad \text{and} \qquad p^i \rightarrow -i\hbar\partial_i\,, \tag{3-3}$$

one finds, from the RHS of (3-2),

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[1] Actually, Schrödinger first attempted to find a wave equation that was relativistic and came up with what later came to be known as the Klein-Gordon equation, which we will study in this chapter. He discarded it because of problems discussed later on herein, and because it gave wrong answers for the hydrogen atom. Shortly thereafter, he deduced the non-relativistic Schrödinger equation we are familiar with. Some time afterwards, other researchers then tried to "relativize" that equation, as discussed herein.

$$H = \sqrt{-\hbar^2 c^2 \partial_i \partial_i + m^2 c^4} \,, \tag{3-4}$$

Bad news: Relativistic H has square root of a differential operator

seemingly the only form a relativistic Hamiltonian could take. Unfortunately, taking the square root of terms containing a derivative is problematic, and difficult to correlate with the physical world.

The solution to the problem of finding a relativistic Schrödinger equation has been found, however, and as we will see in the next three chapters, turns out to be different for different spin types. This was quite unexpected at first, but has since become a cornerstone of relativistic quantum theory. (See first row of Wholeness Chart 1-2 in Chap. 1, pg. 7.)

But answer has been found, as we will see

Particles with zero spin, such as π-mesons (pions) and the famous Higgs boson, are known as scalars, and are governed by one particular relativistic Schrödinger equation, deduced by (after Schrödinger, actually), and named after, Oscar Klein and Walter Gordon. Particles with ½ spin, such as electrons, neutrinos, and quarks, and known as spinors, by a different relativistic Schrödinger equation, discovered by Paul Dirac. And particles with spin 1, such as photons and the W's and Z's that carry the weak charge, and known as vectors, by yet another relativistic Schrödinger equation, discovered by Alexandru Proça. The Proça equation reduces, in the massless (photon) case, to Maxwell's equations.

Each spin type has its own relativistic wave equation

We will devote a separate chapter to each of these three spin types and the wave equation associated with each. We begin in this chapter with scalars.

3.0.2 Chapter Overview

RQM first,

RQM overview (scalars)

where we will look at

- deducing the Klein-Gordon equation, the first relativistic Schrödinger equation, using the relativistic H^2,
- solutions (which are states = wave functions) to the Klein-Gordon equation,
- probability density and its connection to the funny normalization constant in the solutions, and
- the problem with negative energies in the relativistic solutions.

Then QFT,

QFT overview (scalars)

- using the classical relativistic $\mathcal{L}$ (Lagrangian density) for scalar fields, and the Legendre transformation to get $\mathcal{H}$ (Hamiltonian density),
- from $\mathcal{L}$ and the Euler-Lagrange equation, finding the same Klein-Gordon equation, with the same mathematical form for the solutions, but this time the solutions are fields, not states,
- from 2^{nd} quantization, finding the commutation relations for QFT,
- determining relevant operators in QFT: $H = \int \mathcal{H}\, d^3x$, number, creation/destruction, etc.,
- showing this approach avoids negative energy states,
- seeing how the vacuum is filled with quanta of energy $\frac{1}{2}\hbar\omega$,
- deriving other operators (probability density, 3-momentum, charge) and
- picking up relevant loose ends (scalars = bosons, Fock (multiparticle) space).

And then,

- seeing quantum fields in a different light, as harmonic oscillators.

With finally, and importantly,

- finding the Feynman propagator, the mathematical expression for virtual particles.

Free (no force) Fields

In this chapter, as well as Chaps. 4 (spin ½) and 5 (spin 1), we will deal only with fields/particles that are not interacting, i.e., feel no force = "free". Thus, we will take potential energy $V = 0$. In Chap. 7, which begins Part 2 of the book, we will begin to investigate interactions.

We study free (no interactions) case first

3.1 Relativistic Quantum Mechanics: A History Lesson

3.1.1 Two Possible Routes to RQM

Recall from Chaps. 1 and 2, that 1^{st} quantization, for both non-relativistic and relativistic particle theories, entails i) using the classical form of the Hamiltonian as the quantum form of the

Hamiltonian, and ii) changing Poisson brackets to commutators. We recall also from Prob. 6 of Chap. 1 that non-commutation of dynamical variables means those variables are operators (because ordinary numbers commute.) For example,

Non-commutating variables must be operators

$$\left[p^i , x^j \right] = -i\hbar \delta_i^{\ j} \quad \xleftrightarrow{\text{equivalent}} \quad p^i = -i\hbar \partial_i \tag{3-5}$$

as the RHS above is the only form that satisfies the LHS, and it is an operator.

One might expect that this is the route we would follow to obtain RQM, i.e., 1st quantization of relativistic classical particle theory. However, historically, it was done differently. That is, RQM was first extrapolated from NRQM, not from classical theory. As illustrated in Fig. 3-1, it can be done either way.

In this book, to save space and time, we will only show one of these paths, the historical one represented by the lowest arrow in Fig. 3-1.

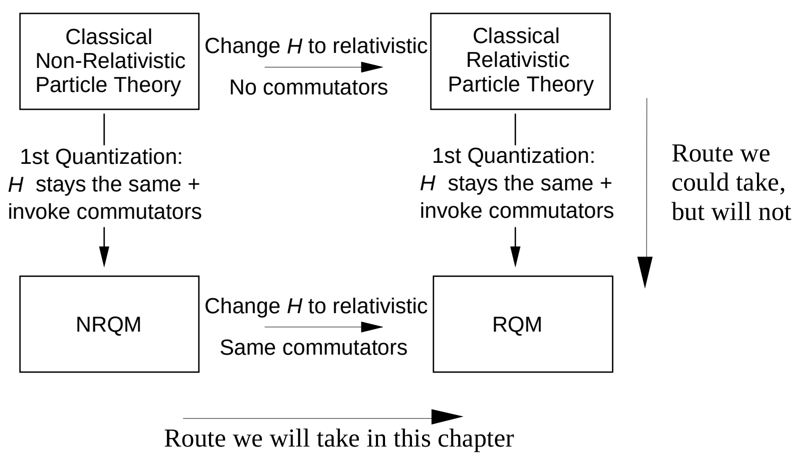

Figure 3-1. Different Routes to Relativistic Quantum Mechanics

3.1.2 Deducing the Klein-Gordon Equation

As we saw in Sect. 3.0.1, when we try to use a relativistic Hamiltonian in the Schrödinger equation, we have the problem of the partial derivative operator (see (3-4)) being under a square root sign. So, rather than use *H*, Klein and Gordon, in 1927, did the next best thing. They used H^2 instead. That is, they squared the operators (operate on each side twice rather than once) in the original Schrödinger equation (3-1) and thus from (3-2), obtained

Let's square operators on both sides of Schrödinger eq

$$\left(i\hbar \frac{\partial}{\partial t} \right)\left(i\hbar \frac{\partial}{\partial t} \right)\phi = H^2 \phi = \left(\mathbf{p}_{oper}^2 c^2 + m^2 c^4 \right)\phi , \tag{3-6}$$

Then use operator form for H^2

which becomes from the square of (3-4)

$$-\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t^2}\phi = \left(-\hbar^2 \frac{\partial}{\partial X_i}\frac{\partial}{\partial X_i} + m^2 c^2 \right)\phi \;\rightarrow\; -\frac{\partial}{\partial x^0}\frac{\partial}{\partial x_0}\phi = \left(\frac{\partial}{\partial x^i}\frac{\partial}{\partial x_i} + \underbrace{\frac{m^2 c^2}{\hbar^2}}_{\mu^2} \right)\phi . \tag{3-7}$$

To get the Klein-Gordon equation

Re-arranging, we have the Klein-Gordon equation (expressed in two equivalent ways with slightly different notation)

$$\left(\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x_\mu} + \mu^2 \right)\phi = 0 \quad \text{or} \quad \left(\partial_\mu \partial^\mu + \mu^2 \right)\phi = 0 , \qquad \mu^2 = \frac{m^2 c^2}{\hbar^2}\left(= m^2 \text{ in nat. units} \right). \tag{3-8}$$

As noted in Chap. 2, Prob. 4, the operation $\partial_\mu \partial^\mu = \partial^\mu \partial_\mu$ is called the d'Alembertian operator, and is the 4D Minkowski coordinates analogue of the 3D Laplacian operator $\partial_i \partial_i = \partial^i \partial^i$ of Cartesian coordinates.

In 1934, Pauli and Weisskopf [1] showed that the Klein-Gordon equation specifically describes a spin-0 (scalar) particle. This should become evident to us as we study the Dirac and Proça equations, for spin ½ and spin 1, later on, and compare them to the Klein-Gordon equation.

Klein-Gordon equation is specifically for scalars

3.1.3 The Solutions to the Klein-Gordon Equation

A solution set to (3-8), readily checked by substitution into (3-8) (which is good practice when using contravariant/covariant notation), is

$$\phi(x) = \sum_{n=1}^{\infty} \frac{1}{\sqrt{2VE_n / \hbar}} \left(A_n e^{-\frac{i}{\hbar}(E_n t - \mathbf{p}_n \bullet \mathbf{x})} + \underbrace{B_n^\dagger e^{\frac{i}{\hbar}(E_n t - \mathbf{p}_n \bullet \mathbf{x})}}_{\text{absent in NRQM}} \right), \qquad (3\text{-}9)$$

Solutions to Klein-Gordon equation (discrete)

where we will discuss the funny looking normalization factor in front, containing the volume V and the energy of the nth solution, later. The coefficients A_n and $B_n^\dagger$ are constants, and a complex conjugate form for the coefficient of the last term above, i.e., $B_n^\dagger$, is used because it will prove advantageous later.

This is a discrete set of solutions, typical for cases with waves constrained inside a volume V, though V can be taken as large as one wishes. Each discrete wavelength in the summation of (3-9) fits an integer number of times inside the volume V. Continuous (integral rather than sum) solutions, for waves not constrained inside a specific volume V, exist for (3-8) as well, but we are not concerned with them at this point.

Continuous solutions also exist

This solution set is also specifically for plane waves. We will not consider alternative solution forms for other wave shapes that would exist in problems with cylindrical or spherical geometries.

Only plane wave solutions here

The solution (3-9), because we are working in RQM, is a state, i.e., $\phi(x)$ above = $|\phi(x)\rangle$, for a single particle. Each individual term in the summation is an eigenstate. $\phi(x)$ is a general state superposition of eigenstates.

Solutions in RQM are states (particles)

Note that in NRQM, we only had terms in the counterpart to (3-9) that had the exponential form of $-i(E_n t - \mathbf{p}_n \cdot \mathbf{x})/\hbar$, because that was the only form that satisfied the non-relativistic Schrödinger equation. Because we are using the square of the relativistic Hamiltonian in RQM, we get additional solutions of exponential form $+i(E_n t - \mathbf{p}_n \cdot \mathbf{x})/\hbar$ that also solve the relativistic Klein-Gordon equation. You should do Prob. 1, at the end of the chapter, to justify the statements in this paragraph to yourself.

Relativistic form has extra set of solutions

With an aim towards using natural units, we note the following relations, where wave number $k_i = 2\pi/\lambda_i$ and we use the deBroglie relation $p^i = \hbar k^i$,

$$p_\mu = \begin{bmatrix} E/c \\ p_i \end{bmatrix} = \begin{bmatrix} E/c \\ -p^i \end{bmatrix} = \hbar k_\mu = \begin{bmatrix} \hbar\omega/c \\ -\hbar k^i \end{bmatrix} \xrightarrow{\text{nat. units}} p_\mu = \begin{bmatrix} E \\ -p^i \end{bmatrix} = k_\mu = \begin{bmatrix} \omega \\ -k^i \end{bmatrix}, \qquad (3\text{-}10)$$

Relations for p_μ and k_μ

and recall the notation introduced in Chap. 2,

$$px = p_\mu x^\mu = Et - p^i x^i = Et - \mathbf{p} \bullet \mathbf{x} \qquad \left(= p^\mu x_\mu\right)$$

$$kx = k_\mu x^\mu = \omega t - k^i x^i = \frac{Et}{\hbar} - \frac{p^i x^i}{\hbar} = \frac{p_\mu}{\hbar} x^\mu \qquad \left(= k^\mu x_\mu\right) \qquad (3\text{-}11)$$

$$\text{in nat. units} \rightarrow \; E = \omega, \quad p_i = k_i, \quad p_\mu = k_\mu, \quad px = kx.$$

Notation review

It is then common to re-write (3-9) in natural units with the above notation. In doing so, we also switch the dummy summation variable n, which represents each individual wave in the summation, to the 3D vector quantity $\mathbf{k}$, representing the wave number and direction of each possible wave. For free fields, a given wave with wave number vector $\mathbf{k}$ has a particular energy (see (3-2) with $\mathbf{p} = \mathbf{k}$ in natural units), and we can designate that energy via either $E_\mathbf{k}$ or $\omega_\mathbf{k}$. It is common practice for scalars to use $\mathbf{k}$ (rather than $\mathbf{p}$) and $\omega_\mathbf{k}$ (rather than $E_\mathbf{p}$ or $E_\mathbf{k}$.)

[1] Pauli, W. and Weisskopf, V., Helv. Phys. Acta 7, 709 (1934). Translation in Miller, A. I., *Early Quantum Electrodynamics: A Source Book*, Cambridge U. Press, New York (1994)

The Klein-Gordon equation solutions (3-9) then become, in natural units

$$\phi(x)=\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}\left(A_{\mathbf{k}}e^{-ikx}+B_{\mathbf{k}}^{\dagger}e^{ikx}\right)\quad . \tag{3-12}$$

Natural units form of Klein-Gordon solutions

Except for Box 3-1, which reviews NRQM, we will henceforth, in this chapter, use natural units.

Definition of Eigensolutions

As noted previously, in RQM, the solution ϕ of (3-12) is that of a general (sum of eigenstates) single particle state. Each eigenstate has mathematical form (where we are going to omit the $2\omega_{\mathbf{k}}$ part here, because of what is coming)

Eigenstates of Klein-Gordon equation

$$\phi_{\mathbf{k},A}=\frac{e^{-ikx}}{\sqrt{V}}\quad\text{or}\quad\phi_{\mathbf{k},B^{\dagger}}=\frac{e^{ikx}}{\sqrt{V}}\ . \tag{3-13}$$

Each of these forms has what is called unit norm. That is, for $\phi_{\mathbf{k},A}$ (and similarly, for $\phi_{\mathbf{k},B^{\dagger}}$),

$$\int\phi_{\mathbf{k},A}^{\dagger}\phi_{\mathbf{k},A}d^3x=\frac{1}{V}\int_V e^{ikx}e^{-ikx}d^3x=1\,, \tag{3-14}$$

Eigenstates have unit norm

or more generally, all such eigenstates are orthonormal, i.e., their inner products are

$$\int\phi_{\mathbf{k},A}^{\dagger}\phi_{\mathbf{k}',A}d^3x=\frac{1}{V}\int_V e^{ikx}e^{-ik'x}d^3x=\delta_{\mathbf{k}\mathbf{k}'}\,. \tag{3-15}$$

and are orthogonal

Similar relations to (3-15) exist for $\phi_{\mathbf{k},B^{\dagger}}$, and every $\phi_{\mathbf{k},A}$ is orthogonal to every $\phi_{\mathbf{k},B^{\dagger}}$. Work this out by doing Prob.2.

Relations (3-13) to (3-15) should look familiar from NRQM. There, (3-14) was the integral of the probability density for a particle in an eigenstate. In RQM, however, things are a little different, as we will see, and we use the term "unit norm" for the property displayed in (3-14).

Unit norm eigenstates were advantageous in NRQM, and they will be in QFT as well. That is the reason we omitted the $2\omega_{\mathbf{k}}$ part of our solutions (3-12) in forming our definitions (3-13). By so doing, the eigenstates then have unit norm, and things just turn out easier later on.

We defined eigenstates to have unit norm because it will be advantageous

3.1.4 Probability Density in RQM

We are going to investigate probability density in RQM, but first look over Box 3-1, and be sure you understand how probability density is derived in NRQM.

Probability Density Using the Klein-Gordon Equation

For RQM, we start with the Klein-Gordon equation rather than Schrödinger equation. First post-multiply it by $\phi^{\dagger}$, then subtract the complex conjugate equation post-multiplied by ϕ, i.e.,

Deduce RQM probability density using relativistic wave equation

$$\begin{aligned}&\left\{\frac{\partial^2}{\partial t^2}\phi=\left(\nabla^2-\mu^2\right)\phi\right\}\phi^{\dagger}\\ -&\left\{\frac{\partial^2}{\partial t^2}\phi^{\dagger}=\left(\nabla^2-\mu^2\right)\phi^{\dagger}\right\}\phi,\end{aligned} \tag{3-16}$$

and note that $\mu^2\phi^{\dagger}\phi-\mu^2\phi\phi^{\dagger}=0$. The LHS of the result can be replaced with the new LHS in (3-17) below, and the RHS with (3-18).

$$\underbrace{\frac{\partial^2\phi}{\partial t^2}\phi^{\dagger}-\frac{\partial^2\phi^{\dagger}}{\partial t^2}\phi}_{\text{LHS of result above}}+\underbrace{\frac{\partial\phi}{\partial t}\frac{\partial\phi^{\dagger}}{\partial t}-\frac{\partial\phi^{\dagger}}{\partial t}\frac{\partial\phi}{\partial t}}_{=0}=\underbrace{\frac{\partial}{\partial t}\left(\frac{\partial\phi}{\partial t}\phi^{\dagger}-\frac{\partial\phi^{\dagger}}{\partial t}\phi\right)}_{\text{new LHS}} \tag{3-17}$$

$$\underbrace{\left(\nabla^2\phi\right)\phi^{\dagger}-\left(\nabla^2\phi^{\dagger}\right)\phi}_{\text{RHS of result above}}+\underbrace{\nabla\phi\cdot\nabla\phi^{\dagger}-\nabla\phi^{\dagger}\cdot\nabla\phi}_{=0}=\underbrace{\nabla\cdot\left(\left(\nabla\phi\right)\phi^{\dagger}-\left(\nabla\phi^{\dagger}\right)\phi\right)}_{\text{new RHS}} \tag{3-18}$$

Box 3-1. Review of Non-Relativistic QM Probability Density

In non-relativistic quantum mechanics (NRQM), we encountered 1) the wave function solution to the Schrödinger equation Ψ, and 2) the particle probability density $\rho = \Psi^\dagger\Psi$ (or equivalently when Ψ is a scalar quantity, $\Psi^*\Psi$.) We review here the derivation of that relation for probability density.

Conserved quantities in field theory:

Recall the continuity equation of continuum mechanics and electromagnetism,

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0 \qquad \left(\xrightarrow{\text{implies}} \int_V \rho\, d^3x = \text{constant in time}\right), \tag{B3-1.1}$$

where ρ is density (mass or charge density), $\mathbf{j}$ is the 3D current density (mass/area-sec or charge/area-sec), and V is all space, or at least large enough so that everywhere outside it, for all time, $\rho = 0$. V is fixed in space and time, whereas ρ can change in space and time inside V. Any conserved quantity (such as total mass M or total charge Q) obeys (B3-1.1).

The general procedure:

Use the governing quantum wave equation to deduce another equation having the form of the continuity equation (B3-1.1), and we will then know that ρ, whatever it turns out to be in that case, must represent a conserved quantity. Its integral over all space is constant in time. If we normalize ρ such that when integrated over all space, the result equals one, we can conjecture that ρ is the particle probability density (which when integrated over all space equals the probability that we will find the particle somewhere in all space, i.e., one.) Then throughout time, as our particle evolves, moves, and rearranges its probability density distribution, the total probability of finding it somewhere in space is always one. It turns out, from experiment, that the conjecture that this quantity ρ in NRQM equals probability density is true.

Probability Density Using the Schrödinger Equation:

First, pre-multiply the Schrödinger equation by the complex conjugate of the wave function, i.e.,

$$\Psi^\dagger\left\{\frac{\partial}{\partial t}\Psi = \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2M}\nabla^2 + V\right)\Psi\right\} \tag{B3-1.2}$$

Then, post-multiply the complex conjugate of the Schrödinger equation by the wave function

$$\left\{\frac{\partial}{\partial t}\Psi^\dagger = \frac{-1}{i\hbar}\left(-\frac{\hbar^2}{2M}\nabla^2 + V^\dagger\right)\Psi^\dagger\right\}\Psi \tag{B3-1.3}$$

where the potential V is real so $V=V^\dagger$. Adding (B3-1.2) to (B3-1.3), we get

$$\Psi^\dagger\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^\dagger}{\partial t}\Psi = \Psi^\dagger\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2M}\nabla^2 + V\right)\Psi + \left(\frac{-1}{i\hbar}\left(-\frac{\hbar^2}{2M}\nabla^2\Psi^\dagger + V^\dagger\Psi^\dagger\right)\right)\Psi \tag{B3-1.4}$$

or

$$\frac{\partial\left(\Psi^\dagger\Psi\right)}{\partial t} = \frac{-\hbar}{2iM}\underbrace{\left(\Psi^\dagger\left(\nabla^2\Psi\right) - \left(\nabla^2\Psi^\dagger\right)\Psi\right)}_{\nabla\cdot\left[\Psi^\dagger(\nabla\Psi) - \left(\nabla\Psi^\dagger\right)\Psi\right]} + \underbrace{\frac{\Psi^\dagger V\Psi}{i\hbar} - \frac{V^\dagger\Psi^\dagger\Psi}{i\hbar}}_{=0 \text{ since } V^\dagger = V} \tag{B3-1.5}$$

This is the same as the continuity equation (B3-1.1) if we take as our probability density

$$\rho = \Psi^\dagger\Psi\ , \tag{B3-1.6}$$

and as our probability current

$$\mathbf{j} = \frac{\hbar}{2iM}\left\{\Psi^\dagger\left(\nabla\Psi\right) - \left(\nabla\Psi^\dagger\right)\Psi\right\}\ . \tag{B3-1.7}$$

This is how the commonly used relation (B3-1.6) is found.

Equating the new LHS of (3-17) to the new RHS of (3-18), and to make future work easier, multiplying both sides by the constant *i*, gives the form of the continuity equation

Manipulations of the wave equation lead to an equation like the continuity equation

$$i\frac{\partial}{\partial t}\left(\frac{\partial \phi}{\partial t}\phi^{\dagger}-\frac{\partial \phi^{\dagger}}{\partial t}\phi\right)=i\nabla\cdot\left(\left(\nabla\phi\right)\phi^{\dagger}-\left(\nabla\phi^{\dagger}\right)\phi\right) \quad\rightarrow\quad \frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{j}=0\,, \tag{3-19}$$

where probability density and the probability current for a Klein-Gordon particle are

From that, we deduce form of RQM probability density

$$\rho=j^{0}=i\left(\frac{\partial \phi}{\partial t}\phi^{\dagger}-\frac{\partial \phi^{\dagger}}{\partial t}\phi\right),\text{ and} \tag{3-20}$$

$$\mathbf{j}=-i\left(\left(\nabla\phi\right)\phi^{\dagger}-\left(\nabla\phi^{\dagger}\right)\phi\right) \qquad j^{i}=-i\left(\phi_{,i}\,\phi^{\dagger}-\phi^{\dagger}{}_{,i}\,\phi\right)=i\left(\phi^{,i}\phi^{\dagger}-\phi^{\dagger,i}\phi\right). \tag{3-21}$$

Importantly, and perhaps surprisingly, the relativistic form of the probability density (3-20) is <u>not</u> the same as (B3-1.6), the NRQM probability density.

<u>4 Currents</u>

We introduce 4D notation for the scalar and 3D vector of (3-19) and define the <u>scalar 4-current</u>

$$j^{\mu}=\begin{bmatrix}\rho\\ \mathbf{j}\end{bmatrix}=\begin{bmatrix}\rho\\ j^{i}\end{bmatrix}=\begin{bmatrix}j^{0}\\ j^{i}\end{bmatrix}=i\left(\phi^{,\mu}\phi^{\dagger}-\phi^{\dagger,\mu}\phi\right)\quad . \tag{3-22}$$

4-current and 4D form of continuity equation

The <u>4D continuity equation</u> form of (3-19) is then

$$\boxed{\frac{\partial j^{\mu}}{\partial x^{\mu}}=\partial_{\mu}j^{\mu}=j^{\mu}{}_{,\mu}=0}\,, \tag{3-23}$$

where we have shown three common notational ways to designate partial derivative. (3-23) tells us the *important fact* that the <u>4-divergence</u> *of the 4-current of any conserved quantity* (total probability in this case) *is zero.*

4-divergence of 4-current of conserved quantity always = 0

<u>Probability for Klein-Gordon Discrete Solutions</u>

For a single particle state in RQM, we are going to <u>assume at first</u>, for simplicity, that the solution (3-12), has <u>only terms with coefficients $A_{\mathbf{k}}$</u>, i.e., the general state ϕ contains no eigenstates shown with coefficients $B_{\mathbf{k}}^{\dagger}$. Probability density (3-20) is then (where primes do *not* denote derivatives with respect to spatial coordinates, merely different summation dummy variables)

Scalar probability density in terms of first Klein-Gordon solution set

$$\rho=\left(\sum_{\mathbf{k}}\frac{\omega_{\mathbf{k}}A_{\mathbf{k}}}{\sqrt{2\omega_{\mathbf{k}}}}\frac{e^{-ikx}}{\sqrt{V}}\right)\left(\sum_{\mathbf{k}'}\frac{A^{\dagger}_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{ik'x}}{\sqrt{V}}\right)+\left(\sum_{\mathbf{k}'}\frac{\omega_{\mathbf{k}'}A^{\dagger}_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{ik'x}}{\sqrt{V}}\right)\left(\sum_{\mathbf{k}}\frac{A_{\mathbf{k}}}{\sqrt{2\omega_{\mathbf{k}}}}\frac{e^{-ikx}}{\sqrt{V}}\right), \tag{3-24}$$

where the $\omega_{\mathbf{k}}$ and $\omega_{\mathbf{k}'}$ came from the time derivatives.

If we integrate ρ over the volume V (which is large enough to encompass the entire state), the result must equal 1. When we do so, all terms with $\mathbf{k}'\neq\mathbf{k}$ go to zero, so the $\omega_{\mathbf{k}'}\rightarrow\omega_{\mathbf{k}}$ and cancel out. The V term in the denominator cancels in the integration over the volume V, and the two terms result in a factor of 2 that cancels with the 2 in the denominator. The result is

Square of absolute value of coefficient $A_{\mathbf{k}}$ = probability of finding **k***th eigenstate*

$$\int\rho d^{3}x=\sum_{\mathbf{k}}|A_{\mathbf{k}}|^{2}=1\,. \tag{3-25}$$

Thus $|A_{\mathbf{k}}|^2$ is the probability of measuring the **k**th eigenstate, similar to what the coefficients of eigenstates represented in NRQM.

<u>Difference from NRQM</u>

Note that in RQM

Comparing probability in NRQM and RQM

$$\int\underbrace{\phi^{\dagger}\phi}_{\neq\rho}d^{3}x=\sum_{\mathbf{k}}\frac{\left(A_{\mathbf{k}}\right)^{2}}{2\omega_{\mathbf{k}}}\neq 1\quad\text{but}\quad\int\underbrace{i\left(\frac{\partial\phi}{\partial t}\phi^{\dagger}-\frac{\partial\phi^{\dagger}}{\partial t}\phi\right)}_{=\rho}d^{3}x=\sum_{\mathbf{k}}|A_{\mathbf{k}}|^{2}=1\qquad\text{(RQM)}\,, \tag{3-26}$$

whereas in NRQM, we had

$$\int \underbrace{\phi^{\dagger}\phi}_{=\rho} d^3x = \sum_{\mathbf{k}} |A_{\mathbf{k}}|^2 = 1 \qquad \text{(NRQM)} . \tag{3-27}$$

Normalization Factors

Obtaining the RHS of (3-26) is the reason for the normalization factors $1/\sqrt{2\omega_{\mathbf{k}}V}$ used in the solution ϕ of (3-12) and (3-9). Those factors result in a total probability of one for a single particle and $|A_{\mathbf{k}}|^2$ as the probability for measuring the respective eigenstate. That is, the form of the relativistic field equation gave us the form of the probability density in (3-20) (and (3-26)), and the need to have total probability of unity gave us the normalization factors in the solutions.

RQM normalization factors arise from need to have total probability = 1 *and* $|A_{\mathbf{k}}|^2$ = *probability of* **k***th state*

Relativistic Invariance of Probability

This total probability value of unity in (3-25) (and (3-26)) is a relativistic invariant (i.e., a world scalar.) If we change our frame, the energy spectrum (i.e., the $\omega_{\mathbf{k}}$ values) will change (kinetic energy for each energy-momentum eigenstate looks different). But these changes cancel out in the probability calculation, since the $\omega_{\mathbf{k}}$ cancel, and always result in a total probability of one for any frame. Further, the $A_{\mathbf{k}}$ here are constants that do not vary with frame, so the probability of finding any particular state is also independent of what frame the measurements are taken in.

Total probability and $A_{\mathbf{k}}$ *are frame independent* (*relativistically invariant*)

Note that this means the normalization factors chosen provide relativistic invariance of total probability, which we would not have had with any other choice.

3.1.5 Negative Energies in RQM

If we take our traditional operator form for H as $i\partial/\partial t$ and operate on one of our Klein-Gordon solution eigenstates of (3-12) and (3-13), we should get the energy eigenvalue $\omega_{\mathbf{k}}$. When we do this for the eigenstates with exponents in $-ikx$, all looks as expected.

$$H\phi_{\mathbf{k},A} = E_{\mathbf{k},A}\phi_{\mathbf{k},A} \;\rightarrow\; i\frac{\partial\phi_{\mathbf{k},A}}{\partial t} = i\frac{\partial}{\partial t}\frac{e^{-ikx}}{\sqrt{V}} = \omega_{\mathbf{k}}\frac{e^{-ikx}}{\sqrt{V}} = \omega_{\mathbf{k}}\phi_{\mathbf{k},A} = E_{\mathbf{k},A}\phi_{\mathbf{k},A} . \tag{3-28}$$

However, when we do it for the eigenstates with exponents in $+ikx$, we have an "uh-oh", i.e.,

$$H\phi_{\mathbf{k},B^{\dagger}} = E_{\mathbf{k},B^{\dagger}}\phi_{\mathbf{k},B^{\dagger}} \;\rightarrow\; i\frac{\partial\phi_{\mathbf{k},B^{\dagger}}}{\partial t} = i\frac{\partial}{\partial t}\frac{e^{ikx}}{\sqrt{V}} = -\omega_{\mathbf{k}}\frac{e^{ikx}}{\sqrt{V}} = -\omega_{\mathbf{k}}\phi_{\mathbf{k},B^{\dagger}} = E_{\mathbf{k},B^{\dagger}}\phi_{\mathbf{k},B^{\dagger}} . \tag{3-29}$$

Half of our RQM eigenstates have negative energy

Since $\omega_{\mathbf{k}}$ is always a positive number, we have states with negative energies in RQM. We might have expected this, since we used the square of the Hamiltonian as the basis of RQM, and square roots typically have both positive and negative signs.

The bottom line: This is not an attribute of what a good theory has been expected to have, i.e., solely positive energies as we see in our world. As we will shortly see, QFT solved this dilemma (as well as others delineated in Chap. 1.)

3.1.6 Negative Probabilities in RQM

Do Prob. 3 to prove to yourself that a particle ϕ containing only eigenstates of the exponential form $+i(E_n t - \mathbf{p}_n\cdot\mathbf{x})/\hbar = ikx$ (i.e., those with coefficients $B_{\mathbf{k}}^{\dagger}$ in (3-12)) has total probability of being measured of –1. The extra states in RQM have physically untenable negative probabilities!

Half of our RQM eigenstates have negative probability density

Time to move on to QFT.

3.2 The Klein-Gordon Equation in Quantum Field Theory

3.2.1 States vs Fields

It should come as no surprise, to those who have read Chap. 1, that the fundamental scalar wave equation of RQM, the Klein-Gordon equation (3-8), is also the fundamental scalar wave equation of QFT, except that ϕ therein is considered a field, instead of a state. The word "field" in classical theory means an entity that, unlike a particle, is spread out, i.e., is a function of space (it has different values at different spatial locations) and typically also a function of time. The state ϕ of NRQM and RQM certainly fills that bill, but in quantum theory we don't use the word "field" for this, we use the word "state" (or "wave function" or "ket" or "particle".)

States & fields both spread out in space. But in quantum theories, "field" also means "operator"

The word "field" in quantum theory refers to a quantity that is spread out in space, but also, importantly, as we will soon see, is an operator in QFT. More properly, it is called a quantum field or an operator field, though the short term field is far more common. Confusingly, we use the same symbol ϕ in QFT for a field as we used for a state in NRQM and RQM.

Notation

Notational difference between states and fields. In QFT, ϕ is not a state, but a field

In QFT, symbols such as ϕ, which are not part of a ket symbol, do not represent states, but fields. Unless otherwise explicitly noted, in QFT notation,

$|\phi\rangle$ symbolizes a state (particle) and ϕ symbolizes a field (operator),

On the other hand, in NRQM and RQM, both symbols above represented the same thing, a state.

We will understand these distinctions a little better later, but for now understand that formally, the Klein-Gordon equation in QFT is called a field equation, because its solution ϕ is a (quantum or operator) field. See the second and third rows of Wholeness Chart 1-2 in Chap. 1, pg. 7.

There are two common ways to derive this equation, which we present in the following two sections, plus a third, which is a good check on the theory and can be found in the Appendix A.

3.2.2 From RQM to QFT

Fig. 3-2 illustrates, schematically, the two basic routes to QFT. The quickest is at the bottom of the figure, for which we simply postulate that the solution ϕ of the Klein-Gordon equation (3-8) describes a field (instead of a particle). This is reasonable, since ϕ is a function of spatial location (and often time), i.e., it is a field in the formal mathematical sense.

Two different routes to QFT

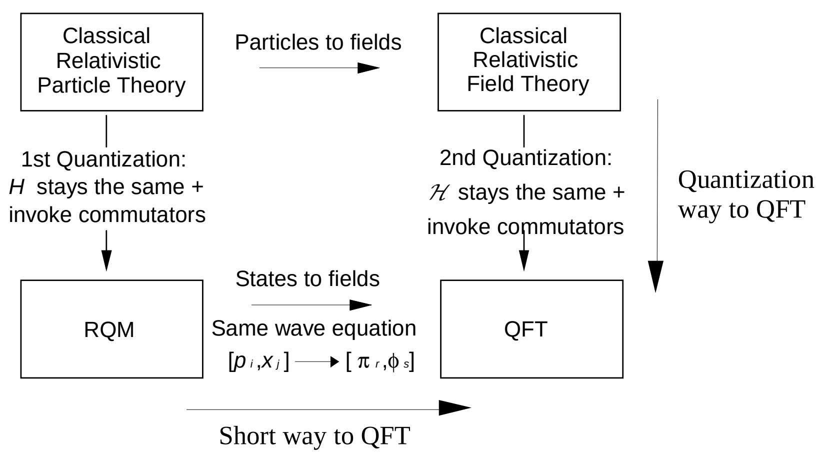

Figure 3-2. Different Routes to Quantum Field Theory

Short route: RQM → QFT. Similar math as 2^{nd} quantization below

We then must apply the commutation relations for fields (see Chap. 2, pg. 31, Wholeness Chart 2-5, 6^{th} column = 3^{rd} column on right hand page), instead of the commutation relations for particle properties (same chart, 3^{rd} column on left hand page). When we do this, and simply crank the mathematics, we obtain QFT. Because the QFT we then obtain describes the real world so well, it justifies the original postulate.

The formal mathematics are much the same as for the alternative route, illustrated on the RHS of Fig. 3-2, and treated in the next section.

3.2.3 From Classical Relativistic Fields to QFT

2^{nd} quantization route: Classical fields → QFT

Classical Scalar Fields

Start with classical Lagrangian density for free scalar field

The classical Lagrangian density for a free (no forces), real, relativistic scalar field ϕ has form

$$\mathcal{L}_0^0 = K\left(\partial_\alpha\phi\partial^\alpha\phi - \mu^2\phi\phi\right) = K\left(\dot\phi\dot\phi + \partial_i\phi\partial^i\phi - \mu^2\phi\phi\right) = K\left(\dot\phi\dot\phi - \underbrace{\partial_i\phi\partial_i\phi}_{\nabla\phi\cdot\nabla\phi} - \mu^2\phi\phi\right), \qquad (3\text{-}30)$$

where ϕ, since it is a classical field, is real (not complex), μ is a constant to be determined by experiment, K is an arbitrary constant, the superscript "0" on $\mathcal{L}$ stands for scalar (with spin 0), and the subscript "0" means "free". This is not the place to do classical theory, so we will not derive (3-30) here. We do note in passing that (3-30) is a general result derived by insisting that ϕ and $\mathcal{L}$ are Lorentz invariants (i.e., world scalars – see Chap. 2 including appendix) and that the associated Euler-Lagrange equation is also Lorentz invariant in form. (3-30) is the only form that satisfies these conditions and results in a linear field equation (i.e., ϕ appears only to first power.) A non-linear field equation might work, but is far more complicated. For free fields, we will find a linear equation works well.

Using the Legendre transformation, we can readily use (3-30) to find the Hamiltonian density, where $\pi_0^{\,0}$ is the field conjugate momentum,

Find Hamiltonian density from Legendre transformation

$$\mathcal{H}_0^0 = \pi_0^0\dot{\phi} - \mathcal{L}_0^0 = \underbrace{\frac{\partial \mathcal{L}_0^0}{\partial \dot{\phi}}}_{2K\dot{\phi}}\dot{\phi} - \mathcal{L}_0^0 = K\left(\dot{\phi}\dot{\phi} + \nabla\phi\cdot\nabla\phi + \mu^2\phi\phi\right). \tag{3-31}$$

We may be tempted at this point to proceed with quantization, and simply use the $\mathcal{H}$ and $\mathcal{L}$ above along with the appropriate commutators. However, we know that in quantum mechanics most meaningful things are complex, not real. Quite the reverse of the macroscopic world we live in, and for which real fields of form ϕ generally apply.

Classical field taken as complex

So, we adopt one more postulate, which is that our field ϕ be complex. This means re-expressing our values for $\mathcal{H}$ and $\mathcal{L}$ in terms of a complex field, but such that $\mathcal{H}$ and $\mathcal{L}$ remain real (energy, and energy density $\mathcal{H}$, must be real numbers.) Doing this, where we choose to take K=1, yields the free, complex scalar field Lagrangian and Hamiltonian densities

Re-express Lagrangian and Hamiltonian densities in terms of complex fields

$$\boxed{\mathcal{L}_0^0 = \left(\partial_\alpha\phi^\dagger\,\partial^\alpha\phi - \mu^2\phi^\dagger\phi\right) = \left(\dot{\phi}^\dagger\dot{\phi} - \nabla\phi^\dagger\cdot\nabla\phi - \mu^2\phi^\dagger\phi\right)}\text{, and} \tag{3-32}$$

$$\boxed{\mathcal{H}_0^0 = \frac{\partial \mathcal{L}_0^0}{\partial \dot{\phi}^r}\dot{\phi}^r - \mathcal{L}_0^0 = \underbrace{\frac{\partial \mathcal{L}_0^0}{\partial \dot{\phi}}}_{\pi_0^0=\dot{\phi}^\dagger}\dot{\phi} + \underbrace{\frac{\partial \mathcal{L}_0^0}{\partial \dot{\phi}^\dagger}}_{\pi_0^{0\dagger}=\dot{\phi}}\dot{\phi}^\dagger - \mathcal{L}_0^0 = \dot{\phi}\dot{\phi}^\dagger + \nabla\phi^\dagger\cdot\nabla\phi + \mu^2\phi^\dagger\phi}\,. \tag{3-33}$$

Take care to realize that ϕ and $\phi^\dagger$ are considered *separate fields in the summation over field types r*, and note the definitions of their respective conjugate momenta. That is, $\pi_0^{\,0}$ equals the complex conjugate of the time derivative of the field (not the time derivative of the field.) $\pi_0^{0\dagger}$ equals the time derivative of the field, not its complex conjugate.

If, as we progress, we find situations where real, rather than complex, fields are involved, we can simply deal with the special case of a complex field where the imaginary part is zero. Assuming a complex field above means we assumed the most general case.

Deriving the Klein-Gordon Field Equation

Substituting the Lagrangian density (3-32) into the Euler-Lagrange field equation,

$$\frac{\partial}{\partial x^\mu}\left(\frac{\partial \mathcal{L}}{\partial \phi^r{}_{,\mu}}\right) - \frac{\partial \mathcal{L}}{\partial \phi^r} = 0\ . \tag{3-34}$$

Use $\mathcal{L}$ in Euler-Lagrange equation to get Klein-Gordon equation

yields the Klein-Gordon equation for fields, where again, the values r=1,2 signify, respectively, the field ϕ and its complex conjugate transpose $\phi^\dagger$ (also called the Hermitian conjugate) which, for scalars, is simply the complex conjugate,

$$\boxed{\begin{aligned}\left(\partial_\mu\partial^\mu + \mu^2\right)\phi\ &= \left(\Box^2 + \mu^2\right)\phi\ = 0 \qquad \text{(a)}\\ \left(\partial_\mu\partial^\mu + \mu^2\right)\phi^\dagger &= \left(\Box^2 + \mu^2\right)\phi^\dagger = 0. \qquad \text{(b)}\end{aligned}} \tag{3-35}$$

In the above, we have introduced the $\Box^2$ symbol for the D'Alembertian, the 4D equivalent of the 3D Laplacian, $\nabla^2 = \partial^i\partial^i = \partial_i\partial_i = -\partial^i\partial_i$. (Note, some authors use $\Box$ instead of $\Box^2$.) We could, of course, also have obtained (3-35)(b) by taking the complex conjugate transpose of (3-35)(a), since everything inside the parentheses is real.

Recall from Chap. 2, that given any one of $\mathcal{H}$, $\mathcal{L}$, or the field equation, we can deduce any of the others (via the Legendre transformation and the Euler-Lagrange equation). So knowing any one of these is equivalent to knowing any of the others, and our first postulate of 2nd quantization could have stipulated the same $\mathcal{L}$ in classical theory and QFT, or the same field equation, instead of $\mathcal{H}$.

The discrete plane wave solutions to (3-35) are the same as (3-12), and its Hermitian conjugate, from RQM, i..e.,[1]

$$\begin{aligned}
\phi(x) &= \underbrace{\sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} a(\mathbf{k}) e^{-ikx}}_{} + \underbrace{\sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} b^{\dagger}(\mathbf{k}) e^{ikx}}_{} && \text{(a)} \\
&= \qquad \phi^{+} \qquad + \qquad \phi^{-} \\
\phi^{\dagger}(x) &= \underbrace{\sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} b(\mathbf{k}) e^{-ikx}}_{} + \underbrace{\sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} a^{\dagger}(\mathbf{k}) e^{ikx}}_{} && \text{(b)} \\
&= \qquad \phi^{\dagger +} \qquad + \qquad \phi^{\dagger -} \; .
\end{aligned} \qquad (3\text{-}36)$$

Discrete plane wave solutions to Klein-Gordon field equation

Note the new symbolism for each of the solution forms. We use lower case coefficients in QFT because, as we will see, the coefficients play a much different role in QFT than they did in RQM, and we need to distinguish them.

The continuous plane wave solutions to (3-35) are

$$\begin{aligned}
\phi(x) &= \underbrace{\int \frac{d^3\boldsymbol{k}}{\sqrt{2(2\pi)^3\omega_{\mathbf{k}}}} a(\mathbf{k}) e^{-ikx}}_{} + \underbrace{\int \frac{d^3\boldsymbol{k}}{\sqrt{2(2\pi)^3\omega_{\mathbf{k}}}} b^{\dagger}(\mathbf{k}) e^{ikx}}_{} && \text{(a)} \\
&= \qquad \phi^{+} \qquad + \qquad \phi^{-} \\
\phi^{\dagger}(x) &= \underbrace{\int \frac{d^3\boldsymbol{k}}{\sqrt{2(2\pi)^3\omega_{\mathbf{k}}}} b(\mathbf{k}) e^{-ikx}}_{} + \underbrace{\int \frac{d^3\boldsymbol{k}}{\sqrt{2(2\pi)^3\omega_{\mathbf{k}}}} a^{\dagger}(\mathbf{k}) e^{ikx}}_{} && \text{(b)} \\
&= \qquad \phi^{\dagger +} \qquad + \qquad \phi^{\dagger -} \; .
\end{aligned} \qquad (3\text{-}37))$$

Continuous plane wave solutions to Klein-Gordon field equation

The continuous solutions represent waves that are not constrained to a specific volume. Wavelengths for such solutions do not have to fit an integer number of times inside a particular volume, and thus are not limited to discrete values.

Note also the shorthand notation for each of the four different solution sets underneath the brackets. You will see these symbols again and again, so you might want to consider making a copy of (3-36), pasting it above your desk, and doing memorization tests with yourself every day until they become ingrained in your consciousness. Try to remember that $\phi^{\dagger +}$ is *not* the complex conjugate of ϕ^{+}, for example, contrary to what you might expect. The + sign refers to a term with positive energy in the RQM sense (i.e., – sign before the energy in the exponent.) It might help to think that because † changes the sign of the imaginary part of every complex quantity, it also changes the sign of the symbol ϕ^{-}. So, $(\phi^{-})^{\dagger} = \phi^{\dagger +}$.

Learn the shorthand notation for the four types of solutions

[1] These solutions have the familiar $\pm\, i(\omega_{\mathbf{k}} t - \mathbf{k}\cdot\mathbf{x})$ form in the exponent. There are actually additional solutions to the Klein-Gordon equation having form $\pm\, i(\omega_{\mathbf{k}} t + \mathbf{k}\cdot\mathbf{x})$, but these have been widely ignored. These solutions, and their impact on QFT, are discussed in R. D. Klauber, “Mechanism for Vanishing Zero-Point Energy”, http://arxiv.org/abs/astro-ph/0309679 (2003) and “Supplemental Solutions to the Field Equations: Norms, Observables, and Propagators”, www.quantumfieldtheory.info/suppl_soltns.pdf.

However you do it, being able to readily recall the definitions of the symbols in (3-36) and (3-37) will help in the future.

Finding μ^2

Do Prob. 4 to prove to yourself that the value of μ^2, which appeared as an unknown constant in the theoretical determination of (3-30), has the same value it did in RQM, i.e.,

μ^2 has same value in QFT as in RQM

$$\boxed{\mu^2 = \frac{m^2 c^2}{\hbar^2} \quad \left(= m^2 \text{ in nat. units}\right)}. \tag{3-38}$$

Third Way to Klein-Gordon Equations: A Consistency Check

Recall from Chap 2. and Wholeness Charts 2-2 and 2-5 (pgs. 20 and 30), that we could express the equations of motion for classical fields in terms of Poisson brackets in the former chart, and for Heisenberg picture quantum fields, in terms of commutators in the latter chart. The commutator-based equation of motion for a quantum field in the next to last box in the right hand column of Wholeness Chart 2-5 (reproduced below on the LHS of (3-39)) is in terms of the Hamiltonian and the field. For scalar fields, this equation of motion for ϕ should be essentially the same as the Klein-Gordon equation for ϕ. That is,

There is yet a third way to derive the field equation of motion, this time from a variational math relation

Heisenberg Picture Field Equation of Motion — Klein-Gordon Field Equation

$$\dot{\phi} = -i\left[\phi, H\right] \quad \xleftrightarrow{\text{should be same thing}} \quad \left(\partial_\mu \partial^\mu + \mu^2\right)\phi = 0 \tag{3-39}$$

In the Appendix A of this chapter, we show that this is indeed true, and thus our theory is self consistent. It also proves that the Klein-Gordon field equation of QFT (3-35) (and (3-39)) derived above applies to the Heisenberg, not Schrödinger, picture.

This is a parallel path to do second quantization that is included in the route represented by the vertical arrow on the RHS of Fig. 3-2, but it uses a different, though related, part of the theory.

3.2.4 Summary Chart

All that we have done in this Sect. 3.2, and what we will do in the remainder of this and the next two chapters, is summarized in Wholeness Chart 5-4 at the end of Chap. 5.

Note the summary is at the end of Chap. 5 because each column in it lists the key components in the development of QFT for one of the three spin types (spin 0, ½, and 1), and we won't be doing the latter two until Chaps. 4 and 5.

Be sure to use the summary wholeness chart, as you study this chapter and the next two

You can follow along in the chart, as we develop the theory for scalars, by reading the blocks in the Spin 0 column. You may want to stick a Post-It on that page as a book marker, so you can easily flip to it as you read along in this, and the following two, chapters.

3.3 Commutation Relations: The Crux of QFT

We will soon see how the commutation relations encompassed in the <u>second part of 2nd quantization</u>, found in the last box in the right hand column of Wholeness Chart 2-5 of Chap. 2, pg. 31, and reproduced in (3-40) below, lie at the root of, and structure, all of QFT. For scalars, they are

$$\left[\phi^r(\mathbf{x},t), \pi_s(\mathbf{y},t)\right] = \phi^r \pi_s - \pi_s \phi^r = i\delta^r{}_s \delta(\mathbf{x}-\mathbf{y}) \qquad \left[\phi^r, \phi^s\right] = \left[\pi_r, \pi_s\right] = \left[\phi^r, \pi_s{}^\dagger\right] = 0. \tag{3-40}$$

Note, in passing, that a complex conjugate of a field is considered a different field. In effect, if $\phi^r = \phi$, then $\phi^s = \phi^\dagger$, where $r \neq s$, so that $\left[\phi, \phi^\dagger\right] = 0$.

2^{nd} quantization commutation relations determine coefficient commutation

Of overriding importance in the theory, as we will see, are the following <u>coefficient commutation relations</u>, which we will derive below from the 2nd quantization postulate of (3-40).

$$\boxed{\left[a(\mathbf{k}), a^\dagger(\mathbf{k}')\right] = \left[b(\mathbf{k}), b^\dagger(\mathbf{k}')\right] = \delta_{\mathbf{k}\mathbf{k}'} \text{ (discrete)}; \quad = \delta(\mathbf{k}-\mathbf{k}') \text{ (continuous)}}. \tag{3-41}$$

The form of (3-41) should tell us immediately that the Klein-Gordon solution coefficients $a(\mathbf{k})$, $b(\mathbf{k})$, etc. in QFT of (3-36) and (3-37) are far different animals than the $A_{\mathbf{k}}$, $B_{\mathbf{k}}$, etc. in RQM of (3-12). The latter are merely numbers, which commute. We must, therefore, suspect that the $a(\mathbf{k})$, $b(\mathbf{k})$, etc. are operators, and as we will see, this suspicion will turn out to be correct.

Coefficient com rels 1) play fundamental role in QFT, and 2) imply coefficients are operators

Proof of coefficient commutation relations

To prove (3-41), start with (3-40) and take different spatial coordinates **x** and **y**, but the same time coordinate t, for ϕ and $\pi^0{}_0$. This results in the equal time commutation relations

$$\left[\phi(\mathbf{x},t)\pi_0^0(\mathbf{y},t)-\pi_0^0(\mathbf{y},t)\phi(\mathbf{x},t)\right]=\left[\phi(\mathbf{x},t)\dot{\phi}^\dagger(\mathbf{y},t)-\dot{\phi}^\dagger(\mathbf{y},t)\phi(\mathbf{x},t)\right]=i\delta(\mathbf{x}-\mathbf{y})\,, \qquad (3\text{-}42)$$

Proving coefficient commutation relations

which are only important at this point as a step in our proof. Then, plugging the discrete solutions (3-36) into the middle part of (3-42), where to save space we use the compressed notation $a_{\mathbf{k}} = a(\mathbf{k})$, etc., we get

$$\left(\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}a_{\mathbf{k}}e^{-i(\omega_{\mathbf{k}}t-\mathbf{k}\bullet\mathbf{x})}+\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}b^\dagger_{\mathbf{k}}e^{i(\omega_{\mathbf{k}}t-\mathbf{k}\bullet\mathbf{x})}\right)\left(\sum_{\mathbf{k}'}\frac{-i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}}b_{\mathbf{k}'}e^{-i(\omega_{\mathbf{k}'}t-\mathbf{k}'\bullet\mathbf{y})}+\sum_{\mathbf{k}'}\frac{i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}}a^\dagger_{\mathbf{k}'}e^{i(\omega_{\mathbf{k}'}t-\mathbf{k}'\bullet\mathbf{y})}\right)$$
$$-\left(\sum_{\mathbf{k}'}\frac{-i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}}b_{\mathbf{k}'}e^{-i(\omega_{\mathbf{k}'}t-\mathbf{k}'\bullet\mathbf{y})}+\sum_{\mathbf{k}'}\frac{i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}}a^\dagger_{\mathbf{k}'}e^{i(\omega_{\mathbf{k}'}t-\mathbf{k}'\bullet\mathbf{y})}\right)\left(\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}a_{\mathbf{k}}e^{-i(\omega_{\mathbf{k}}t-\mathbf{k}\bullet\mathbf{x})}+\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}b^\dagger_{\mathbf{k}}e^{i(\omega_{\mathbf{k}}t-\mathbf{k}\bullet\mathbf{x})}\right)$$
$$=\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\frac{i\omega_{\mathbf{k}'}}{2V\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\begin{pmatrix}-a_{\mathbf{k}}b_{\mathbf{k}'}e^{-i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\bullet\mathbf{x}+\mathbf{k}'\bullet\mathbf{y})}+a_{\mathbf{k}}a^\dagger_{\mathbf{k}'}e^{-i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\bullet\mathbf{x}-\mathbf{k}'\bullet\mathbf{y})}\\ -b^\dagger_{\mathbf{k}}b_{\mathbf{k}'}e^{i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{-i(\mathbf{k}\bullet\mathbf{x}-\mathbf{k}'\bullet\mathbf{y})}+b^\dagger_{\mathbf{k}}a^\dagger_{\mathbf{k}'}e^{i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{-i(\mathbf{k}\bullet\mathbf{x}+\mathbf{k}'\bullet\mathbf{y})}\\ +b_{\mathbf{k}'}a_{\mathbf{k}}e^{-i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\bullet\mathbf{x}+\mathbf{k}'\bullet\mathbf{y})}+b_{\mathbf{k}'}b^\dagger_{\mathbf{k}}e^{i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{-i(\mathbf{k}\bullet\mathbf{x}-\mathbf{k}'\bullet\mathbf{y})}\\ -a^\dagger_{\mathbf{k}'}a_{\mathbf{k}}e^{-i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\bullet\mathbf{x}-\mathbf{k}'\bullet\mathbf{y})}-a^\dagger_{\mathbf{k}'}b^\dagger_{\mathbf{k}}e^{i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{-i(\mathbf{k}\bullet\mathbf{x}+\mathbf{k}'\bullet\mathbf{y})}\end{pmatrix}=i\delta(\mathbf{x}-\mathbf{y}).$$

K-G solutions into equal time commutator

(3-43)

Using the math identity for the 3D Dirac delta function

$$\delta(\mathbf{x}-\mathbf{y})=\frac{1}{V}\sum_{n=-\infty}^{+\infty}e^{-i\mathbf{k}_n\cdot(\mathbf{x}-\mathbf{y})}\qquad\begin{pmatrix}\text{in our notation}=\dfrac{1}{V}\sum_{\mathbf{k}}e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\\ \text{or equivalently, }\dfrac{1}{2V}\sum_{\mathbf{k}}\left(e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}+e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\right)\end{pmatrix}\qquad(3\text{-}44)$$

Re-express Dirac delta function

on the RHS of the last row in (3-43), and matching terms, we see that all terms where $\mathbf{k}' \neq \pm\,\mathbf{k}$ must equal zero, since (3-44) has no terms in both **k** and **k′**. These particular terms reduce to the following form, summed over **k** and **k′**.

$$\frac{i\omega_{\mathbf{k}'}}{2V\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\begin{pmatrix}\underbrace{\left(b_{\mathbf{k}'}a_{\mathbf{k}}-a_{\mathbf{k}}b_{\mathbf{k}'}\right)}_{\text{must}=0}e^{-i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\bullet\mathbf{x}+\mathbf{k}'\bullet\mathbf{y})}+\underbrace{\left(a_{\mathbf{k}}a^\dagger_{\mathbf{k}'}-a^\dagger_{\mathbf{k}'}a_{\mathbf{k}}\right)}_{\text{must}=0}e^{-i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\bullet\mathbf{x}-\mathbf{k}'\bullet\mathbf{y})}\\ +\underbrace{\left(b_{\mathbf{k}'}b^\dagger_{\mathbf{k}}-b^\dagger_{\mathbf{k}}b_{\mathbf{k}'}\right)}_{\text{must}=0}e^{i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{-i(\mathbf{k}\bullet\mathbf{x}-\mathbf{k}'\bullet\mathbf{y})}+\underbrace{\left(b^\dagger_{\mathbf{k}}a^\dagger_{\mathbf{k}'}-a^\dagger_{\mathbf{k}'}b^\dagger_{\mathbf{k}}\right)}_{\text{must}=0}e^{i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{-i(\mathbf{k}\bullet\mathbf{x}+\mathbf{k}'\bullet\mathbf{y})}\end{pmatrix}=0\qquad(3\text{-}45)$$

$$\left(\text{All terms in summations with }\mathbf{k}'\neq\pm\mathbf{k}\text{ equal 0, as no terms on RHS in }\mathbf{k}\text{ and }\mathbf{k}'\right)$$

Terms where $\mathbf{k}' \neq \pm\,\mathbf{k}$

These must vanish, so their commutators must = 0

So, all possible coefficient commutators with $\mathbf{k}' \neq \mathbf{k}$ or $-\,\mathbf{k}$ vanish. The remaining terms all have $\mathbf{k}' = \pm\,\mathbf{k}$, which means $\omega_{\mathbf{k}} = \omega_{\mathbf{k}'}$. Some of these have an exponential form $i(\omega_{\mathbf{k}} + \omega_{\mathbf{k}'})t$, and those terms give us a summation of terms over **k** having form, for each possible **k′**, of

$$\frac{i\omega_{\mathbf{k}}}{2V\omega_{\mathbf{k}}}\begin{pmatrix}\underbrace{\left(b_{\mathbf{k}}a_{\mathbf{k}}-a_{\mathbf{k}}b_{\mathbf{k}}\right)}_{\text{must}=0}\underbrace{e^{-i2\omega_{\mathbf{k}}t}}_{\neq 0}e^{i\mathbf{k}\bullet(\mathbf{x}+\mathbf{y})}+\underbrace{\left(b^\dagger_{\mathbf{k}}a^\dagger_{\mathbf{k}}-a^\dagger_{\mathbf{k}}b^\dagger_{\mathbf{k}}\right)}_{\text{must}=0}e^{i2\omega_{\mathbf{k}}t}e^{-i\mathbf{k}\bullet(\mathbf{x}+\mathbf{y})}\qquad(\leftarrow\mathbf{k}'=\mathbf{k})\\ +\underbrace{\left(b_{-\mathbf{k}}a_{\mathbf{k}}-a_{\mathbf{k}}b_{-\mathbf{k}}\right)}_{\text{must}=0}e^{-i2\omega_{\mathbf{k}}t}e^{i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}+\underbrace{\left(b^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}}-a^\dagger_{-\mathbf{k}}b^\dagger_{\mathbf{k}}\right)}_{\text{must}=0}e^{i2\omega_{\mathbf{k}}t}e^{-i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}\qquad(\leftarrow\mathbf{k}'=-\mathbf{k})\end{pmatrix}=0\qquad(3\text{-}46)$$

$$\left(\text{All time dependent terms with }\mathbf{k}'=\pm\mathbf{k}\text{ equal 0, as no time dependence on RHS}\right)$$

Terms where $\mathbf{k}' = \pm\,\mathbf{k}$*, i.e., those of form* $exp(i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}})t)$

Commutators must = 0

For these terms, the coefficient commutators must vanish because the exponential in $\omega_{\mathbf{k}}$ varies in time, whereas there is no such variation on the RHS of the last row in (3-43).

The remaining terms have exponential form $i(\omega_{\mathbf{k}} - \omega_{\mathbf{k}'})t$ and $\mathbf{k}' = \pm\,\mathbf{k}$. Adding those terms for $\mathbf{k}' = \mathbf{k}$ with the terms for $\mathbf{k}' = -\mathbf{k}$ yields, with the relevant terms on the RHS of (3-43) (see 2nd row in parentheses of (3-44)) on the RHS below,

Remaining terms where $\mathbf{k}' = \pm\,\mathbf{k}$, *i.e., those of form* $exp(i(\omega_{\mathbf{k}} - \omega_{\mathbf{k}})t)$

$$\frac{i}{2V}\begin{pmatrix} \underbrace{\left(a_{\mathbf{k}}a_{\mathbf{k}}^{\dagger} - a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\right)}_{\text{must}=1}\underbrace{e^{-i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}})t}}_{=1}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} + \underbrace{\left(b_{\mathbf{k}}b_{\mathbf{k}}^{\dagger} - b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}\right)}_{\text{must}=1}e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \quad (\leftarrow \mathbf{k}'=\mathbf{k}) \\ + \underbrace{\left(a_{\mathbf{k}}a_{-\mathbf{k}}^{\dagger} - a_{-\mathbf{k}}^{\dagger}a_{\mathbf{k}}\right)}_{\text{must}=0}e^{i\mathbf{k}\cdot(\mathbf{x}+\mathbf{y})} + \underbrace{\left(b_{-\mathbf{k}}b_{\mathbf{k}}^{\dagger} - b_{\mathbf{k}}^{\dagger}b_{-\mathbf{k}}\right)}_{\text{must}=0}e^{-i\mathbf{k}\cdot(\mathbf{x}+\mathbf{y})} \quad (\leftarrow \mathbf{k}'=-\mathbf{k}) \end{pmatrix} = \frac{i}{2V}\begin{pmatrix} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \\ +e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \end{pmatrix} \tag{3-47}$$

Key commutators must = 1

(All time independent terms in summation with $\mathbf{k}' = \pm\,\mathbf{k}$ must equal RHS).

All terms with ($\mathbf{x} + \mathbf{y}$) in the exponents of the LHS must equal zero, as the RHS only has terms in ($\mathbf{x} - \mathbf{y}$). The LHS of (3-47) matches the RHS if each coefficient commutator in the first row equals one. Subtleties in justifying that as the only way to interpret (3-47) are shown in Appendix E.

The commutation relations for $a_{\mathbf{k}}a_{\mathbf{k}'}^{\dagger}$ and $b_{\mathbf{k}}b_{\mathbf{k}'}^{\dagger}$ in (3-45) to (3-47) are the same as (3-41). QED.

If you are ambitious, have extra time, and/or simply have to prove everything to yourself, do Prob. 7 to derive the continuous solution commutators of (3-41).

End of coefficient commutation relations proof

With the coefficient commutator relations in hand, we are finally ready to dive into the real core of QFT.

3.4 The Hamiltonian in QFT

We find the Hamiltonian by integrating the Hamiltonian density $\mathcal{H}$ over all space (a volume V containing the discrete solutions, which we can make as large as we like.) In QFT, we express $\mathcal{H}$ in terms of a complex field and substitute our field equation solutions.

$H = \int \mathcal{H}\, dV$

3.4.1 The Free Scalar Hamiltonian in Terms of the Coefficients

For a free scalar field $\mathcal{H} = \mathcal{H}_0^{\,0}$, as in (3-33), where we employ our discrete, plane wave solutions (3-36) we get

$H = \int \mathcal{H}\, dV$ in terms of the fields

$$H_0^0 = \int \mathcal{H}_0^0 d^3x = \int\left(\dot{\phi}\dot{\phi}^{\dagger} + \nabla\phi^{\dagger}\cdot\nabla\phi + \mu^2\phi^{\dagger}\phi\right)d^3x =$$

$$\int\left(\sum_{\mathbf{k}}\frac{\partial}{\partial t}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}\left(a(\mathbf{k})e^{-ikx} + b^{\dagger}(\mathbf{k})e^{ikx}\right)\right)\left(\sum_{\mathbf{k}'}\frac{\partial}{\partial t}\frac{1}{\sqrt{2V\omega_{\mathbf{k}'}}}\left(b(\mathbf{k}')e^{-ik'x} + a^{\dagger}(\mathbf{k}')e^{ik'x}\right)\right)d^3x \tag{3-48}$$

$$+\int\left(-\partial_i\phi^{\dagger}\partial^i\phi + \mu^2\phi^{\dagger}\phi\right)d^3x.$$

Deriving H in terms of the coefficients ↓

The middle line of (3-48), i.e., the $\int\dot{\phi}\dot{\phi}^{\dagger}d^3x$ part, becomes

$$\int\left(\sum_{\mathbf{k}}\frac{i\omega_{\mathbf{k}}}{\sqrt{2V\omega_{\mathbf{k}}}}\left(-a(\mathbf{k})e^{-ikx} + b^{\dagger}(\mathbf{k})e^{ikx}\right)\right)\left(\sum_{\mathbf{k}'}\frac{i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}}\left(-b(\mathbf{k}')e^{-ik'x} + a^{\dagger}(\mathbf{k}')e^{ik'x}\right)\right)d^3x. \tag{3-49}$$

or

$$\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\frac{-\sqrt{\omega_{\mathbf{k}}}\sqrt{\omega_{\mathbf{k}'}}}{2V}\int\begin{pmatrix} a(\mathbf{k})b(\mathbf{k}')e^{-ikx}e^{-ik'x} - a(\mathbf{k})a^{\dagger}(\mathbf{k}')e^{-ikx}e^{ik'x} \\ -b^{\dagger}(\mathbf{k})b(\mathbf{k}')e^{ikx}e^{-ik'x} + b^{\dagger}(\mathbf{k})a^{\dagger}(\mathbf{k}')e^{ikx}e^{ik'x} \end{pmatrix}d^3x. \tag{3-50}$$

The sum over $\mathbf{k}$ and $\mathbf{k}'$ is from negative infinity to positive infinity in the x, y, and z directions.

All terms in the integration in (3-50) result in zero except when $\mathbf{k}' = \mathbf{k}$ or $\mathbf{k}' = -\,\mathbf{k}$, because we are integrating orthogonal functions between their boundaries. (This is similar to $sin(2X)sin(4X)$ integrated with respect to X along a complete number of wavelengths, where here $\mathbf{k} = 2$ and $\mathbf{k}' = 4$.) Since the volume of integration in (3-50) equals V, we end up with

$$\begin{aligned}\int\dot{\phi}\dot{\phi}^{\dagger}d^3x &= \sum_{\mathbf{k}}\frac{\omega_{\mathbf{k}}}{2}\left(-a(\mathbf{k})b(-\mathbf{k})e^{-2i\omega_{\mathbf{k}}t} + a(\mathbf{k})a^{\dagger}(\mathbf{k}) + b^{\dagger}(\mathbf{k})b(\mathbf{k}) - b^{\dagger}(\mathbf{k})a^{\dagger}(-\mathbf{k})e^{2i\omega_{\mathbf{k}}t}\right) \\ &= \sum_{\mathbf{k}}\frac{(\omega_{\mathbf{k}})^2}{2\omega_{\mathbf{k}}}\left(-a(-\mathbf{k})b(\mathbf{k})e^{-2i\omega_{\mathbf{k}}t} + a(\mathbf{k})a^{\dagger}(\mathbf{k}) + b^{\dagger}(\mathbf{k})b(\mathbf{k}) - b^{\dagger}(-\mathbf{k})a^{\dagger}(\mathbf{k})e^{2i\omega_{\mathbf{k}}t}\right).\end{aligned} \tag{3-51}$$

In the second row of (3-51), the sign change on the **k** in the first and last terms is justified since we are summing over all **k**, so for every term with **k** in it, there is another with – **k**. This modification will make things easier a bit later.

Following similar steps for the next term in (3-48) we get

$$
\begin{aligned}
&-\int \partial_i \phi^\dagger \partial^i \phi d^3x = \int \partial_i \phi^\dagger \partial_i \phi d^3x \\
&= \int \left(\sum_{\mathbf{k}} \frac{ik_i}{\sqrt{2V\omega_{\mathbf{k}}}} \left(b(\mathbf{k}) e^{-ikx} - a^\dagger(\mathbf{k}) e^{ikx} \right) \right) \left(\sum_{\mathbf{k}'} \frac{ik'_i}{\sqrt{2V\omega_{\mathbf{k}'}}} \left(a(\mathbf{k}') e^{-ik'x} - b^\dagger(\mathbf{k}') e^{ik'x} \right) \right) d^3x \quad (3\text{-}52) \\
&= \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2\omega_{\mathbf{k}}} \left(b(\mathbf{k}) a(-\mathbf{k}) e^{-2i\omega_{\mathbf{k}} t} + a^\dagger(\mathbf{k}) a(\mathbf{k}) + b(\mathbf{k}) b^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k}) b^\dagger(-\mathbf{k}) e^{2i\omega_{\mathbf{k}} t} \right)
\end{aligned}
$$

where we note that terms in the summation with both **k** and – **k** have an extra sign change since $k_i = -k'_i$ in the multiplication in the second line of (3-52).

Similarly, for the mass term in (3-48), we get (do Prob. 8 at the end of the chapter to prove it)

$$
\int \mu^2 \phi^\dagger \phi d^3x = \sum_{\mathbf{k}} \frac{\mu^2}{2\omega_{\mathbf{k}}} \left(b(\mathbf{k}) a(-\mathbf{k}) e^{-2i\omega_{\mathbf{k}} t} + b(\mathbf{k}) b^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k}) a(\mathbf{k}) + a^\dagger(\mathbf{k}) b^\dagger(-\mathbf{k}) e^{2i\omega_{\mathbf{k}} t} \right). \quad (3\text{-}53)
$$

Adding the final parts of (3-51), (3-52), and (3-53), and using $\mathbf{k}^2 + \mu^2 = (\omega_{\mathbf{k}})^2$ along with the coefficient commutation relations (3-41), we end up with

$$
\begin{aligned}
H_0^0 &= \sum_{\mathbf{k}} \frac{\omega_{\mathbf{k}}}{2} \Big(\underbrace{a(\mathbf{k}) a^\dagger(\mathbf{k})}_{\text{use commutator}} + a^\dagger(\mathbf{k}) a(\mathbf{k}) + b^\dagger(\mathbf{k}) b(\mathbf{k}) + \underbrace{b(\mathbf{k}) b^\dagger(\mathbf{k})}_{\text{use commutator}} \Big) \\
&= \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(a^\dagger(\mathbf{k}) a(\mathbf{k}) + \tfrac{1}{2} + b^\dagger(\mathbf{k}) b(\mathbf{k}) + \tfrac{1}{2} \right).
\end{aligned} \quad (3\text{-}54)
$$

or simply

$$
\boxed{H_0^0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(N_a(\mathbf{k}) + \tfrac{1}{2} + N_b(\mathbf{k}) + \tfrac{1}{2} \right)}\,, \quad (3\text{-}55)
$$

$H = \int \mathcal{H}\, dV$ in terms of the coefficients

where

$$
\boxed{N_a(\mathbf{k}) = a^\dagger(\mathbf{k}) a(\mathbf{k}) \qquad N_b(\mathbf{k}) = b^\dagger(\mathbf{k}) b(\mathbf{k})}\ . \quad (3\text{-}56)
$$

Expressions (3-55) and (3-56) lie at the heart of QFT, as we are about to see.

3.4.2 Number Operators

Consider what we must get if the Hamiltonian of (3-55) operates on a state (a ket) comprised of two free scalar particles, each in the same eigenstate of energy $\omega_{\mathbf{k}_1}$. We would expect that (multiparticle) state to have an energy eigenvalue equal to its total energy $2\omega_{\mathbf{k}_1}$ i.e.,

$$
H_0^0 \left| 2\phi_{\mathbf{k}_1} \right\rangle = 2\omega_{\mathbf{k}_1} \left| 2\phi_{\mathbf{k}_1} \right\rangle . \quad (3\text{-}57)
$$

But from (3-55), that means

$$
\sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(N_a(\mathbf{k}) + \tfrac{1}{2} + N_b(\mathbf{k}) + \tfrac{1}{2} \right) \left| 2\phi_{\mathbf{k}_1} \right\rangle = 2\omega_{\mathbf{k}_1} \left| 2\phi_{\mathbf{k}_1} \right\rangle . \quad (3\text{-}58)
$$

How can we make sense of (3-58)? The answer is that it is not quite true, and that we can make sense of it all if, instead of (3-57) and (3-58), we consider

$$
H_0^0 \left| 2\phi_{\mathbf{k}_1} \right\rangle = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \Big(\underbrace{N_a(\mathbf{k}) + \tfrac{1}{2}}_{a\text{ type particles}} + \underbrace{N_b(\mathbf{k}) + \tfrac{1}{2}}_{b\text{ type particles}} \Big) \underbrace{\left| 2\phi_{\mathbf{k}_1} \right\rangle}_{a\text{ type particles}} = \left(2\omega_{\mathbf{k}_1} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(\frac{1}{2} + \frac{1}{2} \right) \right) \left| 2\phi_{\mathbf{k}_1} \right\rangle, \quad (3\text{-}59)
$$

$H = \int \mathcal{H}\, dV$ in terms of number operators

with the following interpretation.

$N_a(\mathbf{k})$ = number operator with eigenvalue $n_a(\mathbf{k})$ = number of *a* particles with 3-mom **k** in the ket, $N_b(\mathbf{k})$ = number operator with eigenvalue $n_b(\mathbf{k})$ = number of *b* particles with 3-mom **k** in the ket, and, the vacuum has ½ quantum of energy for each **k** for *a* particles, and also for *b* particles.

This might, at first, be considered a separate postulate, but if the $\mathcal{H}_0^0$ derived by 2nd quantization for quantum scalar fields is correct, this is the only possible interpretation of (3-59) that works. The part about the vacuum would be surprising to anyone who had not already heard that the vacuum is a seething caldron of virtual quanta. More on this shortly.

For $H = \int \mathcal{H}\, dV$ to work, the vacuum must be filled with ½ quanta

We also anticipate that the *b* type particles will be antiparticles, and the *a* types, normal particles. More on this later, as well.

Examples of number operators and kets

In light of the above, the following examples should be relatively straightforward. Note we designate *b* type particles with an overbar.

Example #1: 10 particle state

$$
\begin{aligned}
H_0^0 \,|5\phi_{\mathbf{k}_1}, 2\phi_{\mathbf{k}_2}, \underbrace{3\bar{\phi}_{\mathbf{k}_3}}_{\substack{b \text{ type} \\ \text{particles}}} \rangle &= \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(N_a(\mathbf{k}) + \tfrac{1}{2} + N_b(\mathbf{k}) + \tfrac{1}{2} \right) \left| 5\phi_{\mathbf{k}_1}, 2\phi_{\mathbf{k}_2}, 3\bar{\phi}_{\mathbf{k}_3} \right\rangle \\
&= \left(5\omega_{\mathbf{k}_1} + 2\omega_{\mathbf{k}_2} + 3\omega_{\mathbf{k}_3} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(\frac{1}{2} + \frac{1}{2} \right) \right) \left| 5\phi_{\mathbf{k}_1}, 2\phi_{\mathbf{k}_2}, 3\bar{\phi}_{\mathbf{k}_3} \right\rangle .
\end{aligned} \tag{3-60}
$$

Every state has vacuum as part of it, so every state has huge vacuum energy

and so we see that *b* type particles in our theory have positive energy. This resulted from our interpretation of H_0^0 in (3-59), i.e., from our postulate for the properties of $N_b(\mathbf{k})$ in (3-59) and the box following it. We know from experiment that antiparticles have positive energy, and this interpretation will lead to *b* particles filling the role of antiparticles. We will see later that *b* particles have opposite charge from the *a* particles, and so they fit nicely into our theory as antiparticles.

Example #2: Vacuum state

$$
H_0^0 \underbrace{|0\rangle}_{\substack{\text{vacuum} \\ \text{state}}} = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(N_a(\mathbf{k}) + \tfrac{1}{2} + N_b(\mathbf{k}) + \tfrac{1}{2} \right) |0\rangle = \underbrace{\sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(\frac{1}{2} + \frac{1}{2} \right)}_{\text{infinite energy}} |0\rangle . \tag{3-61}
$$

Note that every state is superimposed on the vacuum, so every state actually has infinite energy. We saw this in Example #1.

3.4.3 Zero Point (Vacuum) Energy

The infinite sum of ½ quanta in (3-61) represents the now famous perspective on the vacuum as being almost inconceivably crammed with energy, known as zero point energy (ZPE.) In actuality, the sum, while enormous, is usually not considered infinite, but for reasons beyond the scope of our current discussion, to terminate at a very high level, known as the Planck scale.

Zero point (vacuum) energy results from 2nd quantization postulate of non-commutation

It is important to recognize that this *vacuum energy arose from our postulate of 2nd quantization*, that a field and its conjugate momentum don't commute (see (3-40). Because of this we got the coefficient commutation relations (3-41), and those were used in our derivation of the form of the Hamiltonian (see (3-54), which resulted in the appearance of $\frac{1}{2}\omega_{\mathbf{k}}$ terms.

The field commutation relations of QFT are siblings to the particle commutation relations for NRQM and RQM. (See Wholeness Chart 2-5 in Chap. 2, pg. 30.) In the latter, particle position and momentum do not commute and this results in the renowned Heisenberg uncertainty relation between position and momentum. In QFT, the field and its conjugate momentum do not commute, implying a parallel uncertainty relationship between them. This, in this sense, may be partially behind the oft heard statement that the uncertainty principle is the cause of the zero point energy. In Chap. 10, we cover another sense commonly meant.

Non-commutation leads to uncertainty. Source of statements that uncertainty principle results in ZPE

Are the ½ Quanta Effervescent?

One often also hears that the ½ quanta "pop" in and out of the vacuum effervescently in particle/antiparticle pairs. I submit that this is a heuristic, at best, representation for the popular media. According to (3-55), there is no "popping", no evanescent physical reality alternated with nothingness, no pairing of particles at a creation event followed by a common mutual destruction event as one might see in a Feynman diagram (different from, but similar in nature to, what we saw in Fig. 1-1 of Chap. 1, pg. 2) Via our fundamental QFT relation for H_0^0, the ½ quanta are simply

Ruminations on vacuum effervescence

sitting in the vacuum. They may be virtual in some sense, and not real, but the QFT H operator does not suggest any intermittent sort of existence.

Further, our derivation of $H_0^{\,0}$ has been exclusively for free fields, where no interactions are included (more on interactions in later chapters). The particles (and antiparticles), for which $H_0^{\,0}$ determines the energy, do not interact with other particles or antiparticles. This means they can't create or destroy in pairs, since that is, above all, an interaction between the associated particles and antiparticles. So $H_0^{\,0}$ specifically does not measure the energy of such pairs and the ½ energy terms therein must be for free fields that are not "popping" in and out of the vacuum in pairs.

Some argue that experimental measurements of Casimir plate forces, the Lamb shift, and the anomalous magnetic moment of the electron demonstrate the existence of vacuum fluctuations. However, Casimir forces are generally computed by considering the ½ quanta such as those in (3-61) to be standing waves between the plates. That is, they do *not need*, in those analyses, to be "popping" in and out of the vacuum, but merely be sitting there continually. Further, the Casimir force can be computed without reference to zero-point energies at all, and thus may not be the conclusive proof for their existence it is widely taken to be. (See R. L. Jaffe, "Casimir Effect and the Quantum Vacuum", Phys. Rev. D72 021301(R) (2005) http://arxiv.org/abs/hep-th/0503158 .)

Casimir plates do not prove ZPE existence

The Lamb shift calculation involves so-called "vacuum fluctuations", but they are actually higher order corrections to propagators for interacting fields (which we study in later chapters), not the ½ quanta vacuum energy of free fields (which we study in this chapter.) The same is true of the QFT correction to the magnetic moment of the electron (the famed "anomalous magnetic moment".)

Neither are Lamb shift nor anomalous magnetic moment solution due to free field ½ quanta (ZPE)

As a caveat, I note that the remarks in this sub-section entitled "Are the ½ Quanta Effervescent" reflect my personal position on vacuum energy. The majority of physicists believe quanta are continually "bubbling" in and out of existence in the vacuum. I simply have not seen a sound derivation of this in the literature, and don't believe it is supported by the formal derivation of ZPE.

We will discuss this issue further when we get to interaction theory. (See Chap. 10.)

3.4.4 Positive Energy in QFT

Note that unlike RQM, all particles in QFT have positive energy. The QFT energy operator $H_0^{\,0}$ operating on states yields positive eigenvalues for both *a* and *b* types of particles. The RQM energy operator operating on states did not do that, as we saw in Sect. 3.1.5 (pg. 47).

$H = \int \mathcal{H}\, dV$ leads to positive energy for both QFT particle types

Continuation of Wholeness Chart 1-2. Comparison of Three Quantum Theories

	NRQM	**RQM**	**QFT**
Hamiltonian	$i\dfrac{\partial}{\partial t}$	$i\dfrac{\partial}{\partial t}$	$H = \int \mathcal{H}\, d^3x$
Sign of Energy *E*	positive	positive & negative	positive

3.4.5 Unit Norms and Orthogonality for Multiparticle States

Recall from NRQM, that it was advantageous to normalize states, i.e., change the constant in front of the ket such that the inner product of the state and its complex conjugate transpose (the bracket of the bra and ket) equaled unity. That is, we defined

$$\left\langle \phi_{\mathbf{k}} \middle\| \phi_{\mathbf{k}} \right\rangle = \int_V \underbrace{\phi_{\mathbf{k}}^{\dagger}(\mathbf{x},t)\phi_{\mathbf{k}}(\mathbf{x},t)}_{\text{states}} d^3x = 1 \quad \text{and} \quad \left\langle \phi_{\mathbf{k}} \middle\| \phi_{\mathbf{k}'} \right\rangle = \int_V \underbrace{\phi_{\mathbf{k}}^{\dagger}(\mathbf{x},t)\phi_{\mathbf{k}'}(\mathbf{x},t)}_{\text{states}} d^3x = 0, \;\; \mathbf{k} \neq \mathbf{k}'. \tag{3-62}$$

As aside, note that in (3-62), it is assumed that the ket is expressed in the position basis. For example, a plane wave momentum eigenstate in that basis would have form[1]

---

[1] The ket symbol $|\phi\rangle$ in general represents a particle state, but the form of the ket when we write it out mathematically, such as we did in the RHS of (3-63), changes with the basis we care to use. For example we could express the ket in the momentum basis (in momentum space) instead of the position basis x; or in a number of other ways. Mathematically, (3-63) is really $|\phi\rangle_{x\,\text{basis}} = \langle x|\phi\rangle = Ae^{-i(Et-\mathbf{k}\cdot\mathbf{x})}$.

$$\left|\phi_{\mathbf{k}}\right\rangle = Ae^{-i(Et-\mathbf{k}\cdot\mathbf{x})} \qquad \left(\left|\phi_{\mathbf{k}}\right\rangle \text{ here is expressed in the position basis}\right). \tag{3-63}$$

In this book, unless otherwise stated, when we express $|\phi\rangle$ mathematically, we will assume the position basis as in (3-63). At such times, $|\phi\rangle$ will = $|\phi\rangle_{\text{x basis}}$. Now, back to the main point.

In NRQM and RQM, states are single particle states. In QFT, they are typically multiparticle, but we will also find it advantageous therein to normalize. So, we define our symbols for multiparticle states so that every such state is normalized (i.e, has unit norm.) For example, for a state comprising two *a* particles of 3-momentum **k**, one of 3-momentum **k**′, and five *b* particles of 3-momentum **k**″, we would have (where the middle part is just a reminder of what we mean by the bracket notation[1])

Multiparticle states in QFT have unit norm

$$\left\langle 2\phi_{\mathbf{k}},\phi_{\mathbf{k}'},5\bar{\phi}_{\mathbf{k}''}\middle|\middle|2\phi_{\mathbf{k}},\phi_{\mathbf{k}'},5\bar{\phi}_{\mathbf{k}''}\right\rangle = \int_V \Big(\underbrace{2\phi_{\mathbf{k}}\phi_{\mathbf{k}'}5\bar{\phi}_{\mathbf{k}''}}_{\text{states}}\Big)^{\dagger}\Big(\underbrace{2\phi_{\mathbf{k}}\phi_{\mathbf{k}'}5\bar{\phi}_{\mathbf{k}''}}_{\text{states}}\Big)d^3x = 1 \ . \tag{3-64}$$

Note that any (multiparticle) state is orthogonal to every other state that is not identical to it in particle types, particle numbers, and **k** values for each. For examples, where $\mathbf{k} \neq \mathbf{k}'$,

Different multiparticle states in QFT are orthogonal

$$\left\langle 2\phi_{\mathbf{k}},\phi_{\mathbf{k}'},5\bar{\phi}_{\mathbf{k}''}\middle|\middle|\phi_{\mathbf{k}'},5\bar{\phi}_{\mathbf{k}''}\right\rangle = 0 \qquad \left\langle 2\phi_{\mathbf{k}}\middle|\middle|\phi_{\mathbf{k}}\right\rangle = 0 \qquad \left\langle 5\phi_{\mathbf{k}''}\middle|\middle|5\bar{\phi}_{\mathbf{k}''}\right\rangle = 0 \qquad \left\langle \phi_{\mathbf{k}}\middle|\middle|\phi_{\mathbf{k}'}\right\rangle = 0 \ . \tag{3-65}$$

Note on Notation

It is common practice in QFT to employ the bracket notation of the LHS of (3-64), and virtually never, the integral form shown between the equal signs. As noted earlier, in QFT, symbols such as $\phi_{\mathbf{k}}$, which are not part of a ket symbol, normally do not represent states, but operators/fields. When they play the role of states, as in (3-62), we must label them specifically, as there and in (3-64).

QFT virtually never uses $\phi_{\mathbf{k}}$ to represent a state, nor an integral to represent an inner product of states

3.5 Expectation Values and the Hamiltonian

Note that the expectation value relation for an operator $\mathcal{O}$ in QFT for a single particle state is the same as that in the rest of quantum mechanics, i.e., provided $|\phi\rangle$ has unit norm,

Expectation value for single particle in QFT like those in NRQM and RQM

$$\bar{\mathcal{O}} = \langle\phi|\mathcal{O}|\phi\rangle \ . \tag{3-66}$$

where we don't confuse the overbar (used here outside a bra or ket) for expectation (or average) value with its use inside a bra or ket, where it signifies *b* type particles. The expectation value is the average value we would measure over a large number of measurements of the state. If the particle is in an eigenstate of an observable (an operator), then every measurement of that observable for that state would be the same (the eigenvalue), and thus equal to the expectation value. An eigenstate of energy would measure the same value for energy upon every measurement. This is true for a single particle state, such as in (3-66).

It is also true for a multiparticle state, such as those we run into in QFT. For example, the multiparticle state in (3-60) is in an eigenstate of energy (the sum of the energies from each of the ten particles in the state.) Each particle therein has fixed mass plus a fixed momentum **k**, and hence fixed total energy. Thus, the energy expectation value for the state in (3-60) is

$$\begin{aligned}
\bar{H}_0^0 &= \left\langle 5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_3}\middle|H_0^0\middle|5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_3}\right\rangle = \\
&= \left\langle 5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_3}\right|\underbrace{\left(5\omega_{\mathbf{k}_1}+2\omega_{\mathbf{k}_2}+3\omega_{\mathbf{k}_3}+\sum_{\mathbf{k}}\omega_{\mathbf{k}}\left(\tfrac{1}{2}+\tfrac{1}{2}\right)\right)}_{\text{a number, not an operator, so can move outside}}\left|5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_3}\right\rangle \\
&= \left(5\omega_{\mathbf{k}_1}+2\omega_{\mathbf{k}_2}+3\omega_{\mathbf{k}_3}+\sum_{\mathbf{k}}\omega_{\mathbf{k}}\left(\tfrac{1}{2}+\tfrac{1}{2}\right)\right)\underbrace{\left\langle 5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_3}\middle|5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_3}\right\rangle}_{=1} \\
&= 5\omega_{\mathbf{k}_1}+2\omega_{\mathbf{k}_2}+3\omega_{\mathbf{k}_3}+\sum_{\mathbf{k}}\omega_{\mathbf{k}}\left(\tfrac{1}{2}+\tfrac{1}{2}\right).
\end{aligned} \tag{3-67}$$

[1] For the purists, we note that (3-64) can be taken as an invariant relationship if we define our states properly. That is, we can define our multiparticle eigenstate with a factor of $1/\sqrt{V}$ in front, so the integrand in (3-64) yields a factor $1/V$. The integral over 3D space then yields a factor of V. V is non-invariant, but one in the numerator and one in the denominator cancel, leaving an invariant final result.

In general, for any operator $\mathcal{O}$, the expectation value for any multiparticle state is

Expectation value for multiparticle state has same form as single particle state

$$\boxed{\bar{\mathcal{O}} = \langle \phi_1, \phi_2, \phi_3, ... | \mathcal{O} | \phi_1, \phi_2, \phi_3, ... \rangle} \,, \tag{3-68}$$

where we will typically find the operator expressed in terms of number operators.

A concept that becomes important later on in QFT is that of the vacuum expectation value, or simply the VEV, whose symbol and mathematical expression are

Expectation value for the vacuum, VEV

$$\langle \mathcal{O} \rangle = \langle 0 | \mathcal{O} | 0 \rangle . \tag{3-69}$$

If you don't see it right away, do Prob. 9 to prove to yourself that the VEV of the free field scalar Hamiltonian is

Hamiltonian VEV

$$\left\langle H_0^0 \right\rangle = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \,. \tag{3-70}$$

We expect to measure infinite (or enormous, if nature has a maximum |**k**|) energy in the vacuum.

3.6 Creation and Destruction Operators

In this section, we will prove what is perhaps the most fundamental aspect of QFT, which we foreshadowed in Chap. 1, that the Klein-Gordon solution coefficients $a(\mathbf{k})$, $a^\dagger(\mathbf{k})$, $b(\mathbf{k})$, and $b^\dagger(\mathbf{k})$ are not numbers, but operators that create and destroy particles. Since certain combinations of them do not commute, we should expect them to be operators of some kind.

The coefficients are creation and destruction operators

3.6.1 Proving It

Proof that $a(\mathbf{k})$ is a Particle Destruction Operator

With the notation $|n_{\mathbf{k}}\rangle$ denoting a multiparticle state of $n_{\mathbf{k}}$ a type particles (no b types for now), all with the same 4-momentum k^μ, what can we say about the state

Proving it.

$$a(\mathbf{k}) | n_{\mathbf{k}} \rangle = | m_{\mathbf{k}} \rangle \; ? \tag{3-71}$$

To see, first operate on this state with our number operator $N_a(\mathbf{k}) = a^\dagger(\mathbf{k})\, a(\mathbf{k})$

$$N_a(\mathbf{k}) | m_{\mathbf{k}} \rangle = N_a(\mathbf{k}) a(\mathbf{k}) | n_{\mathbf{k}} \rangle = \underbrace{a^\dagger(\mathbf{k}) a(\mathbf{k})}_{\text{use commutator}} a(\mathbf{k}) | n_{\mathbf{k}} \rangle . \tag{3-72}$$

Then, where noted above, use the commutation relations from (3-41), to find (3-72) equals

$$\begin{aligned} &\left(a(\mathbf{k}) a^\dagger(\mathbf{k}) - 1\right) a(\mathbf{k}) | n_{\mathbf{k}} \rangle = a(\mathbf{k}) a^\dagger(\mathbf{k}) a(\mathbf{k}) | n_{\mathbf{k}} \rangle - a(\mathbf{k}) | n_{\mathbf{k}} \rangle = a(\mathbf{k}) N_a(\mathbf{k}) | n_{\mathbf{k}} \rangle - a(\mathbf{k}) | n_{\mathbf{k}} \rangle \\ &= a(\mathbf{k}) n_{\mathbf{k}} | n_{\mathbf{k}} \rangle - a(\mathbf{k}) | n_{\mathbf{k}} \rangle = n_{\mathbf{k}} a(\mathbf{k}) | n_{\mathbf{k}} \rangle - a(\mathbf{k}) | n_{\mathbf{k}} \rangle = (n_{\mathbf{k}} - 1) a(\mathbf{k}) | n_{\mathbf{k}} \rangle = (n_{\mathbf{k}} - 1) | m_{\mathbf{k}} \rangle . \end{aligned} \tag{3-73}$$

So

$$N_a(\mathbf{k}) | m_{\mathbf{k}} \rangle = (n_{\mathbf{k}} - 1) | m_{\mathbf{k}} \rangle = m_{\mathbf{k}} | m_{\mathbf{k}} \rangle \qquad m_{\mathbf{k}} = n_{\mathbf{k}} - 1 \,. \tag{3-74}$$

Since the number operator operating on $|m_{\mathbf{k}}\rangle$ gives a number of particles one less than it did when operating on $|n_{\mathbf{k}}\rangle$, the operation of $a(\mathbf{k})$ on $|n_{\mathbf{k}}\rangle$ in (3-71) reduces the number of particles in the state by one. We conclude that $a(\mathbf{k})$ is a particle destruction operator.

End of Proof

Do Prob. 10, or at least part of it, to prove one or more of the last three relations below to yourself.

Summary of operator functions of coefficients

$$\begin{aligned} N_a(\mathbf{k})\left(a(\mathbf{k}) | n_{\mathbf{k}} \rangle\right) &= (n_{\mathbf{k}} - 1)\left(a(\mathbf{k}) | n_{\mathbf{k}} \rangle\right) && a(\mathbf{k}) \text{ destroys an } a \text{ particle with momentum } \mathbf{k} \\ N_a(\mathbf{k})\left(a^\dagger(\mathbf{k}) | n_{\mathbf{k}} \rangle\right) &= (n_{\mathbf{k}} + 1)\left(a^\dagger(\mathbf{k}) | n_{\mathbf{k}} \rangle\right) && a^\dagger(\mathbf{k}) \text{ creates an } a \text{ particle with momentum } \mathbf{k} \\ N_b(\mathbf{k})\left(b(\mathbf{k}) | \bar{n}_{\mathbf{k}} \rangle\right) &= (\bar{n}_{\mathbf{k}} - 1)\left(b(\mathbf{k}) | \bar{n}_{\mathbf{k}} \rangle\right) && b(\mathbf{k}) \text{ destroys a } b \text{ particle with momentum } \mathbf{k} \\ N_b(\mathbf{k})\left(b^\dagger(\mathbf{k}) | \bar{n}_{\mathbf{k}} \rangle\right) &= (\bar{n}_{\mathbf{k}} + 1)\left(b^\dagger(\mathbf{k}) | \bar{n}_{\mathbf{k}} \rangle\right) && b^\dagger(\mathbf{k}) \text{ creates a } b \text{ particle with momentum } \mathbf{k} . \end{aligned} \tag{3-75}$$

Creation operators $a^\dagger(\mathbf{k})$ and $b^\dagger(\mathbf{k})$ are sometimes called raising operators, because they raise the number of particles in a state. Destruction operators $a(\mathbf{k})$ and $b(\mathbf{k})$ are sometimes called lowering operators, for what should be obvious reasons. States that have been operated on by a raising operator are sometimes called raised states; those by a lowering operator, lowered states.

3.6.2 Normalization Factors for Raised and Lowered States

Raising and lowering particle number results in a factor in front of the new ket

When a raising operator operates on a ket, the resulting raised ket does not generally have unit norm (is not normalized.) Consider

$$a^{\dagger}(\mathbf{k})\left|n_{\mathbf{k}}\right\rangle = A\left|n_{\mathbf{k}}+1\right\rangle \; , \tag{3-76}$$

where A is some constant (which is a number, not an operator, and could be complex). The original ket $|n_{\mathbf{k}}\rangle$ and the ket $|n_{\mathbf{k}}+1\rangle$ (without the constant A) in (3-76) have unit norm. (See (3-64) for one example.) Also, by taking the complex conjugate transpose of (3-76), we see the $a(\mathbf{k})$ acting leftward on the bra has the same raising effect as the $a^{\dagger}(\mathbf{k})$ acting on the ket,

$$\left(A\left|n_{\mathbf{k}}+1\right\rangle\right)^{\dagger} = \left(a^{\dagger}(\mathbf{k})\left|n_{\mathbf{k}}\right\rangle\right)^{\dagger} = \left\langle n_{\mathbf{k}}\right|a(\mathbf{k}) = \left\langle n_{\mathbf{k}}+1\right|A^{\dagger} \; . \tag{3-77}$$

Note that

$$\underbrace{\left\langle n_{\mathbf{k}}\right|a(\mathbf{k})}_{\left\langle n_{\mathbf{k}}+1\right|A^{\dagger}}a^{\dagger}(\mathbf{k})\left|n_{\mathbf{k}}\right\rangle = \left\langle n_{\mathbf{k}}+1\right|A^{\dagger}A\left|n_{\mathbf{k}}+1\right\rangle = A^{\dagger}A\underbrace{\left\langle n_{\mathbf{k}}+1\middle|\middle|n_{\mathbf{k}}+1\right\rangle}_{1} = A^{\dagger}A \, . \tag{3-78}$$

(3-78) also equals

$$\left\langle n_{\mathbf{k}}\right|\underbrace{a(\mathbf{k})a^{\dagger}(\mathbf{k})}_{\text{use commutator}}\left|n_{\mathbf{k}}\right\rangle = \left\langle n_{\mathbf{k}}\right|\underbrace{a^{\dagger}(\mathbf{k})a(\mathbf{k})}_{N_a(\mathbf{k})}+1\left|n_{\mathbf{k}}\right\rangle = \left\langle n_{\mathbf{k}}\right|n_{\mathbf{k}}+1\left|n_{\mathbf{k}}\right\rangle = n_{\mathbf{k}}+1 \; . \tag{3-79}$$

Equating the RHS's of (3-78) and (3-79), and for simplicity taking A as real (complex would also work, but be more complicated) yields

$$A = \sqrt{n_{\mathbf{k}}+1} \; . \tag{3-80}$$

From (3-76), we then have the first line in (3-81) below. Identical logic leads to the third line. Do Prob. 11 if you can't just accept the second and fourth lines without seeing for yourself how they are obtained.

Factors arising from action of creation and destruction operators

$$\boxed{\begin{aligned} a^{\dagger}(\mathbf{k})\left|n_{\mathbf{k}}\right\rangle &= \sqrt{n_{\mathbf{k}}+1}\left|n_{\mathbf{k}}+1\right\rangle \\ a(\mathbf{k})\left|n_{\mathbf{k}}\right\rangle &= \sqrt{n_{\mathbf{k}}}\left|n_{\mathbf{k}}-1\right\rangle \\ b^{\dagger}(\mathbf{k})\left|\bar{n}_{\mathbf{k}}\right\rangle &= \sqrt{\bar{n}_{\mathbf{k}}+1}\left|\bar{n}_{\mathbf{k}}+1\right\rangle \\ b(\mathbf{k})\left|\bar{n}_{\mathbf{k}}\right\rangle &= \sqrt{\bar{n}_{\mathbf{k}}}\left|\bar{n}_{\mathbf{k}}-1\right\rangle \end{aligned}} \tag{3-81}$$

2nd quantization responsible for creation/ destruction operators

Note that the above results are ultimately due to 2nd quantization. The non-commutation of fields and their conjugate momenta resulted in the coefficient commutation relations, which was a crucial part in the proof that the coefficients create and destroy states, as well as the derivation of the normalization constants shown above. *Second quantization turned the solution coefficients in RQM, which were merely constants, into creation and destruction operators in QFT.*

3.6.3 Annihilating the Vacuum

The vacuum state has unit norm

Note that the vacuum $|0\rangle$ has unit norm, like any other state, i.e.,

$$\left\langle 0\middle|\middle|0\right\rangle = 1 \, . \tag{3-82}$$

Note also that 0 (zero) is a number representing nothing, and is different from $|0\rangle$, the vacuum state, which actually is something. From (3-81), the action of a destruction operator on the vacuum results in zero. That is,

A destruction operator annihilates the vacuum, i.e., leaves 0

$$a(\mathbf{k})\left|0\right\rangle = \sqrt{0}\left|-1\right\rangle = 0 \; . \tag{3-83}$$

Don't worry about the funny looking ket in the middle (which is actually meaningless and not something you will ever see in the literature). The root of zero controls the final result.

In QFT lingo, one says "a lowering operator destroys (or annihilates) the vacuum".

3.6.4 Total Particle Number

For future use, we define the total particle number as the number of particles (i.e. *a* types) minus the number of antiparticles (*b* types). For scalars, the total particle number operator is

Total particle number is number of particles minus number of antiparticles

$$N(\phi) = \sum_{\mathbf{k}} \left(N_a(\mathbf{k}) - N_b(\mathbf{k}) \right). \tag{3-84}$$

Note the subtle difference in phraseology in that we commonly use the term "number of particles" as being equal to the number of particles *plus* the number of antiparticles. "Total particle number" on the other hand refers to a negative value for the number of antiparticles.

We will soon see that *b* particles have opposite charge from *a* particles, and thus, in many senses, represent their negatives. So designating them as having negative total particle number seems reasonable.

3.6.5 ϕ(x) and $\phi^\dagger$(x) as Operator Fields

Since the field solutions $\phi(x)$ and $\phi^\dagger(x)$ contain the operator coefficients, they are then also operators, or more properly, operator fields or quantum fields. As noted in Chap. 1 and earlier in the present chapter, this is often shortened in QFT to simply fields. At long last, we have proven our earlier statements about the solutions to the wave equation in QFT being operators (fields).

ϕ and $\phi^\dagger$ are operator fields since they contain coefficient operators

Note that for our field solutions of (3-36), ϕ acts as a total particle number lowering operator, because it destroys particles (via $a(\mathbf{k})$) and creates antiparticles (via $b^\dagger(\mathbf{k})$). The former decreases a positive total particle number, whereas the latter increases the magnitude of a negative total particle number. For $\phi^\dagger$, the situation is reversed: $a^\dagger(\mathbf{k})$ creates particles and $b(\mathbf{k})$ destroys antiparticles, both actions increasing the total particle number.

Thus, the total particle lowering operator field is (see (3-36) for full expression)

ϕ is a total particle number lowering operator field

$$\phi = \underbrace{\phi^+}_{\substack{\text{destroys} \\ \text{particles}}} + \underbrace{\phi^-}_{\substack{\text{creates} \\ \text{anti-particles}}} , \tag{3-85}$$

and the total particle raising operator field is

$\phi^\dagger$ is a total particle number raising operator field

$$\phi^\dagger = \underbrace{\phi^{\dagger +}}_{\substack{\text{destroys} \\ \text{anti-particles}}} + \underbrace{\phi^{\dagger -}}_{\substack{\text{creates} \\ \text{particles}}} . \tag{3-86}$$

When we originally saw the field solutions (3-36), it was suggested, as a mnemonic, that you make a copy of them and stick it over your desk. It would be good now to insert (3-85) and (3-86) into that copy and make them part of it, as we will be using those symbols and what they represent, over and over.

3.6.6 Normal Ordering

When the infinite sum of ½ quanta energy in (3-59) was first found, physicists wanted desperately to make it go away. The amount of energy involved should, via general relativity, curve the universe to such an enormous degree that the light emanating from your finger would be bent so much that it would never reach your eyes. But that isn't what happens in our world, so something isn't correct. In fact, the difference in mass-energy level of the vacuum, between what is predicted by theory and what is observed, is on the order of a factor of 10^{120}, the biggest discrepancy between theory and experiment in the history of science.

One approach to solving ("hiding" may be a better word) this problem is something called normal ordering. Normal ordering, in any term, consists of moving all destruction operators to the right hand side of that term. This has little impact for operators that commute, such as $a(\mathbf{k})$ and $b^\dagger(\mathbf{k})$, for example. That is, changing the term $a(\mathbf{k})b^\dagger(\mathbf{k})$ to $b^\dagger(\mathbf{k})a(\mathbf{k})$ is not an issue, since the factors commute, i.e., $a(\mathbf{k})b^\dagger(\mathbf{k}) = b^\dagger(\mathbf{k})a(\mathbf{k})$. However, the term $a(\mathbf{k})a^\dagger(\mathbf{k})$ is a different story, since $a(\mathbf{k})a^\dagger(\mathbf{k}) \neq a^\dagger(\mathbf{k})a(\mathbf{k})$.

Normal ordering puts all destruction operators in any term on the RHS

In particular, note the effect of normal ordering in our derivation of the number operator form of the Hamiltonian in (3-54). Instead of employing the commutator relations for the $a(\mathbf{k})a^\dagger(\mathbf{k})$ and $b(\mathbf{k})b^\dagger(\mathbf{k})$ terms as done in (3-54), we simply move all the destruction operators to the RHS, so those terms become $a^\dagger(\mathbf{k})a(\mathbf{k})$ and $b^\dagger(\mathbf{k})b(\mathbf{k})$. Thus, we never end up with the $\frac{1}{2}\omega_{\mathbf{k}}$ terms, the Hamiltonian is finite, just what we would originally have expected it to be, and the vacuum has zero energy, i.e.,

Normal ordering makes vacuum energy go away

$$H_0^0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(a^\dagger(\mathbf{k}) a(\mathbf{k}) + b^\dagger(\mathbf{k}) b(\mathbf{k}) \right) \quad \text{(normal ordered = what is observed)}. \qquad (3\text{-}87)$$

The Hamiltonian only has number operators yielding $n_{\mathbf{k}}\omega_{\mathbf{k}}$ energy for $n_{\mathbf{k}}$ particles, each having 3-momentum $\mathbf{k}$.

Although use of normal ordering became quite widespread, it suffers from a pretty fundamental problem. It violates the foundational postulate of non-commutation of certain operators, upon which all of QFT stands. Invoking normal ordering means assuming, in this one area of QFT, that $a(\mathbf{k})$ and $a^\dagger(\mathbf{k})$ (as well as $b(\mathbf{k})$ and $b^\dagger(\mathbf{k})$) commute! But they don't. And the fact that they don't is fundamental to every other part of QFT[1]. In normal ordering, we simply suspend commutation long enough to get a zero energy for the vacuum, then bring it back for the rest of the theory. It is not unreasonable to conclude that use of normal ordering for this purpose is questionable, at best.

Some argue that using normal ordering in this way is internally inconsistent

Caveat: The position expressed in the above paragraph is not widespread, and normal ordering to remove the ½ quanta terms is often invoked with questionable (in my mind) justification. (See next paragraph.) I, and a handful of others[2] I am aware of, contend it should simply be jettisoned.

Note that normal ordering is often justified because particle/field behavior in our theories of classical mechanics, electromagnetism, and special relativity depends on energy difference, so we can take our reference as the vacuum energy level and all energies of interest are relative to that. In those theories, it is ΔE that is important, not E. So, why not assume our Hamiltonian represents $\Delta E = E - \infty$ instead of E? The answer, I and others submit, is because in general relativity, the theory depends on E. (See above.) To be consistent with all of physics, we need H representing E, not ΔE.

In any case, in spite of common use of normal ordering to "clean up" the Hamiltonian, the huge vacuum energy issue has not gone away in most physicists eyes, and it remains a widely discussed, unsolved problem as of the year of this version of this book (though I offer a possible solution in the article cited in the footnote on page 50).

Paradoxically both 1) normal ordering is widely used to eliminate vacuum energy, and 2) vacuum energy is generally accepted as a fact

It may seem to you the reader that the entire issue is fraught with ambiguity, and that is probably a reasonable assessment. In spite of that, virtually everyone considers vacuum energy to be a reality.

3.6.7 The Observable Hamiltonian

One can distinguish observables, which in quantum theories are represented by operators, from the theoretically obtained expressions for the corresponding operators. That is, the $\frac{1}{2}\omega_{\mathbf{k}}$ terms in $H_0{}^0$ are not observed, so for reasons of practicality, we can consider the normal ordered Hamiltonian of of (3-87) to be what we will call the observable Hamiltonian.

The normal ordered Hamiltonian is the observable Hamiltonian.

The relation (3-87), even though derived via the *ad hoc* and mathematically questionable normal ordering process, results in what is actually observed. This is why normal ordering persists.

Since we will not do a lot with the vacuum, we will find it more convenient and streamlined to use (3-87) for the Hamiltonian, except when we are specifically interested in vacuum energy. Just don't forget, as we do that, what the complete Hamiltonian, as derived via our theory, looks like.

3.7 Probability, Four Currents, and Charge Density

Probability in QFT is found in essentially the same way as we did for NRQM (see Box 3-1) and RQM (see Sect. 3.1.4, pg. 44.) That is, we use the governing wave equation and manipulate it to obtain a relationship like the continuity equation (3-19) (or (3-23) in 4D notation). The integral over all space of the quantity ρ in that relationship is conserved, and since total probability (of finding one or more particles) is also conserved, ρ has a good chance of being probability density. Experiment can confirm, or deny, that.

Probability in QFT found in similar way as in NRQM and RQM, i.e., from wave equation

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[1] As an example of one such part, see Sect. 3.6.1, where commutation relations result in $a(\mathbf{k})$ and $b(\mathbf{k})$ being destruction operators, and $a^\dagger(\mathbf{k})$ and $b^\dagger(\mathbf{k})$ being creation operators.

[2] P. Teller, *An Interpretive Introduction to Quantum Field Theory,* Princeton University Press (1995). Teller submits that a complete and true theory would not have such an artificial, and arbitrarily imposed, feature as normal ordering. On page 130, with reference to normal ordering he states, "If, as appears to be the case, at this point one must use mathematically illegitimate tricks, concern is an appropriate response."

3.7.1 Four Currents, Operators, and Probability Density in QFT

In the present case, the solutions to the governing equation are operator fields, not states, so we would expect the resulting density ρ to be an operator density, rather than a numeric density. Our expectation will turn out to be true, as we see below.

Since our governing equation is the Klein-Gordon equation, and that is the same as in RQM, similar steps (3-16) to (3-20) can be followed. The result is the same 4-current relations as (3-22) and (3-23), except that ϕ and $\phi^\dagger$ are now operator fields (or simply, in QFT lingo "fields"),

Same wave equation as RQM → same form for probability 4-current

$$\boxed{j^{\mu}{}_{,\mu} = 0 \quad \text{with} \quad j^{\mu} = i\left(\phi^{,\mu}\phi^{\dagger} - \phi^{\dagger,\mu}\phi\right) \qquad j^{\mu} \text{ is an operator}}, \tag{3-88}$$

so

$$\rho = j^0 = i\left(\frac{\partial\phi}{\partial t}\phi^{\dagger} - \frac{\partial\phi^{\dagger}}{\partial t}\phi\right). \tag{3-89}$$

But now 4-current is an operator

Since (3-89) is an operator, we need its expectation value to find measurable probability density,

So, need to find expectation value of probability operator

$$\bar{\rho} = \langle\phi_1,\phi_2,\phi_3,....|\rho|\phi_1,\phi_2,\phi_3,....\rangle. \tag{3-90}$$

To evaluate (3-90), we need first to substitute our free field solutions (3-36) into (3-89). Do Prob. 12 to prove to yourself that if we restrict ourselves to particles in **k** eigenstates (which is typically the case in QFT), then this results in an effective density operator

Probability operator expressed in terms of number operators

$$\rho = \frac{1}{V}\sum_{\mathbf{k}}\left(a^{\dagger}(\mathbf{k})a(\mathbf{k}) - b^{\dagger}(\mathbf{k})b(\mathbf{k})\right) = \frac{1}{V}\sum_{\mathbf{k}}\left(N_a(\mathbf{k}) - N_b(\mathbf{k})\right). \tag{3-91}$$

3.7.2 Single Particle State

Let's now find the expectation value of ρ for a single a type particle state $|\phi_{\mathbf{k}'}\rangle$. We find all the number operators except the one for an a type particle with momentum $\mathbf{k}'$ yield zero, so

Probability expectation value for single type a particle = 1, no surprise

$$\bar{\rho} = \left\langle\phi_{\mathbf{k}'}\middle|\rho\middle|\phi_{\mathbf{k}'}\right\rangle = \left\langle\phi_{\mathbf{k}'}\middle|\frac{1}{V}\sum_{\mathbf{k}}\left(N_a(\mathbf{k}) - N_b(\mathbf{k})\right)\middle|\phi_{\mathbf{k}'}\right\rangle = \left\langle\phi_{\mathbf{k}'}\middle|\frac{1}{V}\middle|\phi_{\mathbf{k}'}\right\rangle = \frac{1}{V}. \tag{3-92}$$

For a plane wave, this is exactly our probability density, a flat distribution over the volume, whose integral over the volume equals one. So far, ρ looks like it could well be a probability distribution.

3.7.3 Multiparticle State

But now let's look at a multiparticle state.

Probability expectation value for four type a particles = 4 > 1 !

$$\begin{aligned}\bar{\rho} &= \left\langle 3\phi_{\mathbf{k}_1},\phi_{\mathbf{k}_2}\middle|\rho\middle|3\phi_{\mathbf{k}_1},\phi_{\mathbf{k}_2}\right\rangle = \left\langle 3\phi_{\mathbf{k}_1},\phi_{\mathbf{k}_2}\middle|\frac{1}{V}\sum_{\mathbf{k}}\left(N_{\mathbf{a}}(\mathbf{k}) - N_{\mathbf{b}}(\mathbf{k})\right)\middle|3\phi_{\mathbf{k}_1},\phi_{\mathbf{k}_2}\right\rangle \\ &= \left\langle 3\phi_{\mathbf{k}_1},\phi_{\mathbf{k}_2}\middle|\frac{4}{V}\middle|3\phi_{\mathbf{k}_1},\phi_{\mathbf{k}_2}\right\rangle = \frac{4}{V}.\end{aligned} \tag{3-93}$$

When (3-93) is integrated over V, we get 4, the number of particles in the state! Since total probability is never greater than 1, our interpretation of ρ as a probability density seems to be in trouble for multiparticle states.

So, QFT deals with number of particles instead of probability

Partially for this reason, QFT rarely deals with probability densities for states. It concerns itself, instead, with *numbers* of particles (and antiparticles) in a state. Thus, the number operators play a major role. As we will see, this works well, and allows us to solve the kinds of problems in QFT we need to solve.

3.7.4 Antiparticles (Type b Particles)

Now consider the expectation value of ρ on a b type single particle state.

Probability expectation value for single type b particle = − 1 < 0 !!

$$\bar{\rho} = \left\langle\bar{\phi}_{\mathbf{k}'}\middle|\rho\middle|\bar{\phi}_{\mathbf{k}'}\right\rangle = \left\langle\bar{\phi}_{\mathbf{k}'}\middle|\frac{1}{V}\sum_{\mathbf{k}}\left(N_a(\mathbf{k}) - N_b(\mathbf{k})\right)\middle|\bar{\phi}_{\mathbf{k}'}\right\rangle = \left\langle\bar{\phi}_{\mathbf{k}'}\middle|\frac{-1}{V}\middle|\bar{\phi}_{\mathbf{k}'}\right\rangle = -\frac{1}{V}. \tag{3-94}$$

So total probability of a b type particle would be negative! And for 3 such particles, it would be -3.

This was another tip to early researchers that the density they were dealing with was more readily related to charge density, and the b particles were antiparticles, with opposite charge (and charge density) from particles.

Thus, we have started to see that the concept of probability density, and the mathematics associated with it, seem to lose some applicability in QFT. Particle number, however, takes on significance, as now antiparticles would simply be designated as having negative total particle numbers.

Led to conclusion that $\rho \propto$ charge probability density, and its spatial integral is total charge

3.7.5 Charge Density Not Probability Density

If we multiply our four current operator (3-88) by the charge of a scalar particle q it behaves like a charge density operator, which we will designate by s^{μ}.

Multiply 4-current operator by particle charge to get charge 4-current operator

$$s^{\mu}{}_{,\mu} = 0 \quad \text{with} \quad s^{\mu} = qj^{\mu} = iq\left(\phi^{,\mu}\phi^{\dagger} - \phi^{\dagger,\mu}\phi\right) \ , \tag{3-95}$$

so

$$\rho_{charge} = qj^{0} = iq\left(\frac{\partial \phi}{\partial t}\phi^{\dagger} - \frac{\partial \phi^{\dagger}}{\partial t}\phi\right). \tag{3-96}$$

This makes sense, as charge would be distributed in parallel fashion to probability density, i.e., denser charge where the particle is more concentrated. Further, total charge using (3-93) multiplied by q would yield 4q, the charge on the state. Similarly, the total charge on the state in (3-94) would be $-q$.

Thus, re-interpreting the operator ρ, as charge density, and the 3D part of the four current as charge current density is consistent. In actuality, it is demanded in order for our theory to agree with experiment. That empirical reality also forces us to accept b type particles as antiparticles.

Take care that in the future, we may use the symbol ρ as simply charge density, without a subscript. Since we will rarely, if ever, deal again with probability density, hopefully, there will be little confusion.

3.7.6 Caution in Evaluating Expectation Values of Density Operators

Some care must be taken in the evaluation of expectation values similar to that of (3-90). The bracket, expressed in the position basis, is an integration over space. But for operators with a spatial dependence such as ρ often has (and which is typical of charge, mass or any type of density), the spatial dependence in the operator is <u>not</u> included in the integration. That is, writing out the expectation value as an integral, we integrate over the $\mathbf{x}'$ of the state, but not the $\mathbf{x}$ of the operator.

Integration implied in expectation value is over ket $\mathbf{x}'$, not over operator $\mathbf{x}$

$$\left\langle \rho(\mathbf{x},t)\right\rangle = \left\langle \phi_{\mathbf{k}}(\mathbf{x}',t)\,|\,\rho(\mathbf{x},t)\,|\phi_{\mathbf{k}}(\mathbf{x}',t)\right\rangle = \int \phi^{\dagger}_{\mathbf{k},state}(\mathbf{x}',t)\rho(\mathbf{x},t)\phi_{\mathbf{k},state}(\mathbf{x}',t)\,d^{3}x' \ . \tag{3-97}$$

This was not evident in (3-92) and similar relations above, because there (for plane waves, specifically) the operator ρ was not a function of space.

The point in (3-97) generalizes to other types of operator functions that would be sandwiched inside a bra and a ket. We will run into these in the future.

3.7.7 The ϕ and $\phi^{\dagger}$ Normalization Constants Again

We just assumed, in all of our discussion so far, that the normalization constants in our solutions, $1/\sqrt{2\omega_{\mathbf{k}}V}$, that we derived in RQM, are also valid in QFT. Since our field solutions ϕ and $\phi^{\dagger}$ in QFT had the same form as the state solutions in RQM, and our 4 current $j^{\mu} = (\rho, \mathbf{j})$ in each case had the same form as well, this seems like a reasonable assumption. The assumption can be considered justified by our results in the above few sections. For example, (3-91) worked out as a correct form for density (probability or charge) only because of the form chosen for our constants. The square root of $2\omega_{\mathbf{k}}$ dropped out in getting (3-91) because of the two terms, each with two field factors multiplied, and the time derivatives in (3-89).

ϕ and $\phi^{\dagger}$ normalization constants from RQM work for QFT

We can therefore consider the results of the sections above as justification for the choice of normalization constants in the field solutions to the Klein-Gordon equation. All of so many other results, yet to be seen in our studies, will be further justification.

3.8 More on Observables

QFT, like the quantum theories studied before it, is interested in observable quantities, such as energy, 3-momentum, charge, and spin, which are represented in each of those theories by operators. The eigenvalues of those operators are what we measure. Expectation values of those operators are the averages of what we measure over many trials.

Finding operators other than H in terms of number operators

Regarding energy, we have already discussed the observable operator corresponding to it. See (3-87). Regarding spin, scalar particles have none, so we will put off discussion of particles that do have it to later chapters.

3.8.1 Charge Operator

Regarding charge, we need merely to integrate our charge density operator qj^0 of (3-96) and (3-91) over the entire volume, to get the charge operator

$$Q = \int s^0 d^3x = q\int j^0 d^3x = q\sum_{\mathbf{k}}\left(N_a(\mathbf{k}) - N_b(\mathbf{k})\right). \tag{3-98}$$

Total charge operator yields total charge of a (multiparticle) state

A typical multiparticle state is in a charge eigenstate with an eigenvalue of charge equal to the sum of the charges of all particles in the state. Hence, the eigenvalue equals the charge expectation value, since we will measure the same charge with each measurement. For a sample state,

$$\bar{Q} = \langle 7\phi_{\mathbf{k}_1}, \phi_{\mathbf{k}_2}, 5\bar{\phi}_{\mathbf{k}_3} | \underbrace{q\sum_{\mathbf{k}}\left(N_a(\mathbf{k}) - N_b(\mathbf{k})\right)}_{Q} | 7\phi_{\mathbf{k}_1}, \phi_{\mathbf{k}_2}, 5\bar{\phi}_{\mathbf{k}_3} \rangle = 7q + q - 5q = +3q\,. \tag{3-99}$$

Note, we derived (3-98) using (3-91). If you did Prob. 12, you saw that in deriving (3-91) we summed terms in ½ and – ½ that cancelled to net zero. In other words, (3-98) actually has a $+q/2$ and a $-q/2$ term for each **k**. Thus, Q acting on the vacuum would sum up an infinite number of half charge quanta for both particles (positive charge) and anti-particles (negative charge), leaving zero total vacuum charge. (Thankfully, it does. If it didn't, our theory would be bound for the trash heap.)

Vacuum has zero charge

3.8.2 Three Momentum Operator

The three momentum operator can be found using the relationship for physical momentum density at the bottom of Box 2-2 in Chap. 2, pg. 23, and integrating over the volume. (Also shown in the 9th block under the title in the RH column of Wholeness Chart 2-2, pg. 21.) That is,

$$p^i = \int \not{p}^i d^3x = -\int \pi_r \frac{\partial \phi^r}{\partial x^i} d^3x = -\int\left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}}\frac{\partial \phi}{\partial x^i} + \frac{\partial \mathcal{L}}{\partial \dot{\phi}^\dagger}\frac{\partial \phi^\dagger}{\partial x^i}\right) d^3x\,. \tag{3-100}$$

Substituting the Klein-Gordon solutions (3-36) and their conjugate momenta into (3-100), one obtains the 3-momentum operator (do Prob. 13 to prove it)

$$\mathbf{P} = \sum_{\mathbf{k}} \mathbf{k}\left(N_a(\mathbf{k}) + N_b(\mathbf{k})\right), \tag{3-101}$$

Total 3-momentum operator yields total 3-momentum of a (multiparticle) state

which is pretty much what we would have expected. **P** operating on a multiparticle ket, with all particles in **k** eigenstates, would yield an eigenvalue equal to the number of particles and antiparticles with 3-momentum **k** multiplied by **k**. If this is less than obvious to you, do Prob. 14.

It is interesting that, similar to what happened to charge, we have ½ quanta in the vacuum with 3-momentum, but the total for the vacuum sums to zero. That is, in deriving (3-101), we get terms in the summation of ½ **k** + ½ **k** = **k** (one ½ quanta for each particle and one for each antiparticle), similar to what we had for energy. But unlike energy, this is a vector summation, and for every 3-momentum **k** in the sum, there is a 3-momentum – **k**, as well. The net is nil 3-momentum for the vacuum, which again, is a welcome result.

Vacuum has zero 3-momentum

So far in our theory, only energy has proved problematic in having a non-zero vacuum expectation value (VEV.)

3.8.3 The Four Momentum Operator

As discussed in the Appendix of Chap. 2, and elsewhere, the four momentum has energy in the 0th component (E/c in non-natural units) and 3-momentum for the other three components. Given (3-87) for H_0^0, and (3-101) for the free scalar field p^i, the four momentum operator is

$$\underbrace{P^{\mu}=K^{\mu}}_{\substack{\text{operators}\\ \text{here}}}=\underbrace{\begin{pmatrix}H\\ \mathbf{P}\end{pmatrix}}_{\substack{\text{for free}\\ \text{scalars}}}=\sum_{\mathbf{k}}\underbrace{\begin{pmatrix}\omega_{\mathbf{k}}\\ \mathbf{k}\end{pmatrix}}_{\substack{\text{usually what}\\ \text{we mean by}\\ \text{symbol } k^{\mu}}}\left(N_a(\mathbf{k})+N_b(\mathbf{k})\right), \qquad (3\text{-}102)$$

4-momentum operator includes energy and 3-momentum

where we note that k^{μ} usually refers to the numeric (not operator) 4 vector ($\omega_{\mathbf{k}}$,**k**).

3.9 Real Fields

So far, we have only dealt with complex fields. It is possible to have real fields, and in fact, we will see they play a key role in the theory. They turn out to be associated with neutral particles, which are, in fact, their own antiparticles.

To see this, look at a special case for our general field equation solutions (3-36) where $\phi = \phi^{\dagger}$, i.e., ϕ is real. In order for this to be true, we must have $a(\mathbf{k}) = b(\mathbf{k})$, and of course, $a^{\dagger}(\mathbf{k}) = b^{\dagger}(\mathbf{k})$. Thus, for this case,

$$\phi=\phi^{\dagger}=\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}a(\mathbf{k})e^{-ikx}+\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}a^{\dagger}(\mathbf{k})e^{ikx}\quad(\text{for }\phi\text{ real}), \qquad (3\text{-}103)$$

which makes sense, since adding a complex number and its complex conjugate yields a real number.

In the charge operator (3-98), we would then have $N_a(\mathbf{k}) = N_b(\mathbf{k})$ (i.e., $a^{\dagger}(\mathbf{k})a(\mathbf{k}) = b^{\dagger}(\mathbf{k})b(\mathbf{k})$), so charge would be zero for any such particle(s) state. Each *b* type particle operator (creation, destruction, charge, energy, etc.) will be the same operator as that for *a* particles. There is only one type of particle (for a real field), so that particle must be its own antiparticle.

Real (not complex) fields create and destroy neutral charge particles

<u>Conclusion:</u> Real fields are associated with charge-neutral particles, which are their own anti-particles.

<u>Note on nomenclature:</u> The term "<u>real field</u>" refers to the (operator) field solution to the field equation (Klein-Gordon for scalars) that are not complex. The term "<u>real particle</u>" refers to a particle that is not virtual, but manifest and detectable.

Terminology difference between real fields and real particles

3.10 Characteristics of Klein-Gordon States

3.10.1 Bosons vs Fermions

Although at this point in your career, you should be familiar with bosons and fermions, and their behavior, Wholeness Chart 3-1 can serve as a refresher course. It should need no further comment.

Wholeness Chart 3-1. Bosons vs Fermions

	<u>Bosons</u>	**<u>Fermions</u>**
What role	typically forces	typically matter
Some examples	elementary: photons, Higgs composite: mesons	elementary: electrons, neutrinos, quarks composite: baryons (e.g., proton, neutron)
Behavior	can occupy same state	can't occupy same state
Spin	integer spin Scalars: spin 0 Vectors (e.g. photons): spin 1 Graviton: spin 2	half integer spin Spinors: spin ½ Gravitinos: spin 3/2

3.10.2 Klein-Gordon States are Bosons

The same scalar creation operator that operates repeatedly on a state results in a raised state containing a number of the same particle with the same **k** (and thus the same energy and identical in all regards.) For example, using the creation operator of the first line of (3-81) acting first on the vacuum, then repeatedly on the newly created states, we have

$$a(\mathbf{k})^{\dagger}|0\rangle = |\phi_{\mathbf{k}}\rangle \;\rightarrow\; a(\mathbf{k})^{\dagger}|\phi_{\mathbf{k}}\rangle = \sqrt{2}|2\phi_{\mathbf{k}}\rangle \;\rightarrow\; a(\mathbf{k})^{\dagger}|2\phi_{\mathbf{k}}\rangle = \sqrt{3}|3\phi_{\mathbf{k}}\rangle \rightarrow ..... \tag{3-104}$$

Scalar kets can have > 1 particle in same state, so scalars are bosons, not fermions

We are not concerned, for this discussion, with the square root numeric coefficients, but with the fact that we can have multiparticle states with more than one individual particle in the same individual state.

This means Klein-Gordon states must be bosons. We sort of knew this because we were told that they have zero spin. But here we prove it.

As we will see in the next chapter, spinors do not have the characteristic displayed by (3-104).

3.10.3 Commutators with Scalars, Not Anti-Commutators

Let's see what happens if anti-commutators were used instead of commutators with the Klein-Gordon field equation solutions. That is, in the derivation of our number operator form of the Hamiltonian, in equation (3-54), try the anti-commutators

$$\begin{aligned} \left[a(\mathbf{k}), a^{\dagger}(\mathbf{k}')\right]_{+} &= a(\mathbf{k})a^{\dagger}(\mathbf{k}') + a^{\dagger}(\mathbf{k}')a(\mathbf{k}) = \delta_{\mathbf{kk}'} \\ \left[b(\mathbf{k}), b^{\dagger}(\mathbf{k}')\right]_{+} &= b(\mathbf{k})b^{\dagger}(\mathbf{k}') + b^{\dagger}(\mathbf{k}')b(\mathbf{k}) = \delta_{\mathbf{kk}'} . \end{aligned} \tag{3-105}$$

A minus sign is then introduced, such that instead of (3-55), we would get

$$H_0^0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(\tfrac{1}{2} + \tfrac{1}{2}\right) \;, \tag{3-106}$$

Using anti-commutator instead of commutator → theory with faulty energy prediction (wrong)

or for an observable Hamiltonian (ignoring vacuum energy)

$$H_0^0 = 0 \quad \text{and thus,} \quad H_0^0|\phi_{\mathbf{k}_1}\rangle = 0 . \tag{3-107}$$

Every real state would have zero energy, which is certainly not physically true. Therefore, we can only use commutators with spin 0 boson fields, and not anti-commutators.

We will find in the next chapter, that fermions in QFT are governed by anti-commutators in parallel fashion to the way in which bosons (scalars, at least, to this point in our studies) are governed by commutators. Just as anti-commutators can't work for bosons (scalars), as we saw above, we will also see later that commutators can't work for fermions.

Klein-Gordon scalars:
1) *must be bosons, and*
2) *can only use commutation relations*

3.11 Odds and Ends

3.11.1 Usefulness of 3-Momentum Discrete Eigenstates

As you will see in time, QFT can find real world experimental values, for things like scattering cross sections and decay half lives, using only discrete **k** eigenstate forms for real states. These eigenstates, unlike wave packets, typically extend indefinitely in the **k** direction. But for experimental predictions, the particle states, which are actually wave packets, can be approximated to extremely high precision by such discrete **k** eigenstates.

Discrete form of solutions (not wave packets) suffice for extremely accurate real particle predictions

One exception is the propagator, the mathematical representation of virtual particles, which is best derived, as shown in Sect. 3.13, and most useful practically, via incorporation of the continuous (integral) form of the field equation solutions. This is, at least in part, because virtual particles are not constrained by boundary conditions to discrete **k** values and in certain cases must be integrated over all possible, continuous values of **k**.

Except, we will need continuous solutions to find Feynman propagator (for virtual particles)

3.11.2 Nevertheless, What about Non-eigen States?

In NRQM (and RQM) we commonly dealt with general states, i.e., non-eigen states, which were superpositions of two or more eigenstates. Granted, as noted above, that we can solve almost all QFT problems using **k** eigenstates, we might still ask "how does QFT compare in this regard to what we learned in NRQM?" It is a good question, troubling many students, no doubt, and not treated in any other text I am aware of.

A closely related question is "what is created or destroyed by the general solutions $\phi(x)$ (or $\phi^{\dagger}(x)$), which for discrete eigenstates, is a summation of terms, each containing a single particle eigenstate creation/destruction operator?" Does operation of $\phi^{\dagger}(x)$ on the vacuum, for instance, create an infinite number of single particles, or a single particle comprising an infinite number of momentum eigenstates? If the latter, what amplitudes (whose absolute values squared are probabilities) are assigned to each such eigenstate?

Creating a General Single Particle State (Discrete Solution Form)

To create a general single particle state, , we would need a creation operator of form

Creation operator for single particle general (non-eigen) state, discrete case.

$$C = \sum_{\mathbf{k}} A_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}^{\dagger} , \tag{3-108}$$

so that operation of C on the vacuum results in a sum of eigenstates,

$$C|0\rangle = \sum_{\mathbf{k}} A_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}^{\dagger} |0\rangle = A_1|\phi_1\rangle + A_2|\phi_2\rangle + A_3|\phi_3\rangle + ... = |\phi\rangle . \tag{3-109}$$

In (3-108) and (3-109) $A_{\mathbf{k}}$ is a numerical coefficient, the square of the absolute value of which (for proper normalization of the ket eigenstates) equals the probability of finding the $\mathbf{k}$ eigenstate.

If only one term in C is used, then only one eigenstate with $|A_{\mathbf{k}}| = 1$ is created. If a more general state, comprising a sum of eigenstates, is created, then we are free to select the $A_{\mathbf{k}}$ as we please in order to create the particular general state we like, provided (for conservation of probability and correct normalization so total probability is unity)

$$\sum_{\mathbf{k}} | A_{\mathbf{k}} |^2 = 1 . \tag{3-110}$$

Destroying a General Single Particle State (Discrete)

Destruction operator for single particle general (non-eigen) state, discrete case.

Note that the general single particle destruction operator

$$D = \sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}} \tag{3-111}$$

acting on any single particle general state will lower that state to the vacuum. That is,

$$\begin{aligned} \left(\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}\right)|\phi\rangle &= \left(\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}\right)\left(A_1|\phi_1\rangle + A_2|\phi_2\rangle + A_3|\phi_3\rangle + ...\right) \\ &= \left(\left(\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}\right)A_1|\phi_1\rangle + \left(\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}\right)A_2|\phi_2\rangle + \left(\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}\right)A_3|\phi_3\rangle + \dots\right) \\ &= A_1 \underbrace{\mathbf{a}_1|\phi_1\rangle}_{|0\rangle} + A_1 \underbrace{\mathbf{a}_2|\phi_1\rangle}_{0} + A_1 \underbrace{\mathbf{a}_3|\phi_1\rangle}_{0} + ... + A_2 \underbrace{\mathbf{a}_1|\phi_2\rangle}_{0} + A_2 \underbrace{\mathbf{a}_2|\phi_2\rangle}_{|0\rangle} + 0 + ... = \underbrace{(A_1 + A_2 + ...)}_{\text{can normalize} = 1} |0\rangle . \end{aligned} \tag{3-112}$$

Creating and Destroying Multi-particle State (Discrete)

Applying operators similar in form to (3-108) (with typically different values for $A_{\mathbf{k}}$ in each operator) twice in succession creates a two particle state where each particle is a single particle general state (i.e., each is a summation of momentum eigenstates.) Any number of such operators may be applied to create a state of any number of particles, each in a general (not necessarily eigen) state.

For multiparticle general states, repeatedly apply C and D operators

Applying (3-111) repeatedly will destroy one general state single particle upon each application.

What $\phi(x)$ and $\phi^{\dagger}(x)$ Create When Acting on the Vacuum

$\phi(x)$ acting on the vacuum will create a single general antiparticle state comprising a superposition of an infinite number of eigenstates, each with a constant coefficient in front of it, i.e.,

$$\phi(x)|0\rangle = \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} e^{-ikx} \underbrace{a(\mathbf{k})|0\rangle}_{0} + \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} e^{ikx} \underbrace{b^{\dagger}(\mathbf{k})|0\rangle}_{|\bar{\phi}_{\mathbf{k}}\rangle} = \sum_{\mathbf{k}} \underbrace{\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}}_{\text{constant}} \underbrace{e^{ikx}}_{\substack{\text{phase}\\ \text{factor}}} |\bar{\phi}_{\mathbf{k}}\rangle . \tag{3-113}$$

Similarly, $\phi^{\dagger}(x)$ acting on the vacuum will create a single particle general state comprising a superposition of particle eigenstates. For discrete solutions, these operations have little use in QFT.

Creating and Destroying Continuous Solution Forms of States

In analogous fashion, the continuous form of $\phi(x)$ (or $\phi^{\dagger}(x)$) acting on the vacuum yields a single antiparticle (particle) wave packet, i.e., an integral over all $\mathbf{k}$, rather than a sum. You don't need to know more now, but for the future, details are in this book's web site (address on pg. xvi, opposite pg. 1) at the link titled Non Eigen States, Wave Packets, and the Hamiltonian in QFT. A summary of that can be found in Appendix C of Chap. 10 herein. We will work more with these operations when we derive the Feynman propagator in Sect. 3.13.

3.11.3 c-numbers vs q-Numbers

The terms c-number and q-number were introduced by Paul Dirac to distinguish between *classical numbers* (real or complex), which commute, and *quantum operators*, which do not always commute. The term *q*-number can equally apply to the *eigenvalue* of a given quantum operator.

q-numbers are quantum numbers (operators or their eigenvalues);

c-numbers are classical numbers

Thus, the 3-momentum of a classical particle is a *c*-number. The 3-momentum of a quantum state, in a 3-momentum eigenstate, is a *q*-number.

Eigenstates are often labeled by their *q*-numbers (eigenvalues). For example, the *n, l,* and *m* numbers for electron levels in the hydrogen atom are quantum, or *q*-, numbers. *n* represents the energy level number (which is simpler than specifying the energy itself); *l*, the angular momentum magnitude; and *m*, the *z* component of angular momentum. By specifying *n*, *l*, and *m*, one specifies the eigenstate of the electron in the atom.

3.11.4 Fock Space and Hilbert Space

As you should (hopefully) remember, a quantum state in NRQM is an abstract vector in an abstract vector space, analogous to a physical vector in 3D physical space. The same thing is true in RQM and QFT. This is summarized in Wholeness Chart 3-2.

In all quantum theories, basis vectors (which are typically eigenstates) are abstractions of the unit basis vectors along the 3D axes. A general state is a vector sum of certain amounts of each basis vector state. Operators in each kind of space act on the states in that space.

In NRQM and RQM, the states are single particle states and the abstract space they inhabit is called Hilbert space, which has a different single particle eigenstate as the basis vector of each "axis". The dimension of the Hilbert space for a given system is simply the number of linearly independent eigenstates in that system. This can, for many systems, be infinite.

In QFT, states are multiparticle, so the basis eigenstate of each "axis" is a multiparticle state. One "axis" basis vector might be an electron and a photon, each with particular 3-momentum. Another might be 2 photons and a positron with particular 3-momenta. Yet another might be an electron and photon like the first, except that at least one of them has different 3-momentum from the first. The multiparticle abstract state space of QFT is called Fock space, which is simply an extension of Hilbert space to multiparticle states.

Fock space is Hilbert space generalized to multiparticle states

Wholeness Chart 3-2. Physical, Hilbert, and Fock Spaces

	3D Physical Space	**Hilbert Space**	**Fock Space**
Character of a vector	Position vector in 3D	State vector $\|\Psi\rangle$ in NRQM, RQM Single particle	State vector $\|\phi_1, \phi_2, \dots\rangle$ in QFT Multi particle
Orthonormal basis vectors along "axes"	$\hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \hat{\mathbf{i}}_3$	Normalized eigenvectors $\|\Psi_1\rangle, \|\Psi_2\rangle, \|\Psi_3\rangle, \|\Psi_4\rangle, \dots$	Normalized eigenvectors $\|0\rangle, \|\phi_1\rangle, \|\phi_2\rangle, .. \|\phi_1, \phi_2\rangle, ..\|\phi_1, \phi_2, \phi_3\rangle, \dots$
Inner product	$\hat{\mathbf{i}}_i \cdot \hat{\mathbf{i}}_j = \delta_{ij}$	$\langle\Psi_r\|\Psi_s\rangle = \delta_{rs}$	$\langle\phi_1\|\phi_1, \phi_2\rangle = 0;\ \langle\phi_1, \phi_2\|\phi_1, \phi_2\rangle = 1$; etc.
General state vector	$\mathbf{r} = x^1\hat{\mathbf{i}}_1 + x^2\hat{\mathbf{i}}_2 + x^3\hat{\mathbf{i}}_3$	$\|\Psi\rangle = C_1\|\Psi_1\rangle + C_2\|\Psi_2\rangle + C_3\|\Psi_3\rangle + \dots$	$\|\Phi\rangle = C_1\|\phi_1\rangle + C_2\|\phi_2\rangle + \dots + C_{12}\|\phi_1, \phi_2\rangle + C_{13}\|\phi_1, \phi_3\rangle + \dots + C_{123}\|\phi_1, \phi_2, \phi_3\rangle + \dots$
State vector & its components	point in 3D space = amount along each basis vector	"point" in Hilbert Space = amount of each single particle basis vector	"point" in Fock Space = amount of each multi particle basis vector
Operators	Matrices operate on vectors	Hamiltonian H, 3-momentum $\mathbf{P}$, etc operate on states	Hamiltonian H, $\mathbf{P}$, creation $a^\dagger(\mathbf{k})$, $b^\dagger(\mathbf{k})$, destruction $a(\mathbf{k})$,$b(\mathbf{k})$, charge Q operate on states

3.11.5 *a*(k) *Destroys Any State without Single a Type Particle in* k *Eigenstate*

Keep in mind (as we actually already did in the last row of (3-112)) that, for example,

$$\mathbf{a}_2 \left| \phi_1, 4\phi_3, 7\bar{\phi}_2 \right\rangle = 0\,, \tag{3-114}$$

which is zero, not the vacuum state. In general, a particular type particle destruction operator of given **k** acting on a state that has no particles of that type of the same 3-momentum **k** results in zero.

Destruction operators of given kind and **k** *destroy any state not having like kind of particle in a* **k** *eigenstate*

3.12 Harmonic Oscillators and QFT

One sometimes hears that particles in QFT can be considered to be harmonic oscillators. The reason for this can be seen with the aid of Wholeness Chart 3-3, which summarizes the states of the NRQM harmonic oscillator (relativistic form is similar, but more complicated, so we won't bother with it) and particles in QFT.

One sees immediately that the energy levels of the two look very similar. Each level is $\hbar\omega$ above the one below it. (We keep the symbol $\hbar$ for this discussion, since it makes the NRQM summary look more familiar.) And strikingly, each also has a lowest level of energy, when n = 0 ($n_{\mathbf{k}}$ = 0 in QFT, to be precise), of ½ quantum (½$\hbar\omega$ or ½$\hbar\omega_{\mathbf{k}}$.) More striking still, each has raising and lowering operators that raise and lower energy levels by $\hbar\omega$ (or $\hbar\omega_{\mathbf{k}}$ for each extra particle in QFT.)

QFT particle states have similarities to harmonic oscillator energy states

These similarities led people to think in terms of QFT particles as harmonic oscillators. The vacuum was the lowest excitation of the quantum field. (Really, one should say the "state", not the "field", but people commonly express it this way. Confusing? Yes.) Each state above (in QFT, each additional particle) was simply a more excited state of the lowest state (in QFT, the vacuum state.) Operators acting on states raise or lower the number of particles, and thus the energy level, and so excite, or de-excite, the vacuum. Particles are just excitations of an underlying vacuum field.

Wholeness Chart 3-3. Quantum Harmonic Oscillator Compared to QFT Free States

	NRQM Harmonic Oscillator	**QFT Free States**
Energy Levels	$(n + ½)\,\hbar\omega$	$(n_{\mathbf{k}} + ½)\,\hbar\omega_{\mathbf{k}}$
Interpretation of n and $n_{\mathbf{k}}$	single particle energy level 0,1,2,…	number of particles at $\hbar\omega_{\mathbf{k}}$ energy
Interpretation of ω and ω_{k}	natural angular frequency of classical oscillator	angular frequency of particle of energy $\hbar\omega_{\mathbf{k}}$
Lowest energy level	½ $\hbar\omega$	½ $\hbar\omega_{\mathbf{k}}$
Interpretation of ↑	real particle in lowest state	vacuum, virtual particle
Raising operator	raises single particle energy one level	raises number of particles by one and thus, also raises energy one level
Lowering operator	lowers single particle energy one level	lowers number of particles by one and thus, also lowers energy one level
Wave form	Hermite polynomial	$e^{\pm ikx}$
Nature of wave form	real, non-sinusoid	complex, sinusoid
Motion	oscillates in one place	wave that moves
Spatial constraints	bound state, local region	unbound state, unlimited volume
Free or interaction	harmonic oscillator potential → force	free, no force

3.12.1 *"Derivation" of QFT via Harmonic Oscillators*

Some "derive" QFT from harmonic oscillator assumption

Some treatments actually introduce QFT via assuming states therein are harmonic oscillators. I submit this assumption can only be made after one already knows the form of the Hamiltonian (3-55) and the raising/lowering operators (3-75) as we derived them in Sect. 3.4 (pg. 53.) Otherwise, how could anyone understand they should simply assume the QFT states have energy levels similar to those of the harmonic oscillator?

I contend that assuming harmonic oscillator behavior in QFT is an unreasonable, and unfounded, assumption, but that starting with 2nd quantization (a parallel track to what was known to work in NRQM) is a reasonable assumption. However, the former approach is common.

3.12.2 Harmonic Oscillators Have Different Behavior than States

But there are differences between QFT particle states and harmonic oscillator states

Note that the wave form for the harmonic oscillator is a Hermite polynomial, far different from the complex sinusoid of $e^{\pm ikx}$ that fields (and states) have in QFT. And, a harmonic oscillator doesn't move in space (other than up and down, or side to side, in one location), whereas waves (particles = states) do, i.e., they travel from place to place. Further, the free fields (and particles) we have been dealing with in QFT are unrestricted in space (for discrete solutions, volume V can be as large as the universe; for continuous solutions, there is no volume constraint), whereas harmonic oscillators are confined to a local region. Still further, harmonic oscillators are not free states like those we have treated, but feel force/interaction (due to the harmonic oscillator potential).[1]

For discussion of a counter argument that might be made here for the vacuum, see Appendix B.

Note the caveat: This section and the one above it are my personal position on this matter, and not, to my knowledge, shared by many others. You, the reader, should make your own call.

3.12.3 Vacuum Excitations = Real Particles

States can be thought of as excitations of the vacuum (the least excited, or ground, state)

In spite of the foregoing, one can still think of real states as stable, excited states of the vacuum, since our raising operators can create a particle state from that vacuum, i.e.,

$$a^{\dagger}(\mathbf{k})|0\rangle = |\phi_{\mathbf{k}}\rangle . \qquad (3\text{-}115)$$

The RHS above can be considered as the next highest state above the ground state (above the vacuum), and thus, an excited state of the vacuum. Considering such excited states specifically as *harmonic oscillator* excited states is a different matter.

3.13 The Scalar Feynman Propagator

Feynman propagator not simple to understand

The Feynman propagator, the mathematical formulation representing a virtual particle, such as the one represented by the wavy line in Fig. 1-1 of Chap. 1, pg. 2, is one of the toughest things, in my opinion, to learn and feel comfortable with in QFT. If you don't feel comfortable with it right away, don't worry about it. That is how virtually everyone feels. Over time, it will become more familiar, and if you are lucky and work hard, maybe even easy.

Use wholeness chart as you study the derivation

I have tried to take the derivation of the propagator one step at a time, and emphasize what each step entails. Wholeness Chart 5-4 (at the end of Chap. 5) breaks these steps out clearly, and should be used as an aid when studying the propagator derivation.

Propagators: NRQM vs QFT and Real vs Virtual Particles

Feynman propagator for QFT virtual particles is different from propagator for real particles of NRQM & RQM

Note that the propagator for real particles, which you may have studied in NRQM, is *not* the same as the Feynman propagator, which is explicitly for virtual particles in QFT. It may be confusing, but the Feynman propagator is often simply called, "the propagator". You will have to get used to discerning the difference from context.

In QFT, as we will see when we study interactions, a propagator for real particles is not generally needed, and we will not derive one here.

3.13.1 The Approach

We'll use the Feynman propagator when we get to interaction theory

The first part of QFT is a free particle theory (no interactions, as in this chapter and the next three). After this, interactions are introduced. In the course of deriving the interaction theory, a mathematical relationship arises that is called the Feynman propagator. Physically, it can be visualized as representing a virtual particle that exists fleetingly and carries energy, momentum, and

[1] All of this harmonic oscillator business confused me greatly as a student. I simply could not understand how QFT states could possibly be essentially identical to harmonic oscillators. I was not confident enough to bring up the counter points mentioned herein, and they were never addressed. So if you have seen and been confused by the harmonic oscillator approach, you are not alone.

in some cases, charge from one real particle to another. Thus, it is the carrier, or mediator, of force (interaction.) See the virtual photon of Fig. 1-1 in Chap. 1, pg. 2.

It will help us pedagogically to derive the Feynman propagator now, rather than when we get to interactions. The derivation of interaction theory is fairly complicated and it will be easier, as we develop it, if we already know the mathematical relation for the Feynman propagator, rather than diverting our attention for several pages to derive it then.

But it's easier in the long run if we derive it here

Heuristically, it may help to consider the virtual particle as created at a particular spacetime point and destroyed at a later spacetime point, and this is how Feynman diagrams portray it. From this (heuristic) perspective the operator field $\phi^{\dagger}(y)$ can be considered to create a virtual scalar particle at event y (we used the symbol x_2 in Fig. 1-1), and the field operator $\phi(x)$ destroys that virtual particle at event x (x_1 in Fig. 1-1.) The scalar propagator incorporates these two field operators in a sort of "short-hand" way.

Note that the above "creation/destruction at a point" perspective can help initially in understanding the derivation of the propagator, but we caution that it will have to be modified and refined. We will save that to the end when, after digesting the derivation to follow, this modification will be easier to understand.

We will now derive a relationship for the propagator using the field operators acting on the vacuum, and will later see (Chap. 7) that this derived relationship arises naturally in the full mathematical development of the interaction theory.

3.13.2 Milestones in the Derivation

Start with a physical visualization of the propagator and follow 5 *distinct steps*

We develop the Feynman propagator in five distinct steps, starting with a physical interpretation. We represent that interpretation mathematically and then "massage" it in subsequent steps with more mathematics, until we obtain the form of the propagator that is most useful (in QFT interaction analysis).

The entire derivation is for continuous (not discrete) eigenstate solutions of the field equation (Klein-Gordon here), since the propagator represents a virtual particle in the vacuum and the vacuum is not confined to a volume V. We represent the scalar Feynman propagator with the symbol $i\Delta_F\left(x-y\right)$. (Including the imaginary factor i is common practice.)

Step 1: Math interpretation of the physical propagator

Steps 2, 3, and 4: Math manipulation of relations for particle and anti-particle

Step 5: Combining two integrals in complex space into one over real space

<u>Step 1</u>: Express the Feynman propagator $i\Delta_F$ as a mathematical representation of a particle or antiparticle created at one point in space and time in the vacuum and destroyed at another place and time.

<u>Step 2</u>: Express $i\Delta_F$ in terms of two commutators (one for particles and one for anti-particles).

<u>Step 3</u>: Express those two commutators as real integrals.

<u>Step 4</u>: Re-express those two real integrals as two contour (complex plane) integrals.

<u>Step 5</u>: Re-express the two contour integrals as a single integral over real, not complex, space, the form most suitable for analysis.

<u>Step 1: The Feynman Propagator as the Vacuum Expectation Value of a Time Ordering Operator</u>

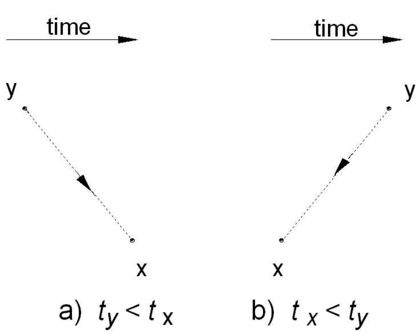

Figure 3-3. Creation & Destruction of Virtual Particle/Antiparticle

Fig 3-3a represents creation of a particle, which will be virtual, at y and destruction of it at x. Fig. 3-3b represents creation of an antiparticle at x and destruction of it at y. Virtual particles are never detected when real particles interact, so the same effect on the real particles could be realized by either of the processes in Fig. 3-3. That is, a virtual particle carrying charge from y to x would represent the same charge exchanges as a virtual antiparticle carrying opposite charge from x to y. Thus, we need a relationship for the propagator that includes both scenarios as possibilities.

Step 1, first part, defining the time ordering operator T and seeing how it represents creation of either a virtual particle or antiparticle followed by its destruction

That is, we need an operator that will create a particle first if $t_y < t_x$, but create an antiparticle first if $t_x < t_y$. Our Klein-Gordon solutions (3-37), (3-85), and (3-86) provide the means for the desired creation and destruction operations. But these have to be arranged to provide us with the time ordering dependence of Fig. 3-3. To this end, consider the time ordering operator T, defined as follows.

If $t_y < t_x$, $\phi^\dagger(y)$ operates first (creates a particle) and is placed on the right, with $\phi(x)$ operating second (destroys the particle) and placed on the left.

$$\text{for } t_y < t_x \quad \text{(particle)} \qquad T\left\{\phi(x)\phi^\dagger(y)\right\} = \phi(x)\phi^\dagger(y)\,. \tag{3-116}$$

Of course, from (3-85), and (3-86), in (3-116), $\phi(x)$ also creates an antiparticle and $\phi^\dagger(x)$ also destroys an anti-particle, but we will see this effect ultimately drops out and does not play a role in the Feynman propagator.

If $t_x < t_y$, $\phi(x)$ operates first (creates an antiparticle) and is placed on the right with $\phi^\dagger(y)$ operating second (destroying the antiparticle) and placed on the left (where the effects of these operators for particles will drop out, as we will see.)

Step 1, second part,defining the transition amplitude as equal to the VEV of time ordering operator T

$$\text{for } t_x < t_y \quad \text{(anti-particle)} \qquad T\left\{\phi(x)\phi^\dagger(y)\right\} = \phi^\dagger(y)\phi(x)\,. \tag{3-117}$$

We now define what is called the transition amplitude, which equals the vacuum expectation value (VEV) of the above time ordering operator. It is an amplitude, similar to the amplitude of a wave function in NRQM, because, as we will shortly see, the square of its magnitude equals the probability density of it being observed. (As the square of the magnitude of the amplitude for a component of the wave function equals the probability of it being observed.)

This transition amplitude is

$$\langle 0|T\left\{\phi(x)\phi^\dagger(y)\right\}|0\rangle\,, \tag{3-118}$$

We use the VEV because we will be interested in the expectation of finding a virtual particle traveling in the vacuum

which is the vacuum expectation value (VEV) of T, and this, as we will see below, represents both possible scenarios of Fig. 3-3. In wave mechanics for the position basis, the bracket above is an integration over all space. This is still true, but note carefully that the integration variable is over the space variable of the bra and ket (think $\mathbf{x}'$), but not the time ordering variables $\mathbf{x}$ and $\mathbf{y}$. (See Sect. 3.7.6, pg 63.) In QFT notation, we tend to merely think of a bracket as equaling zero unless the bra and ket represent the same state.

To gain insight into (3-118), consider the transition amplitude operating on the vacuum when a virtual particle is propagated. Then, from (3-85), and (3-86), where an overbar in a state represents an antiparticle,

Gaining insight into the time ordering operator T acting on the vacuum

$$\begin{aligned} T\left\{\phi(x)\phi^\dagger(y)\right\}|0\rangle &= \phi(x)\phi^\dagger(y)|0\rangle \qquad\qquad \text{for } t_y < t_x \quad \text{(particle)} \\ &= \Big(\underbrace{\phi^+(x)}_{\substack{\text{destroys}\\ \text{particle}}} + \underbrace{\phi^-(x)}_{\substack{\text{creates}\\ \text{antiparticle}}}\Big)\Big(\underbrace{\cancel{\phi^{\dagger+}(y)|0\rangle}}_{\substack{\text{destroys antiparticle,}\\ \text{annihilates vacuum}}} + \underbrace{\phi^{\dagger-}(y)}_{\substack{\text{creates}\\ \text{particle}}}|0\rangle\Big) \\ &= \left(\phi^+(x) + \phi^-(x)\right)F(y)|\phi\rangle \\ &= G(x)F(y)|0\rangle + H(x)F(y)|\bar{\phi}\phi\rangle. \end{aligned} \tag{3-119}$$

G, F, and H are numeric factors that result from the creation and destruction operations (such as the normalization coefficients that are part of the field operators), which we will not express explicitly here. Thus, we have a general ket left, which in this case is part vacuum state, with the amplitude of the vacuum state part being GF, and the amplitude of the multiparticle state (scalar plus anti-scalar) part being HF. As we (hopefully) remember from NRQM, and which is true for all quantum theories, for appropriate normalization, the square of the magnitude of the amplitude of a state equals the probability of finding that state. Thus $(GF)^\dagger(GF)$ represents the probability of observing the vacuum state (no particles left after the transition.) To find the amplitude GF, we need only form an inner product of the last line of (3-119) with $\langle 0|$, i.e.,

Taking the inner product of the above $T|0\rangle$ with $\langle 0|$ to get the transition amplitude

$$\begin{aligned} \langle 0|T\left\{\phi(x)\phi^\dagger(y)\right\}|0\rangle &= \langle 0|G(x)F(y)|0\rangle + \langle 0|H(x)F(y)|\bar{\phi}\phi\rangle \\ &= G(x)F(y)\underbrace{\langle 0|0\rangle}_{=1} + H(x)F(y)\underbrace{\langle 0|\bar{\phi}\phi\rangle}_{=0} = G(x)F(y)\,\cdot \end{aligned} \tag{3-120}$$

Note in (3-119) that the $\phi^{\dagger-}(y)$ part of $\phi^{\dagger}(y)$, which created a particle, left the $F(y)$ factor, but the $\phi^{\dagger+}(y)$ part, which destroys an anti-particle or, in this case, annihilates the vacuum, resulted in zero. Also, the $\phi^{+}(x)$ part of $\phi(x)$, which destroyed a particle, left us with the $G(x)$ factor, but the $\phi^{-}(x)$ part created an anti-particle in the ket, and thus left zero (because the particle + antiparticle ket was orthogonal to the vacuum, the bra, leaving a bracket = 0.)

So, as we said above with reference to our original definition (3-116) of the time ordering operator, only the part of $\phi(x)$ that destroys a particle and the part of $\phi^{\dagger}(y)$ that creates a particle will be relevant.

In a similar way, the same time ordering operator can be used for antiparticle propagation (with time for x and y reversed) as in Fig 3-3b and (3-117). You can prove this by doing Prob. 17.

The square of the absolute value of the transition amplitude is a probability density (for the transition to occur)

So, the VEV of the time ordering operator is an amplitude, the square of whose magnitude is the probability of the transition from the vacuum initially (represented by $|0\rangle$) to the vacuum finally (represented by $\langle 0|$). Actually, $|G(x)F(y)|^2$ is a probability density (to be precise, a double density), because it is a function of **x** and **y**. That is, the location **y** where the virtual particle is created could be anywhere, and so could the location **x** where it is destroyed. We would need to integrate the probability density over all possible **x** and all possible **y** to get the actual probability, and this is what one does in interaction theory to calculate probabilities and cross sections.

Redefine the transition amplitude as the Feynman propagator

Given all of this, we can define our mathematical relationship for the processes shown in Fig. 3-3 as the VEV of the time ordering operator T. This is called, in honor of its discoverer, the Feynman propagator $i\Delta_F$ (where we insert a factor of i because it makes things easier later on),

$$\boxed{i\Delta_F(x-y) = \langle 0|T\{\phi(x)\phi^{\dagger}(y)\}|0\rangle}. \qquad (3\text{-}121)$$

Step 2, expressing Feynman propagator in terms of commutators

Step 2: Expressing $i\Delta_F$ in Terms of Commutators

Note for $t_y < t_x$, the case for a virtual particle (not antiparticle), the Feynman propagator equals

Step 2, first part, finding Feynman propagator for virtual particle (not antiparticle) in terms of a commutator

$$\begin{aligned} i\Delta_F(x-y) &= \langle 0|\phi(x)\phi^{\dagger}(y)|0\rangle \\ &= \langle 0|\phi^{+}(x)\underbrace{\phi^{\dagger+}(y)|0\rangle}_{=0} + \langle 0|\phi^{+}(x)\underbrace{\phi^{\dagger-}(y)|0\rangle}_{=(factor)|\phi\rangle} + \langle 0|\phi^{-}(x)\underbrace{\phi^{\dagger+}(y)|0\rangle}_{=0} + \langle 0|\phi^{-}(x)\underbrace{\phi^{\dagger-}(y)|0\rangle}_{=(factor)|\phi\rangle} \qquad (3\text{-}122) \\ &= \langle 0|\underbrace{\phi^{+}(x)\phi^{\dagger-}(y)|0\rangle}_{=(factor)|0\rangle} + \underbrace{\langle 0|\phi^{-}(x)|\phi\rangle}_{=(factor)\langle 0|\bar{\phi}\phi\rangle=0} = \langle 0|\phi^{+}(x)\phi^{\dagger-}(y)|0\rangle . \end{aligned}$$

where "factor" represents the non-operator quantities in each field operator term that are left unchanged when the creation and destruction coefficient operators act on a ket. To the last part of (3-122), we can add zero in the form of

By adding a term equal to zero, we can use a commutator

$$0 = \langle 0|-\phi^{\dagger-}(y)\underbrace{\phi^{+}(x)|0\rangle}_{=0} . \qquad (3\text{-}123)$$

Doing that, we find (3-122) becomes

$$i\Delta_F(x-y) = \langle 0|\phi^{+}(x)\phi^{\dagger-}(y) - \phi^{\dagger-}(y)\phi^{+}(x)|0\rangle = \langle 0|\left[\phi^{+}(x),\phi^{\dagger-}(y)\right]|0\rangle \qquad (3\text{-}124)$$

Step 2, second part, expressing Feynman propagator for virtual antiparticle in terms of a commutator

In similar fashion, for $t_x < t_y$, the case for a virtual antiparticle, one finds, by doing Prob. 18, that

$$i\Delta_F(x-y) = \langle 0|\left[\phi^{\dagger+}(y),\phi^{-}(x)\right]|0\rangle . \qquad (3\text{-}125)$$

In summary for Step 2, we have shown the Feynman propagator can be expressed in terms of commutators as

Step 2, summary

$$\begin{aligned} i\Delta_F(x-y) &= \langle 0|\left[\phi^{+}(x),\phi^{\dagger-}(y)\right]|0\rangle \quad \text{if } t_y < t_x \quad \text{(virtual particle)} \\ &= \langle 0|\left[\phi^{\dagger+}(y),\phi^{-}(x)\right]|0\rangle \quad \text{if } t_x < t_y \quad \text{(virtual anti-particle)}. \end{aligned} \qquad (3\text{-}126)$$

Step 3: Expressing Commutator Forms of $i\Delta_F$ as Integrals

Define the symbol $i\Delta^+$ as the commutator of the field type *a* solutions (for particle) of the first line of (3-126), i.e.,

Step 3, first part, find $i\Delta^+$ = commutation relation for type a fields (particles) as an integral

$$i\Delta^+(x-y)=\left[\phi^+(x),\phi^{\dagger -}(y)\right], \tag{3-127}$$

where the solutions used on the RHS are the integral (continuous) form for the Klein-Gordon solutions (3-37). It is common usage to use a + sign to designate (3-127), rather than the letter *a*, which would be easier to remember. Just think "*a* type field" when you see +. Equation (3-127) is thus

$$\begin{aligned} i\Delta^+(x-y) &= \frac{1}{2(2\pi)^3}\iint\left[a(\mathbf{k}),a^\dagger(\mathbf{k}')\right]\frac{e^{-ikx}e^{ik'y}}{\sqrt{\omega_\mathbf{k}\omega_{\mathbf{k}'}}}d^3\mathbf{k}\,d^3\mathbf{k}' \\ &= \frac{1}{2(2\pi)^3}\int\left(\int\frac{e^{ik'y}}{\sqrt{\omega_\mathbf{k}\omega_{\mathbf{k}'}}}\delta(\mathbf{k}-\mathbf{k}')\,d^3\mathbf{k}'\right)e^{-ikx}d^3\mathbf{k}, \end{aligned} \tag{3-128}$$

and hence,

$$i\Delta^+(x-y)=\frac{1}{2(2\pi)^3}\int\frac{e^{-ik(x-y)}}{\omega_\mathbf{k}}d^3\mathbf{k}. \tag{3-129}$$

Similarly, where a minus sign stands for *b* type fields (since they are associated with antiparticles, the minus makes some sense), we define the commutator in the second line of (3-126),

Step 3, second part, find $i\Delta^-$ = commutation relation for type b fields (anti-particles)

$$\begin{aligned} i\Delta^-(x-y) &= \left[\phi^{\dagger +}(y),\phi^-(x)\right]=\frac{1}{2(2\pi)^3}\iint\left[b(\mathbf{k}),b^\dagger(\mathbf{k}')\right]\frac{e^{ikx}e^{-ik'y}}{\sqrt{\omega_\mathbf{k}\omega_{\mathbf{k}'}}}d^3\mathbf{k}\,d^3\mathbf{k}' \\ &= \frac{1}{2(2\pi)^3}\int\frac{e^{ik(x-y)}}{\omega_\mathbf{k}}d^3\mathbf{k}, \end{aligned} \tag{3-130}$$

Thus, (note different authors may define the symbols $i\Delta^+$ and $i\Delta^-$ somewhat differently)

Step 3, final part, combine above parts into one symbol $i\Delta^\pm$

$$i\Delta^\pm(x-y)=\frac{1}{2(2\pi)^3}\int\frac{e^{\mp ik(x-y)}}{\omega_\mathbf{k}}d^3\mathbf{k}. \tag{3-131}$$

Note that though our earlier expressions for $i\Delta$ and $i\Delta^\pm$, contained operators that operated on the ket part of the VEV in (3-126), because the commutator of these operators in (3-128) (and similarly, in (3-130)) is a number, $i\Delta^\pm$ are simply numbers, not operators. Since the expectation value of a number is a number, $i\Delta_F$ of (3-126) is only that, a number. (To be precise it is a numeric *function*, not an operator *function*.) The bottom line is: We don't have to worry about operators, their effects, or VEV brackets any more, but can simply evaluate the Feynman propagator $i\Delta_F$ as a numeric mathematical relation.

Our VEV of operators expression of the propagator has become a simple numeric function

Step 4: Expressing the Two Real Integrals $i\Delta^\pm$ as Contour Integrals

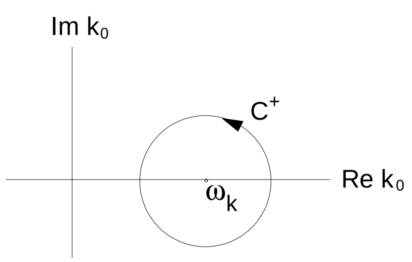

Figure 3-4. Contour Integral for Real, Positive Frequency

It will prove advantageous if we express (3-131) as contour integrals. Before doing so, we first review complex integral theory.

Consider the complex plane for a function *f* of the complex variable k_0, i.e., $f(k_0)$. Here, the symbol k_0 is not a pole (poles are usually designated with null subscript), but represents a complex number generalization of the zeroth component (the energy) of 4-momentum *k*. We concern ourselves with the particular case where k_0 takes on the real value $\omega_\mathbf{k}$.

Review of integral in the complex plane

From complex variable theory,

$$f\left(\omega_{\mathbf{k}}\right)=\frac{1}{i2\pi}\int_{C^+}\frac{f\left(k_0\right)}{k_0-\omega_{\mathbf{k}}}dk_0 . \tag{3-132}$$

Step 4, first part, express $i\Delta^+$ as a contour integral

Now, re-express (3-129) as a regular (not complex plane) integral as

$$i\Delta^+\left(x-y\right)=\frac{1}{\left(2\pi\right)^3}\int e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\underbrace{\left\{\frac{e^{-i\omega_{\mathbf{k}}\left(t_x-t_y\right)}}{2\omega_{\mathbf{k}}}\right\}}_{f\left(\omega_{\mathbf{k}}\right)}d^3\mathbf{k} , \tag{3-133}$$

where we take the bracketed quantity as equal to $f\,(\omega_{\mathbf{k}})$, and where

$$f\left(k_0\right)=\frac{e^{-ik_0\left(t_x-t_y\right)}}{k_0+\omega_{\mathbf{k}}}\qquad\left(\text{so } f\left(\omega_{\mathbf{k}}\right)=\frac{e^{-i\omega_{\mathbf{k}}\left(t_x-t_y\right)}}{\omega_{\mathbf{k}}+\omega_{\mathbf{k}}}\text{ as above}\right). \tag{3-134}$$

We can then use (3-134) in (3-132) to re-express $f\,(\omega_{\mathbf{k}})$ in terms of a contour integral. Using this for the bracket in (3-133), we find (3-133) becomes

$$\begin{aligned}
i\Delta^+\left(x-y\right)&=\frac{1}{\left(2\pi\right)^3}\int e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\left\{\frac{1}{i2\pi}\int_{C^+}\frac{f\left(k_0\right)}{k_0-\omega_{\mathbf{k}}}dk_0\right\}d^3\mathbf{k}\\
&=\frac{1}{\left(2\pi\right)^3}\int e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\left\{\frac{1}{i2\pi}\int_{C^+}\frac{e^{-ik_0\left(t_x-t_y\right)}}{\left(k_0-\omega_{\mathbf{k}}\right)\left(k_0+\omega_{\mathbf{k}}\right)}dk_0\right\}d^3\mathbf{k}\\
&=\frac{-i}{\left(2\pi\right)^4}\int_{C^+}\frac{e^{-ik(x-y)}}{\left(k_0\right)^2-\left(\omega_{\mathbf{k}}\right)^2}d^4k .
\end{aligned} \tag{3-135}$$

where the integral notation now implies integration over four dimensions of the 4-momentum, with the 3-momentum part from $-\infty$ to $+\infty$ in real space and the energy part a contour integral in complex space. Note that the integral does not "blow up" because $k_0 \neq \omega_{\mathbf{k}}$ over the contour integral. We are using a mathematical trick that works, though it jars our usual understanding that, for real particles, the zeroth component of 4-momentum equals energy. k_0 has at this point become, for us, a variable that generally does not equal energy $\omega_{\mathbf{k}}$.

Modifying terms in our result a little

We modify (3-135) a little by noting what is always true mathematically for any four vector, and thus true for 4-momentum components,

$$k^2=\left(k_0\right)^2-\left(\mathbf{k}\right)^2\quad\rightarrow\quad\left(k_0\right)^2=k^2+\left(\mathbf{k}\right)^2 \tag{3-136}$$

and what is physically true relativistically for rest mass, energy, and 3-momentum (see (3-2)),

$$\omega_{\mathbf{k}}^2-\left(\mathbf{k}\right)^2=\mu^2\quad\rightarrow\quad\omega_{\mathbf{k}}^2=\mu^2+\left(\mathbf{k}\right)^2 . \tag{3-137}$$

Substitute the RH expressions of (3-136) and (3-137) into the last line of (3-135) to get

$$i\Delta^+\left(x-y\right)=\frac{-i}{\left(2\pi\right)^4}\int_{C^+}\frac{e^{-ik(x-y)}}{k^2-\mu^2}d^4k . \tag{3-138}$$

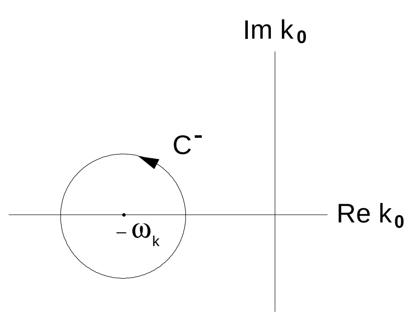

Figure 3-5. Contour Integral for Real, Negative Frequency

Step 4, second part, express $i\Delta^-$ as a contour integral

For $i\Delta^-\,(x-y)$, we carry out similar steps except that the contour integral (still counter clock-wise [ccw], as in Fig. 3-4) is now about $-\,\omega_{\mathbf{k}}$. In Appendix C, we carry out these steps. When all is said and done, we find the only differences from (3-138) to be the sign and the contour, which is now about the negative frequency value and designated by C^-.

$$i\Delta^{-}(x-y)=\frac{i}{(2\pi)^4}\int_{C^-}\frac{e^{-ik(x-y)}}{k^2-\mu^2}d^4k. \tag{3-139}$$

Step 5: Re-express $i\Delta_F$ in Most Convenient Form

Step 5, expressing Feynman propagator as integral over real, not complex space

We would like two things more: 1) express the propagator as a single function so we don't have to keep track (while we are integrating over spacetime and doing other things) of whether the virtual field is a particle or antiparticle (i.e., whether to use the Δ^+ or Δ^- function), and 2) have all our integrations over real numbers rather than deal with contour integrals.

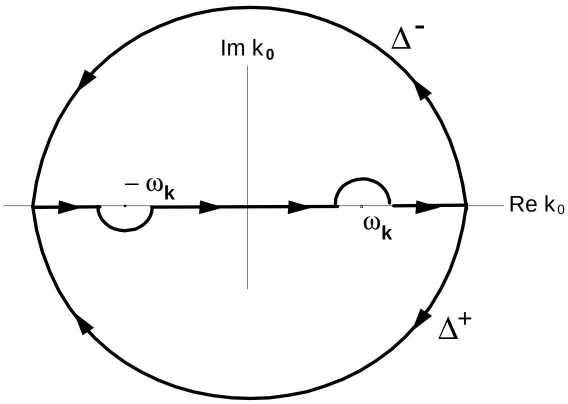

Figure 3-6. Contour Integrals for Δ^- and Δ^+

To do this, consider Fig. 3-6, where we have shown two contour integrals and the quantity being integrated in both cases is the integrand of (3-139). The top loop represents Δ^- (we have left out a factor of $(2\pi)^4$ in the figure) and encloses $-\omega_{\mathbf{k}}$ with a ccw path. The lower loop encloses $+\omega_{\mathbf{k}}$, but since it has a cw integration path, the result will have a sign change, and hence equals the ccw integration in (3-138). Thus, the lower loop represents Δ^+.

This means we can define the Feynman propagator Δ_F of (3-138) and (3-139) as proportional to the same integral over the two different loops of Fig. 3-6. We say "proportional" because we also have to include the concomitant integration over the 3D space of $\mathbf{k}$ not shown in Fig. 3-6, as well as the various constants involved.

Two different contours for the Feynman propagator written with same integral, different meaning for path C_F

So we can then re-write the Feynman propagator of (3-138) and (3-139) with Fig. 3-6, as

$$i\Delta_F(x-y)=\frac{i}{(2\pi)^4}\int_{C_F}\frac{e^{-ik(x-y)}}{k^2-\mu^2}d^4k\ , \tag{3-140}$$

where the C_F on the integral defines the route we take in the plane of Fig. 3-6.

Extending outer semicircle parts of contours to ∞

Now, consider enlarging the outer hemispheric parts of the two loops in Fig. 3-6, so they extend essentially to infinity. The value of the contour integrals over them will remain unchanged. But the k^2 value in the denominator of (3-140) will become so large that any contribution to the integral over those parts of the path will become negligible. (See Appendix D.) Thus, we can effectively take the integral (3-140) as extending only along the real axis from $-\infty$ to $+\infty$ as in Fig. 3- 7.

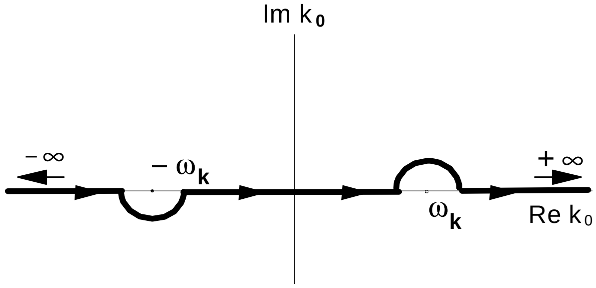

Fig. 3-7. Contour C_F for Δ_F

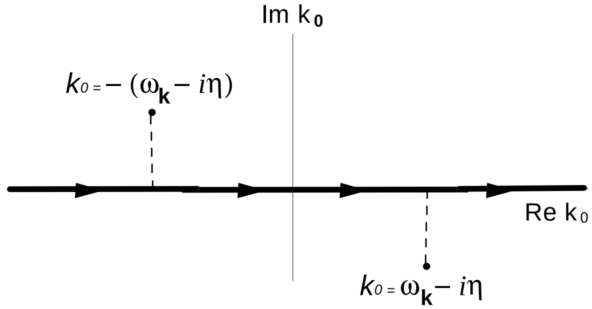

Fig. 3-8. Contour and Displaced Poles for Δ_F

Instead of integrating around poles on the axis, move poles slightly off the axis

We can further simplify by moving the poles an infinitesimal distance η off the real axis as shown in Fig. 3-8 and deform the contour so that it is all along the real axis. In the limit as $\eta \to 0$, the integral will have the same value, though we must now include this slight pole shift in the propagator expression (3-140). We do this by recalling from (3-136) and (3-137) that we used

$$k^2 - \mu^2 = (k_0)^2 - (\omega_{\mathbf{k}})^2 \tag{3-141}$$

to obtain the denominator of (3-140), so we must temporarily restate (3-140) using the right hand side of (3-141), then shift the poles. Thus, (3-140) becomes

$$i\Delta_F(x-y) = \frac{i}{(2\pi)^4}\int_{-\infty}^{+\infty} \frac{e^{-ik(x-y)}}{(k_0)^2 - (\omega_{\mathbf{k}} - i\eta)^2} d^4k. \tag{3-142}$$

Yields a single integral over real space representing both virtual particle & antiparticle, the most convenient form for the Feynman propagator

If we then use (3-141) again, ignore second order terms in η, and take $\varepsilon = 2\eta\omega_{\mathbf{k}}$, we have our final result for the Feynman scalar propagator

$$\boxed{i\Delta_F(x-y) = \frac{i}{(2\pi)^4}\int_{-\infty}^{+\infty} \frac{e^{-ik(x-y)}}{k^2 - \mu^2 + i\varepsilon} d^4k.} \tag{3-143}$$

Note the advantages of this form. We now have a single mathematical relationship that automatically describes both a particle propagating from y to x *and* an antiparticle propagating from x to y. We also have done away with the cumbersome contour integrals in favor of a simple 4D integral over the entire real (not complex) 4-momentum space. In principle, we can evaluate this integral then take ε to zero after the integration is carried out.

Summary of propagator derivation

Summary of Steps 1 to 5

Steps 1 to 4

Steps 1 to 4 for the virtual particle Feynman propagator were

$$\begin{aligned} i\Delta_F(x-y) &= \langle 0|T\{\phi(x)\phi^\dagger(y)\}|0\rangle = \langle 0|\phi(x)\phi^\dagger(y)|0\rangle \quad \text{if } t_y < t_x \ (\text{particle}) \\ &= \langle 0|\underbrace{\left[\phi^+(x),\phi^{\dagger-}(y)\right]}_{i\Delta^+(x-y),\text{ a number}}|0\rangle = \left[\phi^+(x),\phi^{\dagger-}(y)\right]\langle 0||0\rangle = \left[\phi^+(x),\phi^{\dagger-}(y)\right] \\ &= i\Delta^+(x-y) = \frac{1}{2(2\pi)^3}\int \frac{e^{-ik(x-y)}}{\omega_{\mathbf{k}}} d^3\mathbf{k} = \frac{-i}{(2\pi)^4}\int_{C^+} \frac{e^{-ik(x-y)}}{k^2-\mu^2} d^4k \ , \end{aligned} \tag{3-144}$$

and for the virtual anti-particle Feynman propagator,

$$\begin{aligned} i\Delta_F(x-y) &= \langle 0|T\{\phi(x)\phi^\dagger(y)\}|0\rangle = \langle 0|\phi^\dagger(y)\phi(x)|0\rangle \quad \text{if } t_x < t_y \ (\text{anti-particle}) \\ &= \langle 0|\underbrace{\left[\phi^{\dagger+}(y),\phi^-(x)\right]}_{i\Delta^-(x-y),\text{ a number}}|0\rangle = \left[\phi^{\dagger+}(y),\phi^-(x)\right]\langle 0||0\rangle = \left[\phi^{\dagger+}(y),\phi^-(x)\right] \\ &= i\Delta^-(x-y) = \frac{1}{2(2\pi)^3}\int \frac{e^{ik(x-y)}}{\omega_{\mathbf{k}}} d^3\mathbf{k} = \frac{i}{(2\pi)^4}\int_{C^-} \frac{e^{-ik(x-y)}}{k^2-\mu^2} d^4k \ . \end{aligned} \tag{3-145}$$

Step 5

The two contour integrals of (3-144) and (3-145) were combined in Step 5 to yield the single integral over real space of (3-143).

3.13.3 Comments on the Propagator and Its Derivation

The Propagator and Interaction Theory

Our definition of Feynman propagator here will pop up in our formal derivation of interaction theory

The derivation above was formulated with an eye to interaction theory. In that theory, amplitudes are derived for various kinds of interactions between various particles. The square of the magnitude of each amplitude turns out to be the probability of that particular interaction (transition) occurring. These transition amplitudes each depend on the initial real particles, the final real particles, and the virtual particle(s) that mediate the transition. It turns out that the factor in the amplitude representing the virtual particle contribution is identical to the Feynman propagator Δ_F as we defined it in the VEV of the time ordering operator (3-121). Thus, it is also equal to (3-143), so we can simply plug the RHS of (3-143) into the overall transition amplitude as part of our analysis.

This is one reason we started with the relation $\phi\phi^\dagger$ to create and destroy a virtual scalar particle, rather than what one might initially expect, the simpler creation and destruction operator relation

$a(\mathbf{k})a^\dagger(\mathbf{k})$. Our heuristic approach was tailored to match what we knew would be coming in the mathematical development of interaction theory.

Meaning of Spacetime Points y and x

In Fig. 3-3a, we imply the virtual particle is created at y and destroyed at x. In Feynman diagrams virtual particles are depicted in this way, and at least one real incoming particle can be thought of as being destroyed at y, as in Fig. 1-1 of Chap. 1, pg.2, with a virtual particle created simultaneously at y. At x the virtual particle is destroyed, with the simultaneous creation of at least one outgoing real particle at x.

Feynman diags, & our derivation, imply creation/ destruction at a point, but more properly, waves created/destroyed & they spread out over space.

To be precise, it is more correct to think of the incoming, outgoing, and virtual particles as moving waves spread out in space. What we calculate for a given y and x is the probability density for the interaction as a function of the coordinates y and x. If $\mathbf{y}$ and $\mathbf{x}$ are closer, one would find the probability density for the interaction to occur is greater; if farther away, the probability density is less. Integrating over all $\mathbf{x}$ and $\mathbf{y}$ gives the total probability for observing the interaction.

We are really finding probability density as function of $\mathbf{x}$, $\mathbf{y}$

Momentum Space Form of the Propagator

From (3-143), we can readily write down the 4-momentum space form of the propagator, the Fourier transform of (3-143), which will be very useful,

$$\boxed{\Delta_F(k) = \frac{1}{k^2 - \mu^2 + i\varepsilon}}. \qquad (3\text{-}146)$$

Momentum space form of the propagator

Earlier version was physical space form

Green's Functions, Correlation Functions, and Propagators

Feynman propagators have the form of functions known in mathematics as Green's functions, and you will sometimes see them referred to in that way. You may also see them referred to as correlation functions for free fields, because there is a correlation implied between events x and y.

Feynman propagator = Green function or correlation function

3.14 Chapter Summary

Scalars and Relativistic Quantum Mechanics (RQM)

Do Prob. 20 to create your own Wholeness Chart summary of scalars and RQM as in Sect. 3.1.

Scalars and Quantum Field Theory (QFT)

This part of the chapter is key. Know it, and you know most of the basic principles in QFT. Spin ½ and spin 1 field theory closely parallel that of scalars, so most of the conceptual battle is waged in this Chap. 3.

Free scalar QFT is summarized in the second column of Wholeness Chart 5-4 at the end of Chap. 5. If you can, more or less, reproduce that Wholeness Chart column without looking at it (that is, derive the essence of QFT), you have achieved something few have achieved.

QFT Grounded in 2nd Quantization

It is important to understand how the entire theory springs out of the two 2nd quantization postulates. All the operators (number, Hamiltonian, creation/destruction, 3-momentum, charge, etc) are a direct result of these postulates. So is the vacuum energy. Wholeness Chart 5-4 can help to make that transparent.

In particular, starting with the classical Lagrangian density (or Hamiltonian density), the commutation postulate gives us the rest of the theory, step-by-step, as illustrated below (where we use only a type particles to save space).

Although the steps shown below are specifically for scalars, the developments of QFT for spin ½ and spin 1 particles follow precisely the same conceptual steps.

Steps to QFT

$[\phi^r(\mathbf{x},t), \pi_s(\mathbf{y},t)] = i\delta^r{}_s\,\delta(\mathbf{x}-\mathbf{y}) \;\rightarrow\; [a(\mathbf{k}), a^\dagger(\mathbf{k}')] = \delta_{\mathbf{kk}'} \;\rightarrow\; H_0^0$ & vacuum energy $\rightarrow$

$N_a(\mathbf{k}) = a^\dagger(\mathbf{k})a(\mathbf{k})$ as number operator $\rightarrow$ $a^\dagger(\mathbf{k})$, $a(\mathbf{k})$ as creation/destruction operators

↓ (from number operator) form of observable operators (for real particles)

↙ (from creation/destruction operators) the propagator (for virtual particles)

↘ (from creation/destruction operators) interaction theory – to be studied (for real & virtual particles)

Kinds of Operators in QFT

In QFT there are two kinds of operators. One kind is the usual one from NRQM and RQM representing the dynamical variables of classical theory, such as the Hamiltonian (energy), the 3-momentum operator, charge, etc. The other kind comprises creation and destruction operators.

The first kind, when operating on an eigenstate, re-produces the original state multiplied by an eigenvalue. The second kind changes the state to another state (raising or lowering the number of particles in the state.) The second kind comprises the coefficients $a(\mathbf{k})$, $a^\dagger(\mathbf{k})$, $b(\mathbf{k})$, $b^\dagger(\mathbf{k})$, as well as the fields of which they are a part, ϕ and $\phi^\dagger$. Note that operators of this kind do not have eigenvalues, since their operation on a state changes that state, rather than re-producing it (times an eigenvalue), and hence they are generally *not* observable.

Wholeness Chart 3-4. Different Kinds of Operators in QFT

	Examples	Effect on Eigenstate	Observable?
Dynamical Variable Operators	H, $\mathbf{P}$, Q, $N_a(\mathbf{k})$	eigenvalue times original eigenstate	Yes
Raising and Lowering Operators	$a^\dagger(\mathbf{k})$, $a(\mathbf{k})$, $b^\dagger(\mathbf{k})$, $b(\mathbf{k})$	new eigenstate, one more/less particle	No
Fields	ϕ and $\phi^\dagger$	as above	No

Odds and Ends

For a summary of bosons vs fermions, and Fock space, see Wholeness Charts 3-1 and 3-2.

3.15 Appendix A: Klein-Gordon Equation from H.P. Equation of Motion

3.15.1 Background Math Needed for Delta Function Relation

From Arfken and Weber, *Mathematical Methods for Physicists*, 4th ed (Academic Press 1995), pg 85,

$$\int \frac{d\delta(x'-a)}{dx'} f(x')\,dx' = -\int \frac{df(x')}{dx'}\delta(x'-a)\,dx' = -\left.\frac{df(x)}{dx}\right|_{x=a}, \qquad (3\text{-}147)$$

where in our case we will have

$$x' \to \mathbf{x}' \qquad a \to \mathbf{x} \qquad f(x') \to \nabla'\phi(\mathbf{x}') \qquad \frac{d\delta(x'-a)}{dx'} \to \nabla'\delta(\mathbf{x}'-\mathbf{x}), \qquad (3\text{-}148)$$

so that (3-147) becomes

$$\int \nabla'\delta(\mathbf{x}'-\mathbf{x}) \cdot \nabla'\phi(\mathbf{x}',t)\,d^3x' = -\nabla\cdot\nabla\phi(\mathbf{x},t). \qquad (3\text{-}149)$$

3.15.2 Deriving the Scalar Field Equation

The Heisenberg equation of motion for any operator is

$$i\frac{\partial}{\partial t}\mathcal{O} = [\mathcal{O}, H], \qquad (3\text{-}150)$$

and for a complex scalar field, this is

$$i\frac{\partial}{\partial t}\phi = [\phi, H]. \qquad (3\text{-}151)$$

Thus, using (3-33) for $\mathcal{H}$ to find $H = \int \mathcal{H} d^3x$, we have

$$i\frac{\partial}{\partial t}\phi(\mathbf{x},t) = \Big[\phi(\mathbf{x},t), \int d^3x' \Big\{ \underbrace{\pi^\dagger\pi}_{\substack{\text{only non}\\ \text{-zero result}}} + \nabla'\phi^\dagger \cdot \nabla'\phi + \mu^2\phi^\dagger\phi \Big\}\Big] \qquad (3\text{-}152)$$

where the quantities inside the integral are all functions of $\mathbf{x}'$ and t. Since $\phi(\mathbf{x},t)$ is not a function of $\mathbf{x}'$, we can evaluate the commutator inside the integral. The second and third terms inside the integral of (3-152) commute with ϕ, and thus drop out. Writing out the independent variable dependence only when needed for clarity, and using the field commutation relations for ϕ and π (reproduced below from Chap. 2, Wholeness Chart 2-5, pg. 31, last box in RH column) of

$$\left[\pi_s,\phi^r\right]=-i\,\delta^r{}_s\,\delta\left(\mathbf{x}'-\mathbf{x}\right), \tag{3-153}$$

in the second line below, where it says "subs", we find (3-152) becomes

$$\begin{aligned} i\frac{\partial}{\partial t}\phi(\mathbf{x},t) &= \int d^3\mathbf{x}'\left[\phi(\mathbf{x},t),\pi^\dagger(\mathbf{x}',t)\pi(\mathbf{x}',t)\right]=\int d^3\mathbf{x}'\{\underbrace{\phi\pi^\dagger}_{\text{commute}}\pi-\pi^\dagger\underbrace{\pi\phi}_{\text{subs}}\} \\ &= \int d^3\mathbf{x}'\{\underbrace{\pi^\dagger\phi\pi-\pi^\dagger\phi\pi}_{0}+\pi^\dagger(\mathbf{x}',t)\,i\delta(\mathbf{x}'-\mathbf{x})\} \\ &= i\pi^\dagger(\mathbf{x},t). \end{aligned} \tag{3-154}$$

Next, using (3-150) when the operator is the complex conjugate of the canonical momentum,

$$i\frac{\partial}{\partial t}\pi^\dagger(\mathbf{x},t)=[\underbrace{\pi^\dagger(\mathbf{x},t)}_{\substack{\text{function}\\ \text{of }\mathbf{x}}},\underbrace{\int d^3\mathbf{x}'\{\underbrace{\pi^\dagger\pi}_{\substack{\to 0\text{ in}\\ \text{commutator}}}+\nabla'\phi^\dagger\cdot\nabla'\phi+\mu^2\phi^\dagger\phi\}}_{\text{functions of }\mathbf{x}'}]\ . \tag{3-155}$$

Note that $\nabla'\pi^\dagger(\mathbf{x},t)=0$, because the derivative of a function of $\mathbf{x}$ is with respect to a primed $\mathbf{x}'$, and we can move $\pi^\dagger$ inside and outside of any quantity the 3D spatial derivative operates on. We use this several times in what follows. We then focus on the second term in (3-155) and substitute (3-149) in the third line below where it says "use math relation above". That second term is

$$\begin{aligned} &\int d^3\mathbf{x}'\{\underbrace{\pi^\dagger\nabla'\phi^\dagger}_{\nabla'(\pi^\dagger\phi^\dagger)}\cdot\nabla'\phi-\nabla'\phi^\dagger\cdot\underbrace{(\nabla'\phi)\pi^\dagger}_{\nabla'\underbrace{(\phi\pi^\dagger)}_{\text{commute}}}\}=\int d^3\mathbf{x}'\{\nabla'\underbrace{(\pi^\dagger\phi^\dagger)}_{\substack{\text{use com}\\ \text{relations}}}\cdot\nabla'\phi-\underbrace{\nabla'\phi^\dagger\cdot\nabla'(\pi^\dagger\phi)}_{\nabla'(\phi^\dagger\pi^\dagger)\cdot\nabla'\phi}\} \\ &=\int d^3\mathbf{x}'\{\nabla'(\phi^\dagger\pi^\dagger)\cdot\nabla'\phi-\underbrace{\nabla' i\delta(\mathbf{x}'-\mathbf{x})\cdot\nabla'\phi}_{\text{use math relation above}}-\nabla'(\phi^\dagger\pi^\dagger)\cdot\nabla'\phi\}=i\nabla^2\phi(\mathbf{x},t). \end{aligned} \tag{3-156}$$

By doing Prob. 6 at the end of the chapter, the reader can verify that evaluation of the third term in the RHS of (3-155), using similar (but simpler) steps, leads to

$$i\frac{\partial}{\partial t}\pi^\dagger(\mathbf{x},t)=i\left(\nabla^2-\mu^2\right)\phi(\mathbf{x},t). \tag{3-157}$$

Substituting the time derivative of (3-154) into (3-157), one gets the Klein-Gordon equation

$$\frac{\partial^2}{\partial t^2}\phi=\left(\nabla^2-\mu^2\right)\phi\ , \tag{3-158}$$

thus showing that the equation of motion of a scalar field in the Heisenberg picture, expressed in terms of commutation relations, is equivalent to the Klein-Gordon equation.

3.16 Appendix B: Vacuum Quanta and Harmonic Oscillators

One might argue that two vacuum quanta traveling waves of energy $\frac{1}{2}\hbar\omega_{\mathbf{k}}$ with 3-momenta $\mathbf{k}$ and $-\mathbf{k}$ could be superimposed to yield a vacuum standing wave, i.e., a harmonic oscillator (distributed in space). But the total energy of the standing wave would then be $\hbar\omega$, which is not the ground state of a quantum oscillator, and thus the parallel disappears. Further, the wave form would still be sinusoidal in nature, not that of a Hermite polynomial. Nor is any potential involved.

One might instead argue that the two traveling wave eigenstates are superimposed to comprise a general quantum state, wherein the probability of measuring each of the states is ½. In this case, the expectation value for energy of the standing wave would be $\frac{1}{2}(\frac{1}{2}\hbar\omega_{\mathbf{k}})+\frac{1}{2}(\frac{1}{2}\hbar\omega_{\mathbf{k}})=\frac{1}{2}\hbar\omega_{\mathbf{k}}$. But, this violates (3-55), which tells us the energy must be $\hbar\omega_{\mathbf{k}}$. Thus, this interpretation is inconsistent with contemporary QFT. The lack of Hermite polynomial form and potential points apply here, as well.

Still further, this logic implies the entire vacuum state is one general state comprised of all the ½ energy eigenstates. This would mean the expectation value for the energy of the vacuum is the average energy of all those eigenstates, not the sum of them. So, if one assumes (which is common) an upper limit on these energies of the Planck scale energy (see Appendix A of Chap. 10), the total vacuum energy of the universe could then not exceed the Planck energy, which is about that of a very small bit of dust and hardly anything to make a fuss about.

3.17 Appendix C: Propagator Derivation Step 4 for Real, Negative Frequency

We derive (3-139) from the scalar propagator derivation step 3, (3-131),

$$i\Delta^-(x-y)=\frac{1}{2(2\pi)^3}\int\frac{e^{ik(x-y)}}{\omega_{\mathbf{k}}}d^3\mathbf{k}=\frac{1}{2(2\pi)^3}\int\frac{e^{i\omega_{\mathbf{k}}(t_x-t_y)}}{\omega_{\mathbf{k}}}e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}d^3\mathbf{k}$$

$$=\frac{1}{2(2\pi)^3}\int_{-\infty}^{\infty}\underbrace{\frac{e^{i\omega_{\mathbf{k}}(t_x-t_y)}}{\omega_{\mathbf{k}}}}_{\substack{\text{even, same value}\\ \text{for }\mathbf{k}\text{ or }-\mathbf{k}}}\underbrace{\Big(\underbrace{\cos(-\mathbf{k})\cdot(\mathbf{x}-\mathbf{y})}_{\substack{\text{even, same value}\\ \text{for }\mathbf{k}\text{ or }-\mathbf{k}}}+\underbrace{i\sin(-\mathbf{k})\cdot(\mathbf{x}-\mathbf{y})}_{\substack{\text{odd, integral of this}\\ \text{contribution}=0\text{ for }\mathbf{k}\text{ or }-\mathbf{k}}}\Big)}_{\text{integral same if take this}=\cos\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})+i\sin\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})=e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}d^3\mathbf{k} \qquad (3\text{-}159)$$

$$=\frac{1}{(2\pi)^3}\int\underbrace{\frac{e^{i\omega_{\mathbf{k}}(t_x-t_y)}}{2\omega_{\mathbf{k}}}}_{=g(-\omega_{\mathbf{k}})}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}d^3\mathbf{k}\ .$$

From complex variable theory

$$g(-\omega_{\mathbf{k}})=\frac{1}{i2\pi}\int_{C^-}\frac{g(k_0)}{k_0-(-\omega_{\mathbf{k}})}dk_0\quad\text{with}\quad g(k_0)=\frac{e^{-ik_0(t_x-t_y)}}{-k_0+\omega_{\mathbf{k}}}, \qquad (3\text{-}160)$$

which we can check is correct (i.e., equals the underbracket quantity in the last part of (3-159)) via

$$g(-\omega_{\mathbf{k}})=\frac{e^{-i(-\omega_{\mathbf{k}})(t_x-t_y)}}{-(-\omega_{\mathbf{k}})+\omega_{\mathbf{k}}}\overset{\text{checks}}{=}\frac{e^{i\omega_{\mathbf{k}}(t_x-t_y)}}{2\omega_{\mathbf{k}}}. \qquad (3\text{-}161)$$

Putting the RH quantity in (3-160) into the LH quantity in (3-160), we have

$$g(-\omega_{\mathbf{k}})=\frac{1}{i2\pi}\int_{C^-}\frac{1}{k_0+\omega_{\mathbf{k}}}\frac{e^{-ik_0(t_x-t_y)}}{-k_0+\omega_{\mathbf{k}}}dk_0=\frac{i}{2\pi}\int_{C^-}\frac{e^{-ik_0(t_x-t_y)}}{(k_0)^2-(\omega_{\mathbf{k}})^2}dk_0\,. \qquad (3\text{-}162)$$

Using (3-162) in the last part of (3-159) results in

$$i\Delta^-(x-y)=\frac{i}{(2\pi)^4}\int_{C^-}\frac{e^{-ik(x-y)}}{\underbrace{(k_0)^2-(\omega_{\mathbf{k}})^2}_{=k^2-\mu^2}}d^4k\,, \qquad (3\text{-}163)$$

where the underbracket part comes from (3-136) and (3-137). (3-163) is (3-139).

3.18 Appendix D: Enlarging the Integration Path of Fig. 3-6

The integral of Fig. 3-6 expressed in (3-140), can be written as

$$i\Delta_F(x-y)=\frac{i}{(2\pi)^4}\int_{C_F}\frac{e^{-ik_0(t_x-t_y)}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{k^2-\mu^2}dk_0d^3k=\frac{i}{(2\pi)^4}\int_{C_F}\frac{e^{-i(\text{Re}k_0+i\text{Im}k_0)(t_x-t_y)}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{k^2-\mu^2}dk_0\,d^3k$$

$$=\frac{i}{(2\pi)^4}\int_{C_F}\frac{e^{-i(\text{Re}k_0)(t_x-t_y)}e^{(\text{Im}k_0)(t_x-t_y)}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{k^2-\mu^2}dk_0\,d^3k. \qquad (3\text{-}164)$$

The factor with Re k_0 in the exponent oscillates and will be swamped by the denominator wherever $k_0^{\,2} \rightarrow \infty$. But the factor with Im$k_0$ in the exponent is real, so we have to be careful about it.

For the lower half plane of Fig. 3-6, the integral $i\Delta_F\,(x-y)$ represents $\Delta^+(x-y)$, where $t_x > t_y$ and Imk_0 is negative. That means in (3-164) the factor with Imk_0 has a negative value in the exponent and will go to zero as Im $k_0 \rightarrow -\infty$.

For the upper half plane of Fig. 3-6, the integral $i\Delta_F\,(x-y)$ represents $\Delta^-\,(x-y)$, where $t_y > t_x$ and Imk_0 is positive. That means in that half of the plane that the factor with Imk_0 has a negative value in the exponent too and will go to zero as Im $k_0 \rightarrow +\infty$.

Thus the integral over the contour vanishes whenever $k_0^{\,2} \rightarrow \infty$.

Appendix E: Justifying (3-47) Conclusions

Note that (3-47) is one term in a sum over **k**, where for each term in **k** there is an additional one in – **k**. Writing out two such terms leads to

$$
\begin{aligned}
&\left[a_{\mathbf{k}},a_{\mathbf{k}}^{\dagger}\right]e^{i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}+\left[b_{\mathbf{k}},b_{\mathbf{k}}^{\dagger}\right]e^{-i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}+\left[a_{\mathbf{k}},a_{-\mathbf{k}}^{\dagger}\right]e^{i\mathbf{k}\bullet(\mathbf{x}+\mathbf{y})}+\left[b_{-\mathbf{k}},b_{\mathbf{k}}^{\dagger}\right]e^{-i\mathbf{k}\bullet(\mathbf{x}+\mathbf{y})}\\
&\left[a_{-\mathbf{k}},a_{-\mathbf{k}}^{\dagger}\right]e^{-i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}+\left[b_{-\mathbf{k}},b_{-\mathbf{k}}^{\dagger}\right]e^{i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}+\left[a_{-\mathbf{k}},a_{\mathbf{k}}^{\dagger}\right]e^{-i\mathbf{k}\bullet(\mathbf{x}+\mathbf{y})}+\left[b_{\mathbf{k}},b_{-\mathbf{k}}^{\dagger}\right]e^{i\mathbf{k}\bullet(\mathbf{x}+\mathbf{y})}\\
&\quad=e^{i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}+e^{-i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}+e^{i-\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}+e^{i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}=2e^{i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})}+2e^{-i\mathbf{k}\bullet(\mathbf{x}-\mathbf{y})},
\end{aligned}
\tag{3-165}
$$

and thus,

$$
\begin{aligned}
&\left[a_{\mathbf{k}},a_{\mathbf{k}}^{\dagger}\right]+\left[b_{-\mathbf{k}},b_{-\mathbf{k}}^{\dagger}\right]=2 \qquad\qquad \left[b_{\mathbf{k}},b_{\mathbf{k}}^{\dagger}\right]+\left[a_{-\mathbf{k}},a_{-\mathbf{k}}^{\dagger}\right]=2\\
&\left[a_{\mathbf{k}},a_{-\mathbf{k}}^{\dagger}\right]+\left[b_{\mathbf{k}},b_{-\mathbf{k}}^{\dagger}\right]=0 \qquad\qquad \left[b_{-\mathbf{k}},b_{\mathbf{k}}^{\dagger}\right]+\left[a_{-\mathbf{k}},a_{\mathbf{k}}^{\dagger}\right]=0
\end{aligned}
\tag{3-166}
$$

At this point, we could adopt a reasonable postulate that coefficients in (3-166) not having the same 3-momentum have zero commutators, and those that do have the same 3-momentum all have the same commutator values. That would give us (3-41) and lead to our present (good) theory of QFT.

If we were to be thorough, however, and repeat the process of (3-42) to (3-47) for other commutators, such as $\left[\phi,\phi^{\dagger}\right]=0$, we would find other relations between coefficient commutators that would lead inevitably to (3-41). You can take my word for this, work it out yourself (which is tedious), or see it on the book website under Auxiliary Material (URL on pg. xvi, opposite pg. 1).

3.19 Problems

1. Substitute (3-9) into the non-relativistic Schrödinger equation (3-1), and also the relativistic Klein-Gordon equation (3-8), to prove to yourself that only terms with exponential form $-i(E_n t - \mathbf{p}_n\cdot\mathbf{x})/\hbar$ solve the Schrödinger equation, but all terms in (3-9) solve the Klein-Gordon equation. Do you see that the single time derivative in the former equation, and the second order time derivative in the latter, are responsible for this?

2. Prove that the orthonormality conditions (3-15) of states $\phi_{\mathbf{k},A}$ also apply to states $\phi_{\mathbf{k},B^{\dagger}}$.

3. Repeat steps (3-24) and (3-25) using the terms with coefficients $B_{\mathbf{k}}^{\dagger}$ in (3-12) instead of those with $A_{\mathbf{k}}$. You should find total probability is negative.

4. Express the Klein-Gordon equations (3-35) and their discrete solutions (3-36) in cgs units (i.e., with c and $\hbar \neq 1$) and plug the latter into the former to show that $\mu^2 = m^2c^2/\hbar^2$.

5. Prove that the continuous solutions (3-37) solve the Klein-Gordon equations.

6. Show that the 3rd term in (3-155) of the Appendix equals $-\,i\mu^2\phi(\mathbf{x},t)$.

7. Derive the commutators for the continuous solutions to the Klein-Gordon field equation from the second postulate of 2nd quantization. (Warning: This problem may not be worth the significant investment in time needed.)

8. Starting with the mass term in (3-48), derive (3-53).

9. Find the VEV (vacuum expectation value) of the free field scalar Hamiltonian.

10. Show that $a^{\dagger}(\mathbf{k})$ creates an *a* type particle with 3-momentum **k**, $b(\mathbf{k})$ destroys a *b* type particle with 3-momentum **k**, and $b^{\dagger}(\mathbf{k})$ creates a *b* type particle with 3-momentum **k**. Follow steps similar to those in (3-71) to (3-74).

11. Show $a(\mathbf{k})\left|n_{\mathbf{k}}\right\rangle = \sqrt{n_{\mathbf{k}}}\left|n_{\mathbf{k}}-1\right\rangle$. Does it follow in a heart beat that $b(\mathbf{k})\left|\bar{n}_{\mathbf{k}}\right\rangle = \sqrt{\bar{n}_{\mathbf{k}}}\left|\bar{n}_{\mathbf{k}}-1\right\rangle$?

12. Substitute the free field solutions (3-36) to the Klein-Gordon equation into the probability density operator relation (3-89) and then insert that into (3-90) to find the effective probability density operator expressed in terms of number operators (3-91). It will help you in doing so to note that for any term where $\mathbf{k} \neq \mathbf{k}'$, the destruction and creation operators will cause the ket to be different from (orthogonal to) the bra, so the resulting term in the expectation value $\bar{\rho}$ will be zero. Hence, those terms can be ignored in determining an effective ρ.

    Note that the result you get is restricted to situations where all particles (in the ket) are in **k** eigenstates, which is almost invariably the case in QFT problems and applications. With particles in general (non **k** eigen) states, ρ becomes more complicated.

13. Using (3-100), the expression for 3-momentum in terms of the fields and their conjugate momenta, and the Klein-Gordon field equation solutions, prove (3-101), the number operator form of the 3-momentum operator.

14. For the state $\left|2\phi_{\mathbf{k}_1}, 3\bar{\phi}_{\mathbf{k}_1}, \bar{\phi}_{\mathbf{k}_2}\right\rangle$, determine the expectation value of **P**, the 3-momentum operator.

15. Show that for real (not complex) scalar fields, in order for π to be equal to $\dot{\phi}$, the constant *K* in the scalar Lagrangian density (3-30) must be ½. In general, in QFT, for real fields, we take *K*=½.

16. Show that if instead of the 2nd quantization, postulate #2 of commutator relations (3-40), we had anti-commutators between the field and its conjugate momentum, i.e.,

$$\left[\phi^r(\mathbf{x},t), \pi_s(\mathbf{y},t)\right]_+ = \phi^r \pi_s + \pi_s \phi^r = i\delta^r{}_s \delta(\mathbf{x}-\mathbf{y}) \tag{3-167}$$

    then the coefficient commutators would be anti-commutator relations, i.e.,

$$\left[a(\mathbf{k}), a^{\dagger}(\mathbf{k}')\right]_+ = -\left[b(\mathbf{k}), b^{\dagger}(\mathbf{k}')\right]_+ = \delta_{\mathbf{k}\mathbf{k}'} \;. \tag{3-168}$$

    (Hint: Just use opposite signs in (3-43) 2nd row and then in last two rows inside the bracket just before the last equal sign. Then, all commutators in (3-45) to (3-47) become anti-commutators.

17. Find the transition amplitude operating on the vacuum when a virtual anti-particle is propagated as shown in Fig. 3-3b. Use symbols for numeric factors resulting from creation and destruction operators acting on the vacuum and other states.

18. Prove (3-125).

19. Reproduce the essence, with the best detail you can muster, of the Spin 0 column in Wholeness Chart 5-4 without looking at it. That is, prove to yourself that you know how the free field part of QFT is developed.

20. Create your own Wholeness Chart summary of RQM, as presented in Sect. 3.1. Take each sub-section heading of Sect. 3.1 as a block in the left hand column of your chart. Put the main result(s) of that section in the block just to its right in the next column. In between main results insert blocks with short notes on how one gets from the material above to the result in the block below. If there are other comments you wish to add, put them in another column to the right of the others.