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.

Joe Cocker
Lyrics by Leonard Cohen

Chapter 3 *Version Date: March 9, 2010*

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

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

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

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

$$p^\mu p_\mu = m^2c^2 = g_{\mu\nu}p^\mu p^\nu = \begin{bmatrix} E/c & -p_1 & -p_2 & -p_3 \end{bmatrix}\begin{bmatrix} E/c \\ p_1 \\ p_2 \\ p_3 \end{bmatrix} \rightarrow \frac{E^2}{c^2} = \mathbf{p}^2 + m^2c^2\,. \tag{3-2}$$

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

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

[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.

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

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

seemingly the only form a relativistic Hamiltonian could take. Unfortunately, we have a problem, as evaluating operators like ∂_i under a radical is not really feasible. (It is bizarre, really.)

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.)

Particles with zero spin, such as π-mesons (pions) and the famous Higg's 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 1/2 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.

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,

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,

- 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 2nd 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. 6 (?), which begins Part 2 of the book, we will begin to investigate interactions.

3.1 Relativistic Quantum Mechanics: A History Lesson

3.1.1 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 (3-4), obtained

$$\left(i\hbar\frac{\partial}{\partial t}\right)\left(i\hbar\frac{\partial}{\partial t}\right)\phi = H^2\phi = \left(\mathbf{p}_{oper}^2 c^2 + m^2c^4\right)\phi\,, \tag{3-5}$$

which becomes

$$-\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t^2}\phi = \left(-\hbar^2\frac{\partial}{\partial X_i}\frac{\partial}{\partial X_i} + m^2c^2\right)\phi \;\rightarrow\; -\frac{\partial}{\partial x^0}\frac{\partial}{\partial x_0}\phi = \left(\frac{\partial}{\partial x^i}\frac{\partial}{\partial x_i} + \underbrace{\frac{m^2c^2}{\hbar^2}}_{\mu^2}\right)\phi\,. \tag{3-6}$$

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

$$\left(\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x_\mu} + \mu^2\right)\phi = 0 \quad \text{or} \quad \left(\partial_\mu\partial^\mu + \mu^2\right)\phi = 0\,, \qquad \mu^2 = \frac{m^2c^2}{\hbar^2}\left(= m^2 \text{ in nat. units}\right). \tag{3-7}$$

In 1934, Wolfgang Pauli and Victor Weisskopf 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.

3.1.2 The Solutions to the Klein-Gordon Equation

A solution set to (3-7), readily checked by substitution into (3-7) (which is good practice in using contravariant/covariant notation), is

$$\phi(x) = \sum_{n=1}^{\infty}\frac{1}{\sqrt{2VE_n/\hbar}}\left(A_n e^{-\frac{i}{\hbar}\left(E_nt-\mathbf{p}_n\bullet\mathbf{x}\right)} + \underbrace{B_n^\dagger e^{\frac{i}{\hbar}\left(E_nt-\mathbf{p}_n\bullet\mathbf{x}\right)}}_{\text{absent in NRQM}}\right), \tag{3-8}$$

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 $A_\mathbf{k}$ and $B_\mathbf{k}^\dagger$ 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 (3-8) 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 (3-7) as well, but we are not concerned with them at this point.

This solution set is also specifically for plane waves. We will not consider alternative solution forms for other wave shapes, such as one might find in problems with cylindrical or spherical geometries.

The solution (3-8), 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.

Note that in NRQM, we only had terms in the counterpart to (3-8) 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.

With an aim towards using natural units, we note the following relations, where wave number $k_i = 2\pi/\lambda_i$,

$$p_\mu = \begin{bmatrix} E/c \\ p_i \end{bmatrix} = \hbar k_\mu = \begin{bmatrix} \hbar\omega/c \\ \hbar k_i \end{bmatrix} \xrightarrow{\text{nat. units}} p_\mu = \begin{bmatrix} E \\ p_i \end{bmatrix} = k_\mu = \begin{bmatrix} \omega \\ k_i \end{bmatrix}, \tag{3-9}$$

and recall the notation introduced in Chap. 2,

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

$$kx = k_\mu x^\mu = \omega t - k_i x^i = \frac{Et}{\hbar} - \frac{p_i x^i}{\hbar} = \frac{p_\mu}{\hbar} x^\mu \qquad \left(= k^\mu x_\mu\right) \tag{3-10}$$

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

It is then common to re-write (3-8) 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 $E_{\mathbf{k}}$.)

The <u>Klein-Gordon equation solutions</u> (3-8) then become, in <u>natural units</u>

$$\phi(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left(A_{\mathbf{k}} e^{-ikx} + B_{\mathbf{k}}^\dagger e^{ikx} \right) \quad . \tag{3-11}$$

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

<u>Definition of Eigensolutions</u>

As noted previously, in RQM, the solution ϕ of (3-11) is that of a general (sum of eigenstates) single particle state. Each <u>eigenstate</u> has mathematical form (where we are going to omit the $2\omega_{\mathbf{k}}$ part here, because of what is coming)

$$\phi_{\mathbf{k},A} = \frac{e^{-ikx}}{\sqrt{V}} \qquad \text{or} \qquad \phi_{\mathbf{k},B^\dagger} = \frac{e^{ikx}}{\sqrt{V}}. \tag{3-12}$$

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

$$\int \phi_{\mathbf{k},A}^\dagger \phi_{\mathbf{k},A} d^3x = \frac{1}{V} \int_V e^{ikx} e^{-ikx} d^3x = 1, \tag{3-13}$$

or more generally, all such eigenstates are <u>orthonormal</u>, i.e., their inner products are

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

Similar relations to (3-14) 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. 1.

Relations (3-12) to (3-14) should look familiar from NRQM. There, (3-13) 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 (3-13).

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 (3-11) in forming our definitions (3-12). Things just turn out easier that way.

3.1.3 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 Schroedinger equation. First pre-multiply it by $\phi^\dagger$, i.e.,

$$\phi^\dagger \left\{ \frac{\partial^2}{\partial t^2}\phi = \left(\nabla^2 - \mu^2\right)\phi \right\}. \tag{3-15}$$

Then take the complex conjugate Klein-Gordon equation post multiplied by ϕ, i.e.,

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

and subtract the former (3-15) from the latter (3-16). The result (after multiplying by i) and using the identity shown under the first downward bracket of (B-1.5) in Box 3-1, is

$$\frac{\partial}{\partial t}\left\{ i\left(\phi^\dagger \frac{\partial\phi}{\partial t} - \frac{\partial\phi^\dagger}{\partial t}\phi\right)\right\} + \nabla\cdot\left\{-i\left(\phi^\dagger\nabla\phi - \left(\nabla\phi^\dagger\right)\phi\right)\right\} = 0. \tag{3-17}$$

This has the form of the continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0, \tag{3-18}$$

where probability density for a Klein-Gordon particle is then

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

and the probability current is

$$\mathbf{j} = j^i = -i\left(\phi^\dagger\nabla\phi - \left(\nabla\phi^\dagger\right)\phi\right) = -i\left(\phi^\dagger\phi_{,i} - \phi^\dagger{}_{,i}\,\phi\right). \tag{3-20}$$

Importantly, and perhaps surprisingly, the relativistic form of the probability density (3-19) is *not* the same as (B3-1.6), the NRQM probability density.

4 Currents

We introduce 4D notation for the scalar and 3D vector of (3-18) and define the 4-current

$$j^\mu = \begin{bmatrix} \rho \\ \mathbf{j} \end{bmatrix} = \begin{bmatrix} \rho \\ j^i \end{bmatrix} = \begin{bmatrix} j^0 \\ j^i \end{bmatrix} = -i\left(\phi^{\dagger,\mu}\phi - \phi^{,\mu}\phi^\dagger\right). \tag{3-21}$$

The 4D continuity equation form of (3-18) is then

$$\boxed{\frac{\partial j^\mu}{\partial x^\mu} = \partial_\mu j^\mu = j^\mu{}_{,\mu} = 0}, \tag{3-22}$$

where we have shown three common notational ways to designate partial derivative. (3-22) tells us the *important fact* that the 4-divergence *of the 4-current of any conserved quantity* (total probability in this case) *is zero.*

Probability for Klein-Gordon Discrete Solutions

For a single particle state in RQM, we are going to assume at first, for simplicity, that the solution (3-11), has only terms with coefficients $A_{\mathbf{k}}$, i.e., the general state ϕ contains no eigenstates shown with coefficients $B_{\mathbf{k}}^\dagger$. Probability density (3-19) is then

$$\rho = \left(2\sum_{\mathbf{k}} \frac{A_{\mathbf{k}}^\dagger}{\sqrt{2\omega_{\mathbf{k}}}}\frac{e^{ikx}}{\sqrt{V}}\right)\left(\sum_{\mathbf{k}'} \frac{\omega_{\mathbf{k}'}A_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{-ik'x}}{\sqrt{V}}\right), \tag{3-23}$$

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

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,

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

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.,

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

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

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

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

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

or

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

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

$$\rho = \Psi^{\dagger}\Psi \ , \qquad \text{(B3-1.6)}$$

and as our probability current

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

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

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 (as do the factors of 2), leaving

$$\int \rho d^3x = \sum_{\mathbf{k}} |A_{\mathbf{k}}|^2 = 1 . \tag{3-24}$$

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

<u>Normalization Factors</u>

Note that obtaining (3-24) is the reason for the normalization factors $1/\sqrt{2\omega_{\mathbf{k}}V}$ used in the solution ϕ of (3-11) and (3-8). 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 (3-19). The time derivatives in (3-19) gave us a factor of $\omega_{\mathbf{k}}$, and the two terms a factor of 2. These cancel in (3-24) with the $2\omega_{\mathbf{k}}$ in the denominators. The V term in the denominator cancels in the integration over the volume V, and the result is a total probability of 1.

<u>Difference from NRQM</u>

Note that in RQM

$$\int \phi^{\dagger}\phi \, d^3x = \sum_{\mathbf{k}} \frac{(A_{\mathbf{k}})^2}{2\omega_{\mathbf{k}}} \neq 1 , \tag{3-25}$$

because in RQM (unlike in NRQM), the LHS of (3-25) does not represent the integral of the probability density over space.

<u>Relativistic Invariance of Probability</u>

This probability value of unity in (3-24) 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 looks different for each energy-momentum eigenstate). 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.

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

3.1.4 A Note on Quantization

Recall from Chaps. 1 and 2, that 1st 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. 1 of Chap. 1 that non-commutation of dynamical variables means those variables are operators (because ordinary numbers commute.) For example,

$$\left[p_i , x^j \right] = -i\delta_{ij} \quad \xleftrightarrow{\text{equivalent}} \quad p_i = -i\partial_i , \tag{3-26}$$

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

But, you the reader might protest that in the pages above, we didn't use 1st quantization to obtain RQM. Rather, we extrapolated from NRQM. The fact is, as illustrated in Fig. 3-1, that we could have done it either way. We could have gone from classical relativistic particle theory to RQM via quantization (specifically, invoking commutators) or from NRQM to RQM via simply changing the non-relativistic Hamiltonian to the relativistic one. We did the latter because, historically, that is how it was first done.

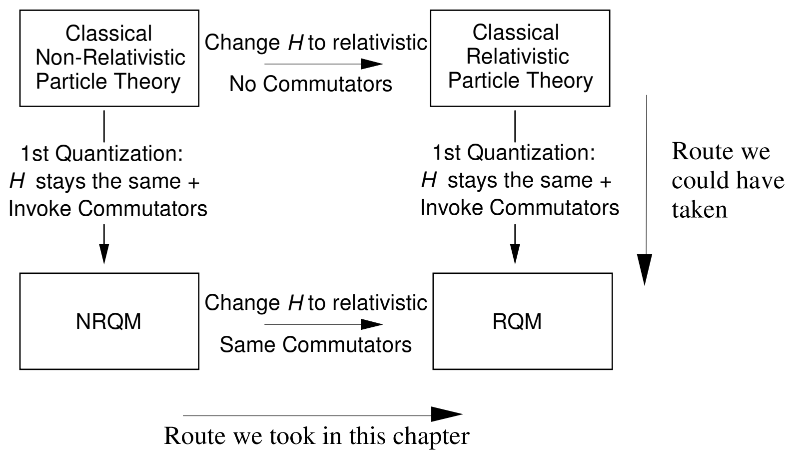

Figure 3-1. Different Routes to Relativistic Quantum Mechanics

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 (3-11) and (3-12), we should get the energy eigenvalue $\omega_{\mathbf{k}}$. When we do this for the eigenstates with exponents in $-ikx$, all looks as expected.

$$H\phi_{\mathbf{k},A} = i\frac{\partial\phi_{\mathbf{k},A}}{\partial t} = E_{\mathbf{k},A}\phi_{\mathbf{k},A} = i\frac{\partial}{\partial t}\frac{e^{-ikx}}{\sqrt{V}} = \omega_{\mathbf{k}}\frac{e^{-ikx}}{\sqrt{V}} = \omega_{\mathbf{k}}\phi_{\mathbf{k},A}\,. \tag{3-27}$$

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

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

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 (3-11)) has total probability of being measured of –1. The extra states in RQM have physically untenable negative probabilities!

Time to move on to QFT.

3.2 The Klein-Gordon Equation in Quantum Field Theory

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 (3-7), is also the fundamental scalar wave equation of QFT, except that ϕ therein is considered a field, instead of a state. (We will understand a little better what that means, shortly.) Formally, the Klein-Gordon equation in QFT is called a field equation.

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 Appendix A.

3.2.1 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 ϕ of the Klein-Gordon equation (3-7) is a field (instead of a state). This is reasonable, since a field value, by definition, is a function of spatial location (and time), and ϕ is such a function.

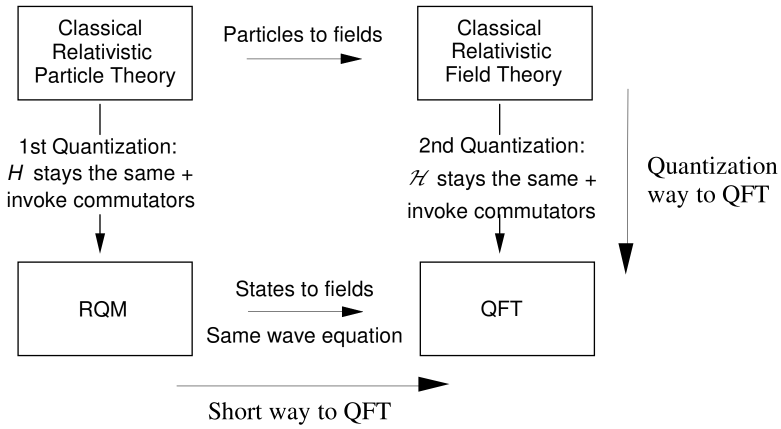

Figure 3-2. Different Routes to Quantum Field Theory

We then must apply the commutation relations for fields (see Chap. 2, Wholeness Chart 2-5, right hand column), instead of the commutation relations for particle properties (same chart, third column). 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.

3.2.2 From Classical Relativistic Fields to QFT

Classical Scalar Fields

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

$$\mathcal{L}_0^0 = K\left(\partial_\alpha\phi\partial^\alpha\phi-\mu^2\phi\phi\right)=K\left(\dot{\phi}\dot{\phi}+\partial_i\phi\partial^i\phi-\mu^2\phi\phi\right)=K\left(\dot{\phi}\dot{\phi}-\underbrace{\partial_i\phi\partial_i\phi}_{(\nabla\phi)\cdot(\nabla\phi)}-\mu^2\phi\phi\right), \qquad (3\text{-}29)$$

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 (3-29) here. We do note in passing that (3-29) 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. (3-29) 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 (3-29) to find the Hamiltonian density, where $\pi_0{}^0$ is the field conjugate momentum,

$$\mathcal{H}_0^0 = \pi_0^0\dot{\phi}-\mathcal{L}_0^0=\underbrace{\frac{\partial\mathcal{L}_0^0}{\partial\dot{\phi}}}_{K2\dot{\phi}}\dot{\phi}-\mathcal{L}_0^0=K\left(\dot{\phi}\dot{\phi}+\nabla\phi\nabla\phi+\mu^2\phi\phi\right). \qquad (3\text{-}30)$$

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

$$\boxed{\mathcal{L}_0^0 = \left(\partial_\alpha \phi^\dagger \partial^\alpha \phi - \mu^2 \phi^\dagger \phi\right) = \left(\dot{\phi}^\dagger \dot{\phi} - \nabla\phi^\dagger \nabla\phi - \mu^2\phi^\dagger\phi\right)}\text{, and} \tag{3-31}$$

$$\boxed{\mathcal{H}_0^0 = \frac{\partial \mathcal{L}_0^0}{\partial \dot{\phi}^r}\dot{\phi}^r - \mathcal{L}_0^0 = \underbrace{\frac{\partial \mathcal{L}_0^0}{\partial \dot{\phi}}}_{\pi_0^0=\dot{\phi}^\dagger}\dot{\phi} + \underbrace{\frac{\partial \mathcal{L}_0^0}{\partial \dot{\phi}^\dagger}}_{\pi_0^{0\dagger}=\dot{\phi}}\dot{\phi}^\dagger - \mathcal{L}_0^0 = \dot{\phi}\dot{\phi}^\dagger + \nabla\phi^\dagger\nabla\phi + \mu^2\phi^\dagger\phi}\ . \tag{3-32}$$

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 (3-31) into the Euler-Lagrange field equation,

$$\frac{d}{dx^\mu}\left(\frac{\partial \mathcal{L}}{\partial \phi^r{}_{,\mu}}\right) - \frac{\partial \mathcal{L}}{\partial \phi^r} = 0\ . \tag{3-33}$$

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) which, for scalars, is simply the complex conjugate,

$$\boxed{\begin{aligned} \left(\partial_\mu \partial^\mu + \mu^2\right)\phi &= \left(\Box^2 + \mu^2\right)\phi = 0 \qquad \text{(a)} \\ \left(\partial_\mu \partial^\mu + \mu^2\right)\phi^\dagger &= \left(\Box^2 + \mu^2\right)\phi^\dagger = 0. \qquad \text{(b)} \end{aligned}} \tag{3-34}$$

In the above, we have introduced the $\Box^2$ symbol, 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 (3-34)(b) by taking the complex conjugate transpose of (3-34)(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 (3-34) are the same as (3-11), and its Hermitian, from RQM, i..e.,[1]

[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).

$$\boxed{\begin{aligned}
\phi(x) &= \underbrace{\sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} a(\mathbf{k}) e^{-ikx}}_{} + \underbrace{\sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} b^{\dagger}(\mathbf{k}) e^{ikx}}_{} \qquad \text{(a)} \\
&= \qquad \phi^{+} \qquad + \qquad \phi^{-} \\
\phi^{\dagger}(x) &= \underbrace{\sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} b(\mathbf{k}) e^{-ikx}}_{} + \underbrace{\sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} a^{\dagger}(\mathbf{k}) e^{ikx}}_{} \qquad \text{(b)} \\
&= \qquad \phi^{\dagger +} \qquad + \qquad \phi^{\dagger -} \; .
\end{aligned}} \tag{3-35}$$

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.

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 (3-35), 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, $(\phi^{-})^{\dagger} = \phi^{\dagger +}$.

However you do it, being able to readily recall the definitions of the symbols in (3-35) will help in the future.

The <u>continuous plane wave solutions</u> to (3-34) are

$$\boxed{\begin{aligned}
\phi(x) &= \underbrace{\int \frac{d^3\boldsymbol{k}}{\sqrt{2(2\pi)^3\omega_{\mathbf{k}}}} a(\mathbf{k}) e^{-ikx}}_{} + \underbrace{\int \frac{d^3\boldsymbol{k}}{\sqrt{2(2\pi)^3\omega_{\mathbf{k}}}} b^{\dagger}(\mathbf{k}) e^{ikx}}_{} \qquad \text{(a)} \\
&= \qquad \phi^{+} \qquad + \qquad \phi^{-} \\
\phi^{\dagger}(x) &= \underbrace{\int \frac{d^3\boldsymbol{k}}{\sqrt{2(2\pi)^3\omega_{\mathbf{k}}}} b(\mathbf{k}) e^{-ikx}}_{} + \underbrace{\int \frac{d^3\boldsymbol{k}}{\sqrt{2(2\pi)^3\omega_{\mathbf{k}}}} a^{\dagger}(\mathbf{k}) e^{ikx}}_{} \; . \qquad \text{(b)} \\
&= \qquad \phi^{\dagger +} \qquad + \qquad \phi^{\dagger -}
\end{aligned}} \tag{3-36)}$$

These 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.

<u>Finding μ^2</u>

Do Prob. 4 to prove to yourself that the value of μ^2, which appeared as an unknown constant in the theoretical determination of (3-29), has the same value it did in RQM, i.e.,

$$\boxed{\mu^2 = \frac{m^2c^2}{\hbar^2} \quad \left(= m^2 \text{ in nat. units}\right)}. \tag{3-37}$$

<u>Third Way to Klein-Gordon Equations: A Consistency Check</u>

Recall from Chap 2. and Wholeness Charts 2-2 and 2-5, 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 (3-38)) 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,

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

$$\dot{\phi} = -i\left[\phi, H\right] \quad \xleftrightarrow{\text{should be same thing}} \quad \left(\partial_\mu \partial^\mu + \mu^2\right)\phi = 0 \tag{3-38}$$

In 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 (3-34) (and (3-38)) 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.

3.2.3 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-X at the end of Chap. 5. XXX Viewers of website www.quantumfieldtheory.info can get this by clicking the Free Fields Wholeness Chart link. For book draft reviewers, a file should be attached with this one. XXX

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.

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 second part of 2nd quantization, found in the last box in the right hand column of Wholeness Chart 2-5 of Chap. 2 and reproduced in (3-39) below, lie at the root of, and structure, all of QFT. For scalars, they are

$$\left[\phi^r(\mathbf{x},t), \pi_s(\mathbf{y},t)\right] = \phi^r \pi_s - \pi_s \phi^r = i\delta^r{}_s \delta(\mathbf{x}-\mathbf{y}). \tag{3-39}$$

Of overriding importance in the theory, as we will see, are the following coefficient commutation relations, which we will derive below from the 2$^{\text{nd}}$ quantization postulate of (3-39).

$$\boxed{\left[a(\mathbf{k}), a^\dagger(\mathbf{k}')\right] = \left[b(\mathbf{k}), b^\dagger(\mathbf{k}')\right] = \delta_{\mathbf{k}\mathbf{k}'} \text{ (discrete);} \quad = \delta(\mathbf{k}-\mathbf{k}') \text{ (continuous)}}\,. \tag{3-40}$$

The form of (3-40) should tell us immediately that the Klein-Gordon solution coefficients $a(\mathbf{k})$, $b(\mathbf{k})$, etc. in QFT of (3-35) and (3-36) are far different animals than the $A_\mathbf{k}$, $B_\mathbf{k}$, etc. in RQM of (3-11). 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.

Proof of coefficient commutation relations

To prove (3-40), start with (3-39) and take different spatial coordinates $\mathbf{x}$ and $\mathbf{y}$, but the same time coordinate t, for ϕ and $\pi^0{}_0$. This results in the equal time commutation relations

$$\left[\phi(\mathbf{x},t)\pi_0^0(\mathbf{y},t) - \pi_0^0(\mathbf{y},t)\phi(\mathbf{x},t)\right] = \left[\phi(\mathbf{x},t)\dot{\phi}^\dagger(\mathbf{y},t) - \dot{\phi}^\dagger(\mathbf{y},t)\phi(\mathbf{x},t)\right] = i\delta(\mathbf{x}-\mathbf{y}), \tag{3-41}$$

which are only important at this point as a step in our proof. Then, plugging the discrete solutions (3-35) into the middle part of (3-41), where to save space we use the compressed notation $a_\mathbf{k} = a(\mathbf{k})$, etc., we get

$$\left(\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}a_{\mathbf{k}}e^{-i(\omega_{\mathbf{k}}t-\mathbf{k}\cdot\mathbf{x})}+\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}b_{\mathbf{k}}^{\dagger}e^{i(\omega_{\mathbf{k}}t-\mathbf{k}\cdot\mathbf{x})}\right)\left(\sum_{\mathbf{k}'}\frac{-i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}}b_{\mathbf{k}'}e^{-i(\omega_{\mathbf{k}'}t-\mathbf{k}'\cdot\mathbf{y})}+\sum_{\mathbf{k}'}\frac{i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}}a_{\mathbf{k}'}^{\dagger}e^{i(\omega_{\mathbf{k}'}t-\mathbf{k}'\cdot\mathbf{y})}\right)$$

$$-\left(\sum_{\mathbf{k}'}\frac{-i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}}b_{\mathbf{k}'}e^{-i(\omega_{\mathbf{k}'}t-\mathbf{k}'\cdot\mathbf{y})}+\sum_{\mathbf{k}'}\frac{i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}}a_{\mathbf{k}'}^{\dagger}e^{i(\omega_{\mathbf{k}'}t-\mathbf{k}'\cdot\mathbf{y})}\right)\left(\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}a_{\mathbf{k}}e^{-i(\omega_{\mathbf{k}}t-\mathbf{k}\cdot\mathbf{x})}+\sum_{\mathbf{k}}\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}b_{\mathbf{k}}^{\dagger}e^{i(\omega_{\mathbf{k}}t-\mathbf{k}\cdot\mathbf{x})}\right)$$

$$=\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\frac{i\omega_{\mathbf{k}'}}{2V\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\begin{pmatrix}-a_{\mathbf{k}}b_{\mathbf{k}'}e^{-i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}+a_{\mathbf{k}}a_{\mathbf{k}'}^{\dagger}e^{-i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\\-b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}'}e^{i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{-i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}+b_{\mathbf{k}}^{\dagger}a_{\mathbf{k}'}^{\dagger}e^{i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{-i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\\+b_{\mathbf{k}'}a_{\mathbf{k}}e^{-i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}+b_{\mathbf{k}'}b_{\mathbf{k}}^{\dagger}e^{i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{-i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\\-a_{\mathbf{k}'}^{\dagger}a_{\mathbf{k}}e^{-i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}-a_{\mathbf{k}'}^{\dagger}b_{\mathbf{k}}^{\dagger}e^{i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{-i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\end{pmatrix}=i\delta(\mathbf{x}-\mathbf{y}). \tag{3-42}$$

Using the math identity for the 3D Dirac delta function

$$\delta(\mathbf{x}-\mathbf{y})=\frac{1}{V}\sum_{n=-\infty}^{+\infty}e^{-i\mathbf{k}_n\cdot(\mathbf{x}-\mathbf{y})}\quad\left(=\frac{1}{V}\sum_{\mathbf{k}}e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\text{ in our notation}\right) \tag{3-43}$$

after the last equal sign in (3-42), and matching terms, we see that all terms where $|\mathbf{k}| \neq |\mathbf{k}'|$ must equal zero. That is,

$$\begin{aligned}&\frac{i\omega_{\mathbf{k}'}}{2V\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\underbrace{\left(b_{\mathbf{k}'}a_{\mathbf{k}}-a_{\mathbf{k}}b_{\mathbf{k}'}\right)}_{\text{must}=0}e^{-i(\omega_{\mathbf{k}}+\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}+\\&\frac{i\omega_{\mathbf{k}'}}{2V\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\underbrace{\left(a_{\mathbf{k}}a_{\mathbf{k}'}^{\dagger}-a_{\mathbf{k}'}^{\dagger}a_{\mathbf{k}}\right)}_{\text{must}=0}e^{-i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}'})t}e^{i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}+\\&\text{... etc. for all terms in }\mathbf{k}\text{ and }\mathbf{k}'\quad=\quad0\quad(\text{no terms on RHS in }\mathbf{k}\text{ and }\mathbf{k}')\end{aligned} \tag{3-44}$$

So, all possible coefficient commutators with different $\mathbf{k}$ vectors vanish. Certain of the remaining terms with $\mathbf{k} = \mathbf{k}'$ have form

$$\begin{aligned}&\frac{i}{2V}\frac{\cancel{\omega_{\mathbf{k}}}}{\cancel{\omega_{\mathbf{k}}}}\underbrace{\left(b_{\mathbf{k}}a_{\mathbf{k}}-a_{\mathbf{k}}b_{\mathbf{k}}\right)}_{\text{must}=0}\underbrace{e^{-i2\omega_{\mathbf{k}}t}}_{\neq0}e^{i\mathbf{k}\cdot(\mathbf{x}+\mathbf{y})}+\\&\frac{i}{2V}\underbrace{\left(b_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}^{\dagger}-a_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}^{\dagger}\right)}_{\text{must}=0}e^{i2\omega_{\mathbf{k}}t}e^{-i\mathbf{k}\cdot(\mathbf{x}+\mathbf{y})}+\\&\text{... etc. for all similar terms}\ =0\qquad(\text{no time dependence on RHS}),\end{aligned} \tag{3-45}$$

and their coefficient commutators must vanish because the exponential in $\omega_{\mathbf{k}}$ varies in time, whereas there is no such variation on the RHS.

The remaining terms have form

$$\begin{aligned}&\frac{i}{2V}\underbrace{\left(a_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}-a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\right)}_{\text{must}=1}\underbrace{e^{-i(\omega_{\mathbf{k}}-\omega_{\mathbf{k}})t}}_{1}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}+\frac{i}{2V}\underbrace{\left(a_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}-a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\right)}_{\text{must}=1}e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}+\\&\frac{i}{2V}\underbrace{\left(b_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}-b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}\right)}_{\text{must}=1}e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}+\frac{i}{2V}\underbrace{\left(b_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}-b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}\right)}_{\text{must}=1}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}=\frac{i}{V}e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}+\frac{i}{V}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})},\end{aligned} \tag{3-46}$$

where we see that the coefficient commutators need to equal unity in order to match corresponding terms on the RHS. (A subtle point for the purists: we also made the reasonable assumption that the commutators in $a_{\mathbf{k}}\,a_{\mathbf{k}}^{\dagger}$ and the commutators in $b_{\mathbf{k}}\,b_{\mathbf{k}}^{\dagger}$ have the same value.)

The commutation relations shown above in (3-44) to (3-46) are the same as (3-40). 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 (3-40).

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.

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 (3-32), where we employ our discrete, plane wave solutions (3-35) we get

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

$$\int \left(\sum_{\mathbf{k}} \frac{\partial}{\partial t} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left(a(\mathbf{k}) e^{-ikx} + b^\dagger(\mathbf{k}) e^{ikx} \right) \right) \left(\sum_{\mathbf{k}'} \frac{\partial}{\partial t} \frac{1}{\sqrt{2V\omega_{\mathbf{k}'}}} \left(b(\mathbf{k}') e^{-ik'x} + a^\dagger(\mathbf{k}') e^{ik'x} \right) \right) d^3x \quad (3\text{-}47)$$

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

The middle line of (3-47), i.e., the $\int \dot{\phi}\dot{\phi}^\dagger d^3x$ part, becomes

$$\int \left(\sum_{\mathbf{k}} \frac{i\omega_{\mathbf{k}}}{\sqrt{2V\omega_{\mathbf{k}}}} \left(-a(\mathbf{k}) e^{-ikx} + b^\dagger(\mathbf{k}) e^{ikx} \right) \right) \left(\sum_{\mathbf{k}'} \frac{i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}} \left(-b(\mathbf{k}') e^{-ik'x} + a^\dagger(\mathbf{k}') e^{ik'x} \right) \right) d^3x. \quad (3\text{-}48)$$

or

$$\sum_{\mathbf{k}} \sum_{\mathbf{k}'} \frac{-\sqrt{\omega_{\mathbf{k}}}\sqrt{\omega_{\mathbf{k}'}}}{2V} \int \begin{pmatrix} a(\mathbf{k}) b(\mathbf{k}') e^{-ikx} e^{-ik'x} - a(\mathbf{k}) a^\dagger(\mathbf{k}') e^{-ikx} e^{ik'x} \\ -b^\dagger(\mathbf{k}) b(\mathbf{k}') e^{ikx} e^{-ik'x} + b^\dagger(\mathbf{k}) a^\dagger(\mathbf{k}') e^{ikx} e^{ik'x} \end{pmatrix} d^3x . \quad (3\text{-}49)$$

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 (3-49) 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 (3-49) equals V, we end up with

$$\int \dot{\phi}\dot{\phi}^\dagger d^3x = \sum_{\mathbf{k}} \frac{\omega_{\mathbf{k}}}{2} \left(-a(\mathbf{k}) b(-\mathbf{k}) + a(\mathbf{k}) a^\dagger(\mathbf{k}) + b^\dagger(\mathbf{k}) b(\mathbf{k}) - b^\dagger(\mathbf{k}) a^\dagger(-\mathbf{k}) \right). \quad (3\text{-}50)$$

Following similar steps for the next term in (3-47) we get

$$-\int \partial_i\phi^\dagger\partial^i\phi d^3x = \int \partial_i\phi^\dagger\partial_i\phi d^3x$$

$$= \int \left(\sum_{\mathbf{k}} \frac{ik_i}{\sqrt{2V\omega_{\mathbf{k}}}} \left(b(\mathbf{k}) e^{-ikx} - a^\dagger(\mathbf{k}) e^{ikx} \right) \right) \left(\sum_{\mathbf{k}'} \frac{ik_i'}{\sqrt{2V\omega_{\mathbf{k}'}}} \left(a(\mathbf{k}') e^{-ik'x} - b^\dagger(\mathbf{k}') e^{ik'x} \right) \right) d^3x \quad (3\text{-}51)$$

$$= \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2\omega_{\mathbf{k}}} \left(b(\mathbf{k}) a(-\mathbf{k}) + a^\dagger(\mathbf{k}) a(\mathbf{k}) + b(\mathbf{k}) b^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k}) b^\dagger(-\mathbf{k}) \right)$$

where we note that terms in the summation with both $\mathbf{k}$ and - $\mathbf{k}$ have an extra sign change since $k_i = -k_i'$ in the multiplication in the second line of (3-51).

Similarly, for the mass term in (3-47), we get (do Prob. 8 at the end of the chapter to prove it)

$$\int \mu^2\phi^\dagger\phi d^3x = \sum_{\mathbf{k}} \frac{\mu^2}{2\omega_{\mathbf{k}}} \left(b(\mathbf{k}) a(-\mathbf{k}) + b(\mathbf{k}) b^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k}) a(\mathbf{k}) + a^\dagger(\mathbf{k}) b^\dagger(-\mathbf{k}) \right). \quad (3\text{-}52)$$

Adding the final parts of (3-50), (3-51), and (3-52), and using $\mathbf{k}^2 + \mu^2 = (\omega_\mathbf{k})^2$ along with the coefficient commutation relations (3-40), we end up with

$$H_0^0 = \sum_\mathbf{k} \frac{\omega_\mathbf{k}}{2}\left(\underbrace{a(\mathbf{k})a^\dagger(\mathbf{k})}_{\text{use commutator}} + a^\dagger(\mathbf{k})a(\mathbf{k}) + b^\dagger(\mathbf{k})b(\mathbf{k}) + \underbrace{b(\mathbf{k})b^\dagger(\mathbf{k})}_{\text{use commutator}} \right)$$
$$= \sum_\mathbf{k} \omega_\mathbf{k}\left(a^\dagger(\mathbf{k})a(\mathbf{k}) + \tfrac{1}{2} + b^\dagger(\mathbf{k})b(\mathbf{k}) + \tfrac{1}{2}\right). \tag{3-53}$$

or simply

$$\boxed{H_0^0 = \sum_\mathbf{k} \omega_\mathbf{k}\left(N_a(\mathbf{k}) + \tfrac{1}{2} + N_b(\mathbf{k}) + \tfrac{1}{2}\right)}, \tag{3-54}$$

where

$$\boxed{N_a(\mathbf{k}) = a^\dagger(\mathbf{k})a(\mathbf{k}) \qquad N_b(\mathbf{k}) = b^\dagger(\mathbf{k})b(\mathbf{k})}. \tag{3-55}$$

Expressions (3-54) and (3-55) 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 (3-54) 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 would have an energy eigenvalue equal to its total energy $2\omega_{\mathbf{k}_1}$ i.e.,

$$H_0^0 \left|2\phi_{\mathbf{k}_1}\right\rangle = 2\omega_{\mathbf{k}_1}\left|2\phi_{\mathbf{k}_1}\right\rangle . \tag{3-56}$$

But from (3-54), that means

$$\sum_\mathbf{k} \omega_\mathbf{k}\left(N_a(\mathbf{k}) + \tfrac{1}{2} + N_b(\mathbf{k}) + \tfrac{1}{2}\right)\left|2\phi_{\mathbf{k}_1}\right\rangle = 2\omega_{\mathbf{k}_1}\left|2\phi_{\mathbf{k}_1}\right\rangle . \tag{3-57}$$

How can we make sense of (3-57)? The answer is that it is not quite true, and that we can make sense of it all if, instead of (3-56) and (3-57), we consider

$$H_0^0\left|2\phi_{\mathbf{k}_1}\right\rangle = \sum_\mathbf{k}\omega_\mathbf{k}\left(\underbrace{N_a(\mathbf{k}) + \tfrac{1}{2}}_{\substack{a\text{ type}\\ \text{particles}}} + \underbrace{N_b(\mathbf{k}) + \tfrac{1}{2}}_{\substack{b\text{ type}\\ \text{particles}}}\right)\underbrace{\left|2\phi_{\mathbf{k}_1}\right\rangle}_{\substack{a\text{ type}\\ \text{particles}}} = \left(2\omega_{\mathbf{k}_1} + \sum_\mathbf{k}\omega_\mathbf{k}\left(\tfrac{1}{2}+\tfrac{1}{2}\right)\right)\left|2\phi_{\mathbf{k}_1}\right\rangle, \tag{3-58}$$

with the following interpretation.

<u>N_a(**k**)</u> = <u>number operator</u> with <u>eigenvalue n_a(**k**)</u> = <u>number of *a* particles with 3-mom **k**</u> in the ket, <u>N_b(**k**)</u> = <u>number operator</u> with <u>eigenvalue n_b(**k**)</u> = <u>number of *b* particles with 3-mom **k**</u> 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 (3-58) 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.

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

<u>Examples of number operators and kets</u>

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

$$H_0^0 \mid 5\phi_{\mathbf{k}_1}, 2\phi_{\mathbf{k}_2}, \underbrace{3\bar{\phi}_{\mathbf{k}_3}}_{\substack{b\text{ type}\\ \text{particles}}} \rangle = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(N_a(\mathbf{k}) + \tfrac{1}{2} + N_b(\mathbf{k}) + \tfrac{1}{2} \right) \left| 5\phi_{\mathbf{k}_1}, 2\phi_{\mathbf{k}_2}, 3\bar{\phi}_{\mathbf{k}_1} \right\rangle$$
$$= \left(5\omega_{\mathbf{k}_1} + 2\omega_{\mathbf{k}_2} + 3\omega_{\mathbf{k}_3} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(\frac{1}{2} + \frac{1}{2} \right) \right) \left| 5\phi_{\mathbf{k}_1}, 2\phi_{\mathbf{k}_2}, 3\bar{\phi}_{\mathbf{k}_1} \right\rangle . \tag{3-59}$$

and so we see that b type particles in our theory have positive energy. Since we know from experiment that antiparticles have positive energy, we might suspect that b particles are antiparticles. We will see later that they have opposite charge from the a particles, and so really do fit the role of antiparticles.

Example #2: Vacuum state

$$H_0^0 \underbrace{\left|0\right\rangle}_{\substack{\text{vacuum}\\ \text{state}}} = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(N_a(\mathbf{k}) + \tfrac{1}{2} N_b(\mathbf{k}) + \tfrac{1}{2} \right) \left|0\right\rangle = \underbrace{\sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(\frac{1}{2} + \frac{1}{2} \right)}_{\text{infinite energy}} \left|0\right\rangle . \tag{3-60}$$

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 (3-60) represents the now famous perspective on the vacuum as being almost inconceivably crammed with energy, known as zero point energy. 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.

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 (3-39). Because of this we got the coefficient commutation relations (3-40), and those were used in our derivation of the form of the Hamiltonian (see (3-53), 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.) 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 is the source of the statements, often heard, that the uncertainty principle is the cause of the zero point energy.

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 (3-54), 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, such as we saw in Fig. 1-1 of Chap. 1. Via our fundamental QFT relation for H_0^0, the ½ quanta are simply 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 and the Lamb shift demonstrate the existence of vacuum fluctuations. However, Casimir forces are generally computed by considering the ½ quanta such as those in (3-60) 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 .)

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.)

As a caveat, I note that the remarks in this sub-section entitled "Are the ½ Quanta Effervescent" are 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 zero point energy shown above.

My mathematical underpinnings for this position are presented in Appendix B, but you should wait to read that until after finishing Sect. 3.8.2.

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.

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

Note that in QFT, we will have positive and negative values of $\omega_{\mathbf{k}}$ and $-\omega_{\mathbf{k}}$ in the exponents of our field equation solutions (3-35), and thus can expect our creation operators will create states with both $\omega_{\mathbf{k}}$ (*a* type particles) and $-\omega_{\mathbf{k}}$ (*b* type particles), as well. However, the energy *E* of both *a* and *b* type particles will be positive.

$\omega_{\mathbf{k}}t$ is the phase angle change in time of the *a* type particle wave, and $-\omega_{\mathbf{k}}t$ is the phase angle change in time of the *b* type particle wave. In Fig. 2-1 of Chap. 2, this corresponds to opposite directions of twist for the "corkscrew" complex wave in the lower RHS.

In QFT, we thus think of $\omega_{\mathbf{k}}$ as energy ($\hbar\omega_{\mathbf{k}}$ in non-natural units) and always a positive quantity, but the sign before it in the exponent denotes the direction of rotation (cw or ccw) in time of the wave in complex space as the wave propagates. Particles and antiparticles can be thought of geometrically as having opposite such directions of rotation, but not oppositely signed energies.

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

$$\langle\phi_{\mathbf{k}}||\phi_{\mathbf{k}}\rangle = \int_V \underbrace{\phi_{\mathbf{k}}{}^{\dagger}\phi_{\mathbf{k}}}_{\text{states}} d^3x = 1 \quad \text{and} \quad \langle\phi_{\mathbf{k}}||\phi_{\mathbf{k}'}\rangle = \int_V \underbrace{\phi_{\mathbf{k}}{}^{\dagger}\phi_{\mathbf{k}'}}_{\text{states}} d^3x = 0, \;\; \mathbf{k} \neq \mathbf{k}'. \tag{3-61}$$

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 <u>symbols for multiparticle states</u> so that every such state is normalized (i.e, has <u>unit norm</u>.) For example, for a state comprising two *a* particles of 3-momentum **k**, one of 3-momentum $\mathbf{k}'$, and five *b* particles of 3-momentum $\mathbf{k}''$, we would have

$$\left\langle 2\phi_{\mathbf{k}},\phi_{\mathbf{k}'},5\bar{\phi}_{\mathbf{k}''}\middle\|2\phi_{\mathbf{k}},\phi_{\mathbf{k}'},5\bar{\phi}_{\mathbf{k}''}\right\rangle = \int_V \left(\underbrace{2\phi_{\mathbf{k}}\phi_{\mathbf{k}'}5\bar{\phi}_{\mathbf{k}''}}_{\text{states}}\right)^{\dagger}\left(\underbrace{2\phi_{\mathbf{k}}\phi_{\mathbf{k}'}5\bar{\phi}_{\mathbf{k}''}}_{\text{states}}\right) d^3x = 1 \ . \tag{3-62}$$

where the middle part is just a reminder as to what we mean by the bracket notation[1].

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,

$$\begin{gathered}\left\langle 2\phi_{\mathbf{k}},\phi_{\mathbf{k}'},5\bar{\phi}_{\mathbf{k}''}\middle\|\phi_{\mathbf{k}'},5\bar{\phi}_{\mathbf{k}''}\right\rangle = 0 \qquad \left\langle 2\phi_{\mathbf{k}}\middle\|\phi_{\mathbf{k}}\right\rangle = 0 \\ \left\langle 5\phi_{\mathbf{k}''}\middle\|5\bar{\phi}_{\mathbf{k}''}\right\rangle = 0 \qquad \left\langle \phi_{\mathbf{k}}\middle\|\phi_{\mathbf{k}'}\right\rangle = 0 \ .\end{gathered} \tag{3-63}$$

Note on Notation

It is common practice in QFT to employ the bracket notation of LHS of (3-62), and virtually never, the integral form shown between the equal signs. In QFT, symbols such as $\phi_{\mathbf{k}}$, which are not part of a ket symbol, do not represent states, but fields. Unless otherwise noted, we shall adhere to this practice from henceforth. That is,

$|\phi_{\mathbf{k}}\rangle$ symbolizes a state and $\phi_{\mathbf{k}}$ symbolizes a field.

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,

$$\bar{\mathcal{O}} = \langle\phi|\mathcal{O}|\phi\rangle \ . \tag{3-64}$$

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 (3-64).

It is also true for a multiparticle state, such as those we run into in QFT. For example, the multiparticle state in (3-59) 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 (3-59) is

$$\begin{aligned}\bar{H}_0^0 &= \left\langle 5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_3}\middle|H_0^0\middle|5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_3}\right\rangle = \\ &= \left\langle 5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_3}\right| \underbrace{\left(5\omega_{\mathbf{k}_1}+2\omega_{\mathbf{k}_2}+3\omega_{\mathbf{k}_3}+\sum_{\mathbf{k}}\omega_{\mathbf{k}}\left(\tfrac{1}{2}+\tfrac{1}{2}\right)\right)}_{\text{a number, not an operator, so can move outside}} \left|5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_1}\right\rangle \\ &= \left(5\omega_{\mathbf{k}_1}+2\omega_{\mathbf{k}_2}+3\omega_{\mathbf{k}_3}+\sum_{\mathbf{k}}\omega_{\mathbf{k}}\left(\tfrac{1}{2}+\tfrac{1}{2}\right)\right)\underbrace{\left\langle 5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_1}\middle|5\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},3\bar{\phi}_{\mathbf{k}_1}\right\rangle}_{=1} \\ &= 5\omega_{\mathbf{k}_1}+2\omega_{\mathbf{k}_2}+3\omega_{\mathbf{k}_3}+\sum_{\mathbf{k}}\omega_{\mathbf{k}}\left(\tfrac{1}{2}+\tfrac{1}{2}\right).\end{aligned} \tag{3-65}$$

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

[1] For the purists, we note that (3-62) 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 (3-62) yields a factor $1/V$. The integral over 3D space then yields a factor of V. V is non-invariant, but there is one in the numerator and one in the denominator, so they cancel, leaving an invariant final result.

$$\boxed{\bar{\mathcal{O}} = \langle \phi_1, \phi_2, \phi_3, \ldots | \mathcal{O} | \phi_1, \phi_2, \phi_3, \ldots \rangle} \,, \tag{3-66}$$

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

$$\langle \mathcal{O} \rangle = \langle 0 | \mathcal{O} | 0 \rangle \,. \tag{3-67}$$

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

$$\left\langle H_0^0 \right\rangle = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \,. \tag{3-68}$$

We expect to measure infinite (or at least enormous, if nature has a maximum $|\mathbf{k}|$ value) 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.

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

$$a(\mathbf{k}) | n_{\mathbf{k}} \rangle = | m_{\mathbf{k}} \rangle \text{ ?} \tag{3-69}$$

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

$$N_a(\mathbf{k}) | m_{\mathbf{k}} \rangle = N_a(\mathbf{k})\, a(\mathbf{k}) | n_{\mathbf{k}} \rangle = \underbrace{a(\mathbf{k})^\dagger a(\mathbf{k})}_{\text{use commutator}} a(\mathbf{k}) | n_{\mathbf{k}} \rangle \,. \tag{3-70}$$

Then use the commutation relations from (3-40), to find (3-70) equals

$$\begin{aligned} &\left(a(\mathbf{k})a(\mathbf{k})^\dagger - 1\right) a(\mathbf{k}) | n_{\mathbf{k}} \rangle = a(\mathbf{k})a(\mathbf{k})^\dagger a(\mathbf{k}) | n_{\mathbf{k}} \rangle - a(\mathbf{k}) | n_{\mathbf{k}} \rangle = a(\mathbf{k}) N_a(\mathbf{k}) | n_{\mathbf{k}} \rangle - a(\mathbf{k}) | n_{\mathbf{k}} \rangle \\ &= a(\mathbf{k}) n_{\mathbf{k}} | n_{\mathbf{k}} \rangle - a(\mathbf{k}) | n_{\mathbf{k}} \rangle = n_{\mathbf{k}} a(\mathbf{k}) | n_{\mathbf{k}} \rangle - a(\mathbf{k}) | n_{\mathbf{k}} \rangle = (n_{\mathbf{k}} - 1) a(\mathbf{k}) | n_{\mathbf{k}} \rangle = (n_{\mathbf{k}} - 1) | m_{\mathbf{k}} \rangle . \end{aligned} \tag{3-71}$$

So

$$N_a(\mathbf{k}) | m_{\mathbf{k}} \rangle = (n_{\mathbf{k}} - 1) | m_{\mathbf{k}} \rangle = m_{\mathbf{k}} | m_{\mathbf{k}} \rangle \qquad m_{\mathbf{k}} = n_{\mathbf{k}} - 1 \,. \tag{3-72}$$

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 (3-69) 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.

$$\begin{aligned} &N_a(\mathbf{k})\left(a(\mathbf{k}) | n_{\mathbf{k}} \rangle\right) = (n_{\mathbf{k}} - 1)\left(a(\mathbf{k}) | n_{\mathbf{k}} \rangle\right) && a(\mathbf{k}) \text{ destroys an } a \text{ particle with momentum } \mathbf{k} \\ &N_a(\mathbf{k})\left(a^\dagger(\mathbf{k}) | n_{\mathbf{k}} \rangle\right) = (n_{\mathbf{k}} + 1)\left(a(\mathbf{k})^\dagger | n_{\mathbf{k}} \rangle\right) && a^\dagger(\mathbf{k}) \text{ creates an } a \text{ particle with momentum } \mathbf{k} \\ &N_b(\mathbf{k})\left(b(\mathbf{k}) | \bar{n}_{\mathbf{k}} \rangle\right) = (\bar{n}_{\mathbf{k}} - 1)\left(b(\mathbf{k}) | \bar{n}_{\mathbf{k}} \rangle\right) && b(\mathbf{k}) \text{ destroys a } b \text{ particle with momentum } \mathbf{k} \\ &N_b(\mathbf{k})\left(b^\dagger(\mathbf{k}) | \bar{n}_{\mathbf{k}} \rangle\right) = (\bar{n}_{\mathbf{k}} + 1)\left(a(\mathbf{k})^\dagger | \bar{n}_{\mathbf{k}} \rangle\right) && b^\dagger(\mathbf{k}) \text{ creates a } b \text{ particle with momentum } \mathbf{k} . \end{aligned} \tag{3-73}$$

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

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

$$a(\mathbf{k})^\dagger |n_\mathbf{k}\rangle = A|n_\mathbf{k}+1\rangle \ , \tag{3-74}$$

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 raised ket $|n_\mathbf{k}+1\rangle$ in (3-74) have unit norm. (See (3-62) for one example.) Also, by taking the complex conjugate transpose of (3-74), 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,

$$\left(A|n_\mathbf{k}+1\rangle\right)^\dagger = \left(a(\mathbf{k})^\dagger|n_\mathbf{k}\rangle\right)^\dagger = \langle n_\mathbf{k}|a(\mathbf{k}) = \langle n_\mathbf{k}+1|A^\dagger \ . \tag{3-75}$$

Note that

$$\underbrace{\langle n_\mathbf{k}|a(\mathbf{k})}_{\langle n_\mathbf{k}+1|A^\dagger} a(\mathbf{k})^\dagger|n_\mathbf{k}\rangle = \langle n_\mathbf{k}+1|A^\dagger A|n_\mathbf{k}+1\rangle = A^\dagger A \underbrace{\langle n_\mathbf{k}+1||n_\mathbf{k}+1\rangle}_{1} = A^\dagger A \, . \tag{3-76}$$

(3-76) also equals

$$\langle n_\mathbf{k}|\underbrace{a(\mathbf{k})a(\mathbf{k})^\dagger}_{\text{use commutator}}|n_\mathbf{k}\rangle = \langle n_\mathbf{k}|\underbrace{a(\mathbf{k})^\dagger a(\mathbf{k})}_{N_a(\mathbf{k})}+1|n_\mathbf{k}\rangle = \langle n_\mathbf{k}|n_\mathbf{k}+1|n_\mathbf{k}\rangle = n_\mathbf{k}+1 \ . \tag{3-77}$$

Equating the RHS's of (3-76) and (3-77), and for simplicity taking A as real (complex would also work, but be more complicated) yields

$$A = \sqrt{n_\mathbf{k}+1} \ . \tag{3-78}$$

From (3-74), we then have the first line in (3-79) 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.

$$\boxed{\begin{aligned} a(\mathbf{k})^\dagger|n_\mathbf{k}\rangle &= \sqrt{n_\mathbf{k}+1}\,|n_\mathbf{k}+1\rangle \\ a(\mathbf{k})|n_\mathbf{k}\rangle &= \sqrt{n_\mathbf{k}}\,|n_\mathbf{k}-1\rangle \\ b(\mathbf{k})^\dagger|\bar{n}_\mathbf{k}\rangle &= \sqrt{\bar{n}_\mathbf{k}+1}\,|\bar{n}_\mathbf{k}+1\rangle \\ b(\mathbf{k})|\bar{n}_\mathbf{k}\rangle &= \sqrt{\bar{n}_\mathbf{k}}\,|\bar{n}_\mathbf{k}-1\rangle \end{aligned}} \tag{3-79}$$

Note that the above results are ultimately due to 2^{nd} 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

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

$$\langle 0||0\rangle = 1 \, , \tag{3-80}$$

and that from (3-79), the action of a destruction operator on the vacuum results in zero (which is different from the vacuum),

$$a(\mathbf{k})|0\rangle = \sqrt{0}\,|-1\rangle = 0 \ . \tag{3-81}$$

Don't worry about the funny looking ket (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

$$N(\phi) = \sum_{\mathbf{k}} \left(N_a(\mathbf{k}) - N_b(\mathbf{k}) \right). \tag{3-82}$$

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.

Since the field solutions $\phi(x)$ and $\phi^\dagger(x)$ contain the operator coefficients, they are then also operators, or more properly, operator fields. As noted in Chap. 1, this is often shortened in QFT to simply fields.

Note that for our field solutions of (3-35), 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 (3-35) for full expression)

$$\phi = \underbrace{\phi^+}_{\substack{\text{destroys}\\ \text{particles}}} + \underbrace{\phi^-}_{\substack{\text{creates}\\ \text{anti-particles}}}, \tag{3-83}$$

and the total particle raising operator field is

$$\phi^\dagger = \underbrace{\phi^{\dagger+}}_{\substack{\text{destroys}\\ \text{anti-particles}}} + \underbrace{\phi^{\dagger-}}_{\substack{\text{creates}\\ \text{particles}}}. \tag{3-84}$$

When we originally saw the field solutions (3-35), 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 (3-83) and (3-84) into that copy and make them part of it, as we will be using those symbols and what they represent, over and over.

3.6.5 Normal Ordering

When the infinite sum of ½ quanta energy in (3-58) 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 10^{118}, 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.

Note the effect of this in our derivation of the number operator form of the Hamiltonian in (3-53). Instead of employing the commutator relations for the $a(\mathbf{k})a^\dagger(\mathbf{k})$ and $b(\mathbf{k})b^\dagger(\mathbf{k})$ terms, 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. That is, the Hamiltonian only has number operators yielding $n_{\mathbf{k}}\omega_{\mathbf{k}}$ energy for $n_{\mathbf{k}}$ particles, each having 3-momentum **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. 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 the very best.

Caveat: The position expressed in the above paragraph is not widespread, and normal ordering to remove the ½ quanta terms is commonly invoked with little comment or qualification. I, and a handful of others[1] I am aware of, contend it should simply be jettisoned.

In any case, the huge vacuum energy issue does remain a widely recognized, unsolved problem as of 2010, the year of this book (though I offer a possible solution in the article cited in the footnote on page 40.)

3.6.6 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 what we will call the <u>observable Hamiltonian</u> of

$$H_0^0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(a^\dagger(\mathbf{k}) a(\mathbf{k}) + b^\dagger(\mathbf{k}) b(\mathbf{k}) \right). \tag{3-85}$$

In fact, from henceforth, unless we are specifically interested in vacuum energy, we will find it more streamlined and efficient to use (3-85) exclusively as our working form for the Hamiltonian. Just don't forget, as we do that, what the complete Hamiltonian looks like.

3.7 Probability, Four Currents, and Charge

Probability in QFT is found in essentially the same way as we did for NRQM (see Box 3-1) and RQM (see Sect. 3.1.3). That is, we use the governing wave equation and manipulate it to obtain a relationship like the continuity equation (3-18) (or (3-22) 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.

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, the same steps (3-15) to (3-19) can be followed. The result is the same 4-current relations as (3-21) and (3-22), except that ϕ and $\phi^\dagger$ are now operator fields (or simply, in QFT lingo "fields"),

$$\boxed{j^\mu{}_{,\mu} = 0 \quad \text{with} \quad j^\mu = -i\left(\phi^{\dagger,\mu}\phi - \phi^{,\mu}\phi^\dagger\right) \qquad j^\mu \text{ is an operator}}, \tag{3-86}$$

so

[1] 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."

$$\rho = j^0 = i\left(\phi^\dagger \frac{\partial \phi}{\partial t} - \frac{\partial \phi^\dagger}{\partial t}\phi\right) . \tag{3-87}$$

Since (3-87) is an operator, we need to look at its expectation value to find measurable probability density, i.e.,

$$\bar{\rho} = \langle \phi_1, \phi_2, \phi_3, \ldots . | \rho | \phi_1, \phi_2, \phi_3, \ldots . \rangle . \tag{3-88}$$

To evaluate (3-88), we need first to substitute our free field solutions (3-35) into (3-87). Do Prob. 12 to prove to yourself that this results in

$$\rho = \frac{1}{V}\sum_{\mathbf{k}}\left(a^\dagger(\mathbf{k})a(\mathbf{k}) - b^\dagger(\mathbf{k})b(\mathbf{k})\right) = \frac{1}{V}\sum_{\mathbf{k}}\left(N_a(\mathbf{k}) - N_b(\mathbf{k})\right). \tag{3-89}$$

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

$$\bar{\rho} = \langle \phi_{\mathbf{k}'} | \rho | \phi_{\mathbf{k}'} \rangle = \langle \phi_{\mathbf{k}'} | \frac{1}{V}\sum_{\mathbf{k}}\left(N_{\mathbf{a}}(\mathbf{k}) - N_{\mathbf{b}}(\mathbf{k})\right) | \phi_{\mathbf{k}'} \rangle = \langle \phi_{\mathbf{k}'} | \frac{1}{V} | \phi_{\mathbf{k}'} \rangle = \frac{1}{V} . \tag{3-90}$$

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.

$$\begin{aligned}\bar{\rho} &= \left\langle 3\phi_{\mathbf{k}_1}, \phi_{\mathbf{k}_2} \left| \rho \right| 3\phi_{\mathbf{k}_1}, \phi_{\mathbf{k}_2} \right\rangle = \left\langle 3\phi_{\mathbf{k}_1}, \phi_{\mathbf{k}_2} \left| \frac{1}{V}\sum_{\mathbf{k}}\left(N_{\mathbf{a}}(\mathbf{k}) - N_{\mathbf{b}}(\mathbf{k})\right) \right| 3\phi_{\mathbf{k}_1}, \phi_{\mathbf{k}_2} \right\rangle \\ &= \left\langle 3\phi_{\mathbf{k}_1}, \phi_{\mathbf{k}_2} \left| \frac{4}{V} \right| 3\phi_{\mathbf{k}_1}, \phi_{\mathbf{k}_2} \right\rangle = \frac{4}{V}.\end{aligned} \tag{3-91}$$

When (3-91) 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.

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 Anti-Particles (Type b Particles)

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

$$\bar{\rho} = \left\langle \bar{\phi}_{\mathbf{k}'} \left| \rho \right| \bar{\phi}_{\mathbf{k}'} \right\rangle = \left\langle \bar{\phi}_{\mathbf{k}'} \left| \frac{1}{V}\sum_{\mathbf{k}}\left(N_{\mathbf{a}}(\mathbf{k}) - N_{\mathbf{b}}(\mathbf{k})\right) \right| \bar{\phi}_{\mathbf{k}'} \right\rangle = \left\langle \bar{\phi}_{\mathbf{k}'} \left| \frac{-1}{V} \right| \bar{\phi}_{\mathbf{k}'} \right\rangle = \frac{-1}{V} . \tag{3-92}$$

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.

3.7.5 Charge Density Not Probability Density

If we multiply our four current operator (3-86) by the charge of a scalar particle q it behaves like a charge density operator, which we will designate by s^μ.

$$s^{\mu}{}_{,\mu} = 0 \quad \text{with} \quad s^{\mu} = qj^{\mu} = -iq\left(\phi^{\dagger,\mu}\phi - \phi^{,\mu}\phi^{\dagger}\right) \;, \tag{3-93}$$

so

$$\rho_{charge} = qj^{0} = iq\left(\phi^{\dagger}\frac{\partial\phi}{\partial t} - \frac{\partial\phi^{\dagger}}{\partial t}\phi\right). \tag{3-94}$$

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 (3-91) multiplied by q would yield $4q$, the charge on the state. Similarly, the total charge on the state in (3-92) 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 (3-88). The bracket, expressed in wave mechanics, 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 not 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.

$$\left\langle \rho(\mathbf{x},t)\right\rangle = \left\langle \phi_{\mathbf{k}}(\mathbf{x}',t)\,|\,\rho(\mathbf{x},t)\,|\,\phi_{\mathbf{k}}(\mathbf{x}',t)\right\rangle = \int \phi^{\dagger}_{\mathbf{k},state}(\mathbf{x}',t)\rho(\mathbf{x},t)\phi_{\mathbf{k},state}(\mathbf{x}',t)\,d^{3}x' \,. \tag{3-95}$$

This was not evident in (3-90) and similar relations above, because there (for plane waves, specifically) the operator ρ was not a function of space.

The point in (3-95) 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, (3-89) 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 (3-89) because of the two terms, each with two field factors multiplied, and the time derivatives in (3-87).

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.

Regarding energy, we have already discussed the observable operator corresponding to it. See (3-85). 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 (3-94) and (3-89) over the entire volume, to get the charge operator

$$Q=\int s^0 d^3x = q\int j^0 d^3x = q\sum_{\mathbf{k}}\left(N_a(\mathbf{k})-N_b(\mathbf{k})\right). \tag{3-96}$$

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,

$$\bar{Q}=\left\langle 7\phi_{\mathbf{k}_1},\phi_{\mathbf{k}_2},5\bar{\phi}_{\mathbf{k}_3}\right|\underbrace{q\sum_{\mathbf{k}}\left(N_a(\mathbf{k})-N_b(\mathbf{k})\right)}_{Q}\left|7\phi_{\mathbf{k}_1},\phi_{\mathbf{k}_2},5\bar{\phi}_{\mathbf{k}_3}\right\rangle = 7q+q-5q=+3q. \tag{3-97}$$

Note, we derived (3-96) using (3-89). If you did Prob. 12, you saw that in deriving (3-89) we summed terms in ½ and – ½ that cancelled to net zero. In other words, (3-96) 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 the total charge of the vacuum as zero. (Thankfully, it does. If it didn't, our theory would be bound for the trash heap.)

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 and integrating over the volume. (Also shown in the 9th block under the title in the RH column of Wholeness Chart 2-2.) That is,

$$p_i=\int \not{p}_i\, d^3x=\int \pi_r \frac{\partial\phi^r}{\partial x^i}d^3x=\int\left(\frac{\partial\mathcal{L}}{\partial\dot{\phi}}\frac{\partial\phi}{\partial x^i}+\frac{\partial\mathcal{L}}{\partial\dot{\phi}^\dagger}\frac{\partial\phi^\dagger}{\partial x^i}\right)d^3x\ . \tag{3-98}$$

Substituting the Klein-Gordon solutions (3-35) and their conjugate momenta into(3-98), one obtains the 3-momentum operator (do Prob. 13 to prove it)

$$\mathbf{P}=\sum_{\mathbf{k}}\mathbf{k}\left(N_a(\mathbf{k})+N_b(\mathbf{k})\right), \tag{3-99}$$

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 (3-99), 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.

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 theAppendix 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 (3-85) for $H_0{}^0$, and (3-99) for the free scalar field p_i, the four momentum operator is

$$\underbrace{P^\mu=K^\mu}_{\substack{\text{operators}\\ \text{here}}}=\underbrace{\begin{pmatrix}H\\ \mathbf{P}\end{pmatrix}}_{\substack{\text{for free}\\ \text{scalars}}}=\sum_{\mathbf{k}}\underbrace{\begin{pmatrix}\omega_{\mathbf{k}}\\ \mathbf{k}\end{pmatrix}}_{\substack{\text{usually what}\\ \text{we mean by}\\ \text{symbol } k^\mu}}\left(N_a(\mathbf{k})+N_b(\mathbf{k})\right), \tag{3-100}$$

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

3.8.4 Vacuum Energy Re-visited

With the 3-momentum operator of Sect. 3.8.2 in hand, we can look again at vacuum energy, this time with regard to the precise mathematical expression of the uncertainty principle. Interested readers can find this in Appendix B.

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 (3-35) 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,

$$\phi = \phi^\dagger \quad = \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} a(\mathbf{k}) e^{-ikx} + \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} a^\dagger(\mathbf{k}) e^{ikx} \quad . \tag{3-101}$$

In the charge operator (3-96), we would then have $N_a(\mathbf{k}) = N_b(\mathbf{k})$ (i.e., $a^\dagger(\mathbf{k})a(\mathbf{k}) = b^\dagger(\mathbf{k})b^\dagger(\mathbf{k})$), so charge would be zero for any real 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.

<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.

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 the 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 (3-79) acting first on the vacuum, then repeatedly on the newly created states, we have

$$a(\mathbf{k})^\dagger |0\rangle = |\phi_\mathbf{k}\rangle \;\to\; a(\mathbf{k})^\dagger |\phi_\mathbf{k}\rangle = \sqrt{2}\,|2\phi_\mathbf{k}\rangle \;\to\; a(\mathbf{k})^\dagger |2\phi_\mathbf{k}\rangle = \sqrt{3}\,|3\phi_\mathbf{k}\rangle \to ..... \tag{3-102}$$

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 (3-102).

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 (3-53), try the anti-commutators

$$\begin{aligned} \left[a(\mathbf{k}),a^\dagger(\mathbf{k}')\right]_+ &= a(\mathbf{k})a^\dagger(\mathbf{k}') + a^\dagger(\mathbf{k}')a(\mathbf{k}) = \delta_{\mathbf{k}\mathbf{k}'} \\ \left[b(\mathbf{k}),b^\dagger(\mathbf{k}')\right]_+ &= b(\mathbf{k})b^\dagger(\mathbf{k}') + b^\dagger(\mathbf{k}')b(\mathbf{k}) = \delta_{\mathbf{k}\mathbf{k}'}\,. \end{aligned} \tag{3-103}$$

A minus sign is then introduced, such that instead of (3-54), we would get

$$H_0^0 = \sum_\mathbf{k} \omega_\mathbf{k}\left(\tfrac{1}{2}+\tfrac{1}{2}\right)\ , \tag{3-104}$$

or for an observable Hamiltonian (ignoring vacuum energy)

$$H_0^0 = 0 \quad \text{and thus,} \quad H_0^0\left|\phi_{\mathbf{k}_1}\right\rangle = 0\,. \tag{3-105}$$

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.

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** eigenstates forms for real states. These, unlike wave packets, have infinite extent in the **k** direction. But for typical experiments, the real particle states, which are not actually infinitely long, can be approximated to extremely high precision by such discrete **k** eigenstates.

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 bounded by a particular volume (as discrete field equation solutions are) and in certain cases must be integrated over all possible, continuous values of **k**.

3.11.2 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.

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 $\lvert\Psi\rangle$ in NRQM, RQM Single particle	State vector $\lvert\phi_1, \phi_2, \ldots\rangle$ in QFT Multi particle
Orthonormal basis vectors along "axes"	$\hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \hat{\mathbf{i}}_3$	Normalized eigenvectors $\lvert\Psi_1\rangle, \lvert\Psi_2\rangle, \lvert\Psi_3\rangle, \lvert\Psi_4\rangle, \ldots$	Normalized eigenvectors $\lvert\phi_1\rangle, \lvert\phi_1, \phi_2\rangle, \lvert\phi_1, \phi_2, \phi_3\rangle, \ldots$
Inner product	$\hat{\mathbf{i}}_i \bullet \hat{\mathbf{i}}_j = \delta_{ij}$	$\langle\Psi_r\lvert\Psi_s\rangle = \delta_{rs}$	$\langle\phi_1\lvert\phi_1, \phi_2\rangle = 0$; $\langle\phi_1, \phi_2\lvert\phi_1, \phi_2\rangle = 1$; etc.
General state vector	$\mathbf{r} = x^1\hat{\mathbf{i}}_1 + x^2\hat{\mathbf{i}}_2 + x^3\hat{\mathbf{i}}_3$	$\lvert\Psi\rangle = C_1\lvert\Psi_1\rangle + X_2\lvert\Psi_2\rangle + C_3\lvert\Psi_3\rangle + \ldots$	$\lvert\Phi\rangle = C_1\lvert\phi_1\rangle + C_2\lvert\phi_1, \phi_2\rangle + C_3\lvert\phi_1, \phi_2, \phi_3\rangle + \ldots$
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

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 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.

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.

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.

3.12 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 quanta (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.)

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.

3.12.1 "Derivation" of QFT via Harmonic Oscillators

Some texts 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 (3-54) and the raising/lowering operators (3-73) as we derived them in Sect. 3.4. 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 very common.

3.12.2 Harmonic Oscillators Have Different Behavior from 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 in one location), whereas waves (particles = states) do. 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).

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

	NRQM Harmonic Oscillator	**QFT 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 $\omega_{\mathbf{k}}$	natural frequency of classical oscillator	frequency of particle of energy $\hbar\omega_{\mathbf{k}}$
Lowest energy level	½ $\hbar\omega$	½ $\hbar\omega_{\mathbf{k}}$
Interpretation of lowest energy level	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

3.12.3 Harmonic Oscillators, QFT, You, and Me

All of this harmonic oscillator business confused me greatly as a student. I simply could not understand how states in QFT could possibly be essentially identical to harmonic oscillators. I was not confident enough to fully fathom, much less bring up, the counter points mentioned herein, and they were never addressed.

So if you have studied QFT in the past, and been confused by the harmonic oscillator approach, rest assured, you are not alone.

Please note the caveat: This section and the two 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.

3.12.4 Vacuum Excitations = Real Particles

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.,

$$a^{\dagger}(\mathbf{k})|0\rangle = |\phi_{\mathbf{k}}\rangle . \qquad (3\text{-}106)$$

The RHS above can be considered as the next highest state above the ground state, 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

The treatment to be included here for the Feynman propagator, the mathematical formulation representing virtual particles, such as the one represented by the wavy line in Fig. 1-1 of Chap. 1, is essentially that found at www.quantumfieldtheory.info under the link Derivation of the Propagator - Step by Baby Step .

The propagator is the toughest thing, in my opinion, to learn and feel comfortable with in QFT. If you don't feel comfortable 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.

I have tried to take the derivation of the propagator one step at a time, and emphasize what each step entails. Wholeness Chart 5-0X (also at Free Fields Wholeness Chart link at www.quantumfieldtheory.info) breaks these steps out clearly, and should be used as an aide when studying the propagator derivation.

3.14 Summary

Scalars and Relativistic Quantum Mechanics (RQM)

Do Prob. 18 to create your own Wholeness Chart summary of scalars and RQM as presented 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-XX at the end of Chap. 5 (Find the equivalent at Free Fields Wholeness Chart link at www.quantumfieldtheory.info.) 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-XX can help make that transparent.

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 comprise the coefficients $a(\mathbf{k})$, $a^\dagger(\mathbf{k})$, $b(\mathbf{k})$, $b^\dagger(\mathbf{k})$ plus the fields of which they are a part ϕ and $\phi^\dagger$.

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

	Examples	**Effect on Eigenstate**
Dynamical Variable Operators	H, $\mathbf{P}$, Q, $N_a(\mathbf{k})$	eigenvalue times original eigenstate
Raising and Lowering Operators	$a(\mathbf{k})$, $a^\dagger(\mathbf{k})$, $b(\mathbf{k})$, $b^\dagger(\mathbf{k})$	new eigenstates (one more or one less particle)
Fields	ϕ and $\phi^\dagger$	as above

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,

$$\int \frac{d\delta(x'-a)}{dx'} f(x')dx' = -\int \frac{df(x')}{dx'}\delta(x'-a)dx' = -\left.\frac{df(x)}{dx}\right|_{x=a}, \tag{3-107}$$

where in our case we will have

$$x' \to \mathbf{x}' \qquad a \to \mathbf{x} \qquad f(x') \to \nabla'\phi(\mathbf{x}') \qquad \frac{d\delta(x-a)}{dx} \to \nabla'\delta(\mathbf{x}'-\mathbf{x}), \tag{3-108}$$

so that (3-107) becomes

$$\int \nabla'\delta(\mathbf{x}'-\mathbf{x})\cdot\nabla'\phi(\mathbf{x}',t)d\mathbf{x}' = -\nabla\cdot\nabla\phi(\mathbf{x},t). \tag{3-109}$$

3.15.2 Deriving the Scalar Field Equation

The Heisenberg equation of motion for any operator is

$$i\frac{\partial}{\partial t}\mathcal{O} = [\mathcal{O}, H], \tag{3-110}$$

and for a complex scalar field, this is

$$i\frac{\partial}{\partial t}\phi = [\phi, H]. \tag{3-111}$$

Thus, using (3-32) for $\mathcal{H}$ to find $H = \int \mathcal{H} d^3x$, we have

$$i\frac{\partial}{\partial t}\phi(\mathbf{x},t) = \left[\phi(\mathbf{x},t), \int d^3\mathbf{x}'\left\{\underbrace{\pi^\dagger \pi}_{\substack{\text{only non}\\\text{-zero result}}} + \nabla'\phi^\dagger \cdot \nabla'\phi + \mu^2\phi^\dagger\phi\right\}\right] \tag{3-112}$$

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 (3-112) 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, last box in RH column) of

$$\left[\pi_s, \phi^r\right] = -i\delta^r{}_s\delta\left(\mathbf{x}' - \mathbf{x}\right), \tag{3-113}$$

in the second line below, where it says "subs", we find (3-112) becomes

$$\begin{aligned}
i\frac{\partial}{\partial t}\phi(\mathbf{x},t) &= \int d^3\mathbf{x}'\left[\phi(\mathbf{x},t), \pi^\dagger(\mathbf{x}',t)\pi(\mathbf{x}',t)\right] \\
&= \int d^3\mathbf{x}'\left\{\underbrace{\phi\pi^\dagger}_{\pi^\dagger\phi}\pi - \pi^\dagger\underbrace{\pi\phi}_{\text{subs}}\right\} \\
&= \int d^3\mathbf{x}'\left\{\underbrace{\pi^\dagger\phi\pi - \pi^\dagger\phi\pi}_{0} + \pi^\dagger(\mathbf{x}',t)\,i\delta(\mathbf{x}' - \mathbf{x})\right\} \\
&= i\pi^\dagger(\mathbf{x},t).
\end{aligned} \tag{3-114}$$

Next, using (3-110) when the operator is the complex conjugate of the canonical momentum, we have

$$i\frac{\partial}{\partial t}\pi^\dagger(\mathbf{x},t) = \left[\underbrace{\pi^\dagger(\mathbf{x},t)}_{\substack{\text{function}\\\text{of }\mathbf{x}}}, \underbrace{\int d^3\mathbf{x}'\left\{\underbrace{\pi^\dagger\pi}_{\substack{\to 0 \text{ in}\\\text{commutator}}} + \nabla'\phi^\dagger \cdot \nabla'\phi + \mu^2\phi^\dagger\phi\right\}}_{\text{functions of }\mathbf{x}'}\right]. \tag{3-115}$$

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 (3-115) and substitute (3-109) in the third line below where it says "use math relation above". That second term is

$$\begin{aligned}
&\int d^3\mathbf{x}'\left\{\underbrace{\pi^\dagger\nabla'\phi^\dagger}_{\nabla'(\pi^\dagger\phi^\dagger)} \cdot \nabla'\phi - \nabla'\phi^\dagger \cdot \underbrace{(\nabla'\phi)\pi^\dagger}_{\nabla'\underbrace{(\phi\pi^\dagger)}_{\text{commute}}}\right\} = \int d^3\mathbf{x}'\left\{\nabla'\underbrace{\left(\pi^\dagger\phi^\dagger\right)}_{\substack{\text{use com}\\\text{relations}}} \cdot \nabla'\phi - \underbrace{\nabla'\phi^\dagger \cdot \nabla'\left(\pi^\dagger\phi\right)}_{\nabla'\left(\phi^\dagger\pi^\dagger\right)\cdot\nabla'\phi}\right\} \\
&= \int d^3\mathbf{x}'\left\{\nabla'\left(\phi^\dagger\pi^\dagger\right) \cdot \nabla'\phi - \underbrace{\nabla' i\delta(\mathbf{x}' - \mathbf{x}) \cdot \nabla'\phi}_{\text{use math relation above}} - \nabla'\left(\phi^\dagger\pi^\dagger\right) \cdot \nabla'\phi\right\} = i\nabla^2\phi(\mathbf{x},t).
\end{aligned} \tag{3-116}$$

By doing Prob. 6 at the end of the chapter, the reader can verify that evaluation of the third term in the RHS of (3-115), using similar (but simpler) steps, leads to

$$i\frac{\partial}{\partial t}\pi^\dagger(\mathbf{x},t) = i\left(\nabla^2 - \mu^2\right)\phi(\mathbf{x},t). \tag{3-117}$$

Substituting the time derivative of (3-114) into (3-117), one ends up with the Klein-Gordon equation

$$\frac{\partial^2}{\partial t^2}\phi = \left(\nabla^2 - \mu^2\right)\phi\,, \tag{3-118}$$

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: The Uncertainty Principle and Vacuum Energy

TO COME

3.17 Problems

1. Substitute (3-8) into the non-relativistic Schrödinger equation (3-1), and also the relativistic Klein-Gordon equation (3-7), 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 (3-8) 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 (3-14) of the set of $\phi_{\mathbf{k},A}$ also apply to the set of $\phi_{\mathbf{k},B^\dagger}$. Then, prove that every $\phi_{\mathbf{k},A}$ is orthogonal to every $\phi_{\mathbf{k},B^\dagger}$.

3. Repeat steps (3-23) and (3-24) using the terms with coefficients $B_{\mathbf{k}}^\dagger$ in (3-11) instead of those with $A_{\mathbf{k}}$. You should find total probability of negative unity.

4. Express the Klein-Gordon equations (3-34) and their discrete solutions (3-35) in cgs units (i.e., with c and $\hbar$ not equal to unity) and plug the latter into the former to show that $\mu^2 = m^2c^2/\hbar^2$.

5. Prove that the continuous solutions (3-36) solve the Klein-Gordon equations.

6. Show that the 3rd term in (3-115) 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.

8. Starting with the mass term in (3-47), derive (3-52).

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 $\mathbf{k}$, $b(\mathbf{k})$ destroys a b type particle with 3-momentum $\mathbf{k}$, and $b^\dagger(\mathbf{k})$ creates a b type particle with 3-momentum $\mathbf{k}$. Follow steps similar to those in (3-69) to (3-72).

11. Show that $a(\mathbf{k})\left|n_{\mathbf{k}}\right\rangle = \sqrt{n_{\mathbf{k}}}\left|n_{\mathbf{k}}-1\right\rangle$. 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 (3-35) to the Klein-Gordon equation into the probability density operator relation (3-87) to find that operator expressed in terms of number operators.

13. Using (3-98), the expression for 3-momentum in terms of the fields and their conjugate momenta, and the Klein-Gordon field equation solutions, prove (3-99), 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 $\mathbf{P}$, 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 (3-29) 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 (3-39), we had anti-commutators between the field and its conjugate momentum, i.e.,

$$\left[\phi^r(\mathbf{x},t),\pi_s(\mathbf{y},t)\right]_+ = \phi^r\pi_s + \pi_s\phi^r = i\delta^r{}_s\delta(\mathbf{x}-\mathbf{y}) \tag{3-119}$$

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

$$\left[a(\mathbf{k}),a^\dagger(\mathbf{k}')\right]_+ = \left[b(\mathbf{k}),b^\dagger(\mathbf{k}')\right]_+ = \delta_{\mathbf{kk}'} \;. \tag{3-120}$$

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

18. 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.

19.