Chapter 3

Scalars: Spin 0 Fields

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

Victor F. Weisskopf
Quarks, Quasars, and Quandaries

3.0 Preliminaries

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

3.0.1 Background

Seeking a relativistic quantum theory?

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

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

Try relativistic Hamiltonian in Schrödinger equation

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

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

Relativistic energy E

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

Relativistic E → relativistic operator H

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

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

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

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

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

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

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

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

But answer has been found, as we will see

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

Each spin type has its own relativistic wave equation

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

3.0.2 Chapter Overview

RQM first,

RQM overview (scalars)

where we will look at

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

Then QFT,

QFT overview (scalars)

- using the classical relativistic $\mathcal{L}$ (Lagrangian density) for scalar fields, and the Legendre transformation to get $\mathcal{H}$ (Hamiltonian density),
- from $\mathcal{L}$ and the Euler-Lagrange equation, finding the same Klein-Gordon equation, with the same mathematical form for the solutions, but this time the solutions are fields, not states,
- from 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. 7, which begins Part 2 of the book, we will begin to investigate interactions.

We study free (no interactions) case first

3.1 Relativistic Quantum Mechanics: A History Lesson

3.1.1 Two Possible Routes to RQM

Recall from Chaps. 1 and 2, that 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. 6 of Chap. 1 that non-commutation of dynamical variables means those variables are operators (because ordinary numbers commute.) For example,

Non-commutating variables must be operators

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

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

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

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

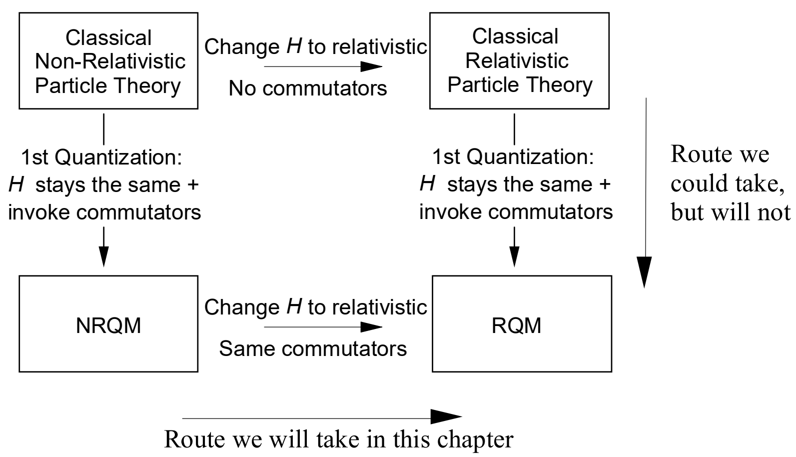

Figure 3-1. Different Routes to Relativistic Quantum Mechanics

3.1.2 Deducing the Klein-Gordon Equation

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

Let's square operators on both sides of Schrödinger eq

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

Then use operator form for H^2

which becomes from the square of (3-4)

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

To get the Klein-Gordon equation

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

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

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

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

Klein-Gordon equation is specifically for scalars

3.1.3 The Solutions to the Klein-Gordon Equation

A solution set to (3-8), readily checked by substitution into (3-8) (which is good practice when using contravariant/covariant notation), is (where $E_n^2 - \mathbf{p}_n^2 = m^2$)

Solutions to Klein-Gordon equation (discrete)

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

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

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

Continuous solutions also exist

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

Only plane wave solutions here

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

Solutions in RQM are states (particles)

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

Relativistic form has extra set of solutions

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

Relations for p_μ and k_μ

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

and recall the notation introduced in Chap. 2,

Notation review

$$\begin{aligned} px &= p_\mu x^\mu = Et - p^i x^i = Et - \mathbf{p} \cdot \mathbf{x} && \left(= p^\mu x_\mu\right) \\ kx &= k_\mu x^\mu = \omega t - k^i x^i = \frac{Et}{\hbar} - \frac{p^i x^i}{\hbar} = \frac{p_\mu}{\hbar} x^\mu && \left(= k^\mu x_\mu\right) \qquad (3\text{-}11) \\ &\text{in nat. units} \rightarrow \; E = \omega, \;\; p_i = k_i, \;\; p_\mu = k_\mu, \;\; px = kx. \end{aligned}$$

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

---

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

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

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

Natural units form of Klein-Gordon solutions

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

Definition of Eigensolutions

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

Eigenstates of Klein-Gordon equation

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

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

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

Eigenstates have unit norm

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

and are orthogonal

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

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

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

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

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

3.1.4 Probability Density in RQM

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

Probability Density Using the Klein-Gordon Equation

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

Deduce RQM probability density using relativistic wave equation

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

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

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

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

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

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

<u>Conserved quantities in field theory</u>:

Recall the <u>continuity equation</u> of continuum mechanics and electromagnetism,

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

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

<u>The general procedure</u>:

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.

<u>Probability Density Using the Schrödinger Equation:</u>

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

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

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

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

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

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

or

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

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

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

and as our <u>probability current density</u> (sometimes just <u>probability current</u>)

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

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

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

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

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

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

From that, we deduce form of RQM probability density

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

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

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

<u>4 Currents</u>

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

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

4-current and 4D form of continuity equation

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

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

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

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

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

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

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

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

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

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

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

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

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

<u>Difference from NRQM</u>

Note that in RQM

Comparing probability in NRQM and RQM

$$\int\underbrace{\phi^{\dagger}\phi}_{\neq\rho}\,d^{3}x=\sum_{\mathbf{k}}\frac{\left(A_{\mathbf{k}}\right)^{2}}{2\omega_{\mathbf{k}}}\neq1\quad\text{but}\quad\int\underbrace{i\left(\frac{\partial\phi}{\partial t}\phi^{\dagger}-\frac{\partial\phi^{\dagger}}{\partial t}\phi\right)}_{=\rho}d^{3}x=\sum_{\mathbf{k}}|A_{\mathbf{k}}|^{2}=1\qquad(\text{RQM})\,,\tag{3-26}$$

whereas in NRQM, we had

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

Normalization Factors

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

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

Relativistic Invariance of Probability

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

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

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

3.1.5 Negative Energies in RQM

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

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

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

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

Half of our RQM eigenstates have negative energy

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

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

3.1.6 Negative Probabilities in RQM

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

Half of our RQM eigenstates have negative probability density

Time to move on to QFT.

3.2 The Klein-Gordon Equation in Quantum Field Theory

3.2.1 States vs Fields

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

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

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

Notation

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

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

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

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

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

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

3.2.2 From RQM to QFT

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

Two different routes to QFT

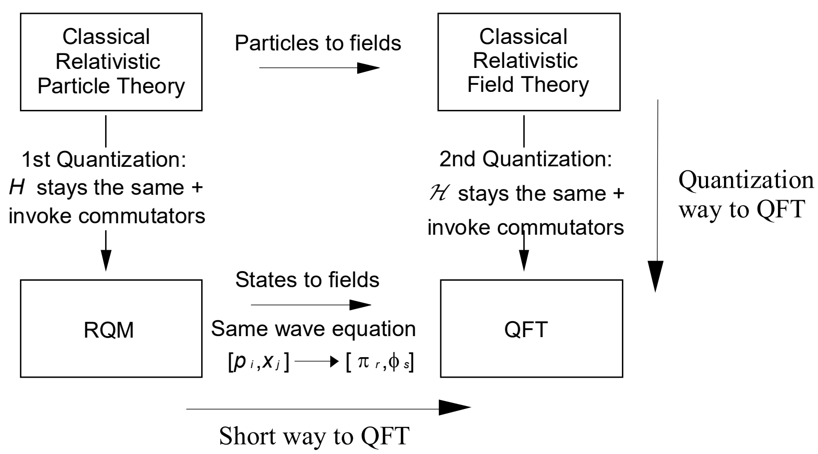

Figure 3-2. Different Routes to Quantum Field Theory

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

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

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

3.2.3 From Classical Relativistic Fields to QFT

2nd quantization route: Classical fields → QFT

Classical Scalar Fields

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

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

Start with classical Lagrangian density for free scalar field