AN INTRODUCTION TO FREE QUANTUM FIELD THEORY THROUGH KLEIN-GORDON THEORY

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ABSTRACT. We provide an introduction to quantum field theory by observing the methods required to quantize the classical form of Klein-Gordon theory.

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1. INTRODUCTION AND OVERVIEW

The phase space for classical mechanics is $\mathbb{R}^3 \times \mathbb{R}^3$, where the first copy of $\mathbb{R}^3$ encodes position of an object and the second copy encodes momentum.

Observables on this space are simply functions on $\mathbb{R}^3 \times \mathbb{R}^3$. The classical dynamics of the system are then given by Hamilton's equations

$$\dot{x} = \{h, x\} \qquad \dot{k} = \{h, k\},$$

where the brackets indicate the canonical Poisson bracket and

$$h(x,k) = \frac{|k|^2}{2m} + V(x)$$

is the classical Hamiltonian.

To quantize this classical field theory, we set our quantized phase space to be $L^2(\mathbb{R}^3)$. Then the observables are self-adjoint operators A on this space, and in a state $\psi \in L^2(\mathbb{R}^3)$, the mean value of A is given by

$$\langle A \rangle_\psi := \langle A\psi, \psi \rangle.$$

The dynamics of a quantum system are then described by the quantized Hamilton's equations

$$\dot{x} = \frac{i}{h}[H, x] \qquad \dot{p} = \frac{i}{h}[H, p]$$

where the brackets indicate the commutator and the Hamiltonian operator H is given by

$$H = h(x,p) = -\frac{|p|^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\Delta + V(x).$$

A question that naturally arises from this construction is then, how do we quantize other classical field theories, and is this quantization as straight-forward as the canonical construction? For instance, how do Maxwell's Equations behave on the quantum scale?

This happens to be somewhat of a difficult problem, with many steps involved. The process can often be rather haphazard, as we will soon see. In fact, there are some classical field theories (such as that of Einstein's field equations) whose quantizations are not known to exist. Conversely, there are a handful of quantum field theories that are known to lack a classical counterpart. The present paper's primary intention is to observe how simple quantizations are performed by observing how Klein-Gordon theory and Maxwell's equations may be quantized.

2. Klein-Gordon Theory as a Hamiltonian System

Before we consider quantum field theory, let us review some classical field theory. In classical field theory, the principle of stationary action tells us that the evolution equations for physical states are the Euler-Lagrange equations of a certain functional called the action.

Let us formulate this concept a bit more rigorously. We consider a space of functions $\{\phi(x,t)\}$ defined on space-time, which we will call "fields". The equation of motion for $\phi(x,t)$ is given by $\partial S(\phi) = 0$, where S is an appropriate functional on the space of fields called the action. In particular, we have S given by:

$$S(\phi) := \int_0^T \int_{\mathbb{R}^d} \mathcal{L}(\phi(x,t), \nabla_x \phi(x,t), \dot{\phi}(x,t)) d^d x dt,$$

where $\phi : \mathbb{R}^d_x \times \mathbb{R}_t \to \mathbb{R}$. We call $\mathcal{L} : \mathbb{R} \times \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$ the Lagrangian density.

Example 2.1. The Klein-Gordon Lagrangian density is given by

$$\mathcal{L}(\phi, \dot{\phi}) = \frac{1}{2}\dot{\phi}^2 - \frac{1}{2}|\nabla_x \phi|^2 - F(\phi),$$

for some continuous function F on $\mathbb{R}$. The corresponding Lagrangian functional is given by

$$L(\phi, \dot{\phi}) = \int_{\mathbb{R}^d} \left(\frac{1}{2}\dot{\phi}^2 - \frac{1}{2}|\nabla_x \phi|^2 - F(\phi) \right)$$

and this is defined on some subspace of $H^1(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$. The critical point equation for $S(\phi)$ is

$$\Box \phi + F' \phi = 0, \tag{2.2}$$

which is the familiar Klein-Gordon equation.

Definition 2.3 (Legendre Transform)**.** Let f be twice-differentiable functional on a reflexive Banach space X (where reflexive means $X = X^{**}$). Furthermore, let f satisfy $\partial^2 f > 0$. Then we define the Legendre transform of f to be a function g on X^* defined by

$$g(\pi) := \sup_{u \in X} (\langle \pi, u \rangle - f(u)) = (\langle \pi, u \rangle - f(u))|_{u : \partial f(u) = \pi}.$$

The second expression is given by solving the variational problem of the first.

As we know from classical mechanics, $\partial^2 g > 0$ and the Legendre transform is its own inverse.

As we observed earlier, in Klein-Gordon classical field theory, the Lagrangian functional is given by

$$L(\phi, \psi) = \int \{ \frac{1}{2}(|\psi|^2 - |\nabla\phi|^2) - F(\phi) \}.$$

Using a Legendre transform in ψ, we get the Hamiltonian for the system

$$H(\phi, \pi) = \int \{ \frac{1}{2}|\pi|^2 + |\nabla\phi|^2) + F(\phi) \}.$$

In more specific terms, the Lagrangian functional of KG theory is defined on a configuration space $X \times V$ so that

$$L : X \times V \to \mathbb{R}.$$

Then through the Legendre transform, the Hamiltonian is a functional

$$H : X \times V^* \to \mathbb{R}.$$

Let Z be a Banach space, which we call a state space. The state space of classical mechanics is $Z = \mathbb{R}^3 \times \mathbb{R}^3$, whereas the Klein-Gordon state space is $Z = H^1(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$. Now that we have determined what the state space for Klein-Gordon theory should be, we need to put a Poisson bracket on this space just as we do in classical mechanics. This will be used to create a system of evolution equations.

Definition 2.4 (Poisson Bracket)**.** A Poisson bracket is a bilinear map $\{\cdot, \cdot\}$ from the space of differentiable functions on Z to itself, satisfying:

$$1)\, \{F, G\} = -\{G, F\},$$

$$2)\, \{F, \{G, H\}\} + \{G, \{H, F\}\} + \{H, \{F, G\}\} = 0.$$

$$3)\, \{F, GH\} = \{F, G\}H + G\{F, H\}.$$

Property 1 is skew-symmetry, Property 2 is the Jacobi Identity, and Property 3 is the Leibniz rule.

Before we create a Poisson bracket on KG-theory, we need to review a few developments from variational calculus:

Definition 2.5. Let X be a Banach space, and let $\phi \in X$. A variation of ϕ along $\xi \in T_\phi X$ is a path ϕ_λ in X, such that $\phi_0 = \phi$ and

$$\frac{\partial \phi_\lambda}{\partial \lambda}|_{\lambda=0} = \xi.$$

Definition 2.6. Let $S : X \to \mathbb{R}$ be a functional on a Banach space X, and let $\phi \in X$. Then we define S to be differentiable at ϕ if there is a linear functional $\partial S(\phi) \in X^*$ satisfying

$$\frac{d}{d\lambda} S(\phi_\lambda)|_{\lambda=0} = \langle \partial S(\phi), \xi \rangle \tag{2.7}$$

for any variation ϕ_λ of ϕ along $\xi \in X$. The function $\partial S(\phi)$ is then called the variational derivative of S at ϕ.

Let us observe two examples of calculations of variational derivatives before we move on. These calculations in particular will help us later when we need to do more complex ones.

Example 2.8. Let $S(\phi) = \int_{\mathbb{R}^d} V(\phi)$ for some differentiable function V. Then we can compute

$$\langle \partial S(\phi), \xi \rangle = \frac{d}{d\lambda} S(\phi_\lambda)|_{\lambda=0} = \frac{d}{d\lambda} \int_{\mathbb{R}^d} \frac{\partial}{\partial \lambda} V(\phi_\lambda)|_{\lambda=0} = \int_{\mathbb{R}^d} \nabla V(\phi) \cdot \xi = \langle \nabla V(\phi), \xi \rangle,$$

so that $\partial S(\phi) = \nabla V(\phi)$.

Example 2.9. Now let $S(\phi) = \frac{1}{2} \int_{\mathbb{R}^d} |\nabla \phi|^2$, and let us additionally assume that $\phi \in L^2(\mathbb{R}^d)$ for each ϕ in our space of functions. We have:

$$\langle \partial S(\phi), \xi \rangle = \frac{d}{d\lambda} S(\phi_\lambda)_{\lambda=0} = \frac{1}{2} \int \frac{\partial}{\partial \lambda} |\nabla \phi_\lambda|^2|_{\lambda=0} = \int \nabla \phi \cdot \nabla \xi = \int (-\Delta \phi) \cdot \xi = \langle -\Delta \phi, \xi \rangle,$$

where we have integrated by parts and used the fact that the functions decay at $+\infty$. It follows that $\partial S(\phi) = -\Delta \phi$.

Theorem 2.10. *If Z is a real inner-product space, the following construction produces a Poisson bracket. Suppose there is a linear operator J on Z such that $J^* = -J$ (so that J is a symplectic operator). Then*

$$\{F, G\} := \langle \partial F, J \partial G \rangle$$

yields a Poisson bracket on Z.

For instance, in classical mechanics, if $Z = \mathbb{R}^3 \times \mathbb{R}^3$, then

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{2.11}$$

is a symplectic operator, so that the assignment

$$\{F, G\} = \nabla_x F \cdot \nabla_k G - \nabla_k F \cdot \nabla_x G$$

is a valid Poisson bracket on the phase space.

In KG theory, we have $Z = H^1(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$. Using (2.11) as our symplectic operator, we get the Poisson bracket

$$\{F, G\} = \int \partial_\pi F \partial_\phi G - \partial_\phi F \partial_\pi G.$$

Definition 2.12 (Hamiltonian Systems)**.** A Hamiltonian system is a Poisson space (that is, a Banach space Z with a Poisson bracket) together with a Hamiltonian defined on that space.

According with this definition, we have derived two such Hamiltonian systems thus far: one corresponding to Klein-Gordon theory and the other corresponding to classical mechanics.

3. Hamilton's Equations

Suppose we have a Hamiltonian system on Z, a Banach space of functions defined on a set X. Given $x \in X$, the functional on Z mapping Φ to $\Phi(x)$ is called the evaluation functional at x. We denote this functional by $\Phi(x)$.

Lemma 3.1. $\partial \Phi(y) = \delta_y$.

Proof.

$$\langle \partial\Phi(y), \xi\rangle = \frac{\partial \Phi_\lambda(y)}{\partial\lambda}\,|_{\lambda=0} = \int \delta_y \frac{\partial\Phi_\lambda(x)}{\partial\lambda}dx = \langle \delta_y, \xi\rangle,$$

so that

$$\partial\Phi(y) = \delta_y.$$

□

Hamilton's equations are given by

$$\dot{\Phi}(x) = \{\Phi(x), H\}. \tag{3.2}$$

Let us put this equation into a more simple form.

If the Poisson structure is given by a symplectic operator J, then

$$\{\Phi(x), H\}(\Phi) = \int (\partial\Phi(x))(y) J\partial H(\Phi)(y)dy = \int \delta_x(y) J\partial H(\Phi)(y) = J\partial H(\Phi)(x).$$

The result is a new form of Hamilton's equation,

$$\dot{\Phi}(x) = J\partial H(\Phi)(x). \tag{3.3}$$

Theorem 3.4. *If $L(\phi,\psi)$ are related by a Legendre transform, then the Euler-Lagrange equations for*

$$S(\phi,\dot{\phi}) = \int_0^T L(\phi,\dot{\phi})dt$$

are equivalent to the Hamilton equation with $\phi = (\phi, \pi)$ and

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

We verify this theorem for Klein-Gordon Theory. Using Examples 2.8 and 2.9, it is easy to see that

$$\partial H(\phi,\pi) = \begin{pmatrix} -\Delta\phi + F'(\phi) \\ \pi \end{pmatrix}.$$

Now, let

$$\Psi = \begin{pmatrix} \phi \\ \psi \end{pmatrix}$$

be a path in $H^1(\mathbb{R}^n) \times L^2(\mathbb{R}^n)$. Equation (3.3) is evaluated to be

$$\begin{pmatrix} \dot{\phi} \\ \dot{\pi} \end{pmatrix} = J \begin{pmatrix} -\Delta\phi + F'(\phi) \\ \pi \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} -\Delta\phi + F'(\phi) \\ \pi \end{pmatrix}.$$

However, this system of equations is equivalent to the Klein-Gordon equation (2.2), so that the theorem is verified in the Klein-Gordon case.

4. Quantization

Let's recall how we quantize classical field theory. We start with our phase space $\mathbb{R}^3 \times \mathbb{R}^3$, and to quantize this, we take $L^2(\mathbb{R}^3)$.

In the Klein-Gordon case, our phase space is

$$Z = H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3),$$

and additionally we have a Poisson bracket attached to this space arising from our previously introduced symplectic matrix J.

(Note: For this section and from here on whenever we are dealing with KG theory in particular, we will use the function $F(\phi) := \frac{1}{2}m^2\phi^2$ as the F as present in the Hamiltonian of the system.)

Let us (naively) attempt to quantize this classical field theory using the same method. Then the quantized space would become the state space

$$L^2(H^1(\mathbb{R}^d), D\phi),$$

where $D\phi$ is a Lebesgue measure on $H^1(\mathbb{R}^3)$. Additionally, the Poisson bracket on the phase space would be transformed into the commutator $\frac{i}{\hbar}[\cdot,\cdot]$ on this state space. The classical observables, which are real-valued functionals on the phase space, become quantum observes - that is, self-adjoint operators on $L^2(H^1(\mathbb{R}^3), D\phi)$. In particular, the classical canonical variables

$$\phi^{cl}(x) \qquad and \qquad \pi^{cl}(x)$$

should become the operators

$$\phi^{op}(x) = \text{ multiplication by } \phi(x) \qquad and \qquad \pi^{op}(x) = -i\hbar\partial_{\phi(x)}.$$

Also, the Hamiltonian of classical Klein-Gordon dynamics, described by

$$H(\phi,\pi) = \frac{1}{2}\int |\pi|^2 + |\nabla\phi|^2 + m^2|\phi|^2,$$

which under quantization should become the Schrodinger operator

$$H = H(\phi^{op}, \pi^{op})$$

on the quantum state space.

However, we can immediately see that there are a number of problems with this approach.

Problem 1. The first thing to notice is that there doesn't exist a Lebesgue measure on infinite-dimensional spaces, so that putting one on $H^1(\mathbb{R}^3)$ is impossible.

We start by replacing $D\phi$ with $d\mu_C(\phi)$, the Gaussian measure of mean 0 and covariance operator C. This operator is defined $L^2(\mathbb{R}^3)$, so it is also defined on $H^1(\mathbb{R}^3)$. Let us observe how this measure is defined. Let

$$\cdots \subset F_n \subset F_{n+1} \subset \cdots$$

be a sequence of finite-dimensional subspaces of $H^1(\mathbb{R}^3)$, the limit of which is $H^1(\mathbb{R}^3)$. Then

$$d\mu_c|_{F_n}(\phi) = M_n(\det C_n)^{-1/2}e^{\langle\phi, C_n^{-1}\phi\rangle/2}D\phi,$$

where $D\phi$ is the usual Lebesgue measure on the finite-dimensional space F_n, C_n is C restricted to F_n, and M_n is a constant chosen so as to force the relation

$$\int_{F_n} d\mu_C(\phi)|_{F_n} = 1.$$

We recall that the expected value of a functional F with respect to $d\mu_C$ is defined to be

$$E(F)L = \int F(\phi)d\mu_C(\phi).$$

We said earlier that $d\mu_C$ should have mean 0 and covariance C. This means that

$$E(\phi(x)) = 0$$

and

$$E(\phi(x)\phi(y)) = C(x,y),$$

where $C(x, y)$ is the integral kernel of C. For KG-theory, we take

$$C = \frac{1}{2}(-\Delta + m^2)^{-1/2}.$$

To see why we make this decision, note that the Klein-Gordon Hamiltonian with $F(\phi) = \frac{m^2|\phi|^2}{2}$ is

$$H(\phi, \pi) = \frac{1}{2}\int \pi^2 + |\nabla\phi|^2 + m^2|\phi|^2.$$

Integrating by parts, we have that

$$\int |\nabla\phi|^2 + m^2|\phi|^2 = \int \phi(-\Delta + m^2)\phi = \int |(-\Delta + m^2)^{1/2}\phi|^2,$$

and so we can write

$$H(\phi, \pi) = \frac{1}{2}\int \pi^2 + |\frac{1}{2}C^{-1}\phi|^2. \tag{4.1}$$

Hence, we have found a measure that works on $H^1(\mathbb{R}^3)$.

Problem 2. Unfortunately, this definition only leads to another problem, namely that $\mu_C(H^1(\mathbb{R}^3))$ must equal 0. To see this, we compute

$$E(\int |\nabla\phi|^2) = \iint \delta(x-y)\nabla_x\nabla_y E(\phi(x)\phi(y) = \iint \delta(x-y)\nabla_x\nabla_y C(x, y).$$

If $C = \check{c}(-i\nabla_x)$, then $C(x, y) = \check{c}(x - y)$ and so

$$E\left(\int |\nabla\phi|^2\right) = \int (\Delta\check{c})(0).$$

Therefore, the integral on the right hand side diverges, since we are integrating over infinite volume. Even if we had finite volume, however, this expression would remain infinite, since if $C = (-\Delta + m^2)^{-1/2}$, we have

$$\check{c}(x) = (2\pi)^{-3/2}\int e^{ik\cdot x}(|k|^2 + m^2)^{-1/2} = K|x|^2 + o(|x|^{-2})$$

for some $K \in \mathbb{R}$ as $|x| \to 0$. It follows that $E(\int |\nabla\phi|^2) = +\infty$, implying that

$$\mu_C(H^1(\mathbb{R}^3)) = 0.$$

This shows that $\check{c}(x)$ must be integrated at least twice to take away the singularity at $x = 0$. We expect then, that

$$E(\int |\nabla^{-s}\phi|^2) < +\infty$$

for $s > 1$. In fact, the following theorem holds.

Theorem 4.2. *If*

$$Q := \left\{f : (1 + |x|^2)^{-t/2}(1 - \Delta)^{-s/2}f \in L^2 \text{ for sufficiently large } s \text{ and } t\right\},$$

then $\mu(Q) = 1$.

Proof. See [1]. □

Members of the space $L^2(Q, d\mu_C)$ are functionals $F(\phi)$ on Q satisfying

$$\int |F(\phi)|^2 d\mu_C(\phi) < +\infty.$$

The following is an example of a functional in Q. Let $f \in H^s$, where we recall that $s > 1$. Then the map

$$\phi \in Q \mapsto \phi(f) := \int f\phi \qquad \left(\text{understood as } \int (1-\Delta)^{s/2} f \cdot (1-\Delta)^{-s/2}\phi \right)$$

is a linear functional on Q which lies in $L^2(Q, d\mu_C)$. To see this, we compute formally that

$$E\left(|\int f\phi|^2 \right) = \iint f(x)f(y)E(\phi(x)\phi(y)) = \langle f, Cf \rangle < +\infty.$$

In summary, we have replaced $L^2(H^1(\mathbb{R}^d), D\phi)$ by $L^2(Q, d\mu_C)$, where $C = (-\Delta + m^2)^{-1/2}$. Unfortunately, this correction has generated yet another problem: $-i\partial_\phi$ is not symmetric on $L^2(Q, d\mu_C)$, which does not fit with our intuition of quantized systems. To see this, we have the following formula by integration by parts:

$$\int \overline{F}(-i\partial_\phi G)d\mu_C(\phi) = \int \overline{(-i\partial_\phi F)} G d\mu_C(\phi) + i\int \overline{F} G \partial_\phi d\mu_C(\phi) = \int \overline{(-i\partial_\phi + iC^{-1}\phi)F} G d\mu_C(\phi),$$

in which we have used the fact that

$$\partial_\phi d\mu_C(\phi) = -C^{-1}\phi d\mu_C(\phi).$$

Hence, we have

$$(-i\partial_\phi)^* = -i\partial_\phi + iC^{-1}\phi,$$

so that we can make a correction via the map

$$i\hbar\partial_\phi \mapsto \pi := -i\hbar\partial_\phi + \frac{i\hbar}{2}C^{-1}\phi.$$

As we can see, $\pi^* = \pi$, as we desired.

Remark 4.3. In the notation of Section 3, we may formally derive following commutation relations.

$$\frac{i}{\hbar}[\pi(x), \phi(y)] = \delta(x-y) \tag{4.4}$$

$$\frac{i}{\hbar}[\pi(x), \pi(y)] = \frac{i}{\hbar}[\phi(x), \phi(y)] = 0.$$

Remark 4.5. Before moving on, however, we need to provide a brief explanation of mathematical rigor. Strictly speaking, ϕ and π are operator-valued distributions. Therefore, $\phi(x)$ is not well-defined, although $\phi(f)$ is well-defined for some test function $f \in C_0^\infty$. We think formally of $\phi(f)$ as $\int \phi(x)f(x)dx$. Particularly, the correct description of (4.4) is

$$\frac{i}{\hbar}[\pi(f), \phi(g)] = \langle \overline{f}, g \rangle.$$

In addition, we have the following theorem, which we will not prove here.

Theorem 4.6. *For each $f \in C_0^\infty$, $\phi(f)$ and $\pi(f)$ are self-adjoint operators on $L^2(Q, d\mu_C)$.*

Proof. See [1]. □

Now we progress to another problem that we must handle:

Problem 3: $H(\phi, \pi) = +\infty$.

This is clearly an undesirable situation, but first we would like to verify the accuracy of this statement. To show this equality, let us first introduce creation and annihilation operators, as they will simplify our calculations and provide a foundation for further steps in our quantization procedure.

5. Creation and Annihilation Operators and Wick Ordering

Remark 5.1. From here on, for simplicity we let $\hbar = 1$.

Definition 5.2. We define the annihilation operator $a(f)$ by

$$a(f) := \frac{1}{2}\phi(C^{-1/2}f) + i\pi(C^{1/2}f).$$

Similarly, we define the creation operator $a^*(f)$ by

$$a^*(f) := \frac{1}{2}\phi(C^{-1/2}f) - i\pi(C^{1/2}f).$$

Lemma 5.3. *The following commutation relations hold for each $f, g \in C_0^\infty$:*

$$[a(f), a^*(g)] = \langle \widehat{f}, g\rangle.$$

$$[a(f), a(g)] = [a^*(f), a^*(g)] = 0.$$

Proof. This is a straightforward calculation, using the results of Remark 4.3. □

Theorem 5.4. *We can write the Hamiltonian operator in terms of the creation and annihilation operators as follows:*

$$H(\phi, \pi) = \frac{1}{2}\int a^* C^{-1} a + \frac{1}{4}\int C^{-1}\delta_x dx. \tag{5.5}$$

Proof. Using the representation (4.1) and the definitions of the creation and annihilation operators, we have

$$\begin{aligned} H(\phi, \pi) &= \frac{1}{2}\int \pi^2 + (\frac{1}{2}C^{-1}\phi)^2 \\ &= \frac{1}{2}\int \left[\frac{i}{2}C^{-1/2}(a^* - a)\right]^2 + \left[\frac{1}{2}C^{-1/2}(a^* + a)\right]^2 \\ &= \frac{1}{4}\int C^{-1/2}a^* C^{-1/2}a + C^{-1/2}aC^{-1/2}a^* \\ &= \frac{1}{2}\int a^* C^{-1} a + \frac{1}{4}\int C^{-1}\delta_x dx. \end{aligned}$$

In this calculation, note that we have used the commutation relation for a and a^* and the self-adjointness of $C^{-1/2}$. □

Now, the first term of the right-hand side of (5.5) is non-negative, while the second is infinite since $C^{-1}\delta_x(x) = \check{c}(0)$. This establishes the fact that $H(\phi, \pi) = +\infty$. This problem may be fixed by Wick Ordering.

Let $A(\phi^{cl}, \pi^{cl})$ be a classical observable that may be written as a power series of ϕ^{cl} and π^{cl}. That is, let A be written as:

$$A = \sum_{m,n} \int A_{m,n}(x_1, \ldots, x_{m+n}) \phi^{cl}(x_1) \cdots \pi^{cl}(x_{m+n}).$$

To simplify notation, we may write

$$A = \sum_{m,n} \int A_{m,n} (\phi^{cl})^m (\pi^{cl})^n.$$

The first step in Wick ordering lies in expressing $A(\phi^{cl}, \pi^{cl})$ in terms of α and α^*, where

$$\alpha := \frac{1}{2} C^{-1/2} \phi^{cl} + i C^{1/2} \pi^{cl}$$

and

$$\alpha^* := \frac{1}{2} C^{-1/2} \phi^{cl} - i C^{1/2} \pi^{cl}$$

are the classical representations of the annihilation and creation operators as expounded earlier. That is, we write

$$A(\phi^{cl}, \pi^{cl}) = B(\alpha, \alpha^*).$$

The next step requires that we move all α^*'s to the left of the α's to obtain an expression of the form

$$B(\alpha, \alpha^*) := \sum_{m,n} B_{m,n} (\alpha^*)^m \alpha^n.$$

The final step is the quantization procedure. We quantize the observable A via the following map:

$$A(\phi^{cl}, \pi^{cl}) \mapsto A(\phi, \pi) := \sum_{m,n} \int B_{m,n} (a^*)^m a^n,$$

where a and a^* are the normal (quantized) annihilation and creation operators.

We denote a Wick-ordered operator by putting it within : marks. For instance, we would denote the Wick-ordered operator π by $: \pi :$. Here are two examples of Wick Ordering.

Example 5.6.

$$\begin{aligned} :\phi^2: &= \; : [C^{-1/2}(a + a^*)]^2 : \\ &= \; : (C^{-1/2}a)^2 + (C^{-1/2}a^*)^2 + C^{-1/2}a * C^{-1/2}a + C^{-1/2}aC^{-1/2}a^* : \\ &= \; (C^{-1/2}a)^2 + (C^{-1/2}a^*)^2 + 2C^{-1/2}a^*C^{-1/2}a. \end{aligned}$$

Example 5.7. If we observe the derivation of the Klein-Gordon Hamiltonian in terms of annihilation and creation operators as given in the previous section, we see that the Wick-ordered Hamiltonian is given by

$$H = \frac{1}{2} \int : \pi^2 + |\nabla \phi|^2 + m^2 \phi^2 : \; = \frac{1}{2} \int a^* C^{-1} a.$$

Now, remember that $C^{-1} = 2\sqrt{-\Delta + m^2}$. Passing to the Fourier transform, we have that

$$a(k) = (2\pi)^{-d/2} \int e^{-k \cdot x} a(x) dx.$$

Using the Plancherel Theorem, we get

$$H = \int \omega(k) a^*(k) a(k) dk,$$

with

$$\omega(k) = \sqrt{|k|^2 + m^2}.$$

To recap and clarify, why is Wick ordering useful to us in general? As in the case presented in the Klein-Gordon Theory, the Hamiltonian may not have a zero expectation value within a vacuum. However, in a vacuum, both a and a^* always have zero expectation value, as we will soon see. Therefore, any Wick-ordered operator has a vacuum expectation value of zero. This tells us that if the Hamiltonian of a theory is Wick-ordered, then the ground state energy will be zero. This presents us with a more desirable situation (and in particular one that does not allow the Hamiltonian to be perpetually infinite as before), so that we alter the quantized Hamiltonian to be Wick-ordered.

6. Fock Space

Note that the annihilation operator

$$a = \frac{1}{2} C^{-1/2} \phi + i C^{1/2} \pi = C^{1/2} \partial_\phi.$$

It follows that the only solution to the equation $a\Omega = 0$ is when $\Omega = c$ for some $c \in \mathbb{R}$. Therefore, we set $\Omega = 1$ and call it the vacuum.

Theorem 6.1. *Let $\phi \in L^2(Q, d\mu_C)$. Then we may write*

$$\phi = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \int \phi_n(x_1, \ldots, x_n) a^*(x_1) \cdots a^*(x_n) \Omega dx_1 \cdots dx_n, \tag{6.2}$$

where

$$\phi_n \in L^2_{sym}(\mathbb{R}^{nd}) = \otimes^n_{1,sym} L^2(\mathbb{R}^d).$$

Here, $\otimes_{sym}$ represents the symmetrized tensor product. Therefore, the functions in the space $L^2_{sym}(\mathbb{R}^{nd})$ are just the functions in $L^2(\mathbb{R}^{nd})$ which happen to be symmetric with respect to the permutations of the n variables $x_j \in \mathbb{R}^d$. As we did earlier, we simplify the right hand side of (6.2) and write

$$\sum_n \frac{1}{\sqrt{n!}} \int \phi_n (a^*)^n \Omega.$$

Below is an additional fact we will use in the proof of this theorem. We will not prove it here.

Lemma 6.3. *The span of vectors which may be written in the form $\prod_{j=1}^n \phi(f_j)\Omega$ for $n \geq 1$, is dense in L^2.*

Remark 6.4. Before we embark on the proof of the theorem, we note that

$$\int \phi_n (a^*)^n \Omega = \int \phi_n^{sym} (a^*)^n \Omega,$$

where

$$\phi^{sym}(x_1, \ldots, x_n) = \frac{1}{n!} \sum_{\pi \in S_n} \phi(x_{\pi(1)}, \ldots, x_{\pi(n)}) \in L^2_{sym}(\mathbb{R}^{nd})$$

is the symmetrization of ϕ.

Proof of Theorem 6.1. Note that

$$\prod_{j=1}^n \phi(f_j)\Omega = \prod_{j=1}^n [a(C^{1/2} f_j) + a^*(C^{1/2} f_j)]\Omega.$$

Using commutation relations, we write $\prod(a + a^*)$ in Wick order as

$$\prod_{j=1}^n (a + a^*)\Omega = \sum_{k+l \leq n} \int A_{kl} (a^*)^k a^l \Omega.$$

However, $(a^*)^k a^l \Omega = 0$ unless $l = 0$, so that

$$\prod_{j=1}^n \phi(f_j)\Omega = \sum_{k \leq n} \int A_{k0} (a^*)^k \Omega.$$

It follows that the vectors of the form

$$\sum_n \frac{1}{n!} \int \phi_n (a^*)^n \Omega$$

are dense in L^2.

We may directly compute that

$$\langle \int \phi_n (a^*)^n \Omega, \int \chi_m (a^*)^n \Omega \rangle = \begin{cases} 0 & n \neq m \\ n! \langle \phi_n, \chi_n \rangle & n = m \end{cases}$$

It then follows that the set

$$\{\phi = \sum_n \frac{1}{\sqrt{n!}} \int \phi_n (a^*)^n \Omega : \phi_n \in L^2_{sym}(\mathbb{R}^{nd})\}$$

is closed and contains a dense set, and hence is the entirety of L^2 space. □

Definition 6.5. The Fock space is

$$\mathcal{F} := \bigoplus_{n=0}^{\infty} \mathcal{F}_n,$$

where

$$\mathcal{F}_n := \bigotimes_{j=1, sym}^{n} L^2(\mathbb{R}^d)$$

is the "section" of $\mathcal{F}$ with n particles. Conventionally, we make $\mathcal{F}_0 = \mathbb{C}$.

The theorem we have just proved shows the existence of a unitary isomorphism between $L^2(Q, d\mu_C)$ and $\mathcal{F}$ given by the map

$$\sum_n \frac{1}{\sqrt{n!}} \int \phi_n (a^*)^n \Omega \leftrightarrow \left\{ \begin{array}{c} \phi_0 \\ \phi_1 \\ \phi_2 \\ \vdots \end{array} \right\}.$$

In fact, we see that on $\mathcal{F}$,

$$a(f) : \phi_n \in \mathcal{F}_n \mapsto \sqrt{n} \langle f, \phi_n \rangle \in \mathcal{F}_{n-1}$$

and

$$a^*(f) : \phi_n \in \mathcal{F}_n \mapsto \sqrt{n+1} f \otimes_{sym} \phi_n \in \mathcal{F}_{n+1},$$

which provides us with a more intuitive understanding of why we call a the annihilation operator and a^* the creation operator.

Using the commutation relations, we may derive the following proposition.

Proposition 6.6. *Let $H = \int a^* C^{-1} a$ be the usual Hamiltonian, and let $N = \int a^* a$ be the particle number operator. We have the following relations between $L^2(Q, d\mu_C)$ and Fock space under the canonical isomorphism:*

$$H\phi \leftrightarrow \frac{1}{2} \left(\sum_{j=1}^{n} C_{x_j}^{-1} \phi_n \right)$$

and

$$N\phi \leftrightarrow (n\phi_n),$$

where the subscript x_j indicates the operator acting on the variable x_j.

In this section, therefore, we have found Fock space to act as a simple realization of our original state space $L^2(Q, d\mu_C)$ which is independent of the covariance operator C. In Fock space, the Klein-Gordon Hamiltonian acts as a direct sum of simple operators in a finite but increasing number of variables:

$$H \approx \bigoplus_{n=0}^{\infty} \left(\sum_{i=1}^{n} \sqrt{-\Delta_{x_i} + m^2} \right).$$

In particular, the spectrum of H is

$$\sigma(H) = \{0\} \cup \{ \bigcup_{n \geq 1} [nm, \infty) \},$$

where the zero eigenfunction is the vacuum Ω. In physical terms, this theory describes non-interacting particles of mass m.

7. Maxwell's Equations and Generalized Free QFT

The Maxwell equations in a vacuum are

$$\nabla \cdot E = 0, \qquad \nabla \times B = \frac{\partial E}{\partial t}. \tag{7.1}$$

$$\nabla \times E = -\frac{\partial B}{\partial t} \qquad \nabla \cdot B = 0 \tag{7.2}$$

for vector fields $E : \mathbb{R}^{3+1} \to \mathbb{R}^3$, the electric field, and $B : \mathbb{R}^{3+1} \to \mathbb{R}$, the magnetic field.

The first step we must take in quantizing these equations is putting this into a Hamiltonian system, which we accomplish below.

The equations (7.2) show that there exist potentials $U : \mathbb{R}^4 \to \mathbb{R}$ and $A : \mathbb{R}^4 \to \mathbb{R}^3$ satisfying

$$B = \nabla \times A, \qquad E = -\frac{\partial A}{\partial t} - \nabla U.$$

In fact, this choice of A and U need not be unique. In particular, if we take any gauge transformation using any $\xi : \mathbb{R}^4 \mapsto \mathbb{R}$, then the result of the mappings

$$A \mapsto A + \nabla \xi \quad \text{and} \quad U \mapsto U - \frac{\partial \xi}{\partial t}$$

give two new potentials A and U which produce the same fields E and B. With an appropriate choice of ξ, in fact, we may assume that

$$U = 0 \quad \text{and} \quad \nabla \cdot A = 0,$$

which we call the Coulomb gauge. Using this gauge, we have

$$E = -\frac{\partial A}{\partial t} \quad \text{and} \quad B = \nabla \times A.$$

Now using the second equation of line (7.1), and using $\nabla \times (\nabla \times A) = \nabla(\nabla \cdot A) - \Delta A$, we have

$$\Box A = 0 \quad \text{and} \quad \nabla \cdot A = 0. \tag{7.3}$$

A vector field $f : \mathbb{R}^3 \to \mathbb{R}^3$ satisfying $\nabla \cdot f = 0$ is called transverse. In fact, Equation (7.3) is the Euler-Lagrange equation for the action

$$S(A) = \frac{1}{2} \int_0^T \int_{\mathbb{R}^3} \{|\dot{A}|^2 - |\nabla \times A|^2\}, \tag{7.4}$$

where the variation lies within transverse vector fields. The Hamiltonian corresponding to this action is

$$H(A, E) = \frac{1}{2} \int \{|E|^2 + |\nabla \times A|^2\} = \frac{1}{2} \int \{|E|^2 + |B|^2\},$$

where E is the dual field to A, and $\nabla \cdot E = 0$.

The phase space corresponding to this Hamiltonian is

$$Z = H^{1,trans}(\mathbb{R}^3; \mathbb{R}^3) \oplus L^{2,trans}(\mathbb{R}^3; \mathbb{R}^3),$$

where "trans" is an abbreviation for the subspace of transverse vector fields.

We can define a Poisson bracket on Z as usual by the relation

$$\{F, G\} := \langle \partial_{A,E} F, J_T \partial_{A,E} G \rangle,$$

where

$$J_T := \begin{pmatrix} 0 & -T \\ T & 0 \end{pmatrix}$$

is our chosen symplectic operator. It is then a simple task to show that Maxwell's equations are equivalent to the Hamiltonian equations

$$\dot{\phi} = J_T \partial_\phi H(\phi), \qquad \phi = (A, E).$$

From here, we quantize Maxwell's equations in precisely the same way that we quantized KG theory. If we assume that the speed of light is $c = 1$, then there are two main differences:

1. Mass is negligible. Therefore, the covariance operator becomes $C = \frac{1}{2}(-\Delta)^{-1/2}$.
2. The quantized $A(x)$ and $E(x)$ are operator-valued transverse vector fields. That is, our state space is $L^2(Q^{trans}, d\mu_C)$.

The Hamiltonian for quantized electromagnetic theory is, as before, just

$$H = \frac{1}{2}\int : |E|^2 + |\nabla \times A|^2 :$$

with commutation relation

$$i[E(x), A(y)] = T(x-y)\mathbf{1},$$

where $T(x-y)$ is the integral kernel of the projection operator onto the transverse vector fields. In this case, we may write

$$H = \int \omega(k) a^*(k) \cdot a(k) dk,$$

with $\omega(k) = |k|$, and where $a(k)$ and $a^*(k)$ are operator-valued transverse vector-fields.

This construction may be generalized. Given a Hamiltonian system with associated positive operator C acting on $L^2(\mathbb{R}^d)$ with densely defined inverse $C^{-1} = 2\Lambda$, we may perform a quantization in exactly the same way as above. This theory is a quantized version of the classical Hamiltonian

$$H_\Lambda(\phi^{cl}, \pi^{cl}) = \frac{1}{2}\int |\pi^{cl}|^2 + \phi^{cl}\Lambda^2\phi^{cl}.$$

We quantize as in the Klein-Gordon case, constructing Fock space analogously in the process.

Now, define the general annihilation operator

$$a(x) := \frac{1}{\sqrt{2}}\Lambda\phi + \frac{i}{\sqrt{2}}\Lambda^{-1}\pi$$

and the general creation operator

$$a^*(x) := \frac{1}{\sqrt{2}}\Lambda\phi - \frac{i}{\sqrt{2}}\Lambda^{-1}\pi.$$

This leads to the quantized Hamiltonian

$$H_\Lambda = \int a^*(x)\Lambda a(x) dx.$$

As with KG-theory, the one-particle operator Λ then determines all the properties of H_Λ, since

$$H_\Lambda \approx \bigoplus_{n=0}^{\infty}\left(\sum_{j=1}^{n}\Lambda_{x_j}\right).$$

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