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What is a Quantum Field?

The Perspective from Physics

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This is for my grandchildren Amber, Emily,
Garrett, and Lacey and my buddy Vinnie.

Preface

It is our ultimate objective to have in hand a mathematically rigorous model of a quantum field theory representing the quantization of the classical Klein-Gordon field. Mathematical rigor and QFT are, however, rather strange bedfellows. Indeed, the very notion that one could (or even should) introduce rigorous methods into QM and QFT came rather late upon the scene. Even a physicist of the stature of Wolfgang Pauli initially disparaged Max Born's efforts to reformulate Heisenberg's ideas in terms of matrices as "futile mathematics" (see page 37 of [VDW]). Rigor is something superimposed upon quantum theory after the fact. In order to understand where the rigorous model comes from and what it is intended to describe one must first have at least a brief look at how these matters are viewed by the physicists. This is what we will try to do here.

The earliest attempt to quantize a classical field appeared in 1926 in the famous "Dreimännerarbeit" [BHJ] of Born, Heisenberg and Jordan. Their real interest was in the electromagnetic field, but as a first step in this direction they chose to consider the much simpler case of a classical vibrating string. We will follow their lead in Section 1.1, emphasizing the heuristic and intuitive aspects of the process in physics rather than the mathematical niceties and we will consider only the non-relativistic case. Although the underlying ideas appear on the surface to be quite similar, the actual gulf separating the vibrating string from the electromagnetic field is enormous, even at the heuristic and intuitive level, and we will not attempt to bridge the gap. Instead we will, in Section 1.2, take a look, again heuristic and intuitive, at the quantization of the classical Klein-Gordon field which, like the vibrating string and unlike the electromagnetic field, is a *scalar field* of *positive mass*.

We will need to assume a familiarity with the canonical quantization procedure proposed by Dirac so we have included appendices in which this is summarized and the two most elementary examples are described; more detailed discussions are available in Sections 7.2, 7.3 and 7.4 of [Nab5]. The example of the harmonic oscillator will be particularly important to us here. In the next installment we will begin constructing some of the mathematical machinery motivated by the vibrating string and the Klein-Gordon field and required in order to proceed to the rigorous treatment of Klein-Gordon based on the Wightman Axioms.

Before getting started, however, we should point out that the Heisenberg picture of quantum mechanics is generally considered to be more natural in quantum field theory than the Schrödinger picture. This is discussed in Section A.4 of [Nab5]. From this point of view the state of a quantum system is represented by a *fixed* element ψ in the Hilbert space $\mathcal{H}$ of the system and the observables are represented by self-adjoint operators $A(t)$ that evolve in time. If H is the Hamiltonian of the system (which is atypical among the observables in the Heisenberg picture in that it is independent of t), then the evolution of an observable from some initial self-adjoint operator $A = A(0)$ is governed by

$$A(t) = e^{itH/\hbar} A e^{-itH/\hbar}.$$

One can prove that, with sufficient regularity assumptions, the evolution $A(t)$ of the observable satisfies the *Heisenberg equation*

$$\frac{dA(t)}{dt}\psi = -\frac{i}{\hbar}[A(t), H]\psi$$

(for a precise statement see Remark A.4.4 and Theorem A.4.3 of [Nab6]).

Caveat Lector: What follows in the next three sections will, on occasion, look like it must be mathematics, but we assure you that there is precious little of that. Here we are attempting, for the purposes of motivation, to follow the path of the physicists, boldly going where no mathematician could comfortably go along a path strewn with purely formal definitions and calculations. As we have said before, mathematical rigor comes (if at all) after the fact and we will return to the problem of constructing the appropriate mathematical foundations later. For the time being we will abide by the physicist's mantra

"Shut up and calculate!"
-N. D. Mermin

(see http://www.gnm.cl/emenendez/uploads/Cursos/callate-y-calcula.pdf). The Exercises in these three sections should be approached in the same spirit.

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Chapter 1
Quantized Fields: Motivation

1.1 The Non-Relativistic Vibrating String

In the classical *Vibrating String Problem* one is asked to describe the small, transverse vibrations $u(x,t)$ of an elastic string, tightly stretched along the x-axis between $x = 0$ and $x = l$ assuming that no external forces act on it. A bit of physics, which one sees in any elementary course on partial differential equations (see, for example, Section 25 of [BC] or Chapter 8 of [Sp3]), shows that $u(x,t)$ satisfies the 1-dimensional wave equation and vanishes at the endpoints of the string for all t, that is,

$$\begin{aligned} \rho\frac{\partial^2 u}{\partial t^2} &= \tau\frac{\partial^2 u}{\partial x^2}, \quad (x,t) \in (0,l)\times(0,\infty) \\ u(0,t) &= u(l,t) = 0, \quad t \in [0,\infty) \end{aligned} \tag{1.1}$$

where ρ is the mass density and τ is the tension of the string, both of which will be assumed constant; in particular, the mass of the string is $m = l\rho$. Since we do not need them at the moment we will not be explicit about the initial displacement $u(x,0)$ and initial velocity $\frac{\partial u}{\partial t}(x,0)$ that one must specify in order to describe a well-posed problem. Standard operating procedure is to separate variables $u(x,t) = X(x)T(t)$ and obtain one Sturm-Liouville problem

$$\begin{aligned} X''(x) - \lambda X(x) &= 0 \\ X(0) = X(l) &= 0 \end{aligned}$$

for $X(x)$ and an ordinary differential equation

$$\ddot{T}(t) - \frac{\lambda\tau}{\rho}T(t) = 0$$

for $T(t)$. The eigenvalues for the Sturm-Liouville problem are $\lambda_k = -\frac{k^2\pi^2}{l^2}$, $k = 1, 2, \ldots$, and the corresponding orthonormal eigenfunctions are

$$X_k(x) = \sqrt{\frac{2}{l}}\, sin\, \frac{k\pi x}{l}, \quad k = 1, 2, \ldots.$$

Here "orthonormal" means in the L^2-sense, that is,

$$\int_0^l X_j(x) X_k(x) dx = \delta_{jk}. \tag{1.2}$$

With $\lambda_k = -\frac{k^2\pi^2}{l^2}$ the equation for $T(t)$ becomes

$$\ddot{T}(t) + \omega_k^2\, T(t) = 0, \quad k = 1, 2, \ldots,$$

where

$$\omega_k = \sqrt{\frac{\tau}{\rho}}\, \frac{k\pi}{l}.$$

These equations for T are also easy to solve, of course, but we prefer to regard them simply as instances of the harmonic oscillator equation and to denote by $T_k(t)$ an arbitrary nontrivial solution to $\ddot{T}(t) + \omega_k^2\, T(t) = 0$. For each k we then obtain a nontrivial solution

$$u_k(x, t) = T_k(t) X_k(x) = T_k(t) \sqrt{\frac{2}{l}}\, sin\, \frac{k\pi x}{l}$$

to (1.1). Notice that, for each $x_0 \in (0, l)$ with $sin\, \frac{k\pi x_0}{l} \neq 0$, the point on the string at location x_0 executes a simple harmonic motion with frequency ω_k and some amplitude determined by $T_k(t)$. The solutions $u_k(x, t)$ therefore represent standing waves and we shall refer to them as *normal modes of vibration* for the string. Since the frequency ω_k and the mass are constant for each normal mode it is sometimes useful to think intuitively of the normal modes themselves as harmonic oscillators, although strictly speaking it is the *amplitude* that satisfies the harmonic oscillator equation.

Superimposing these normal modes (and turning a blind eye to all of the pesky convergence issues it raises) one obtains a "general" motion of the string

$$u(x, t) = \sum_{k=1}^{\infty} T_k(t) \sqrt{\frac{2}{l}}\, sin\, \frac{k\pi x}{l}. \tag{1.3}$$

Classically, the total energy E of the vibration $u(x, t)$ is taken to be

$$E = \frac{1}{2} \int_0^l \left[\rho \left(\frac{\partial u}{\partial t} \right)^2 + \tau \left(\frac{\partial u}{\partial x} \right)^2 \right] dx, \tag{1.4}$$

where $\frac{1}{2}\rho(\partial u/\partial t)^2$ is the kinetic energy density and $\frac{1}{2}\tau(\partial u/\partial x)^2$ is the potential energy density.

Remark 1.1.1. This is not supposed to be obvious. The first term looks about right for a kinetic energy term ($\frac{1}{2}mv^2$), but the second requires more detailed physical considerations. One can find derivations of the string energy as well as some cautionary remarks in [Burko].

Exercise 1.1.1. The Lagrangian for the vibrating string is the difference in the kinetic and potential energies, that is,

$$L = \frac{1}{2}\int_0^l \left[\rho\left(\frac{\partial u}{\partial t}\right)^2 - \tau\left(\frac{\partial u}{\partial x}\right)^2\right] dx.$$

Show that the Euler-Lagrange equation ((1.9) of [Nab7]) is precisely the wave equation

$$\rho\frac{\partial^2 u}{\partial t^2} = \tau\frac{\partial^2 u}{\partial x^2}.$$

Substituting (1.3) into (1.4) and using the orthonormality conditions (1.2) this expression for the energy reduces to

$$E = \sum_{k=1}^{\infty} \frac{\rho}{2}\,[\,\dot{T}_k^2 + \omega_k^2 T_k^2\,].$$

Letting

$$q^k = \sqrt{\rho}\,T_k, \quad \text{and} \quad p_k = \sqrt{\rho}\,\dot{T}_k, \quad k = 1, 2, \ldots$$

this becomes

$$E = \sum_{k=1}^{\infty} \frac{1}{2}\,[p_k^2 + \omega_k^2 (q^k)^2].$$

Each term $\frac{1}{2}\,[p_k^2 + \omega_k^2(q^k)^2]$ in the sum is the canonical form of the classical Hamiltonian for the harmonic oscillator of mass 1 and frequency ω_k. The quantization of such a harmonic oscillator (and any finite sum of independent harmonic oscillators) was described in Appendix B and we will now proceed, heuristically, toward the quantization of the vibrating string by regarding it as a sum of these infinitely many independent harmonic oscillators.

For the canonical quantization of this system we will want to regard q^k, p_k $k = 1, 2, \ldots$, as canonical variables and replace them with the self-adjoint operators Q^k, P_k, $k = 1, 2, \ldots$, of the corresponding quantum harmonic oscillator (see Appendix B). These satisfy the canonical commutation relations

$$[Q^j, Q^k] = [P_j, P_k] = 0, \quad [Q^j, P_k] = i\hbar\delta^j_k, \quad j,k = 1,2,\ldots$$

where the identity operator is understood on the right-hand side of the last relation. Setting aside any qualms we might have about infinite sums of unbounded operators, the energy E of the classical vibrating string becomes the Hamiltonian

$$H = \sum_{k=1}^{\infty} \frac{1}{2}\left[P_k^2 + \omega_k^2 (Q^k)^2\right]$$

of the quantized string.

Remark 1.1.2. What, you might well ask, is the Hilbert space on which this proposed Hamiltonian operator is supposed to act? For a system of finitely many harmonic oscillators we have given a perfectly explicit answer in Appendix B, but the situation becomes rather murky for infinitely many oscillators. We will have a bit more to say about this at the end of this section, but for the time being, let's just compute and see what turns up.

For each $k = 1, 2, \ldots$, the spectrum of $\frac{1}{2}\left[P_k^2 + \omega_k^2 (Q^k)^2\right]$ consists entirely of the simple eigenvalues

$$\mathcal{E}_n^{(k)} = (n + \frac{1}{2})\hbar\omega_k, \quad n = 0, 1, 2, \ldots$$

with corresponding normalized eigenfunctions

$$\psi_n^{(k)}(q^k) = \frac{1}{\sqrt{2^n n!}}\left(\frac{\omega_k}{\hbar\pi}\right)^{1/4} e^{-\omega_k (q^k)^2/2\hbar} H_n\left(\sqrt{\frac{\omega_k}{\hbar}}\, q^k\right), \quad n = 0, 1, 2, \ldots$$

where we have written q^k for the spatial coordinate of the k^{th} oscillator and H_n is the n^{th} Hermite polynomial. Thus,

$$\frac{1}{2}\left[P_k^2 + \omega_k^2 (Q^k)^2\right]\psi_n^{(k)} = \left[(n + \frac{1}{2})\hbar\omega_k\right]\psi_n^{(k)}, \quad n = 0, 1, 2, \ldots$$

$\psi_n^{(k)}$ therefore corresponds to a state of the k^{th} oscillator in which it has energy $\mathcal{E}_n^{(k)} = (n + \frac{1}{2})\hbar\omega_k$. Notice that the state of least energy (the *ground state*) of the k^{th} oscillator is $\psi_0^{(k)}$ and the energy of this state is $\frac{1}{2}\hbar\omega_k$, *which is not zero*. Soon we will see that this causes some problems for our proposed Hamiltonian H. Every other state $\psi_n^{(k)}$ corresponds to an energy level of the k^{th} oscillator that differs from its ground state energy by an integer number of basic *energy quanta* $\hbar\omega_k$.

Now we proceed to formally mimic the procedure for finitely many oscillators in Appendix B. We define, for each $k = 1, 2, \ldots$, lowering and raising operators b_k and $b_k^\dagger$ by

$$b_k = \frac{1}{\sqrt{2\omega_k \hbar}}(\omega_k Q^k + iP_k)$$

and

$$b_k^\dagger = \frac{1}{\sqrt{2\omega_k \hbar}}(\omega_k Q^k - iP_k),$$

respectively. Solving for Q^k and P_k gives

$$Q^k = \sqrt{\frac{\hbar}{2\omega_k}}\,(b_k^\dagger + b_k)$$

$$P_k = i\sqrt{\frac{\omega_k \hbar}{2}}\,(b_k^\dagger - b_k).$$

The operators b_k and $b_k^\dagger$ are adjoints of each other, satisfy the commutation relations

$$[b_j, b_k] = [b_j^\dagger, b_k^\dagger] = 0, \quad [b_j, b_k^\dagger] = \delta_{jk}, \quad j,k = 1,2,\ldots$$

and act on the eigenfunctions $\psi_n^{(k)}$ in the following way. b_k annihilates the ground state $\psi_0^{(k)}$, that is, $b_k\psi_0^{(k)} = 0$ and otherwise

$$b_k\psi_n^{(k)} = \sqrt{n}\,\psi_{n-1}^{(k)}, \quad n = 1,2,\ldots \quad \text{and} \quad b_k^\dagger\psi_n^{(k)} = \sqrt{n+1}\,\psi_{n+1}^{(k)}, \quad n = 0,1,2,\ldots$$

so b_k (respectively, $b_k^\dagger$) decreases (respectively, increases) the energy level of the eigenstates by one energy quantum $\hbar\omega_k$. Furthermore, all of the eigenstates $\psi_n^{(k)}, n = 1,2,\ldots$, can be obtained by repeated application of the raising operator $b_k^\dagger$ to the ground state $\psi_0^{(k)}$. Specifically,

$$\psi_n^{(k)} = \frac{1}{\sqrt{n!}}(b_k^\dagger)^n\psi_0^{(k)}.$$

The k^{th}-number operator N_k is defined by

$$N_k = b_k^\dagger b_k, \quad , k = 1,2,\ldots$$

and satisfies

$$N_k\psi_n^{(k)} = n\psi_n^{(k)}, \quad n = 0,1,2,\ldots$$

Thus, N_k has eigenvalues $n = 0,1,2,\ldots$ and these count the number of energy quanta $\hbar\omega_k$ beyond the ground state energy ($\frac{1}{2}\hbar\omega_k$) in the k^{th} oscillator when it is in state $\psi_n^{(k)}$. In terms of the number operators our vibrating string Hamiltonian can now be written as

$$H = \sum_{k=1}^{\infty} \hbar\omega_k [\, N_k + \frac{1}{2} \,]. \tag{1.5}$$

Remark 1.1.3. We have conscientiously avoided specifying the Hilbert space on which this putative Hamiltonian operator is supposed to be defined. After a few remarks at the end of this section we will address this issue carefully in the next chapter. However, we would like to anticipate the result in order to make an important observation. We will find that this Hilbert space for the string contains a ground state, or vacuum state that is annihilated by every b_k and therefore by every number operator N_k. This is thought of as the state of least energy. According to (1.5), however, the energy of this state is

$$\sum_{k=1}^{\infty} \frac{1}{2} \hbar\omega_k$$

which is clearly infinite. This is, to say the least, rather unfortunate, but seems to be an unavoidable consequence of the formalism we are attempting to build. A mathematician might conclude that we are headed in the wrong direction. Ever the pragmatists, however, physicists simply throw out the offending $\frac{1}{2}$ in H and *redefine the Hamiltonian* to be

$$H' = \sum_{k=1}^{\infty} \hbar\omega_k N_k. \tag{1.6}$$

This no doubt appears rather suspicious. Physicists have offered a number of not-so-convincing arguments to justify the maneuver ("Even classically the Hamiltonian is determined only up to an additive constant so why should an 'infinite constant' be any different?"). H' is referred to as the *renormalized Hamiltonian* of the quantized vibrating string and it certainly does away with the infinite ground state energy. As we will see, however, not all of the "infinities" that plague quantum field theory are so easily wished away.

In the Heisenberg picture of quantum mechanics the time evolution of the observables Q^k and P_k is governed by

$$\begin{aligned} Q^k(t) &= e^{itH/\hbar} Q^k(0) e^{-itH/\hbar} \\ P_k(t) &= e^{itH/\hbar} P_k(0) e^{-itH/\hbar}. \end{aligned} \tag{1.7}$$

Formally manipulating the various commutation relations for Q^k and P_k with $[A, BC] = B[A, C] + [A, B]C$, the Heisenberg equation for $Q^k(t)$ gives

$$\begin{aligned}\frac{d}{dt}Q^k(t) &= -\frac{i}{\hbar}\Big[\, Q^k(t),\ \frac{1}{2}\left[P_k(t)^2 + \omega_k^2 Q^k(t)^2\right]\Big] \\ &= -\frac{i}{2\hbar}[Q^k(t), P_k(t)^2] \quad \text{since} \quad [Q^k(t), Q^k(t)^2] = 0 \\ &= -\frac{i}{2\hbar}P_k(t)(i\hbar) - \frac{i}{2\hbar}(i\hbar)P_k(t) \quad \text{since} \quad [Q^k(t), P_k(t)] = i\hbar\end{aligned}$$

so

$$\frac{d}{dt}Q^k(t) = P_k(t).$$

Exercise 1.1.2. Show, in the same way, that

$$\frac{d}{dt}P_k(t) = -\omega_k^2 Q^k(t).$$

It follows that

$$\frac{d^2}{dt^2}Q^k(t) + \omega_k^2 Q^k(t) = 0.$$

Formally solving this harmonic oscillator equation gives

$$Q^k(t) = Q^k(0)\, cos\, \omega_k t + \frac{1}{\omega_k}P_k(0)\, sin\, \omega_k t \tag{1.8}$$

and then

$$P_k(t) = -Q^k(0)\, \omega_k\, sin\, \omega_k t + P_k(0)\, cos\, \omega_k t. \tag{1.9}$$

In order to obtain our quantized version of the vibrating string we would like to write $Q^k(t)$ in a slightly different form with the lowering and raising operators. For this we will make use of the following exercise.

Exercise 1.1.3. Begin with

$$b_k(t) = e^{it(\hbar\omega_k(N_k+\frac{1}{2}))/\hbar}\, b_k\, e^{-it(\hbar\omega_k(N_k+\frac{1}{2}))/\hbar}$$

and show that

$$\frac{d}{dt}b_k(t) = -i\omega_k b_k(t).$$

Conclude that

$$b_k(t) = e^{-it\omega_k}b_k \quad \text{and} \quad b_k^\dagger(t) = e^{it\omega_k}b_k^\dagger$$

Hint: $\frac{d}{dt}e^{tA} = Ae^{tA} = e^{tA}A$ and $[b_k, N_k] = b_k$.

Now we return to the classical expression $u(x,t) = \sum_{k=1}^{\infty} T_k(t)\sqrt{\frac{2}{l}}\, sin\, \frac{k\pi x}{l}$ for the motion of the string and make the relevant operator substitutions to obtain

$$\begin{aligned} U(x,t) &= \sum_{k=1}^{\infty} \frac{1}{\sqrt{\rho}} Q^k(t) \sqrt{\frac{2}{l}}\, sin\, \frac{k\pi x}{l} \\ &= \sum_{k=1}^{\infty} \frac{1}{\sqrt{\rho}} \Big[\sqrt{\frac{\hbar}{2\omega_k}} (b_k^\dagger(t) + b_k(t)) \Big] \sqrt{\frac{2}{l}}\, sin\, \frac{k\pi x}{l} \end{aligned}$$

which simplifies to

$$U(x,t) = \sqrt{\hbar/m} \sum_{k=1}^{\infty} \frac{1}{\sqrt{\omega_k}} \Big[b_k^\dagger e^{it\omega_k} + b_k e^{-it\omega_k} \Big] sin\, \frac{k\pi x}{l}. \tag{1.10}$$

All of this is highly problematic, of course, since we have allowed ourselves to compute with complete abandon and with no regard for the fact that we have been dealing with unbounded operators on some, as yet unspecified, Hilbert space. Nevertheless, (1.10) is historically the first attempt to write down a "quantized field" and the derivation we have described is a rather simple instance of the no-holds-barred approach that one often encounters in physics. We will conclude this section with a few remarks that may point the way toward the more rigorous view of this process that we will eventually describe in detail.

The first order of business is to say something about an appropriate choice for the Hilbert space of the system. In Appendix B we considered a system of finitely many harmonic oscillators with masses $m_1, \ldots, m_N$ and frequencies $\omega_1, \ldots, \omega_N$. We denoted by $q^1, \ldots, q^N$ the spatial coordinates for the N oscillators and by $L^2(\mathbb{R}, dq^1), \ldots, L^2(\mathbb{R}, dq^N)$ the Hilbert spaces of these oscillators. Then the Hilbert space $\mathcal{H}^{(N)}$ of the system as a whole was taken to be the Hilbert space tensor product

$$\mathcal{H}^{(N)} = L^2(\mathbb{R}, dq^1) \otimes \cdots \otimes L^2(\mathbb{R}, dq^N)$$

which can be identified with

$$L^2(\mathbb{R}^N, d^N q),$$

where $q = (q^1, \ldots, q^N)$ and $d^N q = dq^1 \cdots dq^N$ is the Lebesgue measure on $\mathbb{R}^N$. One might think then that the appropriate choice for the countably infinite collection of oscillators with which we are modeling the vibrating string would be an infinite tensor product of the Hilbert spaces $L^2(\mathbb{R}, dq^k)$, $k = 1, 2, \ldots$ How does one define an infinite tensor product of Hilbert spaces? As it happens, this can be done (see [v.Neu1]), but it is not so simple and the result is generally rather pathological. For example, a tensor product of countably many separable Hilbert spaces of dimension greater than one is *never separable*. Moreover, even if one is willing to forgive the Hilbert space for being non-separable there is yet another issue. The following remark is taken from page 87 of [SW].

... it is characteristic of field theory that some of its observables involve all of the oscillators at once and it turns out that such observables can be naturally defined only on vectors belonging to a tiny separable subset of the infinite tensor product. It is the subspace spanned by such a subset which is the natural state space rather than the whole infinite tensor product itself.

Streater and Wightman do not specify what this "tiny separable subset" is, but it is identified in Section 4 of [ThWin]. Each such subset spans a subspace of the infinite tensor product isomorphic to what is called a "Fock space". These are Hilbert spaces introduced into quantum field theory in 1932 by Vladimir Fock [Fock]. We will describe them carefully in the next chapter.

Once this is done we will find that the expression (1.10) that we have "derived" for the quantized field associated with the vibrating string is, as it stands, mathematically meaningless since it diverges miserably even when applied to the ground state and this time it does not help to throw out the infinite ground state energy by redefining the Hamiltonian (see Remark 1.6). The real problem with $U(x,t)$ as it is defined in (1.10) is more subtle. Here the quantized field U purports to be an *operator-valued function* of (x,t). This suggests that one can attach some physical meaning to the value of a quantized field *at a point* in space or spacetime. But something has physical meaning only if it can be measured, at least in principle in some *gedanken* experiment, and the problem of measurement in quantum mechanics is a very subtle and still contentious one. At very least, however, it should be clear that quantum mechanics (and, in particular, the Uncertainty Principle) will impose restrictions on the measurability of quantities that classical physics would lead one to suspect are, in fact, measurable. This issue was taken up in 1933 by Bohr and Rosenfeld [BR] in the case of the quantized electromagnetic field. Very detailed analyses of the measurements involved led them to conclude that the value of a component of the electromagnetic field *at a point* cannot be regarded as physically meaningful in quantum mechanics. Rather, it is only average values of these components over "small" regions that can be measured.

What seems to be emerging from this discussion is that, whatever the quantum field U is supposed to be mathematically, it cannot reasonably be regarded as a "function" either from the mathematical point of view (it is too singular) or the physical (no physical meaning can be attached to its value at a point). The best one can hope for is that U can be represented mathematically by some sort of "generalized function". Nothing very exotic is being suggested here. Various types of generalized functions are quite common. The elements of $L^2(X,\mu)$, for example, being equivalence classes of functions on X that can differ on sets of μ-measure zero in X, cannot be assigned values at the points of X, but they behave in many ways just like square integrable functions on X. Tempered distributions on $\mathbb{R}^N$ do not take values at the points of $\mathbb{R}^N$, but they are very natural and very useful generalizations of a certain class of functions on $\mathbb{R}^N$, namely, those functions that give rise to regular distributions.

It took some time for the appropriate definition to emerge, but in the end it was determined that a quantum field is most accurately represented mathematically by

an *operator-valued distribution*. We will see the precise definition somewhat later, but essentially this is just a linear map from a Schwartz space to the unbounded operators on a Hilbert space that is continuous in an appropriate sense. We will find that, when quantum fields are viewed as operator-valued distributions, meaningless formulas such as (1.10) can often be salvaged.

Remark 1.1.4. The historical and physical evolution of this view of quantum fields as operator-valued distributions is traced in some detail in [Wight]. This paper also contains more information about the quantized vibrating string.

1.2 The Klein-Gordon Field

In the previous section we tried to follow the line of thought one might find in the physics literature for arriving at a quantized version of the classical field representing the vibrations of a string. This involved some rather dubious mathematical manipulations and the end result appeared to suffer from rather severe difficulties that we briefly described, but made no attempt to resolve. Nevertheless, we would now like continue along this course and try to do something similar for the more interesting example of the classical Klein-Gordon field. We will begin with a brief synopsis of some of what we already know about the classical field and then plunge into the formal arguments used by physicists to quantize it. Following this we will describe, in the next chapter, some of the mathematical machinery required for the rigorous model of the quantum Klein-Gordon field presented in the final chapter.

Throughout this section we will employ natural units ($\hbar = c = 1$). A point x in Minkowski spacetime $\mathbb{R}^{1,3}$ will be written as either (x^0, x^1, x^2, x^3) or $(t, \mathbf{x})$, while a point p in momentum space $\mathbb{P}^{1,3}$ is denoted either (p^0, p^1, p^2, p^3) or $(p^0, \mathbf{p})$. The Klein-Gordon Lagrangian density, action and equation for a *real-valued* function $\varphi(x)$ are

$$\mathcal{L}(\varphi, \partial_\alpha \varphi) = \frac{1}{2}\,(\partial_\alpha \varphi\, \partial^\alpha \varphi - m^2 \varphi^2),$$

$$S[\varphi] = \frac{1}{2} \int_{\mathbb{R}^{1,3}} (\partial_\alpha \varphi\, \partial^\alpha \varphi - m^2 \varphi^2)\, d^4x,$$

and

$$(\partial_\alpha \partial^\alpha + m^2)\, \varphi = 0,$$

or

$$(\Box + m^2)\varphi = 0.$$

The spatial integral of the Lagrangian density $\mathcal{L}$ is denoted

$$L = \int_{\mathbb{R}^3} \mathcal{L}\, d^3\mathbf{x} = \frac{1}{2}\int_{\mathbb{R}^3} (\partial_\alpha\varphi\, \partial^\alpha\varphi - m^2\varphi^2)\, d^3\mathbf{x}$$

and called simply the *Lagrangian*. The action is the time integral of the Lagrangian. The momentum density conjugate to φ is defined by

$$\frac{\partial\mathcal{L}}{\partial(\partial_0\varphi)} = \partial_0\varphi \stackrel{def}{=} \dot{\varphi}.$$

Writing $\nabla\varphi$ for the spatial gradient $(\partial_1\varphi, \partial_2\varphi, \partial_3\varphi)$ this gives, as the analogue of the Hamiltonian in mechanics, the Hamiltonian density

$$\mathcal{H}(\varphi, \dot{\varphi}) = \frac{1}{2}(\, \dot{\varphi}^2 + \nabla\varphi \cdot \nabla\varphi + m^2\varphi^2\,).$$

The spatial integral

$$H(\varphi, \dot{\varphi}) = \int_{\mathbb{R}^3} \mathcal{H}(\varphi, \dot{\varphi})\, d^3\mathbf{x} = \frac{1}{2}\int_{\mathbb{R}^3} (\, \dot{\varphi}^2 + \nabla\varphi \cdot \nabla\varphi + m^2\varphi^2\,)\, d^3\mathbf{x}$$

of the Hamiltonian density is then called simply the Hamiltonian.

Remark 1.2.1. Notice that we have pushed a great many technical issues under the rug here. For example, we have seen that the appropriate domain for the Hamiltonian is $H^1(\mathbb{R}^3;\mathbb{R}) \oplus L^2(\mathbb{R}^3;\mathbb{R})$, but made no mention of the fact. What we propose to do in this section is all quite formal and not to be taken too seriously as mathematics. As a result, we see no need to be scrupulous about such things until we get back to doing mathematics.

"Shut up and calculate!"

Applying the Minkowski Fourier transform $\mathcal{F}_M$ to the Klein-Gordon equation on $\mathbb{R}^{1,3}$ gives its momentum space version

$$(p^2 - m^2)\,\mathcal{F}_M\varphi = 0$$

on $\mathbb{P}^{1,3}$. From this we concluded that the (classical and distributional) solutions to the Klein-Gordon equation on $\mathbb{R}^{1,3}$ are precisely the inverse Fourier transforms of distributions on $\mathbb{P}^{1,3}$ that are supported on the mass hyperboloid $X_m = X_m^+ \sqcup X_m^-$. On the upper branch X_m^+ of X_m one has a Lorentz invariant Borel measure μ_m defined as follows. For any Borel set $B \subseteq X_m^+$, the projection $\pi_+(B)$ of B into $\mathbb{R}^3$ is a Borel subset of $\mathbb{R}^3$ and we define

$$\mu_m(B) = \int_{\pi_+(B)} \frac{d^3\mathbf{p}}{2\omega_{\mathbf{p}}} = \int_{\pi_+(B)} \frac{d^3\mathbf{p}}{2\sqrt{m^2 + \|\mathbf{p}\|^2}}\,,$$

where $d^3\mathbf{p} = dp_1\, dp_2\, dp_3$ denotes integration with respect to Lebesgue measure on $\mathbb{R}^3$. The analogously defined Lorentz invariant measure on X_m^- is also denoted μ_m.

With these one can define distributions $\delta_\pm(p^2 - m^2)$ on $\mathbb{P}^{1,3}$ supported on $X_m^\pm$ and from them, in turn, a class of solutions $\varphi(x)$ to the Klein-Gordon equation on $\mathbb{R}^{1,3}$. In particular, if we let $p = (\omega_{\mathbf{p}}, \mathbf{p})$ denote an arbitrary point of X_m^+, then for any $x = (t, \mathbf{x})$ in $\mathbb{R}^{1,3}$ we define

$$\begin{aligned}\varphi(x) = \varphi(t, \mathbf{x}) &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \frac{1}{2\omega_{\mathbf{p}}} \left(e^{-i(\omega_{\mathbf{p}} t - \mathbf{p}\cdot\mathbf{x})} A(\mathbf{p}) + e^{i(\omega_{\mathbf{p}} t - \mathbf{p}\cdot\mathbf{x})} \overline{A}(\mathbf{p}) \right) d^3\mathbf{p} \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \frac{1}{2\omega_{\mathbf{p}}} \left(e^{-i\langle p, x\rangle} A(\mathbf{p}) + e^{i\langle p, x\rangle} \overline{A}(\mathbf{p}) \right) d^3\mathbf{p},\end{aligned} \tag{1.11}$$

where $A : \mathbb{R}^3 \to \mathbb{C}$ is a smooth function with compact support. In fact, one need only assume that A is a Schwartz function or, indeed, any function with sufficient regularity and sufficiently rapid decay at infinity.

Remark 1.2.2. Note that we have slightly altered the notation used in Section 2.2 of [Nab7] in order to obtain formulas that are more easily compared with those found in the physics literature.

The solution (1.11) is a classical Klein-Gordon field and it is this object that we would like to quantize. What we will describe is essentially the argument one finds in every quantum field theory text (see, for example, Section 4.1 of [Ryd] or Section 12.1 of [BD2]).

Remark 1.2.3. Before getting started, however, we should say a few words about some of the tools physicists use in these calculations. For example, the Dirac delta $\delta(x - y)$ is a singular distribution defined for every $\phi(y) \in \mathcal{S}(\mathbb{R}^N)$ by

$$\delta(x - y)[\phi(x)] = \phi(y)$$

and we have noted that it is not uncommon to write this as if $\delta(x - y)$ were a honest function defining a regular distribution, that is,

$$\int_{\mathbb{R}^N} \delta(x - y)\phi(x)\, d^N x = \phi(y). \tag{1.12}$$

This is mathematical nonsense, of course, since $\delta(x - y)$ is certainly not a function and the integral on the left-hand side is not defined. Its popularity in the physics literature is due to the fact that if one allows oneself to take it seriously as an integral, then many of the integrals one must evaluate in quantum field theory become particularly easy. On the surface of it this does not at all sound like adequate justification for pretending that something makes sense when it does not. The point, however, is that one can often salvage such an argument by regarding it as an abbreviation for a limit statement that we will describe in a moment and that, even if the argument cannot be salvaged, in physics it is the end result that counts. The end result may or

may not be correct, but this is something one checks by looking at its consequences and comparing them with observations.

The procedure for regarding such integral formulas as limit statements goes like this. One chooses a sequence $\delta_n(x-y)$, $n = 1, 2, \ldots$, of (honest) functions with the property that, for every $\phi(y) \in \mathcal{S}(\mathbb{R}^N)$,

$$\lim_{n\to\infty} \int_{\mathbb{R}^N} \delta_n(x-y)\phi(x)\, d^N x = \phi(y). \tag{1.13}$$

These are called *delta sequences* and many such are known (see Example 1.2.1 below). Then one thinks of $\delta(x-y)$ as the limit in $\mathcal{S}'(\mathbb{R}^N)$ of the regular distributions corresponding to $\delta_n(x-y)$ and takes (1.13) as the definition of (1.12).

Example 1.2.1. As an illustration we will exhibit a delta sequence when $N = 1$. For each $n = 1, 2, \ldots$ we define

$$\delta_n(x-y) = \sqrt{\frac{n}{\pi}}\, e^{-n(x-y)^2}$$

Exercise 1.2.1. Show that, for each $y \in \mathbb{R}$,

$$\int_{-\infty}^{\infty} \delta_n(x-y)dx = 1$$

for each $n = 1, 2, \ldots$ *Hint*: These are Gaussian integrals so you may wish to consult Appendix A of [Nab5]; the required integration formulas are on page 520.

Now we must show that, for any $\phi \in \mathcal{S}(\mathbb{R})$,

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} \delta_n(x-y)\phi(x)dx = \phi(y).$$

For this we compute as follows. Fix $\phi \in \mathcal{S}(\mathbb{R})$ and $y \in \mathbb{R}$. Then

$$\begin{aligned}
\left| \int_{-\infty}^{\infty} \delta_n(x-y)\phi(x)dx - \phi(y) \right| &= \left| \int_{-\infty}^{\infty} \delta_n(x-y)\,(\phi(x)-\phi(y))dx \right| \\
&\le \int_{-\infty}^{\infty} \left|\delta_n(x-y)\right| \left|\phi(x)-\phi(y)\right| dx \\
&\le \max_{c\in\mathbb{R}} \left|\phi'(c)\right| \sqrt{\frac{n}{\pi}} \int_{-\infty}^{\infty} e^{-n(x-y)^2} |x-y|\, dx
\end{aligned}$$

Exercise 1.2.2. Show that

$$\sqrt{\frac{n}{\pi}} \int_{-\infty}^{\infty} e^{-n(x-y)^2} |x-y|\, dx = \frac{1}{\sqrt{\pi n}}$$

(Appendix A of [Nab5]) so that

$$\left| \int_{-\infty}^{\infty} \delta_n(x-y)\phi(x)dx - \phi(y) \right| \leq \frac{\max_{c\in\mathbb{R}} \left|\phi'(c)\right|}{\sqrt{\pi n}} \to 0 \quad \text{as} \quad n \to \infty$$

as required.

Thus one thinks of $\delta(x-y)$ intuitively as the limit in $\mathcal{S}'(\mathbb{R})$ of the regular distributions determined by $\sqrt{\frac{n}{\pi}}\, e^{-n(x-y)^2}$. One even writes

$$\delta(x-y) = \lim_{n\to\infty} \sqrt{\frac{n}{\pi}}\, e^{-n(x-y)^2}$$

with the understanding that this is an equality of distributions.

Exercise 1.2.3. Show that the defining property of the distribution $\delta(x-y)$ could equally well be written heuristically as

$$\int_{\mathbb{R}^N} \delta(x-y)\phi(y)\, d^N y = \phi(x)$$

for all $\phi(y) \in \mathcal{S}(\mathbb{R}^N)$ and all $x \in \mathbb{R}^N$.

In the same spirit one finds in the physics literature considerable reliance on what are called *integral representations* of the Dirac delta such as the following (see [LW] for many others).

$$\delta(x-y) = \frac{1}{(2\pi)^N} \int_{\mathbb{R}^N} e^{ip\cdot(x-y)}\, d^N p, \tag{1.14}$$

where the dot in the exponent is the inner product on $\mathbb{R}^N$. One might well wonder what this could possibly mean. After all, the integral on the right clearly diverges and, even if it converged, it would be a function and therefore could not be equal to the singular distribution $\delta(x-y)$. Needless to say, (1.14) is intended to be a shorthand notation for a more complicated statement saying, in effect, that the integral acts on Schwartz functions in the same way as the Dirac delta. Specifically, it means that for any $\phi(y) \in \mathcal{S}(\mathbb{R}^N)$ and for any $x \in \mathbb{R}^N$,

$$\int_{\mathbb{R}^N} \left[\int_{\mathbb{R}^N} \frac{1}{(2\pi)^N} e^{ip\cdot(x-y)} \phi(y)\, d^N y \right] d^N p = \phi(x). \tag{1.15}$$

We will see in a moment that this integral actually makes sense. Notice that if one *formally* reverses the order of the integrations the result can be written

$$\phi(x) = \int_{\mathbb{R}^N} \left[\int_{\mathbb{R}^N} \frac{1}{(2\pi)^N} e^{ip\cdot(x-y)}\, d^N p \right] \phi(y)\, d^N y$$

which doesn't make sense, but should be compared with

$$\phi(x) = \int_{\mathbb{R}^N} \delta(x-y)\phi(y)\, d^N y.$$

This is where (1.14) comes from. To see that the integral (1.15) actually does make sense we simply note that it is essentially a restatement of the Fourier Inversion Theorem for Schwartz functions, that is,

$$\phi(x) = (\mathcal{F}^{-1}(\mathcal{F}\phi))(x) = \frac{1}{(2\pi)^{N/2}} \int_{\mathbb{R}^N} e^{ip\cdot x}\Big[\frac{1}{(2\pi)^{N/2}} \int_{\mathbb{R}^N} e^{-ip\cdot y}\phi(y)\, d^N y\Big] d^N p.$$

Notice that, since the arrangement of signs in the exponents in the definitions of $\mathcal{F}$ and $\mathcal{F}^{-1}$ is a matter of convention and varies with the source, one is also likely to see (1.14) written as

$$\delta(x-y) = \frac{1}{(2\pi)^N} \int_{\mathbb{R}^N} e^{-ip\cdot(x-y)}\, d^N p. \tag{1.16}$$

For future reference we also point out that $\delta(x+y) = \delta(x-(-y))$ satisfies

$$\int_{\mathbb{R}^N} \delta(x+y)\phi(x)\, d^N x = \phi(-y) \tag{1.17}$$

and is given by either one of the following formal expressions.

$$\delta(x+y) = \frac{1}{(2\pi)^N} \int_{\mathbb{R}^N} e^{\pm ip\cdot(x+y)}\, d^N p \tag{1.18}$$

It has been said that one of the differences between mathematicians and physicists is that the former do not like to compute with things that don't exist; in this section we will need to get over that.

With these remarks behind us we will now return to the classical Klein-Gordon field (1.11). We begin by simplifying the form of (1.11) as follows. Define, for each $p = (\omega_{\mathbf{p}}, \mathbf{p}) \in X_m^+$, the function f_p on $\mathbb{R}^{1,3}$ by

$$f_p(x) = \frac{1}{\sqrt{(2\pi)^3 2\omega_{\mathbf{p}}}}\, e^{-i\langle p,x\rangle}.$$

Notice that, since $\omega_{-\mathbf{p}} = \omega_{\mathbf{p}}$,

$$\overline{f}_p = f_{-p}$$

These are, of course, complex solutions to the Klein-Gordon equation and (1.11) can now be written

$$\varphi(x) = \int_{\mathbb{R}^3} \frac{1}{\sqrt{2\omega_{\mathbf{p}}}} \left(f_p(x)A(\mathbf{p}) + \overline{f}_p(x)\overline{A}(\mathbf{p}) \right) d^3\mathbf{p}. \tag{1.19}$$

It will also be convenient to renormalize $A(\mathbf{p})$ by absorbing the factor $\frac{1}{\sqrt{2\omega_{\mathbf{p}}}}$ into it so we will let

$$a(\mathbf{p}) = \frac{1}{\sqrt{2\omega_{\mathbf{p}}}} A(\mathbf{p})$$

and write $\varphi(x)$ as

$$\varphi(x) = \int_{\mathbb{R}^3} \left(f_p(x)a(\mathbf{p}) + \overline{f}_p(x)\overline{a}(\mathbf{p}) \right) d^3\mathbf{p}. \tag{1.20}$$

Next we would like to show that the functions f_p satisfy what the physicists call *generalized orthogonality conditions*. For this they generally introduce the following notation.

$$A \overset{\leftrightarrow}{\partial_0} B = A\left(\frac{\partial B}{\partial t}\right) - \left(\frac{\partial A}{\partial t}\right) B$$

Remark 1.2.4. For some motivation as to where the next definition comes from one should look back to Section 2.3 of [Nab7] for the conserved quantity associated to the internal $U(1)$-symmetry of complex Klein-Gordon fields. Assuming appropriate regularity and decay conditions this is given by

$$\begin{aligned} \int_{\mathbb{R}^3} j^0(x^0, \mathbf{x})\, d^3\mathbf{x} &= i \int_{\mathbb{R}^3} \left[\overline{\varphi}(x)\partial_0\varphi(x) - \partial_0\overline{\varphi}(x)\varphi(x) \right]_{x^0=0} d^3\mathbf{x} \\ &= i \int_{\mathbb{R}^3} \left[\overline{\varphi}(x) \overset{\leftrightarrow}{\partial_0} \varphi(x)\right]_{x^0=0} d^3\mathbf{x}. \end{aligned}$$

where we have evaluated the integrand at $x^0 = 0$, but note that that any other fixed value of x^0 would do just as well since the quantity is conserved.

Exercise 1.2.4. Show that if $\varphi(x) = e^{-i\langle p,x\rangle}$, $p \in X_m$, is a plane wave solution, then this is infinite.

Now, if φ_1 and φ_2 are two solutions, we define the *Klein-Gordon inner product* of φ_1 and φ_2 by

$$(\varphi_1, \varphi_2) = i \int_{\mathbb{R}^3} \left[\overline{\varphi}_1(x) \overset{\leftrightarrow}{\partial_0} \varphi_2(x)\right]_{x^0=0} d^3\mathbf{x}. \tag{1.21}$$

Note that if φ is any solution, then the conserved quantity mentioned in the previous Remark is just (φ, φ). It follows that in (1.21) one could evaluate the integrand at any fixed value of x^0 and the result would be the same. In other words, the definition of

(φ_1, φ_2) is independent of the constant time hypersurface over which the integration takes place. As we just saw, (φ, φ) might well be infinite.

Exercise 1.2.5. Show that, if φ_1 and φ_2 are solutions for which (φ_1, φ_2) is finite and α and β are complex numbers, then $(\alpha\varphi_1, \varphi_2) = \overline{\alpha}(\varphi_1, \varphi_2)$, $(\varphi_1, \beta\varphi_2) = \beta(\varphi_1, \varphi_2)$, and

$$(\varphi_2, \varphi_1) = \overline{(\varphi_1, \varphi_2)}.$$

One of the "orthogonality conditions" to which we referred is then as follows.

$$(f_{p'}, f_p) = \delta(\mathbf{p} - \mathbf{p}') \tag{1.22}$$

for all $p, p' \in X_m^+$. Once again, such apparently nonsensical identities will require some interpretation so we will give the argument in detail; one should keep in mind (1.14) and the meaning we ascribed to it in (1.15). First we will compute

$$\begin{aligned}
\overline{f}_{p'}(x) \overset{\leftrightarrow}{\partial_0} f_p(x) &= \overline{f}_{p'}(x) \frac{\partial f_p(x)}{\partial t} - \frac{\partial \overline{f}_{p'}(x)}{\partial t} f_p(x) \\
&= \frac{1}{\sqrt{(2\pi)^3 2\omega_{\mathbf{p}'}}} e^{i\langle p', x\rangle} (-i\omega_{\mathbf{p}}) \frac{1}{\sqrt{(2\pi)^3 2\omega_{\mathbf{p}}}} e^{-i\langle p, x\rangle} \\
&\quad - (i\omega_{\mathbf{p}'}) \frac{1}{\sqrt{(2\pi)^3 2\omega_{\mathbf{p}'}}} e^{i\langle p', x\rangle} \frac{1}{\sqrt{(2\pi)^3 2\omega_{\mathbf{p}}}} e^{-i\langle p, x\rangle} \\
&= -i \frac{1}{(2\pi)^3} \frac{\omega_{\mathbf{p}} + \omega_{\mathbf{p}'}}{2\sqrt{\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}} e^{i\langle p' - p, x\rangle} \\
&= -i \frac{1}{(2\pi)^3} \frac{\omega_{\mathbf{p}} + \omega_{\mathbf{p}'}}{2\sqrt{\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}} e^{i((\omega_{\mathbf{p}'} - \omega_{\mathbf{p}})t - (\mathbf{p}' - \mathbf{p})\cdot\mathbf{x})}
\end{aligned}$$

At $x^0 = t = 0$ this gives

$$[\overline{f}_{p'}(x) \overset{\leftrightarrow}{\partial_0} f_p(x)]_{t=0} = -i \frac{1}{(2\pi)^3} \frac{\omega_{\mathbf{p}} + \omega_{\mathbf{p}'}}{2\sqrt{\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}} e^{i\mathbf{x}\cdot(\mathbf{p} - \mathbf{p}')}.$$

Consequently,

$$\begin{aligned}
(f_{p'}, f_p) &= \frac{\omega_{\mathbf{p}} + \omega_{\mathbf{p}'}}{2\sqrt{\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}} \int_{\mathbb{R}^3} \frac{1}{(2\pi)^3} e^{i\mathbf{x}\cdot(\mathbf{p} - \mathbf{p}')} \, d^3\mathbf{x} \\
&= \int_{\mathbb{R}^3} \frac{1}{(2\pi)^3} e^{i\mathbf{x}\cdot(\mathbf{p} - \mathbf{p}')} \left(\frac{\omega_{\mathbf{p}} + \omega_{\mathbf{p}'}}{2\sqrt{\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}} \right) d^3\mathbf{x}
\end{aligned}$$

The claim in (1.22) is that this should be "equal to" $\delta(\mathbf{p} - \mathbf{p}')$. We will check this by using the definition (1.15) of (1.14). For this we let $\phi(\mathbf{p}')$ be an arbitrary Schwartz function on $\mathbb{R}^3$ and note that

$$\int_{\mathbb{R}^3}\Big[\int_{\mathbb{R}^3}\frac{1}{(2\pi)^3}\,e^{i\mathbf{x}\cdot(\mathbf{p}-\mathbf{p}')}\Big(\frac{\omega_{\mathbf{p}}+\omega_{\mathbf{p}'}}{2\sqrt{\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}}\Big)\phi(\mathbf{p}')d^3\mathbf{p}'\Big]d^3\mathbf{x}=\frac{\omega_{\mathbf{p}}+\omega_{\mathbf{p}}}{2\sqrt{\omega_{\mathbf{p}}\omega_{\mathbf{p}}}}\,\phi(\mathbf{p})=\phi(\mathbf{p})$$

as required.

Exercise 1.2.6. The second of our "orthogonality conditions" is

$$(\overline{f}_{p'},f_p)=0 \tag{1.23}$$

for all $p,p'\in X_m^+$. Prove this.

Now we consider a Klein-Gordon solution of the form (1.20)

$$\varphi(x)=\int_{\mathbb{R}^3}(\,f_p(x)a(\mathbf{p})+\overline{f}_p(x)\overline{a}(\mathbf{p})\,)\,d^3\mathbf{p}$$

and compute

$$\begin{aligned}(\varphi,f_p)&=\Big(\int_{\mathbb{R}^3}(\,f_{p'}\,a(\mathbf{p}')+\overline{f}_{p'}\,\overline{a}(\mathbf{p}')\,)\,d^3\mathbf{p}',\,f_p\Big)\\&=\int_{\mathbb{R}^3}(\,(f_{p'},f_p)\,\overline{a}(\mathbf{p}')+(\overline{f}_{p'},f_p)\,a(\mathbf{p}')\,)\,d^3\mathbf{p}'\quad\text{(Exercise 1.2.5)}\\&=\int_{\mathbb{R}^3}\delta(\mathbf{p}-\mathbf{p}')\,\overline{a}(\mathbf{p}')\,d^3\mathbf{p}'\\&=\overline{a}(\mathbf{p}).\end{aligned}$$

Thus,

$$\overline{a}(\mathbf{p})=(\varphi,f_p)=i\int_{\mathbb{R}^3}[\varphi(x)\overset{\leftrightarrow}{\partial}_0 f_p(x)]_{x^0=0}\,d^3\mathbf{x} \tag{1.24}$$

because φ is real. Taking conjugates then gives

$$a(\mathbf{p})=\overline{(\varphi,f_p)}=(f_p,\varphi)=i\int_{\mathbb{R}^3}[\overline{f}_p(x)\overset{\leftrightarrow}{\partial}_0\varphi(x)]_{x^0=0}\,d^3\mathbf{x}. \tag{1.25}$$

So far in this section we have just taken another look at the classical Klein-Gordon field (1.11) and have rewritten it in the form (1.20), where $a(\mathbf{p})$ and $\overline{a}(\mathbf{p})$ are given by (1.25) and (1.24), respectively. Why we have bothered to do this may not be so clear at the moment. To understand the significance of (1.20) we must now proceed with the business of quantizing the classical field $\varphi(x)$. How is this done? From the perspective of physics it is all quite clear (see Appendix A). In classical particle mechanics the position q and conjugate momentum p have coordinates that satisfy the commutation relations

$$\{q^j,q^k\}=\{p_j,p_k\}=0\quad\text{and}\quad\{q^j,p_k\}=\delta^j{}_k,\quad j,k=1,\dots n.$$

In quantum mechanics q^j and p_j are promoted to the status of self-adjoint (physicists would say Hermitian) operators Q^j and P_j on some Hilbert space $\mathcal{H}$ that satisfy the corresponding quantum commutation relations

$$[Q^j, Q^k] = [P_j, P_k] = 0 \quad \text{and} \quad [Q^j, P_k] = i\delta^j{}_k, \quad j,k = 1,\dots n, \tag{1.26}$$

where the identity operator is understood on the right-hand side of the last equality and we have taken $\hbar = 1$.

Remark 1.2.5. Keep in mind that in this section (alone) we are setting aside many serious mathematical issues such as domains and commutators for unbounded operators; these are discussed more carefully in Appendix A.

The index j in mechanics labels the number of degrees of freedom in the mechanical problem. In field theory this role is played by $x = (t, \mathbf{x}) \in \mathbb{R}^{1,3}$ so a field is said to have infinitely many degrees of freedom. The field theoretic analogue of the position component Q^j is the value of the field at x. For the Klein-Gordon field this is $\varphi(t, \mathbf{x})$ and the conjugate momentum is $\dot{\varphi}(t, \mathbf{x})$. The canonical quantization of the Klein-Gordon field would have us identify $\varphi(t, \mathbf{x})$ and $\dot{\varphi}(t, \mathbf{x})$ with operators (for which we will use the same symbols) satisfying the analogue of (1.26) which is taken to be the so-called *equal time commutation relations*

$$[\varphi(t, \mathbf{x}), \varphi(t, \mathbf{y})] = [\dot{\varphi}(t, \mathbf{x}), \dot{\varphi}(t, \mathbf{y})] = 0 \quad \text{and} \quad [\varphi(t, \mathbf{x}), \dot{\varphi}(t, \mathbf{y})] = i\delta(\mathbf{x} - \mathbf{y}), \tag{1.27}$$

where the identity operator is understood on the right-hand side of the last equality.

Remark 1.2.6. There is something rather disconcerting about the last of these commutation relations. For each $(t, \mathbf{x}) \in \mathbb{R}^{1,3}$, $\varphi(t, \mathbf{x})$ and $\dot{\varphi}(t, \mathbf{x})$ are intended to be operators on some Hilbert space so the same should be true of their commutator $[\varphi(t, \mathbf{x}), \dot{\varphi}(t, \mathbf{y})]$. On the other hand, $\delta(\mathbf{x} - \mathbf{y})$ is a distribution so it operates on test functions to give multiples of the identity operator. The left- and right-hand sides are of different species and it is not so clear in what sense they can be equal. One should keep in mind, however, that we have already seen that a quantum field cannot really be thought of an operator-valued *function* $\varphi(t, \mathbf{x})$ on $\mathbb{R}^{1,3}$, but rather must be regarded as an operator-valued *distribution*. When we get around to formulating more mathematically precise definitions this issue, at least, will be resolved. What will not be resolved is how one actually represents these commutation relations as operator-valued distributions on some Hilbert space, but we will get around to this as well.

Now suppose the classical solution we have in mind is of the form (1.20). Quantization promotes $\varphi(t, \mathbf{x})$ to the status of an operator (on some as yet unspecified Hilbert space) so it does the same for $a(\mathbf{p})$. For operators, as opposed to functions, however, a "real" solution is one that is self-adjoint since these have a real spectrum. In particular, as quantum mechanical observables, the measured values are real as

all measured values must be. Consequently, the conjugate in $\overline{a}(\mathbf{p})$ is replaced in the quantized field by the adjoint $a^\dagger(\mathbf{p})$. What we intend to do therefore is to look for quantized Klein-Gordon fields of the form

$$\varphi(x) = \int_{\mathbb{R}^3} \left(f_p(x)\, a(\mathbf{p}) + \overline{f}_p(x)\, a^\dagger(\mathbf{p}) \right) d^3\mathbf{p}, \tag{1.28}$$

where

$$a(\mathbf{p}) = i \int_{\mathbb{R}^3} [\overline{f}_p(x) \overset{\leftrightarrow}{\partial_0} \varphi(x)]_{x^0=0}\, d^3\mathbf{x} \tag{1.29}$$

and

$$a^\dagger(\mathbf{p}) = i \int_{\mathbb{R}^3} [\varphi(x) \overset{\leftrightarrow}{\partial_0} f_p(x)]_{x^0=0}\, d^3\mathbf{x} \tag{1.30}$$

are operators on some Hilbert space. Needless to say, even the rather problematic computations that we have allowed ourselves up to this point pale in comparison to the mathematical issues raised by formulas such as these. Nevertheless, we will persevere (*"Shut up and calculate"*) and see if, in the end, we can formulate some precise mathematics that does what we would like to do. The key to this lies with the operators $a(\mathbf{p})$ and $a^\dagger(\mathbf{p})$ so we would first like to compute (still quite formally) the commutation relations for these operators that are implied by the equal time commutation relations (1.27).

$$\begin{aligned}
[a(\mathbf{p}), a^\dagger(\mathbf{p}')] &= \left[i \int_{\mathbb{R}^3} [\overline{f}_p(x) \overset{\leftrightarrow}{\partial_0} \varphi(x)]_{x^0=0}\, d^3\mathbf{x},\ i \int_{\mathbb{R}^3} [\varphi(y) \overset{\leftrightarrow}{\partial_0} f_{p'}(y)]_{y^0=0}\, d^3\mathbf{y} \right] \\
&= -\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \left[\overline{f}_p(x) \overset{\leftrightarrow}{\partial_0} \varphi(x),\ \varphi(y) \overset{\leftrightarrow}{\partial_0} f_{p'}(y) \right]_{x^0=0,\, y^0=0} d^3\mathbf{x}\, d^3\mathbf{y}
\end{aligned}$$

Exercise 1.2.7. Compute the commutator and show that

$$\begin{aligned}
\left[\overline{f}_p(x) \overset{\leftrightarrow}{\partial_0} \varphi(x),\ \varphi(y) \overset{\leftrightarrow}{\partial_0} f_{p'}(y) \right] = &- \overline{f}_p(x) \dot{f}_{p'}(y) \left[\varphi(y), \dot{\varphi}(x)\right] + \dot{\overline{f}}_p(x) f_{p'}(y) \left[\varphi(x), \dot{\varphi}(y)\right] \\
&+ \dot{\overline{f}}_p(x) \dot{f}_{p'}(y) [\varphi(y), \varphi(x)] + \overline{f}_p(x) f_{p'}(y) [\dot{\varphi}(y), \dot{\varphi}(x)].
\end{aligned}$$

From this we conclude that

$$
\begin{aligned}
&- \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \Big[\, \overline{f}_p(x) \overset{\leftrightarrow}{\partial}_0 \varphi(x),\ \varphi(y) \overset{\leftrightarrow}{\partial}_0 f_{p'}(y) \,\Big]_{x^0=0,\, y^0=0} d^3\mathbf{x}\, d^3\mathbf{y} \\
&= i \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \overline{f}_p(x) \dot{f}_{p'}(y)\big|_{x^0=0,\, y^0=0} \delta(\mathbf{y}-\mathbf{x})\, d^3\mathbf{x}\, d^3\mathbf{y} \\
&\quad - i \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \dot{\overline{f}}_p(x) f_{p'}(y)\big|_{x^0=0,\, y^0=0} \delta(\mathbf{x}-\mathbf{y})\, d^3\mathbf{y}\, d^3\mathbf{x} \\
&= i \int_{\mathbb{R}^3} \overline{f}_p(y) \dot{f}_{p'}(y)\big|_{y^0=0}\, d^3\mathbf{y} - i \int_{\mathbb{R}^3} \dot{\overline{f}}_p(x) f_{p'}(x)\big|_{x^0=0}\, d^3\mathbf{x} \\
&= i \int_{\mathbb{R}^3} [\overline{f}_p(x) \overset{\leftrightarrow}{\partial}_0 f_{p'}(x)]_{x^0=0}\, d^3\mathbf{x} \\
&= (f_p, f_{p'})
\end{aligned}
$$

and so

$$
[a(\mathbf{p}), a^\dagger(\mathbf{p}')] = \delta(\mathbf{p}' - \mathbf{p}). \tag{1.31}
$$

Exercise 1.2.8. Show that

$$
[a(\mathbf{p}), a(\mathbf{p}')] = [a^\dagger(\mathbf{p}), a^\dagger(\mathbf{p}')] = 0. \tag{1.32}
$$

The point of these computations can be seen by comparing (1.31) and (1.32) with the commutation relations (B.10)

$$
[b_j, b_k] = [b_j^\dagger, b_k^\dagger] = 0 \quad \text{and} \quad [b_j, b_k^\dagger] = \delta_{jk}, \quad j,k = 1,\dots,N
$$

for the raising and lowering operators of the harmonic oscillator. Taking this analogy seriously would raise the possibility of studying the quantized Klein-Gordon field along the same lines as the harmonic oscillator. One would begin by reinterpreting $a(\mathbf{p})$ and $a^\dagger(\mathbf{p})$ as operator-valued distributions rather than operator-valued functions so that (1.31) at least makes sense and then looking for a Hilbert space $\mathcal{H}$ on which the commutation relations (1.31) and (1.32) could be realized as operators. We will deal with this problem in the next chapter. This done one can mimic the treatment of the harmonic oscillator in terms of raising and lowering operators (outlined in Appendix B and treated in more detail in Section 7.4 of [Nab5]). As a simple illustration we will conclude this section by expressing the Klein-Gordon Hamiltonian

$$
H(\varphi, \dot{\varphi}) = \int_{\mathbb{R}^3} \mathcal{H}(\varphi, \dot{\varphi})\, d^3\mathbf{x} = \frac{1}{2} \int_{\mathbb{R}^3} (\, \dot{\varphi}^2 + \nabla\varphi \cdot \nabla\varphi + m^2\varphi^2 \,)\, d^3\mathbf{x} \tag{1.33}
$$

in terms of a and $a^\dagger$. Thus, we let

$$
\varphi(x) = \int_{\mathbb{R}^3} (\, f_p(x)\, a(\mathbf{p}) + \overline{f}_p(x)\, a^\dagger(\mathbf{p}) \,)\, d^3\mathbf{p}, \tag{1.34}
$$

and compute each of the three terms in the Hamiltonian. Begin by noting that

$$\begin{aligned}
m^2\varphi^2(x) &= m^2 \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} [f_p(x)a(\mathbf{p}) + \overline{f}_p(x)a^\dagger(\mathbf{p})]\,[f_{p'}(x)a(\mathbf{p}') + \overline{f}_{p'}(x)a^\dagger(\mathbf{p}')]\,d^3\mathbf{p}\,d^3\mathbf{p}' \\
&= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} [f_p(x)f_{p'}(x)a(\mathbf{p})a(\mathbf{p}') + f_p(x)\overline{f}_{p'}(x)a(\mathbf{p})a^\dagger(\mathbf{p}') + \\
&\qquad \overline{f}_p(x)f_{p'}(x)a^\dagger(\mathbf{p})a(\mathbf{p}') + \overline{f}_p(x)\overline{f}_{p'}(x)a^\dagger(\mathbf{p})a^\dagger(\mathbf{p}')]\,d^3\mathbf{p}\,d^3\mathbf{p}' \\
&= \frac{m^2}{(2\pi)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{1}{2\sqrt{\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}}\Big[a(\mathbf{p})a(\mathbf{p}')e^{-i\langle p+p',x\rangle} + a(\mathbf{p})a^\dagger(\mathbf{p}')e^{-i\langle p-p',x\rangle} + \\
&\qquad a^\dagger(\mathbf{p})a(\mathbf{p}')e^{i\langle p-p',x\rangle} + a^\dagger(\mathbf{p})a^\dagger(\mathbf{p}')e^{i\langle p+p',x\rangle}\Big]\,d^3\mathbf{p}\,d^3\mathbf{p}'. \qquad (1.35)
\end{aligned}$$

We will eventually insert this into the Hamiltonian $H(\varphi,\dot\varphi)$ and perform the spatial integral. However, just as in classical mechanics the Hamiltonian is conserved so we can evaluate the integrand of $m^2\varphi^2(x)$ at any convenient value of $x^0 = t$ and we might as well do so now. At $x^0 = 0$, (1.35) becomes

$$\begin{aligned}
m^2\varphi^2(0,\mathbf{x}) = \frac{m^2}{(2\pi)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{1}{2\sqrt{\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}}\Big[a(\mathbf{p})a(\mathbf{p}')e^{i\mathbf{x}\cdot(\mathbf{p}+\mathbf{p}')} + a(\mathbf{p})a^\dagger(\mathbf{p}')e^{i\mathbf{x}\cdot(\mathbf{p}-\mathbf{p}')} + \\
a^\dagger(\mathbf{p})a(\mathbf{p}')e^{-i\mathbf{x}\cdot(\mathbf{p}-\mathbf{p}')} + a^\dagger(\mathbf{p})a^\dagger(\mathbf{p}')e^{-i\mathbf{x}\cdot(\mathbf{p}+\mathbf{p}')}\Big]\,d^3\mathbf{p}\,d^3\mathbf{p}'. \qquad (1.36)
\end{aligned}$$

Performing the $\mathbf{x}$-integration of $m^2\varphi^2(0,\mathbf{x})$ each exponential produces $(2\pi)^3$ times a delta function which, in turn, allows us to perform the $\mathbf{p}'$-integral.

$$\begin{aligned}
\int_{\mathbb{R}^3} m^2\varphi^2(0,\mathbf{x})d^3\mathbf{x} &= m^2\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{1}{2\sqrt{\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}}\Big[a(\mathbf{p})a(\mathbf{p}')\delta(\mathbf{p}+\mathbf{p}') + a(\mathbf{p})a^\dagger(\mathbf{p}')\delta(\mathbf{p}-\mathbf{p}') + \\
&\qquad a^\dagger(\mathbf{p})a(\mathbf{p}')\delta(\mathbf{p}-\mathbf{p}') + a^\dagger(\mathbf{p})a^\dagger(\mathbf{p}')\delta(\mathbf{p}+\mathbf{p}')\Big]\,d^3\mathbf{p}'\,d^3\mathbf{p} \\
&= \int_{\mathbb{R}^3}\frac{1}{2\omega_{\mathbf{p}}}\Big[\,m^2[\,a(\mathbf{p})a(-\mathbf{p}) + a^\dagger(\mathbf{p})a^\dagger(-\mathbf{p})\,] + \\
&\qquad m^2[\,a(\mathbf{p})a^\dagger(\mathbf{p}) + a^\dagger(\mathbf{p})a(\mathbf{p})\,]\Big]\,d^3\mathbf{p}
\end{aligned}$$

Exercise 1.2.9. Carry out similar computations for the first and second terms in the Hamiltonian (1.33) to show that

$$\begin{aligned}
H(\varphi,\dot\varphi) &= \frac{1}{2}\int_{\mathbb{R}^3} (\,\dot\varphi^2(0,\mathbf{x}) + \nabla\varphi(0,\mathbf{x})\cdot\nabla\varphi(0,\mathbf{x}) + m^2\varphi^2(0,\mathbf{x})\,)\,d^3\mathbf{x} \\
&= \frac{1}{2}\int_{\mathbb{R}^3}\frac{1}{2\omega_{\mathbf{p}}}\Big[\,(-\omega_{\mathbf{p}}^2 + \mathbf{p}\cdot\mathbf{p} + m^2)[\,a(\mathbf{p})a(-\mathbf{p}) + a^\dagger(\mathbf{p})a^\dagger(-\mathbf{p})\,] + \\
&\qquad (\omega_{\mathbf{p}}^2 + \mathbf{p}\cdot\mathbf{p} + m^2)[\,a(\mathbf{p})a^\dagger(\mathbf{p}) + a^\dagger(\mathbf{p})a(\mathbf{p})\,]\Big]\,d^3\mathbf{p}
\end{aligned}$$

However, since $(\omega_{\mathbf{p}}, \mathbf{p})$ is in X_m^+, $-\omega_{\mathbf{p}}^2 + \mathbf{p}\cdot\mathbf{p} + m^2 = 0$ and $\omega_{\mathbf{p}}^2 + \mathbf{p}\cdot\mathbf{p} + m^2 = 2\omega_{\mathbf{p}}^2$ so this reduces to

$$H(\varphi, \dot{\varphi}) = \int_{\mathbb{R}^3} \omega_{\mathbf{p}}[\, a^\dagger(\mathbf{p})a(\mathbf{p}) + \frac{1}{2}\delta(0)\,]\, d^3\mathbf{p}, \tag{1.37}$$

where, as usual, the identity operator is understood after $\delta(0)$.

Exercise 1.2.10. Verify (1.37).

Notice that, if we introduce the *number density operator* $N(\mathbf{p})$ by

$$N(\mathbf{p}) = a^\dagger(\mathbf{p})a(\mathbf{p}),$$

then the Hamiltonian can be written as

$$H(\varphi, \dot{\varphi}) = \int_{\mathbb{R}^3} \omega_{\mathbf{p}}[\, N(\mathbf{p}) + \frac{1}{2}\delta(0)\,]\, d^3\mathbf{p} \tag{1.38}$$

which should be compared with the corresponding result (1.5) for the vibrating string (with $\hbar = 1$). The term $\frac{1}{2}\delta(0)$ introduces the same difficulties that we saw in this early case (see Remark 1.6). Specifically, once we have specified a Hilbert space on which all of these operators are supposed to be operating we will find that it contains a ground state ψ_0 , that is, a state of least energy, that is annihilated by each $a(\mathbf{p})$ and therefore by each $N(\mathbf{p})$. Applying the Hamiltonian operator to this state, however, gives

$$\Big(\int_{\mathbb{R}^3} \frac{\omega_{\mathbf{p}}}{2}\delta(0)\, d^3\mathbf{p}\Big)\psi_0$$

and the coefficient of ψ_0 is infinite. To see this think of the distribution $\delta(0)$ as acting on a test function ϕ to give $\phi(0)$ and note that

$$\int_{\mathbb{R}^3} \frac{\omega_{\mathbf{p}}}{2}\, d^3\mathbf{p}$$

clearly diverges. Assuming that one has no problem with subtracting infinities one can, as for the vibrating string, proceed in the manner of the physicists to remove this difficulty by simply subtracting the offending term $\frac{\omega_{\mathbf{p}}}{2}\delta(0)$ and redefining the Hamiltonian to be

$$H'(\varphi, \dot{\varphi}) = \int_{\mathbb{R}^3} \omega_{\mathbf{p}} N(\mathbf{p})\, d^3\mathbf{p}$$

(see page 131 of [Ryd] or page 30 of [BD2]).

Remark 1.2.7. In the formalism that we have gotten just a very small taste of in this section and the last these infinities are ubiquitous, particularly when interactions

among various fields are taken into account. The physicists have developed very complex and ingenious techniques, known as *regularization* and *renormalization*, for extracting useful information from them. This is an enormous and technically very demanding subject that we are in no way prepared to deal with here. Those interested in pursuing this might consult Chapter 9 of [Ryd], Chapter 19 of [BD2] or, for a somewhat more mathematical slant on the subject, Chapter 7 of [Fol3].

Exercise 1.2.11. Take the analogy with the harmonic oscillator one step farther by defining operators

$$P(\mathbf{p}) = \sqrt{\frac{\omega_{\mathbf{p}}}{2}}\,(a(\mathbf{p}) + a^\dagger(\mathbf{p})) \quad \text{and} \quad Q(\mathbf{p}) = \frac{i}{\sqrt{2\omega_{\mathbf{p}}}}\,(a(\mathbf{p}) - a^\dagger(\mathbf{p}))$$

and then show that

$$H(\varphi, \dot{\varphi}) = \int_{\mathbb{R}^3} \left[\frac{1}{2}\,P^2(\mathbf{p}) + \frac{\omega_{\mathbf{p}}^2}{2}\,Q^2(\mathbf{p})\right] d^3\mathbf{p}$$

so that one can think of the Klein-Gordon field as a continuous sum of harmonic oscillators, one for each $p = (\omega_{\mathbf{p}}, \mathbf{p}) \in X_m^+$.

At this point we are more than ready to put behind us all of these very formal computations and return to our comfort zone, that is, mathematics. For those who would like to see more of how these ideas are developed by the physicists we refer to Sections 4.1 and 4.2 of [Ryd], Chapter 12 of [BD2], or essentially any other quantum field theory text.

Appendix A
Canonical Quantization

In this section we will assume a familiarity with the foundations of quantum mechanics as laid out, for example, in Appendix A.4 of [Nab6] or, in more detail, in Chapter 6 of [Nab5]. In particular, we refer to the Heisenberg equation

$$\frac{dA}{dt} = -\frac{i}{\hbar}[A, H].$$

((A.19) of [Nab6]) and its striking similarity to the equation

$$\frac{df}{dt} = \{f, H\}$$

describing the time evolution of a classical observable in the Hamiltonian picture of classical mechanics ((A.9) of [Nab6]). This suggested to Paul Dirac [Dirac1] a possible avenue from classical to quantum mechanics, that is, a possible approach to the quantization of classical mechanical systems. The idea is that classical observables f should be replaced by self-adjoint operators A and the Poisson bracket $\{\ ,\ \}$ by the quantum bracket

$$\{\ ,\ \}_\hbar = -\frac{i}{\hbar}[\ ,\ ].$$

The process of implementing Dirac's proposal for obtaining the quantum analogue of a classical mechanical system is known as *canonical quantization* in the physics literature. We will review a few examples of how this is done in Appendix B, but first we must isolate some of the rather substantial mathematical difficulties involved in order to have in hand a rigorous version of Dirac's rather heuristic program. All of this is discussed in much more detail in Sections 7.2, 7.3, and 7.4 of [Nab5] so here we will content ourselves with a schematic.

Dirac is asking us for a "representation" of the algebra of classical observables by self-adjoint operators on some Hilbert space, but we will find that this is much too tall an order so we begin with something less ambitious. We will try to find a "representation" of just the classical canonical commutation relations

$$\{q^i, q^j\} = \{p_i, p_j\} = 0 \quad \text{and} \quad \{q^i, p_j\} = \delta^i{}_j, \quad i, j = 1, \ldots n$$

from classical mechanics by self-adjoint operators. The first order of business is to define precisely what it is we are trying to "represent" and what "representation" means. The abstract context in which the canonical commutation relations live is described as follows.

Let $n \geq 1$ be an integer. The *(2n+1)-dimensional Heisenberg algebra* $\mathfrak{h}_{2n+1}$ is a $(2n+1)$-dimensional, real Lie algebra with a basis $\{X_1, \ldots, X_n, Y_1, \ldots, Y_n, Z\}$ relative to which the bracket $[\,,\,]$ is determined by

$$[X_i, X_j] = [Y_i, Y_j] = [X_i, Z] = [Y_i, Z] = 0, \quad [X_i, Y_j] = \delta_{ij} Z, \quad i, j = 1, \ldots, n.$$

The Heisenberg algebra $\mathfrak{h}_{2n+1}$ can be realized concretely in a number of ways. Here are two such.

1. Let $C^\infty(T^*\mathbb{R}^n; \mathbb{R}) = C^\infty(\mathbb{R}^{2n}; \mathbb{R})$ be the Lie algebra, relative to the Poisson bracket, of classical observables for a mechanical system with configuration space $\mathbb{R}^n$. Then $\mathfrak{h}_{2n+1}$ is isomorphic to the Lie subalgebra of $C^\infty(T^*\mathbb{R}^n; \mathbb{R})$ generated by $\{q^1, \ldots, q^n, p_1, \ldots, p_n, 1\}$. Notice that the elements of this subalgebra are just the classical observables that are *linear* in the canonical coordinates.
2. Let $\mathfrak{gl}(n+2; \mathbb{R})$ be the Lie algebra of all $(n+2) \times (n+2)$ real matrices with the matrix commutator as bracket. Then $\mathfrak{h}_{2n+1}$ is isomorphic to the Lie subalgebra of $\mathfrak{gl}(n+2; \mathbb{R})$ consisting of those matrices of the form

$$\begin{pmatrix} 0 & x^1 & x^2 & \cdots & x^n & z \\ 0 & 0 & 0 & \cdots & 0 & y^1 \\ 0 & 0 & 0 & \cdots & 0 & y^2 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & y^n \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \mathbf{x} & z \\ \mathbf{0} & 0_n & \mathbf{y} \\ 0 & \mathbf{0} & 0 \end{pmatrix},$$

   where 0_n is the $n \times n$ zero matrix, $\mathbf{0}$ is the zero vector in $\mathbb{R}^n$ and $\mathbf{x}$ and $\mathbf{y}$ are arbitrary vectors in $\mathbb{R}^n$ (unless it causes some confusion, we will allow the context to indicate whether the elements of $\mathbb{R}^n$ are to be regarded as row or column vectors).

The simply connected Lie group whose Lie algebra is $\mathfrak{h}_{2n+1}$ is called the *(2n+1)-dimensional Heisenberg group* and denoted H_{2n+1}. This can be described in a number ways. As a matrix group, H_{2n+1} consists precisely of those $(n+2) \times (n+2)$ real matrices of the form

$$\begin{pmatrix} 1 & a^1 & a^2 & \cdots & a^n & c \\ 0 & 1 & 0 & \cdots & 0 & b^1 \\ 0 & 0 & 1 & \cdots & 0 & b^2 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & b^n \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & \mathbf{a} & c \\ \mathbf{0} & I_n & \mathbf{b} \\ 0 & \mathbf{0} & 1 \end{pmatrix},$$

where I_n is the $n \times n$ identity matrix. The matrix exponential map is a bijection of $\mathfrak{h}_{2n+1}$ onto H_{2n+1} and is given by

$$\begin{pmatrix} 0 & \mathbf{x} & z \\ \mathbf{0} & 0_n & \mathbf{y} \\ 0 & \mathbf{0} & 0 \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & \mathbf{x} & z + \frac{1}{2}\langle \mathbf{x}, \mathbf{y} \rangle \\ \mathbf{0} & I_n & \mathbf{y} \\ 0 & \mathbf{0} & 1 \end{pmatrix},$$

where $\langle \mathbf{x}, \mathbf{y} \rangle$ is the usual $\mathbb{R}^n$-inner product.

Alternatively, we can identify $\mathbb{R}^{2n+1}$ with $T^*\mathbb{R}^n \times \mathbb{R} = \mathbb{R}^{2n} \times \mathbb{R}$ and define a nondegenerate, skew-symmetric, bilinear form ω on $T^*\mathbb{R}^n = \mathbb{R}^{2n} = \mathbb{R}^n \times \mathbb{R}^n$ by

$$\omega((\mathbf{x}, \mathbf{y}), (\mathbf{x}', \mathbf{y}')) = \langle \mathbf{x}, \mathbf{y}' \rangle - \langle \mathbf{x}', \mathbf{y} \rangle.$$

Then H_{2n+1} is isomorphic to $T^*\mathbb{R}^n \times \mathbb{R} = \mathbb{R}^{2n} \times \mathbb{R}$ with the group structure defined by

$$(\mathbf{x}, \mathbf{y}, z)(\mathbf{x}', \mathbf{y}', z') = (\mathbf{x} + \mathbf{x}', \mathbf{y} + \mathbf{y}', z + z' + \frac{1}{2}\omega((\mathbf{x}, \mathbf{y}), (\mathbf{x}', \mathbf{y}')).$$

Our problem then is to "represent" the Heisenberg Lie algebra by self-adjoint operators on some Hilbert space. However, the self-adjoint operators we have in mind are generally unbounded and these certainly do not form a Lie algebra under the quantum bracket so the appropriate notion of "representation" is not simply "Lie algebra representation". To hone in on the appropriate definition we will look at the most important example.

Example A.0.1. (*Schrödinger Realization of the Heisenberg Algebra*) We begin with $n = 1$, that is, with the 3-dimensional Heisenberg algebra $\mathfrak{h}_3$. Write $q^1 = q$ and $p_1 = p$ for the canonical coordinates on $T^*\mathbb{R} = \mathbb{R}^2$ and take $\mathcal{H}$ to be the Hilbert space $L^2(\mathbb{R})$. On the Schwartz space $\mathcal{S}(\mathbb{R}) \subseteq L^2(\mathbb{R})$ we define operators Q and P by

$$(Q\psi)(q) = q\psi(q)$$

and

$$(P\psi)(q) = -i\hbar \frac{d}{dq}\psi(q).$$

$\mathcal{S}(\mathbb{R})$ is invariant under both, that is,

$$Q : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$$

and

$$P : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R}).$$

Consequently, the commutator $[Q, P]$ is well-defined on $\mathcal{S}(\mathbb{R})$ and a quick computation shows that

$$[Q, P]\psi = (QP - PQ)\psi = i\hbar\psi \quad \forall \psi \in \mathcal{S}(\mathbb{R}).$$

If we identify X_1 with Q, Y_1 with P and Z with $i\hbar I$ we see that the defining relations for $\mathfrak{h}_3$ are satisfied on $\mathcal{S}(\mathbb{R})$.

Both Q and P are essentially self-adjoint on $\mathcal{S}(\mathbb{R})$ (Exercise 5.2.8 of [Nab5]) so they have unique, unbounded, self-adjoint extensions to $L^2(\mathbb{R})$ that we will denote by the same symbols

$$Q : \mathcal{D}(Q) \subseteq L^2(\mathbb{R}) \to L^2(\mathbb{R})$$

and

$$P : \mathcal{D}(P) \subseteq L^2(\mathbb{R}) \to L^2(\mathbb{R}).$$

Their domains are given by

$$\mathcal{D}(Q) = \left\{ \psi \in L^2(\mathbb{R}) : \| q\psi(q) \|_{L^2}^2 = \int_{\mathbb{R}} q^2 |\psi(q)|^2 dq < \infty \right\}$$

(Example 5.2.3 of [Nab5]) and

$$\mathcal{D}(P) = \left\{ \psi \in L^2(\mathbb{R}) : \psi \in AC[a, b] \, \forall a < b \text{ in } \mathbb{R} \text{ and } \frac{d\psi}{dq} \in L^2(\mathbb{R}) \right\},$$

where $AC[a, b]$ denotes the set of all complex-valued, absolutely continuous functions on the interval $[a, b]$ (Example 5.2.4 o [Nab5]). Q and P are called, respectively, the *position* and *momentum* operators on $L^2(\mathbb{R})$.

Being self-adjoint, each of the operators P and Q determines, by Stone's Theorem, a unique strongly continuous 1-parameter group of unitary operators on $L^2(\mathbb{R})$ which we will denote by

$$\{U_t\}_{t\in\mathbb{R}} = \{e^{itP}\}_{t\in\mathbb{R}}$$

and

$$\{V_s\}_{s\in\mathbb{R}} = \{e^{isQ}\}_{s\in\mathbb{R}},$$

respectively. For future reference we note that in Example 7.2.4 of [Nab5] it is shown that

$$U_t V_s = e^{i\hbar ts} V_s U_t$$

on $L^2(\mathbb{R})$ for all $s, t \in \mathbb{R}$ so that U_t and V_s commute up to a phase factor.

The situation described in this example is essentially the closest one can come to the notion of a "representation" of the Heisenberg Lie algebra $\mathfrak{h}_3$ by unbounded self-adjoint operators so we are led to formulate the following definition. A *realization*

of $\mathfrak{h}_3$ on the separable, complex Hilbert space $\mathcal{H}$ consists of a dense linear subspace $\mathcal{D}$ of $\mathcal{H}$ and two operators Q and P on $\mathcal{H}$ with $\mathcal{D} \subseteq \mathcal{D}(Q)$ and $\mathcal{D} \subseteq \mathcal{D}(P)$ that satisfy

1. $Q : \mathcal{D} \to \mathcal{D}$ and $P : \mathcal{D} \to \mathcal{D}$,
2. $[Q, P]\psi = (QP - PQ)\psi = i\hbar\psi \quad \forall \psi \in \mathcal{D}$, and
3. Q and P are essentially self-adjoint on $\mathcal{D}$.

In this case we say that the unique self-adjoint extensions of Q and P, denoted by the same symbols, *satisfy the canonical commutation relations*. The realization of $\mathfrak{h}_3$ that we have just described is called the *Schrödinger realization* of $\mathfrak{h}_3$.

More generally, a *realization* of $\mathfrak{h}_{2n+1}$ on a separable, complex Hilbert space $\mathcal{H}$ consists of a dense linear subspace $\mathcal{D}$ of $\mathcal{H}$ and operators $Q^1, \ldots, Q^n, P_1, \ldots, P_n$ on $\mathcal{H}$ with $\mathcal{D} \subseteq \mathcal{D}(Q^j)$ and $\mathcal{D} \subseteq \mathcal{D}(P_k)$, $j, k = 1, \ldots, n$, that satisfy

1. $Q^j : \mathcal{D} \to \mathcal{D}$ and $P_k : \mathcal{D} \to \mathcal{D}$ for all $j, k = 1, \ldots, n$,
2. $[Q^j, Q^k]\psi = [P_j, P_k]\psi = 0$ and $[Q^j, P_k]\psi = i\hbar\delta^j_k\psi$ for all $j, k = 1, \ldots, n$, and for all $\psi \in \mathcal{D}$, and
3. $Q^1, \ldots, Q^n, P_1, \ldots, P_n$ are all essentially self-adjoint on $\mathcal{D}$.

In this case we say that the unique self-adjoint extensions of $Q^1, \ldots, Q^n, P_1, \ldots, P_n$, denoted by the same symbols, *satisfy the canonical commutation relations*. The *Schrödinger realization* of $\mathfrak{h}_{2n+1}$ is defined as follows. Let $\mathcal{H} = L^2(\mathbb{R}^n)$ and take $\mathcal{D}$ to be the Schwartz space $\mathcal{S}(\mathbb{R}^n)$. Define Q^j and P_k on $\mathcal{S}(\mathbb{R}^n)$ by

$$(Q^j\psi)(q) = (Q^j\psi)(q^1, \ldots, q^n) = q^j\psi(q^1, \ldots, q^n), \quad j = 1, \ldots, n,$$

and

$$(P_k\psi)(q) = (P_k\psi)(q^1, \ldots, q^n) = -i\hbar\,\frac{\partial}{\partial q^k}\,\psi(q^1, \ldots, q^n), \quad k = 1, \ldots, n.$$

Then $\mathcal{S}(\mathbb{R}^n)$ is invariant under all of the Q^j and P_k for $j, k = 1, \ldots, n$ and each of these is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^n)$ and satisfies the Heisenberg commutation relations there.

Each of the self-adjoint operators $Q^j : \mathcal{D}(Q^j) \to L^2(\mathbb{R}^n)$ and $P_k : \mathcal{D}(P_k) \to L^2(\mathbb{R}^n)$ determines a unique strongly continuous 1-parameter group of unitary operators on $L^2(\mathbb{R}^n)$ which we will denote by

$$\{U^k_t\}_{t\in\mathbb{R}} = \{e^{itP_k}\}_{t\in\mathbb{R}}$$

and

$$\{V^j_s\}_{s\in\mathbb{R}} = \{e^{isQ^j}\}_{s\in\mathbb{R}},$$

respectively and these satisfy

$$U^j_t V^j_s = e^{i\hbar ts} V^j_s U^j_t \tag{A.1}$$

if $k = j$ and, if $k \neq j$,

$$U_t^k V_s^j = V_s^j U_t^k \tag{A.2}$$

on $L^2(\mathbb{R}^n)$ for all $s, t \in \mathbb{R}$. In addition,

$$U_t^j U_s^k = U_s^k U_t^j \quad \text{and} \quad V_t^j V_s^k = V_s^k V_t^j \tag{A.3}$$

on $L^2(\mathbb{R}^n)$ for all $s, t \in \mathbb{R}$ and all $j, k = 1, \ldots, n$.

Manufacturing realizations of Heisenberg algebras is most efficiently done by reversing the procedure in Example A.0.1. Let $\{U_t^k\}_{t\in\mathbb{R}}$ and $\{V_s^j\}_{s\in\mathbb{R}}$, $j, k = 1, \ldots, n$, be a collection of $2n$ strongly continuous 1-parameter groups of unitary operators on the complex, separable Hilbert space $\mathcal{H}$ that satisfy the so-called *Weyl relations* (A.1), (A.2), and (A.3). By Stone's Theorem there exists a unique family of self-adjoint operators $P_1, \ldots, P_n, Q^1, \ldots, Q^n$ on $\mathcal{H}$ for which $U_t^1 = e^{itP_1}, \ldots, U_t^n = e^{itP_n}, V_s^1 = e^{isQ^1}, \ldots, V_s^n = e^{isQ^n}$. One can then prove that there is a dense linear subspace $\mathcal{D}$ of $\mathcal{H}$ with $\mathcal{D} \subseteq \mathcal{D}(P_k)$ and $\mathcal{D} \subseteq \mathcal{D}(Q^j)$ for all $j, k = 1, \ldots, n$ such that

1. $Q^j : \mathcal{D} \to \mathcal{D}$ and $P_k : \mathcal{D} \to \mathcal{D}$ for all $j, k = 1, \ldots, n$,
2. $[Q^j, Q^k]\psi = [P_j, P_k]\psi = 0$ and $[Q^j, P_k]\psi = i\hbar\delta_k^j\psi$ for all $j, k = 1, \ldots, n$, and for all $\psi \in \mathcal{D}$, and
3. $Q^1, \ldots, Q^n, P_1, \ldots, P_n$ are all essentially self-adjoint on $\mathcal{D}$

so we have a realization of $\mathfrak{h}_{2n+1}$ on $\mathcal{H}$. Thus, realizations of the Heisenberg *algebra* $\mathfrak{h}_{2n+1}$ on $\mathcal{H}$ can be constructed from families of 1-parameter groups of unitary operators on $\mathcal{H}$ that satisfy the Weyl relations.

Remark A.0.1. Such families of 1-parameter groups, in turn, can be constructed from a strongly continuous, unitary representation $\pi : H_{2n+1} \to \mathcal{U}(\mathcal{H})$ of the Heisenberg *group* on $\mathcal{H}$ by computing its infinitesimal version $d\pi$ and evaluating $i\hbar\, d\pi$ on the generators of $\mathfrak{h}_{2n+1}$. This is all described in more detail for the case of $\mathfrak{h}_3$ in Section 7.2 of [Nab5] (see, in particular, Theorem 7.2.1 and the discussion that follows). Notice that in the case of $\mathfrak{h}_3$ there are just two 1-parameter groups of unitary operators $\{U_t\}_{t\in\mathbb{R}} = \{e^{itP}\}_{t\in\mathbb{R}}$ and $\{V_s\}_{s\in\mathbb{R}} = \{e^{isQ}\}_{s\in\mathbb{R}}$ so that (A.2) is not relevant and (A.3) follows from the group property. The Weyl relations therefore reduce to $U_t V_s = e^{i\hbar ts} V_s U_t$.

Let $\{U_t^k\}_{t\in\mathbb{R}}$ and $\{V_s^j\}_{s\in\mathbb{R}}$, $j, k = 1, \ldots, n$, be a collection of $2n$ strongly continuous 1-parameter groups of unitary operators on $\mathcal{H}$ that satisfies the Weyl relations. We will say that this collection is *irreducible* if the only closed linear subspaces of $\mathcal{H}$ that are invariant under every U_t^k and every V_s^j are the subspace consisting of the zero vector alone and all of $\mathcal{H}$. This is true, for example, for the Schrödinger realization. One of the most fundamental results in the foundations of quantum mechanics is a theorem of Stone and von Neumann which asserts that every realization of $\mathfrak{h}_{2n+1}$ that arises from such an irreducible family is unitarily equivalent to the Schrödinger realization.

Theorem A.0.1. *(Stone-von Neumann Theorem) Let* $\{U_t^k\}_{t\in\mathbb{R}}$ *and* $\{V_s^j\}_{s\in\mathbb{R}}$, $j, k = 1, \ldots, n$, *be an irreducible collection of* $2n$ *strongly continuous 1-parameter groups*

of unitary operators on the complex, separable Hilbert space $\mathcal{H}$ that satisfies the Weyl relations (A.1), (A.2), and (A.3) . Let $P_1, \ldots, P_n, Q^1, \ldots, Q^n$ be the unique self-adjoint operators on $\mathcal{H}$ for which $U_t^1 = e^{itP_1}, \ldots, U_t^n = e^{itP_n}, V_s^1 = e^{isQ^1}, \ldots, V_s^n = e^{isQ^n}$. Let $\mathcal{D}$ be the dense linear subspace of $\mathcal{H}$ on which $P_1, \ldots, P_n$, $Q^1, \ldots, Q^n$ give a realization of $\mathfrak{h}_{2n+1}$ on $\mathcal{H}$. Then there exists a unitary isomorphism T of $\mathcal{H}$ onto $L^2(\mathbb{R}^n)$ such that, on $T(\mathcal{D})$,

$$TP_jT^{-1}\psi(q^1, \ldots, q^n) = -i\hbar \frac{\partial}{\partial q^j}\psi(q^1, \ldots, q^k), \quad j = 1, \ldots, n$$

and

$$TQ^kT^{-1}\psi(q^1, \ldots, q^n) = q^k\psi(q^1, \ldots, q^n), \quad k = 1, \ldots, n.$$

Remark A.0.2. The uniqueness assertion in Theorem A.0.1 depends crucially on the assumption that the realization of $\mathfrak{h}_{2n+1}$ comes from a family of 1-parameter groups of unitary operators that satisfy the Weyl relations. Such realizations are said to be *integrable*. Not every realization of $\mathfrak{h}_{2n+1}$ is integrable and for these uniqueness fails. We should point out also that it has been implicit in our discussion that $\hbar$ is to be regarded as a fixed positive constant. If one thinks of $\hbar$ as a positive parameter, then different values give different realizations (Exercise 7.2.21 of [Nab5]). There is also a version of the Stone-von Neumann Theorem in which the irreducibility condition is dropped. In this case $\mathcal{H}$ splits into an orthogonal direct sum of closed subspaces on each of which the realization is unitarily equivalent to the Schrödinger realization (see Theorem 7.2.7 of [Nab5]).

At this point we have rather precise information about realizing the classical canonical commutation relations as self-adjoint operators on a Hilbert space and we should pause to ask ourselves how close this has gotten us to Dirac's program for quantizing classical mechanical systems. Sadly, we must admit that the answer is, "not very close." Roughly speaking, Dirac asked for a realization of the algebra $C^\infty(T^*\mathbb{R}^n; \mathbb{R})$ of classical observables and, at this point, we have managed to do this only for the classical observables that live in the Heisenberg subalgebra of $C^\infty(T^*\mathbb{R}^n; \mathbb{R})$ and these are all *linear* in the canonical coordinates. Physically, this is not a particularly interesting class of observables. Classical Hamiltonians, for example, are often *quadratic*. What we need to do then is try to extend our realizations of $\mathfrak{h}_{2n+1}$ to larger Lie subalgebras of $C^\infty(T^*\mathbb{R}^n; \mathbb{R})$ that contain the observables we are interested in quantizing. One would hope that in this way one could work all the way up to $C^\infty(T^*\mathbb{R}^n; \mathbb{R})$ itself. We will see, however, that these hopes are dashed.

In order to suppress a certain amount of notational clutter, but none of the essential ideas, we will limit our remarks to the $n = 1$ case (Section 7.2 of [Nab5] contains a much more detailed discussion of this case). Begin by considering the linear subspace $\mathcal{P}_2(q, p)$ of $C^\infty(\mathbb{R}^2; \mathbb{R})$ spanned by $\{1, q, p, q^2, p^2, qp\}$. These are precisely the quadratic classical observables. Computing Poisson brackets gives, in addition to the commutation relations for $\mathfrak{h}_3$,

$$\{qp, p\} = p, \quad \{qp, q\} = -q, \quad \{p^2, q\} = -2p, \quad \{q^2, p\} = 2q, \tag{A.4}$$

and

$$\left\{\frac{q^2}{2}, \frac{p^2}{2}\right\} = qp, \quad \{qp, p^2\} = 2p^2, \quad \{qp, q^2\} = -2q^2. \tag{A.5}$$

In particular, $\mathcal{P}_2(q, p)$ is closed under Poisson brackets and is therefore a Lie subalgebra of $C^\infty(\mathbb{R}^2; \mathbb{R})$.

Remark A.0.3. In Section 7.2 of [Nab5] it is shown that $\mathcal{P}_2(q, p)$ is isomorphic to the so-called *Jacobi algebra* $\mathfrak{g}^J = \mathfrak{sl}(2, \mathbb{R}) \times_\pi \mathfrak{h}_3$ which is a semi-direct product of $\mathfrak{sl}(2, \mathbb{R})$ and $\mathfrak{h}_3$.

We can view the problem of quantizing the quadratic classical observables as that of extending the Schrödinger realization of $\mathfrak{h}_3$ to $\mathcal{P}_2(q, p)$. The Schrödinger realization sends 1 to the identity operator on $L^2(\mathbb{R})$ and, on $\mathcal{S}(\mathbb{R}) \subseteq L^2(\mathbb{R})$, is given by

$$q \to Q : (Q\psi)(q) = q\psi(q)$$
$$p \to P : (P\psi)(q) = -i\hbar \frac{d}{dq}\psi(q)$$

and satisfies

$$\{p, q\} \to -\frac{i}{\hbar}[P, Q].$$

What we must do is define appropriate images for q^2, p^2 and qp in such a way that $\{\,,\,\} \to -\frac{i}{\hbar}[\,,\,]$. There is certainly an obvious way to start the process.

$$q^2 \to Q^2 : (Q^2\psi)(q) = q^2\psi(q)$$
$$p^2 \to P^2 : (P^2\psi)(q) = -i\hbar \frac{d}{dq}[(P\psi)(q)] = -\hbar^2 \frac{d^2}{dq^2}\psi(q)$$

The element qp presents a problem, however. One might simply try $qp \to QP$. On the other hand, in $C^\infty(T^*\mathbb{R}; \mathbb{R})$, $qp = pq$ so one might just as well try $qp = pq \to PQ$ and these are not the same. This is the infamous *operator ordering problem* of quantization. For quadratic observables the issue is not so serious since we can think of qp as

$$qp = \frac{1}{2}(qp + pq)$$

and take

$$qp \to \frac{1}{2}(QP + PQ) = -i\hbar\,(\,q\frac{d}{dq} + \frac{1}{2}\,)$$

which is symmetric in Q and P. One now checks that the operators Q^2, P^2, and $\frac{1}{2}(QP + PQ)$ are essentially self-adjoint on $\mathcal{S}(\mathbb{R})$ and that the commutation relations (A.4) and (A.5) are satisfied there so we have the desired realization of the quadratic classical observables as self-adjoint operators on $L^2(\mathbb{R})$.

Needless to say, the operator ordering problems that gave us pause in this construction become increasingly severe as the degree of the polynomials increases, but it is not altogether clear that they cannot be somehow resolved as they were for $\mathcal{P}_2(q, p)$. Nevertheless, they cannot. The following is Theorem 7.2.9 of [Nab5].

Theorem A.0.2. *(Groenewold-Van Hove Theorem) Let $\mathcal{O}$ be a Lie subalgebra of $C^\infty(T^*\mathbb{R}; \mathbb{R})$ that properly contains the Lie subalgebra $\mathcal{P}_2(q, p)$ generated by $\{1, q, p, q^2, p^2, qp\}$. Then* ***there does not exist*** *a linear map R from $\mathcal{O}$ to the self-adjoint operators on $L^2(\mathbb{R})$ preserving some fixed dense linear subspace $\mathcal{D} \supseteq \mathcal{S}(\mathbb{R})$ and satisfying all of the following.*

$$
\begin{aligned}
&R(1) = id_{L^2(\mathbb{R})} \\
&R(\{f, g\}) = -\frac{i}{\hbar}[R(f), R(g)]_- \qquad \forall f, g \in \mathcal{O} \\
&R(q) = Q \qquad [\,(Q\psi)(q) = q\psi(q)\,\forall \psi \in \mathcal{S}(\mathbb{R})\,] \\
&R(p) = P \qquad [\,(P\psi)(q) = -i\hbar\frac{d}{dq}\psi(q)\,\forall \psi \in \mathcal{S}(\mathbb{R})\,] \\
&R(q^2) = Q^2 \qquad [\,(Q^2\psi)(q) = q^2\psi(q)\,\forall \psi \in \mathcal{S}(\mathbb{R})\,] \\
&R(p^2) = P^2 \qquad [\,(P^2\psi)(q) = -\hbar^2\frac{d^2}{dq^2}\psi(q)\,\forall \psi \in \mathcal{S}(\mathbb{R})\,].
\end{aligned}
$$

This is, perhaps, a bit depressing. However, the Groenewold-Van Hove Theorem does not imply that it is impossible to quantize, say, quartic polynomials such as q^2p^2 in a manner consistent with the Schrödinger quantization of $\mathcal{P}_2(q, p)$. It says only that the assumptions we have made do not uniquely determine the quantization and it is up to us to use whatever additional information is available to make a choice or to adapt our requirements. Quantization is, as they say, an art not a science and certainly not a theorem. In the next section we will apply the quantization map from the Jacobi algebra $\mathcal{P}_2(q, p) \subseteq C^\infty(T^*\mathbb{R}; \mathbb{R})$ to the self-adjoint operators on $L^2(\mathbb{R})$ to the two simplest examples of classical mechanical systems with quadratic Hamiltonians, that is, the free particle and the harmonic oscillator.

Appendix B
Free Particles and Harmonic Oscillators

In this section we will collect together material on the two most basic examples of quantized classical mechanical systems. The material is taken from Sections 7.3 and 7.4 of [Nab5], but many of the functional analytic preliminaries will be found in Chapter 5 of [Nab5].

A classical free particle of mass m moving in one dimension has configuration space $\mathbb{R}$ and phase space $T^*\mathbb{R} = \mathbb{R}^2$ with coordinates q and (q, p), respectively. The classical Hamiltonian is $\frac{1}{2m}p^2$ which lives in the quadratic Lie subalgebra $\mathcal{P}_2(q, p)$ of $C^\infty(T^*\mathbb{R}; \mathbb{R})$ generated by $1, q, p, q^2, p^2$ and qp. The quantum phase space is taken to be $L^2(\mathbb{R})$ and the map from $\mathcal{P}_2(q, p)$ to the self-adjoint operators on $L^2(\mathbb{R})$ constructed in Appendix A assigns to $1, q, p$ and $\frac{1}{2m}p^2$ the operators $I = id_{L^2(\mathbb{R})}$, Q, P and $H_0 = \frac{1}{2m}P^2$. On the Schwartz space $\mathcal{S}(\mathbb{R})$ these are given by $(Q\psi)(q) = q\psi(q)$, $(P\psi)(q) = -i\hbar\frac{d}{dq}\psi(q)$, and $(H_0\psi)(q) = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2}\psi(q)$, respectively, and they are all essentially self-adjoint on $\mathcal{S}(\mathbb{R})$. The domain of H_0 is the set of all $\psi \in L^2(\mathbb{R})$ for which $\Delta\psi$ is in $L^2(\mathbb{R})$, where $\Delta\psi$ is the second derivative of ψ thought of as a tempered distribution (Example 5.2.14 of [Nab5]), and the spectrum of H_0 is $\sigma(H_0) = [0, \infty)$ (Example 5.4.4 of [Nab5]). From the latter and Postulate QM2 it follows that, just as in the classical case, the energy of a free quantum particle can assume any non-negative real value, that is, the energy is *not* "quantized". According to Postulate QM4, an initial state $\psi(q, 0)$ of the free particle will evolve in time according to

$$\psi(q, t) = e^{-itH_0/\hbar}\psi(q, 0).$$

This evolution is computed explicitly for $\psi(q, 0) = \frac{1}{\pi^{1/4}}e^{-q^2/2}e^{i\alpha q}$ in Example 7.3.1 of [Nab5]. More generally, one can represent the time evolution in terms of an integral kernel. The following is Theorem 7.3.1 of [Nab5].

Theorem B.0.1. *Let $H_0 = -\frac{\hbar^2}{2m}\Delta$ be the free particle Hamiltonian on $L^2(\mathbb{R})$. Then H_0 is self-adjoint on $\mathcal{D}(H_0) = \{\psi \in L^2(\mathbb{R}) : \Delta\psi \in L^2(\mathbb{R})\}$, where Δ is the distributional Laplacian. For any $\psi_0 \in L^2(\mathbb{R})$*

$$(e^{-itH_0/\hbar}\psi_0)(q) = \int_{\mathbb{R}} \sqrt{\frac{m}{2\pi\hbar ti}}\, e^{mi(q-x)^2/2\hbar t}\psi_0(x)\,dx,$$

where $\sqrt{i} = e^{\pi i/4} = \frac{1}{\sqrt{2}}(1+i)$ *and, if* $\psi_0 \in L^2(\mathbb{R}) - L^1(\mathbb{R})$*, the integral must be regarded as an integral in the mean, that is,*

$$\int_{\mathbb{R}} \sqrt{\frac{m}{2\pi\hbar ti}}\, e^{mi(q-x)^2/2\hbar t}\psi_0(x)\,dx = \lim_{M\to\infty} \int_{[-M,M]} \sqrt{\frac{m}{2\pi\hbar ti}}\, e^{mi(q-x)^2/2\hbar t}\psi_0(x)\,dx,$$

where the limit is in $L^2(\mathbb{R})$*. If* $\psi_0(q) = \psi(q,t_0)$ *is the state of the free particle at* $t = t_0$*, then its state at time* t *is*

$$\psi(q,t) = e^{-i(t-t_0)H_0/\hbar}(\psi(q,t_0)) = \int_{\mathbb{R}} K(q,t;x,t_0)\psi(x,t_0)\,dx, \tag{B.1}$$

where

$$K(q,t;x,t_0) = \sqrt{\frac{m}{2\pi\hbar(t-t_0)i}}\, e^{mi(q-x)^2/2\hbar(t-t_0)} \tag{B.2}$$

The function $K(q,t;x,t_0)$ is called the *propagator*, or *integral kernel* for the free particle Hamiltonian H_0, or simply the *Schrödinger kernel* for H_0. Physicists interpret $\left|K(q,t;x,t_0)\right|^2$ as the conditional probability of finding the particle at $q \in \mathbb{R}$ at time t provided it was detected at the point $x \in \mathbb{R}$ at time t_0. $K(q,t;x,t_0)$ itself is interpreted as the probability amplitude for getting from x at time t_0 to q at time t. Thus, for fixed t_0 and t, the integral in (B.1) expresses the probability amplitude $\psi(q,t)$ for detecting the particle at q at time t as the (continuous) weighted sum of the amplitudes $\psi(x,t_0)$ over all $x \in \mathbb{R}$, the weight being just the propagator. Intuitively, there is a contribution to the amplitude $\psi(q,t)$ from every possible location of the particle at time t_0.

Now hold $t_0 = 0$ fixed and define $K_0 : \mathbb{R}\times(0,\infty)\times\mathbb{R} \to \mathbb{C}$ by

$$K_0(q,t,x) = K(q,t;x,0) = \sqrt{\frac{m}{2\pi\hbar ti}}\, e^{mi(q-x)^2/2\hbar t}.$$

Then we can write

$$\psi(q,t) = \int_{\mathbb{R}} K_0(q,t,x)\psi_0(x)\,dx,$$

where $\psi_0(x) = \psi(x,0)$. For each fixed x, $K_0(q,t,x)$ satisfies the free Schrödinger equation

$$i\,\frac{\partial K_0(q,t,x)}{\partial t} = -\frac{\hbar}{2m}\,\frac{\partial^2 K_0(q,t,x)}{\partial q^2} \tag{B.3}$$

on $\mathbb{R}\times(0,\infty)$ (see Exercise 7.3.7 of [Nab5]) and the initial condition

$$\lim_{t\to 0^+}\int_{\mathbb{R}} K_0(q,t,x)\psi_0(x)\,dx = \psi_0(q). \tag{B.4}$$

In the language of partial differential equations one would say that $K_0(q,t,x)$ is the *fundamental solution* to the free Schrödinger equation.

The classical harmonic oscillator has configuration space $\mathbb{R}$ and phase space $T^*\mathbb{R} = \mathbb{R}^2$ with coordinates q and (q,p), respectively. The classical Hamiltonian is $\frac{1}{2m}p^2 + \frac{m\omega^2}{2}q^2$, where m and ω are positive constants. The quantum phase space is taken to be $L^2(\mathbb{R})$. Since the Hamiltonian lives in the Jacobi subalgebra $\mathcal{P}_2(q,p)$ of the Lie algebra $C^\infty(T^*\mathbb{R};\mathbb{R})$ of classical observables we can apply the quantization map described in Appendix A to obtain its quantum analogue

$$H_B = \frac{1}{2m}P^2 + \frac{m\omega^2}{2}Q^2$$

which, on $\mathcal{S}(\mathbb{R})$, is given by

$$H_B\big|_{\mathcal{S}(\mathbb{R})} = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{m\omega^2}{2}q^2.$$

Remark B.0.1. The subscript B is intended to distinguish this *bosonic* harmonic oscillator from the *fermionic* and *supersymmetric* harmonic oscillators that are discussed in Chapter 9 of [Nab5].

In Example 5.3.1 of [Nab5] it is shown that H_B is essentially self-adjoint on $\mathcal{S}(\mathbb{R})$. This followed from the fact that, on $\mathcal{S}(\mathbb{R})$, it is symmetric and has a discrete set of eigenvalues

$$\mathcal{E}_n = (n+\frac{1}{2})\hbar\omega, \quad n = 0,1,2,\ldots$$

with eigenfunctions $\psi_n(q)$, $n = 0,1,2,\ldots$, that live in $\mathcal{S}(\mathbb{R})$ and form an orthonormal basis for $L^2(\mathbb{R})$. Specifically,

$$\psi_n(q) = \frac{1}{\sqrt{2^n n!}}\Big(\frac{m\omega}{\hbar\pi}\Big)^{1/4} e^{-m\omega q^2/2\hbar} H_n\Big(\sqrt{\frac{m\omega}{\hbar}}\,q\Big),$$

where

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}(e^{-x^2})$$

is the n^{th} Hermite polynomial. The eigenvalues $\mathcal{E}_n$ comprise the entire spectrum

$$\sigma(H_B) = \{\mathcal{E}_n\}_{n=0}^\infty = \{\,(n+\frac{1}{2})\hbar\omega\,\}_{n=0}^\infty$$

of H_B (Example 5.4.5 of [Nab5]) and all of the eigenspaces are 1-dimensional. These eigenvalues are therefore all of the allowed energy levels of the quantum oscillator so, unlike the free particle, the energy spectrum of the harmonic oscillator is discrete (quantized). The smallest of these eigenvalues is $\mathcal{E}_0 = \frac{1}{2}\hbar\omega$ and the corresponding eigenstate ψ_0 is called the *ground state* of the oscillator. Notice that the lowest allowed energy level is *not* zero.

Exercise B.0.1. Show that, for the harmonic oscillator, the expected value $\langle Q\rangle_{\psi_0} = \langle \psi_0, Q\psi_0\rangle$ of the position operator Q in the ground state ψ_0 is zero, but its variance $\sigma^2_{\psi_0}(Q) = \|Q\psi_0\|^2 - \langle Q\rangle^2_{\psi_0}$ is nonzero.

Remark B.0.2. The conclusion of Exercise B.0.1 is that the position observable fluctuates about its expected value in the ground state. The same is true in any energy eigenstate ψ_n.

The remaining $\psi_n, n = 1, 2, \ldots$, are called *excited states*. Writing $\psi \in L^2(\mathbb{R})$ as $\psi = \sum_{n=0}^{\infty}\langle\psi_n, \psi\rangle\psi_n$, the domain $\mathcal{D}(H_B)$ of H_B is just the set of ψ for which $\sum_{n=0}^{\infty} \mathcal{E}_n\langle\psi_n, \psi\rangle\psi_n$ converges in $L^2(\mathbb{R})$, that is, for which

$$\sum_{n=0}^{\infty} \mathcal{E}_n^2 \,|\, \langle\psi_n, \psi\rangle \,|^2 < \infty.$$

Since 0 is not an eigenvalue, H_B is invertible. Indeed, its inverse is a bounded operator on all of $L^2(\mathbb{R})$ given by

$$H_B^{-1}\phi = \sum_{n=0}^{\infty} \frac{1}{\mathcal{E}_n}\langle\psi_n, \phi\rangle\psi_n$$

(see (5.40) of [Nab5]). In Example 5.5.4 of [Nab5] it is shown that H_B^{-1} is a compact operator.

The evolution operator $e^{-itH_B/\hbar}$ is given by

$$e^{-itH_B/\hbar}\psi = \sum_{n=0}^{\infty} \langle\, \psi_n, \psi\, \rangle e^{-(i/\hbar)\mathcal{E}_n t}\psi$$

for any $\psi \in L^2(\mathbb{R})$. The time evolution of an initial state $\psi(q, t_0)$ can be written as

$$\psi(q, t) = \sum_{n=0}^{\infty} \Big(\int_{\mathbb{R}} \psi_n(x)\, \psi(x, t_0) dx \Big) e^{-(i/\hbar)\mathcal{E}_n(t-t_0)}\psi_n(q)$$

which, at least for sufficiently nice initial data, can be written in terms of an integral kernel as

$$\psi(q,t) = \int_{\mathbb{R}} K(q,t;x,t_0)\psi(x,t_0)dx,$$

where

$$K(q,t;x,t_0) = \sum_{n=0}^{\infty} e^{-(i/\hbar)\mathcal{E}_n(t-t_0)}\psi_n(q)\,\psi_n(x) = \sum_{n=0}^{\infty} e^{-i(n+\frac{1}{2})\omega(t-t_0)}\psi_n(q)\psi_n(x)$$

(see (6.12) of [Nab5]). $K(q,t;x,t_0)$ is called the *propagator*, or *integral kernel* for the harmonic oscillator, or simply the *Schrödinger kernel* for H_B. A closed form expression for $K(q,t;x,0)$, called the *Feynman-Souriau Formula*, is

$$K(q,t;x,0) =$$
$$\sqrt{\frac{m\omega}{2\pi\hbar\,|sin\,\omega t|}}\; e^{-i(\frac{\pi}{2})(\frac{1}{2}+\lfloor\frac{\omega t}{\pi}\rfloor)}\; exp\Big(\frac{i}{\hbar}\,\frac{m\omega}{2\,sin\,\omega t}\,[\,(q^2+x^2)\,cos\,\omega t - 2qx\,]\Big)$$

which is valid whenever ωt is not an integer multiple of π. This is derived from Mehler's Formula in Section 7.4 of [Nab5] and by evaluating the Feynman path integral in Section 8.3 of [Nab5]. Example 7.4.1 of [Nab5] computes an explicit time evolution from the Feynman-Souriau Formula. As for the free particle one defines

$$K_B(q,t,x) = K(q,t;x,0) \tag{B.5}$$

to obtain a fundamental solution to the Schrödinger equation for the harmonic oscillator.

The analysis of the quantum harmonic oscillator is facilitated by the introduction of the so-called lowering and raising operators b and $b^\dagger$ defined by

$$b = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega Q + iP)$$

and

$$b^\dagger = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega Q - iP),$$

respectively. These are adjoints of each other

$$\langle b\phi,\psi\rangle = \langle\phi,b^\dagger\psi\rangle \quad \text{and} \quad \langle b^\dagger\psi,\phi\rangle = \langle\psi,b\phi\rangle$$

and satisfy various algebraic identities, of which we will record a few (details and additional results are available in Section 5.3 of [Nab5]). Designating them as lowering and raising operators is motivated by

$$b\psi_n = \sqrt{n}\,\psi_{n-1},\ n = 1, 2, \ldots \quad \text{and} \quad b^\dagger\psi_n = \sqrt{n+1}\,\psi_{n+1},\ n = 0, 1, 2, \ldots$$

so that b lowers and $b^\dagger$ raises the energy level of the eigenstates of the harmonic oscillator (b annihilates the ground state, that is, $b\psi_0 = 0$). The excited states can all be obtained from the ground state by repeated application of the raising operator.

$$\psi_n = \frac{1}{\sqrt{n!}}(b^\dagger)^n\psi_0$$

On $\mathcal{S}(\mathbb{R})$ we have $[P, Q] = -i\hbar$ and it follows from this that

$$[b, b^\dagger] = bb^\dagger - b^\dagger b = 1$$

(see (5.32 of [Nab5])). Defining the number operator N_B by $N_B = b^\dagger b$ one obtains

$$N_B\psi_n = n\psi_n,$$

$$H_B = \hbar\omega(N_B + \frac{1}{2}),$$

and various commutation relations such as

$$[N_B, b^\dagger] = b^\dagger \quad \text{and} \quad [N_B, b] = -b,$$

and

$$[H_B, b^\dagger] = \hbar\omega b^\dagger \quad \text{and} \quad [H_B, b] = -\hbar\omega b.$$

Remark B.0.3. We will see that operators analogous to b and $b^\dagger$ exist in quantum field theory where they are called *annihilation operators* and *creation operators* because they are viewed as annihilating and creating particles (more precisely, *quanta*) of a particular energy. The eigenvalues of the number operator N_B count the number of such quanta; hence the name.

Just for reference we should also record how to retrieve the position Q and momentum P operators from the lowering b and raising $b^\dagger$ operators.

$$Q = \sqrt{\frac{\hbar}{2m\omega}}\,(b^\dagger + b)$$

$$P = i\sqrt{\frac{m\omega\hbar}{2}}\,(b^\dagger - b)$$

We will conclude this section by describing a system consisting of a finite number of harmonic oscillators. We will need some basic information about Hilbert space

tensor products available, for example, in Chapter II, Section 6, of [Prug] or Sections II.4 and VIII.10 of [RS1]. Thus, we have positive constants $m_1, \dots, m_N$ and $\omega_1, \dots, \omega_N$. We will denote by $q^1, \dots, q^N$ the spatial coordinates for the N oscillators and by $L^2(\mathbb{R}, dq^1), \dots, L^2(\mathbb{R}, dq^N)$ the Hilbert spaces of these oscillators. Then the Hilbert space $\mathcal{H}^{(N)}$ of the system is taken to be the Hilbert space tensor product

$$\mathcal{H}^{(N)} = L^2(\mathbb{R}, dq^1) \otimes \cdots \otimes L^2(\mathbb{R}, dq^N).$$

This can be identified with

$$L^2(\mathbb{R}^N, d^N q),$$

where $q = (q^1, \dots, q^N)$ and $d^N q = dq^1 \cdots dq^N$ is the Lebesgue measure on $\mathbb{R}^N$.

Remark B.0.4. Specifically, the identification is accomplished in the following way. Each $\phi_1 \otimes \cdots \otimes \phi_N$ in $L^2(\mathbb{R}, dq^1) \otimes \cdots \otimes L^2(\mathbb{R}, dq^N)$ gives rise to an element of $L^2(\mathbb{R}^N, d^N q)$, also denoted $\phi_1 \otimes \cdots \otimes \phi_N$, that is defined by

$$(\,\phi_1 \otimes \cdots \otimes \phi_N\,)(q^1, \dots, q^N) = \phi_1(q^1) \cdots \phi_N(q^N).$$

This extends by linearity to the algebraic tensor product of the $L^2(\mathbb{R}, dq^k)$ and this is dense in $L^2(\mathbb{R}, dq^1) \otimes \cdots \otimes L^2(\mathbb{R}, dq^N)$. One then shows that this linear map on the algebraic tensor product extends uniquely to a unitary map of $L^2(\mathbb{R}, dq^1) \otimes \cdots \otimes L^2(\mathbb{R}, dq^N)$ onto $L^2(\mathbb{R}^N, d^N q)$; this is proved, for example, in Theorem 6.9, Chapter II, of [Prug].

For each $k = 1, \dots, N$ we have an orthonormal basis

$$\psi_n^{(k)}(q^k) = \frac{1}{\sqrt{2^n n!}} \Big(\frac{m_k \omega_k}{\hbar \pi} \Big)^{1/4} e^{-m_k \omega_k (q^k)^2 / 2\hbar} H_n\Big(\sqrt{\frac{m_k \omega_k}{\hbar}}\, q^k \Big), \quad n = 0, 1, 2, \dots$$

for $L^2(\mathbb{R}, dq^k)$ and these give an orthonormal basis

$$\Big\{ \psi_{n_1 \cdots n_N} = \psi_{n_1}^{(1)} \otimes \cdots \otimes \psi_{n_N}^{(N)} : n_1, \dots, n_N = 0, 1, 2, \dots \Big\} \tag{B.6}$$

for $\mathcal{H}^{(N)}$, where, as an element of $L^2(\mathbb{R}^N, d^N q)$,

$$(\,\psi_{n_1}^{(1)} \otimes \cdots \otimes \psi_{n_N}^{(N)}\,)(q^1, \dots, q^N) = \psi_{n_1}^{(1)}(q^1) \cdots \psi_{n_n}^{(N)}(q^N).$$

These are all in the Schwartz space $\mathcal{S}(\mathbb{R}^N)$. An element of $\mathcal{H}^{(N)}$ of the form $\phi_1 \otimes \cdots \otimes \phi_N$ and of norm one is interpreted physically as a state of the system in which the k^{th} oscillator is in the state ϕ_k for each $k = 1, \dots, N$. Other states arising from superpositions of these and limits occur as well.

To define the Hamiltonian $H_B^{(N)}$ on $\mathcal{H}^{(N)}$ we will need some information about operators on tensor products. For each $k = 1, \dots, N$ we will denote by I_k, Q_k, P_k, and H_k the following operators on $L^2(\mathbb{R}, dq^k)$. I_k is the identity operator. Q_k is the

k^{th}-position operator, that is, the self-adjoint extension of multiplication by q^k. P_k is the k^{th}-momentum operator, that is, the self-adjoint extension of $-i\hbar\,\partial_k$, where $\partial_k = \partial/\partial q^k$. H_k is the k^{th}-oscillator Hamiltonian, that is, the self-adjoint extension of

$$-\frac{\hbar^2}{2m_k}\partial_k^2 + \frac{m_k\omega_k^2}{2}(q^k)^2\,,$$

where $\partial_k^2 = \partial^2/\partial(q^k)^2$. To put these together into operators on $\mathcal{H}^{(N)}$ we will need the following result (see the Corollary in Section VIII.10 of [RS1]).

Theorem B.0.2. *Let $\mathcal{H}_1, \ldots, \mathcal{H}_N$ be separable, complex Hilbert spaces. For each $k = 1, \ldots, N$ let $A_k : \mathcal{D}(A_k) \to \mathcal{H}_k$ be a self-adjoint operator on $\mathcal{H}_k$ that is essentially self-adjoint on the dense linear subspace $\mathcal{D}_k \subseteq \mathcal{D}(A_k)$. Let $\mathcal{D}$ be the linear span of the set of all $\phi_1 \otimes \cdots \otimes \phi_N$ with $\phi_k \in \mathcal{D}_k$ for $k = 1, \ldots, N$. Then $\mathcal{D}$ is dense in $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$ and if we define*

$$A_1 \otimes \cdots \otimes A_N : \mathcal{D} \to \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N \tag{B.7}$$

by setting

$$(A_1 \otimes \cdots \otimes A_N)(\phi_1 \otimes \cdots \otimes \phi_N) = A_1\phi_1 \otimes \cdots \otimes A_N\phi_N$$

and extending by linearity to $\mathcal{D}$, then $A_1 \otimes \cdots \otimes A_N$ is essentially self-adjoint on $\mathcal{D}$. Moreover, if $I_1, \ldots, I_N$ are the identity operators on $\mathcal{H}_1, \ldots, \mathcal{H}_N$, respectively, then

$$A_1 \otimes I_2 \otimes \cdots \otimes I_N \;+\; I_1 \otimes A_2 \otimes I_3 \otimes \cdots \otimes I_N \;+\; \cdots \;+\; I_1 \otimes \cdots \otimes I_{N-1} \otimes A_N \tag{B.8}$$

is also essentially self-adjoint on $\mathcal{D}$.

As usual, we will use the same symbols for the unique self-adjoint extensions of the operators (B.7) and (B.8). Notice that (B.8) is really just the sum of $A_1, \ldots, A_N$ with each of these operators thought of as living on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$ so it is common practice to write it simply as

$$A_1 + \cdots + A_N$$

and we will adhere to the custom. In particular, to define the Hamiltonian (total energy) of our system of N harmonic oscillators we will simply add the Hamiltonians of the individual oscillators, that is, we take $H_B^{(N)}$ to be the unbounded, self-adjoint operator on $\mathcal{H}_B^{(N)}$ defined by

$$H_B^{(N)} = H_1 + \cdots + H_N.$$

As an operator on $L^2(\mathbb{R}^N, d^N q)$ one often see this written

$$H_B^{(N)} = \sum_{k=1}^{N} \Big(-\frac{\hbar^2}{2m_k}\partial_k^2 + \frac{m_k\omega_k^2}{2}(q^k)^2 \Big)$$

with the self-adjoint extension taken for granted.

Remark B.0.5. Notice that there is a physical assumption buried in this definition. Since the total energy of the system is just the sum of the energies of the individual oscillators we are assuming none of the oscillators interacts with any of the others, that is, the oscillators are independent or, in the terminology of physics, uncoupled.

Exercise B.0.2. Show that, if $\psi_{n_1\cdots n_N} = \psi_{n_1}^{(1)} \otimes \cdots \otimes \psi_{n_N}^{(N)}$ is an element of the orthonormal basis (B.6) for $\mathcal{H}_B^{(N)}$, then

$$H_B^{(N)}\,\psi_{n_1\cdots n_N} = \Big(n_1 + \cdots + n_N + \frac{N}{2} \Big)\psi_{n_1\cdots n_N}$$

so $\psi_{n_1\cdots n_N}$ is an eigenfunction of the Hamiltonian with eigenvalue, that is, energy $n_1 + \cdots + n_N + \frac{N}{2}$. The ground state of the system is

$$\psi_{0\cdots 0}(q) = \psi_{0\cdots 0}(q^1, \ldots, q^N) = \Big(\frac{m_1\omega_1}{\hbar\pi}\Big)^{1/4} \cdots \Big(\frac{m_N\omega_N}{\hbar\pi}\Big)^{1/4} exp\Big(-\sum_{k=1}^{N} m_k\omega_k(q^k)^2/2\hbar \Big) \tag{B.9}$$

and all of the remaining $\psi_{n_1\cdots n_N}$ are excited states.

Next we define, for each $k = 1, \ldots, N$, lowering and raising operators b_k and $b_k^\dagger$ on $\mathcal{H}_B^{(N)}$ by

$$b_k = \frac{1}{\sqrt{2m\omega_k\hbar}}(m\omega_k Q_k + iP_k)$$

and

$$b_k^\dagger = \frac{1}{\sqrt{2m\omega_k\hbar}}(m\omega_k Q_k - iP_k),$$

respectively. Then

$$Q_k = \sqrt{\frac{\hbar}{2m\omega_k}}\,(b_k^\dagger + b_k)$$

$$P_k = i\sqrt{\frac{m\omega_k\hbar}{2}}\,(b_k^\dagger - b_k).$$

A number of basic properties of these raising and lowering operators follow directly from those of the corresponding 1-dimensional operators. For example, on the Schwartz space $\mathcal{S}(\mathbb{R}^N)$ in $L^2(\mathbb{R}^N, d^N q)$ the operators b_k and $b_k^\dagger$ satisfy the commutation relations

$$[b_j, b_k] = [b_j^\dagger, b_k^\dagger] = 0 \quad \text{and} \quad [b_j, b_k^\dagger] = \delta_{jk} I, \quad j,k = 1, \ldots, N, \tag{B.10}$$

where I is the identity operator. The action of b_k and $b_k^\dagger$ on the basis vectors $\psi_{n_1 \cdots n_N}$ is given by

$$b_k \psi_{n_1 \cdots n_k \cdots n_N} = \sqrt{n_k}\, \psi_{n_1 \cdots (n_k - 1) \cdots n_N}$$

and

$$b_k^\dagger \psi_{n_1 \cdots n_k \cdots n_N} = \sqrt{n_k + 1}\, \psi_{n_1 \cdots (n_k + 1) \cdots n_N}.$$

The excited states $\psi_{n_1 \cdots n_k}$ can all be obtained from the ground state by repeated application of the raising operators $b_k^\dagger$. Specifically,

$$\psi_{n_1 \cdots n_N} = \frac{(b_1^\dagger)^{n_1} \cdots (b_N^\dagger)^{n_N}}{\sqrt{n_1! \cdots n_N!}}\, \psi_{0 \cdots 0}.$$

Defining the k^{th}-number operator by

$$N_k = b_k^\dagger b_k$$

one finds that the Hamiltonian can be written

$$H_B^{(N)} = \sum_{k=1}^{N} \hbar \omega_k \Big(b_k^\dagger b_k + \frac{1}{2} \Big) = \sum_{k=1}^{N} \hbar \omega_k \Big(N_k + \frac{1}{2} \Big).$$

We will see that, for the purposes of quantum field theory, one really requires a system of infinitely many harmonic oscillators and, as the $\frac{1}{2}$ in the preceding expression for the Hamiltonian should make clear, this is likely to present some rather serious technical difficulties. We will take this up again in Section **??** where we transplant all of this information to what is called "bosonic Fock space".

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