The Hamiltonian operator and states

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1 Calculation of the Hamiltonian operator

This is our first typical quantum field theory calculation. They're a bit to keep track of, but not really that hard. Our goal is to compute the expression for the Hamiltonian operator

$$\hat{H} = \frac{\hbar}{2}\int\left(\hat{\pi}^2 + \nabla\hat{\varphi}\cdot\hat{\varphi} + m^2\hat{\varphi}^2\right)d^3x$$

in terms of the mode operators,

$$\hat{a}(\mathbf{k}) = \frac{\sqrt{2\omega}}{2(2\pi)^{3/2}}\int\left(\hat{\varphi}(\mathbf{x},0) - \frac{i}{\omega}\hat{\pi}(\mathbf{x},0)\right)e^{i\mathbf{k}\cdot\mathbf{x}}d^3x \tag{1}$$

$$\hat{a}^\dagger(\mathbf{k}) = \frac{\sqrt{2\omega}}{2(2\pi)^{3/2}}\int\left(\hat{\varphi}(\mathbf{x},0) + \frac{i}{\omega}\hat{\pi}(\mathbf{x},0)\right)e^{-i\mathbf{k}\cdot\mathbf{x}}d^3x \tag{2}$$

Because the techniques involved are used frequently in field theory calculations, we include all the details.

Let's consider one term at a time. The technique is simply to substitute the mode expansions for the field and its momentum, then perform the spatial integral to get Dirac delta functions. For the first,

$$\begin{aligned}
I_\pi &= \frac{1}{2}\int\hat{\pi}^2 d^3x \\
&= -\frac{1}{2(2\pi)^3}\int\left(\int\sqrt{\frac{\omega}{2}}d^3k\left(\hat{a}(\mathbf{k})e^{i(\omega t-\mathbf{k}\cdot\mathbf{x})} - \hat{a}^\dagger(\mathbf{k})e^{-i(\omega t-\mathbf{k}\cdot\mathbf{x})}\right)\right) \\
&\quad\times\left(\int\sqrt{\frac{\omega'}{2}}d^3k'\left(\hat{a}(\mathbf{k}')e^{i\left(\omega' t-\mathbf{k}'\cdot\mathbf{x}\right)} - \hat{a}^\dagger(\mathbf{k}')e^{-i\left(\omega' t-\mathbf{k}'\cdot\mathbf{x}\right)}\right)\right)d^3x \\
&= -\frac{1}{4(2\pi)^3}\int\int\int\sqrt{\omega\omega'}d^3kd^3k'd^3x \\
&\quad\times\left(\hat{a}(\mathbf{k})e^{i(\omega t-\mathbf{k}\cdot\mathbf{x})} - \hat{a}^\dagger(\mathbf{k})e^{-i(\omega t-\mathbf{k}\cdot\mathbf{x})}\right)\left(\hat{a}(\mathbf{k}')e^{i\left(\omega' t-\mathbf{k}'\cdot\mathbf{x}\right)} - \hat{a}^\dagger(\mathbf{k}')e^{-i\left(\omega' t-\mathbf{k}'\cdot\mathbf{x}\right)}\right) \\
&= -\frac{1}{4(2\pi)^3}\int\int\int\sqrt{\omega\omega'}d^3kd^3k'd^3x\left(\hat{a}(\mathbf{k})\hat{a}(\mathbf{k}')e^{i\left(\left(\omega+\omega'\right)t-\left(\mathbf{k}+\mathbf{k}'\right)\cdot\mathbf{x}\right)} - \hat{a}(\mathbf{k})\hat{a}^\dagger(\mathbf{k}')e^{i\left(\left(\omega-\omega'\right)t-\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{x}\right)}\right. \\
&\quad\left. - \hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}')e^{-i\left(\left(\omega-\omega'\right)t-\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{x}\right)} + \hat{a}^\dagger(\mathbf{k})\hat{a}^\dagger(\mathbf{k}')e^{-i\left(\left(\omega+\omega'\right)t-\left(\mathbf{k}+\mathbf{k}'\right)\cdot\mathbf{x}\right)}\right) \\
&= -\frac{1}{4}\int\int\int\sqrt{\omega\omega'}d^3kd^3k'\left(\hat{a}(\mathbf{k})\hat{a}(\mathbf{k}')\delta^3\left(\mathbf{k}+\mathbf{k}'\right)e^{i\left(\omega+\omega'\right)t} - \hat{a}(\mathbf{k})\hat{a}^\dagger(\mathbf{k}')\delta^3\left(\mathbf{k}-\mathbf{k}'\right)e^{i\left(\omega-\omega'\right)t}\right. \\
&\quad\left. - \hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}')\delta^3\left(\mathbf{k}-\mathbf{k}'\right)e^{-i\left(\omega-\omega'\right)t} + \hat{a}^\dagger(\mathbf{k})\hat{a}^\dagger(\mathbf{k}')\delta^3\left(\mathbf{k}+\mathbf{k}'\right)e^{-i\left(\omega+\omega'\right)t}\right)
\end{aligned}$$

where we have used

$$\frac{1}{(2\pi)^3}\int d^3x\ e^{i\mathbf{k}\cdot\mathbf{x}} = \delta^3(\mathbf{k})$$

in the final step. Now, integrate over d^3k', using the Dirac deltas. This replaces each occurrence of $\mathbf{k}'$ with either $+\mathbf{k}$ or $-\mathbf{k}$, but always replaces ω' with ω,

$$\frac{1}{2}\int \hat{\pi}^2 d^3x = -\frac{1}{4}\int \omega d^3k \left(\hat{a}(\mathbf{k})\hat{a}(-\mathbf{k})e^{2i\omega t} - \hat{a}(\mathbf{k})\hat{a}^\dagger(\mathbf{k}) - \hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}) + \hat{a}^\dagger(\mathbf{k})\hat{a}^\dagger(-\mathbf{k})e^{-2i\omega t}\right)$$

Now we press on to the remaining terms. Substitution into the second term gives

$$\begin{aligned}
I_{\nabla\varphi} &= \frac{1}{2}\int \nabla\hat{\varphi}\cdot\nabla\hat{\varphi}d^3x \\
&= \frac{1}{4\left(2\pi\right)^3}\int\int\int \frac{1}{\sqrt{\omega\omega'}}d^3kd^3k'd^3x\,(-i\mathbf{k})\cdot(-i\mathbf{k}') \\
&\quad\times\left(\hat{a}(\mathbf{k})e^{i(\omega t-\mathbf{k}\cdot\mathbf{x})} - \hat{a}^\dagger(\mathbf{k})e^{-i(\omega t-\mathbf{k}\cdot\mathbf{x})}\right)\left(\hat{a}(\mathbf{k}')e^{i\left(\omega' t-\mathbf{k}'\cdot\mathbf{x}\right)} - \hat{a}^\dagger(\mathbf{k}')e^{-i\left(\omega' t-\mathbf{k}'\cdot\mathbf{x}\right)}\right)
\end{aligned}$$

As before, the d^3x integrals of the four terms give four Dirac delta functions and the d^3k' integrals become trivial. The result is

$$I_{\nabla\varphi} = -\frac{1}{4}\int \frac{\mathbf{k}\cdot\mathbf{k}}{\omega}d^3k\ \left(-\hat{a}(\mathbf{k})\hat{a}(-\mathbf{k})e^{2i\omega t} - \hat{a}(\mathbf{k})\hat{a}^\dagger(\mathbf{k}) - \hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}) - \hat{a}^\dagger(\mathbf{k})\hat{a}^\dagger(-\mathbf{k})e^{-2i\omega t}\right)$$

It is not hard to see the pattern that is emerging. The $\frac{\mathbf{k}\cdot\mathbf{k}}{\omega}$ term will combine nicely with the $\omega = \frac{\omega 2}{\omega}$ from the $\hat{\pi}^2$ integral and a corresponding m^2 term from the final integral to give a cancellation. The crucial thing is to keep track of the signs.

The third and final term is

$$\begin{aligned}
\frac{1}{2}\int m^2\hat{\varphi}^2d^3x &= \frac{1}{2}\frac{m^2}{\left(2\pi\right)^3}\int\int\int\frac{d^3k}{\sqrt{2\omega}}\frac{d^3k'}{\sqrt{2\omega'}}d^3x \\
&\quad\times\left(\hat{a}\left(\mathbf{k}\right)e^{i(\omega t-\mathbf{k}\cdot\mathbf{x})} + \hat{a}^\dagger\left(\mathbf{k}\right)e^{-i(\omega t-\mathbf{k}\cdot\mathbf{x})}\right)\left(\hat{a}\left(\mathbf{k}'\right)e^{i\left(\omega' t-\mathbf{k}'\cdot\mathbf{x}\right)} + \hat{a}^\dagger\left(\mathbf{k}'\right)e^{-i\left(\omega' t-\mathbf{k}'\cdot\mathbf{x}\right)}\right) \\
&= \frac{m^2}{4}\int\frac{d^3k}{\omega}\left(\hat{a}\left(\mathbf{k}\right)\hat{a}\left(-\mathbf{k}\right)e^{2i\omega t} + \hat{a}\left(\mathbf{k}\right)\hat{a}^\dagger\left(\mathbf{k}\right) + \hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}\left(\mathbf{k}\right) + \hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}^\dagger\left(-\mathbf{k}\right)e^{-2i\omega t}\right)
\end{aligned}$$

Now we can combine all three terms:

$$\begin{aligned}
\hat{H} &= \frac{\hbar}{2}\int\left(\hat{\pi}^2 + \nabla\hat{\varphi}\cdot\nabla\hat{\varphi} + m^2\hat{\varphi}^2\right)d^3x \\
&= -\frac{\hbar}{4}\int\omega d^3k\left(\hat{a}\left(\mathbf{k}\right)\hat{a}\left(-\mathbf{k}\right)e^{2i\omega t} - \hat{a}\left(\mathbf{k}\right)\hat{a}^\dagger\left(\mathbf{k}\right) - \hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}\left(\mathbf{k}\right) + \hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}^\dagger\left(-\mathbf{k}\right)e^{-2i\omega t}\right) \\
&\quad -\frac{\hbar}{4}\int\frac{\mathbf{k}\cdot\mathbf{k}}{\omega}d^3k\ \left(-\hat{a}\left(\mathbf{k}\right)\hat{a}\left(-\mathbf{k}\right)e^{2i\omega t} - \hat{a}\left(\mathbf{k}\right)\hat{a}^\dagger\left(\mathbf{k}\right) - \hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}\left(\mathbf{k}\right) - \hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}^\dagger\left(-\mathbf{k}\right)e^{-2i\omega t}\right) \\
&\quad +\frac{m^2}{4}\int\frac{d^3k}{\omega}\left(\hat{a}\left(\mathbf{k}\right)\hat{a}\left(-\mathbf{k}\right)e^{2i\omega t} + \hat{a}\left(\mathbf{k}\right)\hat{a}^\dagger\left(\mathbf{k}\right) + \hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}\left(\mathbf{k}\right) + \hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}^\dagger\left(-\mathbf{k}\right)e^{-2i\omega t}\right) \\
&= -\frac{\hbar}{4}\int\frac{d^3k}{\omega}\left(\left(\omega^2 - \mathbf{k}\cdot\mathbf{k} - m^2\right)\hat{a}\left(\mathbf{k}\right)\hat{a}\left(-\mathbf{k}\right)e^{2i\omega t} + \left(-\omega^2 - \mathbf{k}\cdot\mathbf{k} - m^2\right)\left(\hat{a}\left(\mathbf{k}\right)\hat{a}^\dagger\left(\mathbf{k}\right) + \hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}\left(\mathbf{k}\right)\right)\right) \\
&\quad +\left(\omega^2 - \mathbf{k}\cdot\mathbf{k} - m^2\right)\hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}^\dagger\left(-\mathbf{k}\right)e^{-2i\omega t}\Big) \\
&= \frac{1}{2}\int d^3k\left(\hat{a}\left(\mathbf{k}\right)\hat{a}^\dagger\left(\mathbf{k}\right) + \hat{a}^\dagger\left(\mathbf{k}\right)\hat{a}\left(\mathbf{k}\right)\right)\hbar\omega
\end{aligned}$$

This looks extremely close to the harmonic oscillator form,

$$\hat{H}_{almost} = \int d^3k\left(\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}) + \frac{1}{2}\right)\hbar\omega$$

when written in terms of the mode amplitudes $\hat{a}$ and $\hat{a}^\dagger$, and this would make good sense – it is just the energy operator for the quantum simple harmonic oscillator, summed over all modes. However, the two are far from equal. If we use the commutator of the mode amplitudes to rearrange the products, we have

$$\begin{aligned}\hat{H} &= \frac{1}{2}\int d^3k\left(\hat{a}(\mathbf{k})\hat{a}^\dagger(\mathbf{k})+\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k})\right)\hbar\omega \\ &= \int d^3k\left(\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k})+\frac{1}{2}\delta^3(\mathbf{0})\right)\hbar\omega\end{aligned}$$

so we are faced with a divergent integrand. Moreover, even without $\delta^3(0)=\infty^3$, the integral $\int d^3k\,\omega$ also diverges. We have encountered our first infinity.

2 Our first infinity

The form of the Hamiltonian found above displays an obvious problem – the order of the factors makes a difference. If we used the commutator of the mode amplitudes to put the Hamiltonian in the form of the simple harmonic oscillator, we introduce a strongly divergent term. While the constant "ground state energy" of the harmonic oscillator, $\frac{1}{2}\hbar\omega$, causes no probem in quantum mechanics, the presence of such an energy term *for each mode* of quantum field theory leads to an infinite energy for the vacuum state.

Fortunately, a simple rule allows us to eliminate this divergence throughout our calculations. To see how it works, notice that anytime we have a product of two or more fields at the same point, we develop some terms of the general form

$$\hat{\varphi}(\mathbf{x})\hat{\varphi}(\mathbf{x})\sim\hat{a}(\omega,\mathbf{k})\hat{a}^\dagger(\omega,\mathbf{k})+\ldots$$

which have $\hat{a}^\dagger(\omega,\mathbf{k})$ on the right. When such products act on the vacuum state, the $\hat{a}^\dagger(\omega,\mathbf{k})$ gives a nonvanishing contribution, and if we sum over all wave vectors we get a divergence. The solution is to impose a rule that changes the order of the creation and annihilation operators. This is called *normal ordering*, and is denoted by enclosing the product in colons. Thus, we *define* the Hamiltonian to be the normal ordered product

$$\begin{aligned}\hat{H} &= \frac{\hbar}{2}\int :\left(\hat{\pi}^2+\nabla\hat{\varphi}\cdot\nabla\hat{\varphi}+m^2\hat{\varphi}^2\right): d^3x \\ &= \frac{\hbar}{2}\int d^3k :\left(\hat{a}(\mathbf{k})\hat{a}^\dagger(\mathbf{k})+\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k})\right):\omega \\ &= \int d^3k\ \hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k})\ \hbar\omega\end{aligned}$$

We will see that this expression gives zero for the vacuum state, and is finite for all states with a finite number of particles. While this procedure may seem a bit ad hoc, recall that the ordering of operators in any quantum expression is one thing that cannot be determined from the classical framework using canonical quantization. It is therefore reasonable to use whatever ordering convention gives the most sensible results.

2.1 An aside: Working backwards

One might think that we could find a form for the finite Hamiltonian operator in terms of $\hat{\varphi}$ and $\hat{\pi}$ by working backwards from

$$:\hat{H}: \;=\; \int d^3k\ \hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k})\ \hbar\omega$$

However, we again encounter an infinite integral. Substituting

$$\hat{a}(\mathbf{k}) = \frac{\sqrt{2\omega}}{2(2\pi)^{3/2}}\int\left(\hat{\varphi}(\mathbf{x},0)-\frac{i}{\omega}\hat{\pi}(\mathbf{x},0)\right)e^{i\mathbf{k}\cdot\mathbf{x}}d^3x$$

$$\hat{a}^{\dagger}(\mathbf{k}) = \frac{\sqrt{2\omega}}{2(2\pi)^{3/2}} \int \left(\hat{\varphi}(\mathbf{x},0) + \frac{i}{\omega}\hat{\pi}(\mathbf{x},0)\right) e^{-i\mathbf{k}\cdot\mathbf{x}} d^3x$$

into $:\hat{H}:$,

$$\begin{aligned}
:\hat{H}: &= \frac{1}{2(2\pi)^3}\int d^3k\ \hbar\omega^2 \left(\int \left(\hat{\varphi}(\mathbf{x},0) + \frac{i}{\omega}\hat{\pi}(\mathbf{x},0)\right) e^{-i\mathbf{k}\cdot\mathbf{x}} d^3x\right)\left(\int \left(\hat{\varphi}(\mathbf{x}',0) - \frac{i}{\omega}\hat{\pi}(\mathbf{x}',0)\right) e^{i\mathbf{k}\cdot\mathbf{x}'} d^3x'\right) \\
&= \frac{\hbar}{2(2\pi)^3}\int d^3k \int d^3x \int d^3x' \left(\omega\hat{\varphi}(\mathbf{x},0) + i\hat{\pi}(\mathbf{x},0)\right)\left(\omega\hat{\varphi}(\mathbf{x}',0) - i\hat{\pi}(\mathbf{x}',0)\right) e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \\
&= \frac{\hbar}{2(2\pi)^3}\int d^3k \int d^3x \int d^3x' \left(\omega^2\hat{\varphi}(\mathbf{x},0)\hat{\varphi}(\mathbf{x}',0) + i\omega\left[\hat{\pi}(\mathbf{x},0),\hat{\varphi}(\mathbf{x}',0)\right] + \hat{\pi}(\mathbf{x},0)\hat{\pi}(\mathbf{x}',0)\right) e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \\
&= \frac{\hbar}{2(2\pi)^3}\int d^3k \int d^3x \int d^3x' \left(\omega^2\hat{\varphi}(\mathbf{x},0)\hat{\varphi}(\mathbf{x}',0) + i\omega i\delta^3(\mathbf{x}-\mathbf{x}') + \hat{\pi}(\mathbf{x},0)\hat{\pi}(\mathbf{x}',0)\right) e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}
\end{aligned}$$

Consider each of the terms separately.

For the final term, we may carry out the integral over d^3k,

$$\begin{aligned}
I_{\pi\pi} &= \frac{\hbar}{2(2\pi)^3}\int d^3k \int d^3x \int d^3x' \hat{\pi}(\mathbf{x},0)\hat{\pi}(\mathbf{x}',0)\, e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \\
&= \frac{\hbar}{2}\int d^3x \int d^3x' \hat{\pi}(\mathbf{x},0)\hat{\pi}(\mathbf{x}',0)\,\delta^3(\mathbf{x}-\mathbf{x}') \\
&= \frac{\hbar}{2}\int d^3x \hat{\pi}(\mathbf{x},0)\hat{\pi}(\mathbf{x},0)
\end{aligned}$$

For the middle term, we have

$$\begin{aligned}
I_{[\pi,\varphi]} &= \frac{\hbar}{2(2\pi)^3}\int d^3k \int d^3x \int d^3x' \left(-\omega\delta^3(\mathbf{x}-\mathbf{x}')\right) e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \\
&= -\frac{\hbar}{2(2\pi)^3}\int d^3k \int d^3x\,\omega
\end{aligned}$$

which diverges. Finally, if we write the frequency as,

$$\omega^2 = \mathbf{k}^2 + m^2$$

the first term is

$$\begin{aligned}
I_{\varphi\varphi} &= \frac{\hbar}{2(2\pi)^3}\int d^3k \int d^3x \int d^3x' \left(\mathbf{k}^2 + m^2\right)\hat{\varphi}(\mathbf{x},0)\hat{\varphi}(\mathbf{x}',0)\, e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \\
&= -\frac{\hbar}{2(2\pi)^3}\int d^3k \int d^3x \int d^3x' \hat{\varphi}(\mathbf{x},0)\hat{\varphi}(\mathbf{x}',0)\,\nabla^2 e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \\
&\quad + \frac{\hbar m^2}{2(2\pi)^3}\int d^3k \int d^3x \int d^3x' \hat{\varphi}(\mathbf{x},0)\hat{\varphi}(\mathbf{x}',0)\, e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \\
&= -\frac{\hbar}{2(2\pi)^3}\int d^3x \int d^3x' \hat{\varphi}(\mathbf{x},0)\hat{\varphi}(\mathbf{x}',0)\,\nabla^2 \int d^3k\, e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \\
&\quad + \frac{\hbar}{2}m^2 \int d^3x \int d^3x' \hat{\varphi}(\mathbf{x},0)\hat{\varphi}(\mathbf{x}',0)\,\delta^3(\mathbf{x}-\mathbf{x}') \\
&= -\frac{\hbar}{2}\int d^3x \int d^3x' \hat{\varphi}(\mathbf{x},0)\hat{\varphi}(\mathbf{x}',0)\,\nabla^2\delta^3(\mathbf{x}-\mathbf{x}') \\
&\quad + \frac{\hbar}{2}m^2 \int d^3x \hat{\varphi}(\mathbf{x},0)\hat{\varphi}(\mathbf{x}',0)
\end{aligned}$$

We integrate by parts in the first integral,

$$-\frac{\hbar}{2}\int d^3x\int d^3x'\hat{\varphi}(\mathbf{x},0)\hat{\varphi}\left(\mathbf{x}',0\right)\nabla^2\delta^3\left(\mathbf{x}-\mathbf{x}'\right)=\frac{\hbar}{2}\int d^3x\int d^3x'\nabla\hat{\varphi}(\mathbf{x},0)\hat{\varphi}\left(\mathbf{x}',0\right)\cdot\nabla\delta^3\left(\mathbf{x}-\mathbf{x}'\right)$$

then recognizing that $\nabla\delta^3\left(\mathbf{x}-\mathbf{x}'\right)=-\nabla'\delta^3\left(\mathbf{x}-\mathbf{x}'\right)$ we integrate by parts again,

$$\begin{aligned}-\frac{\hbar}{2}\int d^3x\int d^3x'\hat{\varphi}(\mathbf{x},0)\hat{\varphi}\left(\mathbf{x}',0\right)\nabla^2\delta^3\left(\mathbf{x}-\mathbf{x}'\right) &= +\frac{\hbar}{2}\int d^3x\int d^3x'\nabla\hat{\varphi}(\mathbf{x},0)\cdot\nabla'\hat{\varphi}\left(\mathbf{x}',0\right)\delta^3\left(\mathbf{x}-\mathbf{x}'\right) \\ &= +\frac{\hbar}{2}\int d^3x\nabla\hat{\varphi}(\mathbf{x},0)\cdot\nabla\hat{\varphi}\left(\mathbf{x},0\right)\end{aligned}$$

The three non-divergent terms reconstitute the original Hamiltonian,

$$\begin{aligned}:\hat{H}: &= \frac{\hbar}{2}\int d^3x\left(\hat{\pi}^2+\nabla\hat{\varphi}\cdot\nabla\hat{\varphi}+m^2\hat{\varphi}^2-\frac{1}{(2\pi)^3}\int d^3k\int d^3x'\omega\delta^3\left(\mathbf{x}-\mathbf{x}'\right)e^{-i\mathbf{k}\cdot\left(\mathbf{x}-\mathbf{x}'\right)}\right) \\ &= \frac{\hbar}{2}\int d^3x\left(\hat{\mathcal{H}}-\frac{1}{(2\pi)^3}\int d^3k\int d^3x'\omega\delta^3\left(\mathbf{x}-\mathbf{x}'\right)e^{-i\mathbf{k}\cdot\left(\mathbf{x}-\mathbf{x}'\right)}\right)\end{aligned}$$

but again we see the divergent integral.

At the very least, we can see that states for which $:\hat{H}:$ is finite are different from states on which $\hat{H}$ is finite.

3 States of the Klein-Gordon field

The similarity between the field Hamiltonian and the harmonic oscillator makes it easy to interpret this result. We begin the observation that the expectation values of $\hat{H}$ are bounded below. This follows because for *any* normalized state $|\alpha\rangle$ we have

$$\begin{aligned}\langle\alpha|\hat{H}|\alpha\rangle &= \langle\alpha|\int\omega:\left(\hat{a}^\dagger(\mathbf{k})\,\hat{a}(\mathbf{k})+\frac{1}{2}\right):d^3k\,|\alpha\rangle \\ &= \int\omega\ d^3k\ \langle\alpha|\,\hat{a}^\dagger(\mathbf{k})\,\hat{a}(\mathbf{k})\,|\alpha\rangle\end{aligned}$$

But if we let $|\beta\rangle=\hat{a}(\mathbf{k})|\alpha\rangle$, then $\langle\beta|=\langle\alpha|\,\hat{a}^\dagger(\mathbf{k})$, so

$$\begin{aligned}\langle\alpha|\hat{H}|\alpha\rangle &= \int\omega\ d^3k\ \langle\alpha|\,\hat{a}^\dagger(\mathbf{k})\,\hat{a}(\mathbf{k})\,|\alpha\rangle \\ &= \int\omega\ d^3k\ \langle\beta|\beta\rangle \\ &> 0\end{aligned}$$

since the integrand is positive definite. However, we can show that the action of $\hat{a}(\mathbf{k})$ lowers the eigenvalues of $\hat{H}$. For consider the commutator

$$\begin{aligned}\left[\hat{H},\hat{a}(\mathbf{k})\right] &= \left[\int\omega':\left(\hat{a}^\dagger\left(\mathbf{k}'\right)\hat{a}\left(\omega',\mathbf{k}'\right)+\frac{1}{2}\right):d^3k',\hat{a}(\mathbf{k})\right] \\ &= \int\omega'\left[\hat{a}^\dagger\left(\mathbf{k}'\right),\hat{a}(\mathbf{k})\right]\hat{a}\left(\mathbf{k}'\right)d^3k' \\ &= -\int\omega'\delta^3\left(\mathbf{k}-\mathbf{k}'\right)\hat{a}\left(\mathbf{k}'\right)d^3k' \\ &= -\omega\hat{a}(\mathbf{k})\end{aligned}$$

Therefore, if $|\alpha\rangle$ is an eigenstate of $\hat{H}$ with $\hat{H}\,|\alpha\rangle = \alpha\,|\alpha\rangle$ then so is $\hat{a}\,(\mathbf{k})\,|\alpha\rangle$ because

$$\begin{aligned}\hat{H}\left(\hat{a}\,(\mathbf{k})\,|\alpha\rangle\right) &= \left[\hat{H},\hat{a}\,(\mathbf{k})\right]|\alpha\rangle + \hat{a}\,(\mathbf{k})\,\hat{H}\,|\alpha\rangle \\ &= -\omega\hat{a}\,(\mathbf{k})\,|\alpha\rangle + \hat{a}\,(\mathbf{k})\,\alpha\,|\alpha\rangle \\ &= (\alpha-\omega)\left(\hat{a}\,(\mathbf{k})\,|\alpha\rangle\right)\end{aligned}$$

Moreover, the eigenvalue of the new eigenstate is *lower* than α. Since the eigenvalues are bounded below, there must exist a state such that

$$\hat{a}\,(\mathbf{k})\,|0\rangle = 0 \tag{3}$$

for all values of $\mathbf{k}$. The state $|0\rangle$ is called the *vacuum state* and the operators $\hat{a}\,(\mathbf{k})$ are called annihilation operators. From the vacuum state, we can construct the entire spectrum of eigenstates of the Hamiltonian. First, notice that the vacuum state is a minimal eigenstate of $\hat{H}$:

$$\begin{aligned}\hat{H}\,|0\rangle &= \int \omega' : \left(\hat{a}^\dagger\,(\mathbf{k}')\,\hat{a}\,(\mathbf{k}') + \frac{1}{2}\right) : |0\rangle\, d^3k' \\ &= \int \omega'\hat{a}^\dagger\,(\mathbf{k}')\,\hat{a}\,(\mathbf{k}')\,|0\rangle\, d^3k' \\ &= 0\end{aligned}$$

Now, we act on the vacuum state with $\hat{a}^\dagger\,(\mathbf{k})$ to produce new eigenstates.

Exercise: Prove that $|\mathbf{k}\rangle = \hat{a}^\dagger\,(\mathbf{k})\,|0\rangle$ is an eigenstate of $\hat{H}$.

We can build infinitely many states in two ways. First, just like the harmonic oscillator states, we can apply the creation operator $\hat{a}^\dagger\,(\mathbf{k})$ as many times as we like. Such a state contains multiple particles with energy ω. Second, we can apply creation operators of different $\mathbf{k}$,

$$|\mathbf{k}',\mathbf{k}\rangle = \hat{a}^\dagger\,(\mathbf{k}')\,\hat{a}^\dagger\,(\mathbf{k})\,|0\rangle = \hat{a}^\dagger\,(\mathbf{k})\,\hat{a}^\dagger\,(\mathbf{k})\,|0\rangle$$

This state contains two particles, with energies ω and ω'.

As with the harmonic oscillator, we can introduce a number operator to measure the number of quanta in a given state. The number operator is just the sum over all modes of the number operator for a given mode,

$$\begin{aligned}\hat{N} &\equiv \int : \left(\hat{a}^\dagger\,(\mathbf{k})\,\hat{a}\,(\mathbf{k})\right) : d^3k \\ &= \int \hat{a}^\dagger\,(\mathbf{k})\,\hat{a}\,(\mathbf{k})\,d^3k\end{aligned}$$

Exercise: By applying $\hat{N}$, compute the number of particles in the state

$$|\mathbf{k}',\mathbf{k}\rangle = \hat{a}^\dagger(\mathbf{k}')\hat{a}^\dagger(\mathbf{k})\,|0\rangle$$

Notice that creation and annihilation operators for different modes all commute with one another, e.g.,

$$\left[\hat{a}^\dagger(\mathbf{k}'),\hat{a}(\mathbf{k})\right] = 0$$

when $\mathbf{k}' \neq \mathbf{k}$.

4 Poincaré transformations of Klein-Gordon fields

Now let's examine the Lorentz transformation and translation properties of scalar fields. For this we need to construct quantum operators which generate the required transformations. Since the translations are the simplest, we begin with them.

We have observed that the spacetime translation generators forming a basis for the Lie algebra of translations (and part of the basis of the Poincaré Lie algebra) resemble the energy and momentum operators of quantum mechanics. Moreover, Noether's theorem tells us that energy and momentum are conserved as a result of translation symmetry of the action. We now need to bring these insights into the quantum realm.

From our discussion in Chapter 1, using the Klein-Gordon Lagrangian density we have the conserved stress-energy tensor,

$$\begin{aligned} T^{\mu\nu} &= \frac{\partial \mathcal{L}}{\partial\left(\partial_\mu \phi\right)}\partial^\nu \phi - \mathcal{L}\eta^{\mu\nu} \\ &= \partial^\mu \varphi \partial^\nu \varphi - \frac{1}{2}\eta^{\mu\nu}\left(\pi^2 - \nabla\varphi\cdot\nabla\varphi - m^2\varphi^2\right) \end{aligned}$$

which leads to the conserved charges,

$$P^\mu = \int T^{\mu 0} d^3x$$

and the natural extension of this observation is to simply replace the products of fields in $T^{\mu 0}$ with normal-ordered field operators. We therefore define

$$\hat{P}^\mu \equiv \int : \hat{T}^{\mu 0} : d^3x$$

First, for the time component,

$$\begin{aligned} \hat{P}^0 &= \int : \hat{T}^{00} : d^3x \\ &= \int : \partial^0\hat{\varphi}\partial^0\hat{\varphi} - \frac{1}{2}\eta^{00}\left(\hat{\pi}^2 - \nabla\hat{\varphi}\cdot\hat{\varphi} - m^2\hat{\varphi}^2\right) : d^3x \\ &= \frac{1}{2}\int : \hat{\pi}^2 + \nabla\hat{\varphi}\cdot\nabla\hat{\varphi} + m^2\hat{\varphi}^2 : d^3x \\ &= \hat{H} \end{aligned}$$

This is promising!

Now let's try the momentum,

$$\begin{aligned} \hat{P}^i &= \int : \hat{T}^{i0} : d^3x \\ &= \int : \partial^i\hat{\varphi}\partial^0\hat{\varphi} - \frac{1}{2}\eta^{i0}\left(\hat{\pi}^2 - \nabla\hat{\varphi}\cdot\hat{\varphi} - m^2\hat{\varphi}^2\right) : d^3x \\ &= \int : \partial^i\hat{\varphi}\ \hat{\pi} : d^3x \end{aligned}$$

Exercise: By substituting the field operators,

$$\hat{\varphi}(\mathbf{x},t) = \frac{1}{(2\pi)^{3/2}}\int \frac{d^3k}{\sqrt{2\omega}}\left(\hat{a}(\mathbf{k})\, e^{i(\omega t - \mathbf{k}\cdot\mathbf{x})} + \hat{a}^\dagger(\mathbf{k})\, e^{-i(\omega t - \mathbf{k}\cdot\mathbf{x})}\right) \tag{4}$$

$$\hat{\pi}(\mathbf{x},t) = \frac{i}{(2\pi)^{3/2}}\int \sqrt{\frac{\omega}{2}}d^3k\left(\hat{a}(\mathbf{k})\, e^{i(\omega t - \mathbf{k}\cdot\mathbf{x})} - \hat{a}^\dagger(\mathbf{k})\, e^{-i(\omega t - \mathbf{k}\cdot\mathbf{x})}\right) \tag{5}$$

into the integral for $\hat{P}^i$, show that

$$\begin{aligned}\hat{P}^i &= \frac{1}{2}\int k^i \left\{-\hat{a}(\mathbf{k})\,\hat{a}(-\mathbf{k})\,e^{2i\omega t} + \hat{a}(\mathbf{k})\,\hat{a}^\dagger(\mathbf{k})\right. \\ &\quad \left. +\hat{a}^\dagger(\mathbf{k})\,\hat{a}(\mathbf{k}) - \hat{a}^\dagger(\mathbf{k})\,\hat{a}^\dagger(-\mathbf{k})\,e^{-2i\omega t}\right\} d^3k\end{aligned}$$

The calculation is similar to the computation of the Hamiltonian operator above, except there is only one term to consider.

We can simplify this result for $\hat{P}^i$ using a parity argument. Consider the effect of parity on the first integral. Since the volume form together with the limits is invariant under $\mathbf{k} \to -\mathbf{k}$,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^3k \to \int_{\infty}^{-\infty}\int_{\infty}^{-\infty}\int_{\infty}^{-\infty}(-1)^3\,d^3k = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^3k$$

and $\omega(-\mathbf{k}) = \omega(\mathbf{k})$, we have

$$\begin{aligned}I_1 &= \frac{1}{2}\int d^3k\ k_i\ \hat{a}(\mathbf{k})\,\hat{a}(-\mathbf{k})\,e^{2i\omega t} \\ &= \frac{1}{2}\int d^3k\ \ (-k_i)\,\hat{a}(-\mathbf{k})\,\hat{a}(\mathbf{k})\,e^{2i\omega t} \\ &= -\frac{1}{2}\int d^3k\ k_i\ \hat{a}(\mathbf{k})\,\hat{a}(-\mathbf{k})\,e^{2i\omega t} \\ &= -I_1\end{aligned}$$

and therefore $I_1 = 0$. The final term in the same way, so the momentum operator reduces to

$$\begin{aligned}\hat{P}^i &= \int :\partial^i\hat{\varphi}\ \hat{\pi}: d^3x \\ &= \frac{1}{2}\int k^i\!:\left(\hat{a}(\mathbf{k})\,\hat{a}^\dagger(\mathbf{k}) + \hat{a}^\dagger(\mathbf{k})\,\hat{a}(\mathbf{k})\right): d^3k \\ &= \int k^i\ \hat{a}(\mathbf{k})\,\hat{a}^\dagger(\mathbf{k})\,d^3k\end{aligned}$$

Once again, this makes sense; moreover, they are suitable for translation generators since they all commute. We may write all four in the same form,

$$\hat{P}^\alpha = \int \hbar k^\alpha\ \hat{a}(\mathbf{k})\,\hat{a}^\dagger(\mathbf{k})\,d^3k$$

In a similar way, we can compute the operators $\hat{M}^{\alpha\beta}$, and show that the commutation relations of the full set reproduce the Poincaré Lie algebra,

$$\begin{aligned}\left[\hat{M}^{\alpha\beta}, \hat{M}^{\mu\nu}\right] &= \eta^{\beta\mu}\hat{M}^{\alpha\nu} - \eta^{\beta\nu}\hat{M}^{\alpha\mu} - \eta^{\alpha\mu}\hat{M}^{\beta\nu} - \eta^{\alpha\nu}\hat{M}^{\beta\mu} \\ \left[\hat{M}^{\alpha\beta}, \hat{P}^{\mu}\right] &= \eta^{\mu\alpha}\hat{P}^\beta - \eta^{\mu\beta}\hat{P}^\alpha \\ \left[\hat{P}^\alpha, \hat{P}^\beta\right] &= 0\end{aligned}$$

The notable accomplishment here is that we have shown that even after quantization, the symmetry algebra not only survives, but can be built from the quantum field operators. This is far from obvious, because the commutation relations for the field operators are simply imposed by the rules of canonical quantization and have nothing to do, a priori, with the commutators of the symmetry algebra. One consequence, as noted above, is that the Casimir operators of the Poincaré algebra may be used to label *quantum* states.