FREE SCALAR HAMILTONIAN AS AN INTEGRAL OF THE HAMILTONIAN DENSITY

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Reference: References: Robert D. Klauber, *Student Friendly Quantum Field Theory*, (Sandtrove Press, 2013) - Chapter 3, Problem 3.8.

The free-field Hamiltonian density used in the Klein-Gordon equation is, in terms of the field ϕ and the mass μ:

$$\mathcal{H} = \dot{\phi}\dot{\phi}^{\dagger} + \nabla\phi^{\dagger}\cdot\nabla\phi + \mu^{2}\phi^{\dagger}\phi \tag{1}$$

[I've dropped the superscript and subscript 0 to save space, but this is still a scalar Hamiltonian density with no interactions.]

The discrete plane-wave solutions of the Klein-Gordon equation are

$$\phi = \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}\left(a(\mathbf{k})\,e^{-ikx} + b^{\dagger}(\mathbf{k})\,e^{ikx}\right) \tag{2}$$

$$\dot{\phi}^{\dagger} = \sum_{\mathbf{k}'} \frac{1}{\sqrt{2V\omega_{\mathbf{k}'}}}\left(a^{\dagger}(\mathbf{k}')\,e^{ik'x} + b(\mathbf{k}')\,e^{-ik'x}\right) \tag{3}$$

Using these we can find the total Hamiltonian by integrating over 3-d space:

$$H = \int \mathcal{H}d^{3}x \tag{4}$$

In this case, we're dealing with discrete solutions over a finite volume V, such that the values of $\mathbf{k}$ are determined by the condition that an integral number of wavelengths fits into V.

Klauber works out the integral of the first two terms in 1 in his section 3.4.1 and asks us to do the third term, but it's worth looking at the technique used on the first two terms. To do the derivatives, we remember that

$$kx = k_{\mu}x^{\mu} = \omega_{\mathbf{k}}t + k_{i}x^{i} = \omega_{\mathbf{k}}t - \mathbf{k}\cdot\mathbf{x} \tag{5}$$

Therefore

$$\dot{\phi} = \sum_{\mathbf{k}} \frac{i\omega_{\mathbf{k}}}{\sqrt{2V\omega_{\mathbf{k}}}} \left(-a(\mathbf{k})\, e^{-ikx} + b^{\dagger}(\mathbf{k})\, e^{ikx}\right) \tag{6}$$

$$\dot{\phi}^{\dagger} = \sum_{\mathbf{k}'} \frac{i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}} \left(a^{\dagger}\left(\mathbf{k}'\right) e^{ik'x} - b\left(\mathbf{k}'\right) e^{-ik'x}\right) \tag{7}$$

When we calculate $\int \dot{\phi}\dot{\phi}^{\dagger} d^3x$, we get a collection of integrals of the form

$$I_{\mathbf{k}\mathbf{k}'} = \begin{cases} \int e^{ikx+ik'x} d^3x \\ \int e^{ikx-ik'x} d^3x \\ \int e^{-ikx-ik'x} d^3x \\ \int e^{-ikx+ik'x} d^3x \end{cases} \tag{8}$$

If we were integrating over an infinite volume, these would give delta functions, but over a finite volume, with the boundary conditions specified above, the functions e^{ikx} and $e^{ik'x}$ are orthogonal. Therefore, these integrals are zero unless the exponent is zero, in which case we integrate 1 over the volume V, giving V. This means that in the first and third integrals in 8, we must have $\mathbf{k} = -\mathbf{k}'$ and in the second and fourth integrals, we have $\mathbf{k} = +\mathbf{k}'$. Using this condition, and multiplying out 6 and 7 we get

$$\int \dot{\phi}\dot{\phi}^{\dagger} d^3x = \sum_{\mathbf{k}} \frac{(\omega_{\mathbf{k}})^2}{2\omega_{\mathbf{k}}} \left[-a_{\mathbf{k}} b_{-\mathbf{k}} e^{-2i\omega_{\mathbf{k}}t} + a_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} + b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} - b_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} e^{2i\omega_{\mathbf{k}}t}\right] \tag{9}$$

Since we're summing over all $\mathbf{k}$, positive and negative, we can flip the sign of $\mathbf{k}$ in the first and fourth terms to give (remember that $\omega_{\mathbf{k}} = \omega_{-\mathbf{k}}$):

$$\int \dot{\phi}\dot{\phi}^{\dagger} d^3x = \sum_{\mathbf{k}} \frac{(\omega_{\mathbf{k}})^2}{2\omega_{\mathbf{k}}} \left[-a_{-\mathbf{k}} b_{\mathbf{k}} e^{-2i\omega_{\mathbf{k}}t} + a_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} + b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} - b_{-\mathbf{k}}^{\dagger} a_{\mathbf{k}}^{\dagger} e^{2i\omega_{\mathbf{k}}t}\right] \tag{10}$$

To integrate the gradient terms, we have

$$\nabla\phi^{\dagger} \cdot \nabla\phi = -\partial_i \phi^{\dagger} \partial^i \phi = \sum_i \partial_i \phi^{\dagger} \partial_i \phi \tag{11}$$

[The minus sign is because $\partial_i = -\partial^i$ for spatial components.] Klauber gives the details in his equation 3-52, but the procedure is similar to that for calculating $\dot{\phi}$ above. We have, using 5 and $\partial_i e^{ikx} = -ik_i$:

$$\partial_i \phi^\dagger = \sum_{\mathbf{k}'} \frac{-ik'_i}{\sqrt{2V\omega_{\mathbf{k}'}}} \left(a^\dagger \left(\mathbf{k}'\right) e^{ik'x} - b\left(\mathbf{k}'\right) e^{-ik'x} \right) \tag{12}$$

$$\partial_i \phi = \sum_{\mathbf{k}} \frac{-ik_i}{\sqrt{2V\omega_{\mathbf{k}}}} \left(-a\left(\mathbf{k}\right) e^{-ikx} + b^\dagger \left(\mathbf{k}\right) e^{ikx} \right) \tag{13}$$

Multiplying the two terms together and integrating, again using the orthonormality of the exponentials so that $\mathbf{k} = \pm\mathbf{k}'$, depending on the term, gives

$$\int \nabla\phi^\dagger \cdot \nabla\phi d^3x = \sum_{\mathbf{k}} \frac{1}{2\omega_{\mathbf{k}}} \left[k_i(-k_i) \left(-b_{\mathbf{k}} a_{-\mathbf{k}} e^{-2i\omega_{\mathbf{k}}t} - a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} e^{2i\omega_{\mathbf{k}}t} \right) + k_i k_i \left(a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + b_{\mathbf{k}} b^\dagger_{\mathbf{k}} \right) \right] \tag{14}$$

$$= \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2\omega_{\mathbf{k}}} \left[b_{\mathbf{k}} a_{-\mathbf{k}} e^{-2i\omega_{\mathbf{k}}t} + a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} e^{2i\omega_{\mathbf{k}}t} + a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + b_{\mathbf{k}} b^\dagger_{\mathbf{k}} \right] \tag{15}$$

Finally, for the third term in 1 we have

$$\mu^2 \int \phi^\dagger \phi d^3x = \mu^2 \int d^3x \left[\sum_{\mathbf{k}'} \frac{1}{\sqrt{2V\omega_{\mathbf{k}'}}} \left(a^\dagger \left(\mathbf{k}'\right) e^{ik'x} + b\left(\mathbf{k}'\right) e^{-ik'x} \right) \right] \times \left[\sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left(a\left(\mathbf{k}\right) e^{-ikx} + b^\dagger\left(\mathbf{k}\right) e^{ikx} \right) \right] \tag{16}$$

$$\sum_{\mathbf{k}} \frac{\mu^2}{2\omega_{\mathbf{k}}} \left[a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + b_{\mathbf{k}} b^\dagger_{\mathbf{k}} + b_{\mathbf{k}} a_{-\mathbf{k}} e^{-2i\omega_{\mathbf{k}}t} + a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} e^{2i\omega_{\mathbf{k}}t} \right] \tag{17}$$

From the relativistic energy formula (in natural units)

$$\omega^2_{\mathbf{k}} = \mathbf{k}^2 + \mu^2 \tag{18}$$

we can add 15 and 17 to get

$$\mu^2 \int \phi^\dagger \phi d^3x \int \nabla\phi^\dagger \cdot \nabla\phi d^3x + = \sum_{\mathbf{k}} \frac{\omega^2_{\mathbf{k}}}{2\omega_{\mathbf{k}}} \left[a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + b_{\mathbf{k}} b^\dagger_{\mathbf{k}} + b_{\mathbf{k}} a_{-\mathbf{k}} e^{-2i\omega_{\mathbf{k}}t} + a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} e^{2i\omega_{\mathbf{k}}t} \right] \tag{19}$$

To add this to 10, we need to use the commutators

$$\left[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}'} \right] = \left[b_{\mathbf{k}}, b^\dagger_{\mathbf{k}'} \right] = \delta_{\mathbf{k}\mathbf{k}'} \tag{20}$$

Then 10 and 19 become

$$\int \dot{\phi}\dot{\phi}^{\dagger}d^{3}x=\sum_{\mathbf{k}}\frac{(\omega_{\mathbf{k}})^{2}}{2\omega_{\mathbf{k}}}\left[-a_{-\mathbf{k}}b_{\mathbf{k}}e^{-2i\omega_{\mathbf{k}}t}+a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+1+b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}-b_{-\mathbf{k}}^{\dagger}a_{\mathbf{k}}^{\dagger}e^{2i\omega_{\mathbf{k}}t}\right] \tag{21}$$

$$\mu^{2}\int \phi^{\dagger}\phi d^{3}x\int \nabla\phi^{\dagger}\cdot\nabla\phi d^{3}x+=\sum_{\mathbf{k}}\frac{\omega_{\mathbf{k}}^{2}}{2\omega_{\mathbf{k}}}\left[a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}+1+b_{\mathbf{k}}a_{-\mathbf{k}}e^{-2i\omega_{\mathbf{k}}t}+a_{\mathbf{k}}^{\dagger}b_{-\mathbf{k}}^{\dagger}e^{2i\omega_{\mathbf{k}}t}\right] \tag{22}$$

Adding them gives

$$\begin{aligned} H &= \int \mathcal{H}d^{3}x=\sum_{\mathbf{k}}\omega_{\mathbf{k}}\left[a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\frac{1}{2}+b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}+\frac{1}{2}\right] &(23)\\ &= \sum_{\mathbf{k}}\omega_{\mathbf{k}}\left[N_{a}(\mathbf{k})+\frac{1}{2}+N_{b}(\mathbf{k})+\frac{1}{2}\right] &(24)\end{aligned}$$

where N_a and N_b are the number operators that we met earlier, although in a continuous system.

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