Quantum Mechanics II
Solution Sheet 11

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Exercise 11.1 About the one-particle interpretation of the Klein-Gordon equation

a) Using the correspondence principle, the energy-momentum relation in relativistic classical mechanics takes the form $(-\hbar^2\partial_t^2)\Psi = (-c^2\hbar^2\nabla^2 + m^2c^4)\Psi$ which can be written in the covariant form ($c \equiv 1 \equiv \hbar$),

$$[\partial_\mu\partial^\mu + m^2]\Psi(x) = 0, \tag{1}$$

with $x^\mu = (t, \mathbf{r})$, $\partial_\mu = (\partial_t, \nabla)$, and $\partial^\mu = (\partial_t, -\nabla)$. Note that this Klein-Gordon equation, like the Schrödinger equation, is not an operator identity but a differential equation for the wave function $\Psi(x)$.
Taking the classical relation $E = \pm c(\mathbf{p}^2+m^2c^2)^{1/2}$ as a starting point for the corresponding quantum theory would lead to the following differential equation

$$i\hbar\partial_t\Psi(x) = \sqrt{-c^2\hbar^2\nabla^2 + m^2c^4}\,\Psi(x), \tag{2}$$

which is not manifestly covariant; it does not treat the space and time coordinates in an equivalent way. Note that the Schrödinger equation, accounting for nonrelativistic phenomena, must only be invariant with respect to Galilei transformations where space and time coordinates may enter differently. In addition, the expansion of the square root includes derivatives ∇ up to infinite order leading to non-locality and causality problems (for more details see e.g. G. Baym *Lectures on Quantum Mechanics*).
The Klein-Gordon equation (2) has several unusual features. Unlike the nonrelativistic Schrödinger equation, it is second order in time and thus twice as much informationäbout the particle is needed in order to specify its state as nonrelativistically, i.e., both $\Psi(t_0, \mathbf{r})$ and $\partial_t\Psi(t_0, \mathbf{r})$ at some initial time t_0. It turns out that this extra degree of freedom corresponds to specifying the *charge* (see below) of the particle; the Klein-Gordon equation describes both a particle and its antiparticle in one fell swoop. Closely related to this is the fact that Eq. (2) possesses free particle solutions $\propto \exp[i(\mathbf{p}\cdot\mathbf{r} - Et)/\hbar]$ with either sign of the energy, $E = \pm c(\mathbf{p}^2 + m^2c^2)^{1/2}$.

With the substitutions $E \to E - e\Phi$, $\mathbf{p} \to \mathbf{p} - e\mathbf{A}/c$, and the correspondence principle, one finds for the Klein-Gordon equation of a charged particle in the presence of an electromagnetic field,

$$[-(i\partial_\mu - eA_\mu)(i\partial^\mu - eA^\mu) + m^2]\Psi(x) = 0, \tag{3}$$

with the four-vector $A^\mu = (\Phi, \mathbf{A})$.

b) By straight-forward calculation one finds,

$$\begin{aligned}
\partial_t\rho + \nabla\cdot\mathbf{j} =& \frac{i\hbar}{2mc^2}[\partial_t\Psi^*\partial_t\Psi + \Psi^*\partial_t^2\Psi - \partial_t\Psi\partial_t\Psi^* - \Psi\partial_t^2\Psi^*] \\
&+ \frac{\hbar}{2im}[\nabla\Psi^*\cdot\nabla\Psi + \Psi^*\nabla^2\Psi - \nabla\Psi\cdot\nabla\Psi^* - \Psi\nabla^2\Psi^*] \\
=& \frac{i\hbar}{2m}\left\{\Psi^*\left[\frac{1}{c^2}\partial_t^2 - \nabla^2\right]\Psi - \Psi\left[\frac{1}{c^2}\partial_t^2 - \nabla^2\right]\Psi^*\right\} \\
=& \frac{i\hbar}{2m}\left\{\Psi^*\underbrace{\left[\frac{1}{c^2}\partial_t^2 - \nabla^2 + \left(\frac{mc}{\hbar}\right)^2\right]\Psi}_{=0\text{ (KG-Eq.)}} - \Psi\underbrace{\left[\frac{1}{c^2}\partial_t^2 - \nabla^2 + \left(\frac{mc}{\hbar}\right)^2\right]\Psi^*}_{=0\text{ (KG-Eq.)}}\right\} \\
=& 0,
\end{aligned} \tag{4}$$

where in the last line we have made use of the fact that Ψ and Ψ^* are both solutions of the Klein-Gordon equation. With result (4) follows immediately that

$$
\begin{aligned}
\partial_t \int_V d\mathbf{r}\, \rho(t,\mathbf{r}) &= \int_V d\mathbf{r}\, \partial_t \rho(t,\mathbf{r}) \\
&= -\int_V d\mathbf{r}\, \nabla \cdot \mathbf{j}(t,\mathbf{r}) \\
&= -\int_{\partial V} d\mathbf{A} \cdot \mathbf{j}(t,\mathbf{r}) \\
&= 0,
\end{aligned} \tag{5}
$$

since the current density vanishes at the system boundary ∂V. Thus, we have $\int_V d\mathbf{r}\, \rho(t,\mathbf{r}) = const.$ Yet, this constant may be negative as can be seen by explicitly evaluating it for instance for the negative energy solution of a free particle, $\Psi^{(-)}(t,\mathbf{r}) = N \exp\left[i(\mathbf{p}\cdot\mathbf{r} + Et)/\hbar\right]$ with the normalization factor N (up to the sign),

$$
\int_V d\mathbf{r}\, \rho(t,\mathbf{r}) = |N|^2 \int_V d\mathbf{r}\, e^{-i(\mathbf{p}\cdot\mathbf{r}+Et)/\hbar} \Big(\frac{-E}{2mc^2} - \frac{E}{2mc^2}\Big) e^{i(\mathbf{p}\cdot\mathbf{r}+Et)/\hbar} = -1. \tag{6}
$$

Even though a negative probability density does not make sense the Klein-Gordon equation still describes a consistent theory if the one-particle picture is abandoned; the quantities ρ and $\mathbf{j}$ no longer represent the probability density and current but may be reinterpreted as charge density ρ_c and charge current $\mathbf{j}_c$ where, depending on the specific system, the charge stands for electromagnetic charge, the hypercharge, the strangeness,... The continuity equation states the conservation law of this charge. Since particles and their corresponding antiparticles are oppositely charged the theory allows for the creation and annihilation of particle-antiparticle pairs. Within this formalism, the solutions with negative energy and norm represent antiparticles with positive energy and norm.

Exercise 11.2 About the classical Klein-Gordon field and its quantization

a) The verification of the claims is absolutely straight forward if one recalls that $a_\mu a^\mu = a_0^2 - a_1^2 - a_2^2 - a_3^2$.

b) Our goal is the proof of the equivalence of the quantization scheme

$$
\begin{aligned}
&[\phi(t,\mathbf{x}), \pi(t,\mathbf{x}')] = i\delta(\mathbf{x}-\mathbf{x}'), \\
&[\phi(t,\mathbf{x}), \phi(t,\mathbf{x}')] = [\pi(\mathbf{x},t), \pi(\mathbf{x}',t)] = 0
\end{aligned} \tag{7}
$$

on the one hand and

$$
\begin{aligned}
&[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}] = \delta(\mathbf{k}-\mathbf{k}'), \\
&[a_{\mathbf{k}}, a_{\mathbf{k}'}] = [a^\dagger_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}] = 0.
\end{aligned} \tag{8}
$$

on the other hand.

Proof of "⇐":

$$
\begin{aligned}
[\phi(t,\mathbf{x}),\pi(t,\mathbf{y})] &= \frac{i}{2(2\pi)^3}\int\frac{d^3k}{\sqrt{\omega_\mathbf{k}}}\int d^3q\sqrt{\omega_\mathbf{q}}\,[a_\mathbf{k}e^{i(\mathbf{kx}-\omega_\mathbf{k}t)}+a^\dagger_\mathbf{k}e^{-i(\mathbf{kx}-\omega_\mathbf{k}t)},\\
&\quad -a_\mathbf{q}e^{i(\mathbf{qy}-\omega_\mathbf{q}t)}+a^\dagger_\mathbf{q}e^{-i(\mathbf{qy}-\omega_\mathbf{q}t)}]\\
&= \frac{i}{2(2\pi)^3}\int\frac{d^3k}{\sqrt{\omega_\mathbf{k}}}\int d^3q\sqrt{\omega_\mathbf{q}}\,\left(0+e^{i\cdots}[a_\mathbf{k},a^\dagger_\mathbf{q}]-e^{i\cdots}[a^\dagger_\mathbf{k},a_\mathbf{q}]+0\right)\\
&= \frac{i}{2(2\pi)^3}\int\frac{d^3k}{\sqrt{\omega_\mathbf{k}}}\int d^3q\sqrt{\omega_\mathbf{q}}\,\left(e^{i\cdots}\delta(\mathbf{k}-\mathbf{q})+e^{i\cdots}\delta(\mathbf{q}-\mathbf{k})\right)\\
&= \frac{i}{2(2\pi)^3}\int\frac{d^3k}{\sqrt{\omega_\mathbf{k}}}\sqrt{\omega_\mathbf{k}}\,\left(e^{i[\mathbf{k}(\mathbf{x}-\mathbf{y})+0]}-e^{i[-\mathbf{k}(\mathbf{x}-\mathbf{y})+0]}\right)\\
&= \frac{i}{2(2\pi)^3}\left((2\pi)^3\delta(\mathbf{x}-\mathbf{y})+(2\pi)^3\delta(\mathbf{x}-\mathbf{y})\right)\\
&= i\delta(\mathbf{x}-\mathbf{y})
\end{aligned}
$$

Proof of "⇒": Define

$$
f_k(t,\mathbf{x}) := \frac{1}{\sqrt{(2\pi)^3 2\omega_\mathbf{k}}}e^{i(\mathbf{kx}-\omega_\mathbf{k}t)}. \tag{9}
$$

and

$$
F(t)\overleftrightarrow{\partial_0}G(t) := F(t)\frac{\partial G(t)}{\partial t}-\frac{\partial F(t)}{\partial t}G(t). \tag{10}
$$

To show the "⇒"-direction we first have to proof the following four claims:

Claim 1: $\int d^3x\, f_k(t,\mathbf{x})i\overleftrightarrow{\partial_0}f^*_q(t,\mathbf{x}) = -\delta(\mathbf{k}-\mathbf{q})$
Proof:

$$
\begin{aligned}
LHS &= i\int d^3x\, f_k(\partial_0 f^*_q)-(\partial_0 f_k)f^*_q\\
&= i\int d^3x\,\frac{1}{(2\pi)^3\sqrt{2\omega_\mathbf{k}2\omega_\mathbf{q}}}\left[e^{i(\mathbf{kx}-\omega_\mathbf{k}t)}(i\omega_\mathbf{q})e^{-i(\mathbf{qx}-\omega_\mathbf{q}t)}-(-i\omega_\mathbf{k})e^{i(\mathbf{kx}-\omega_\mathbf{k}t)}e^{-i(\mathbf{qx}-\omega_\mathbf{q}t)}\right]\\
&= -\int d^3x\,\frac{1}{(2\pi)^3\sqrt{2\omega_\mathbf{k}}}\sqrt{\frac{2\omega_\mathbf{q}}{2}}e^{i(\mathbf{k}-\mathbf{q})\mathbf{x}}e^{i(\omega_\mathbf{q}-\omega_\mathbf{k})t}-\int d^3x\,\frac{1}{(2\pi)^3\sqrt{2\omega_\mathbf{q}}}\sqrt{\frac{2\omega_\mathbf{k}}{2}}e^{i(\mathbf{k}-\mathbf{q})\mathbf{x}}e^{i(\omega_\mathbf{q}-\omega_\mathbf{k})t}\\
&= -\delta(\mathbf{k}-\mathbf{q})
\end{aligned}
$$

Claim 2a: $\int d^3x\, f_k(t,\mathbf{x})i\overleftrightarrow{\partial_0}f_q(t,\mathbf{x}) = 0$
Proof:

$$
\begin{aligned}
LHS &= i\int d^3x\,\frac{1}{2(2\pi)^3\sqrt{\omega_\mathbf{k}\omega_\mathbf{q}}}\left((-\omega_\mathbf{q})e^{i(\mathbf{k}+\mathbf{q})\mathbf{x}}e^{-i(\omega_\mathbf{k}+\omega_\mathbf{q})t}-(-\omega_\mathbf{k})e^{i(\mathbf{k}+\mathbf{q})\mathbf{x}}e^{-i(\omega_\mathbf{k}+\omega_\mathbf{q})t}\right)\\
&= i\frac{1}{2\sqrt{\omega_\mathbf{k}\omega_\mathbf{q}}}\left((-\omega_\mathbf{q})\delta(\mathbf{k}+\mathbf{q})e^{-i(\omega_\mathbf{k}+\omega_\mathbf{q})t}-(-\omega_\mathbf{k})\delta(\mathbf{k}+\mathbf{q})e^{-i(\omega_\mathbf{k}+\omega_\mathbf{q})t}\right)\\
&= 0
\end{aligned}
$$

Claim 2b: $\int d^3x\, f^*_k(t,\mathbf{x})i\overleftrightarrow{\partial_0}f^*_q(t,\mathbf{x}) = 0$
Proof: cf. proof of claim 2a.

Claim 3: $a^\dagger_\mathbf{k} = \int d^3x\,\phi(t,\mathbf{x})i\overleftrightarrow{\partial_0}f_k(t,\mathbf{x})$

Proof:

$$
\begin{aligned}
RHS &= \int d^3x \left(\int d^3q \, f_q(t,\mathbf{x}) a_{\mathbf{q}} + f_q^*(t,\mathbf{x}) a_{\mathbf{q}}^\dagger \right) i\overleftrightarrow{\partial_0} f_k(t,\mathbf{x}) \\
&= \int d^3q \left(\int d^3x \, f_q(t,\mathbf{x}) i\overleftrightarrow{\partial_0} f_k(t,\mathbf{x}) \right) a_{\mathbf{q}} + \int d^3q \left(\int d^3x \, f_q^*(t,\mathbf{x}) i\overleftrightarrow{\partial_0} f_k(t,\mathbf{x}) \right) a_{\mathbf{q}}^\dagger \\
&= -\int d^3q \int d^3q \left(\int d^3x \, f_k(t,\mathbf{x}) i\overleftrightarrow{\partial_0} f_q^*(t,\mathbf{x}) \right) a_{\mathbf{q}}^\dagger \\
&= -(-\delta(k-q)) a_{\mathbf{k}}^\dagger \\
&= a_{\mathbf{k}}^\dagger
\end{aligned}
$$

In the last equation we have used claim 1 and 2a.

Claim 4: $a_{\mathbf{k}} = \int d^3x \, f_k^*(t,\mathbf{x}) i\overleftrightarrow{\partial_0} \phi(t,\mathbf{x})$

Proof:

$$
\begin{aligned}
RHS &= \int d^3x \, f_k^*(t,\mathbf{x}) i\overleftrightarrow{\partial_0} \left(\int d^3q \, f_q(t,\mathbf{x}) a_{\mathbf{q}} + f_q^*(t,\mathbf{x}) a_{\mathbf{q}}^\dagger \right) \\
&= \int d^3q \int d^3x \, f_k^*(t,\mathbf{x}) i\overleftrightarrow{\partial_0} f_q(t,\mathbf{x}) a_{\mathbf{q}} + 0 \\
&= -\int d^3q \int d^3x \, f_q(t,\mathbf{x}) i\overleftrightarrow{\partial_0} f_k^*(t,\mathbf{x}) a_{\mathbf{q}} \\
&= -\int d^3q \, (-\delta(q-k)) a_{\mathbf{q}} \\
&= a_k
\end{aligned}
$$

Here we have used claim 2b and claim 1.

Now we are ready to go back to the main statement:

$$
\begin{aligned}
[a_{\mathbf{k}}, a_{\mathbf{q}}^\dagger] &= \left[\int d^3x \, f_k^*(t,\mathbf{x}) i\overleftrightarrow{\partial_0} \phi(t,\mathbf{x}), \int d^3y \, \phi(t,\mathbf{y}) i\overleftrightarrow{\partial_0} f_k(t,\mathbf{y}) \right] \\
&= -\int d^3x \int d^3y \, [f_k^*(t,\mathbf{x}) i\overleftrightarrow{\partial_0} \phi(t,\mathbf{x}), \phi(t,\mathbf{y}) i\overleftrightarrow{\partial_0} f_k(t,\mathbf{y})] \\
&= -\int d^3x \int d^3y \, [f_k^*(t,\mathbf{x})(\partial_0\phi)(t,\mathbf{x}) - (\partial_0 f_k^*)(t,\mathbf{x})\phi(t,\mathbf{x}), \phi(t,\mathbf{y})(\partial_0 f_q)(t,\mathbf{y}) - (\partial_0\phi)(t,\mathbf{y}) f_q(t,\mathbf{y})] \\
&= -\int d^3x \int d^3y \, [f_k^*(t,\mathbf{x})\pi(t,\mathbf{x}) - (\partial_0 f_k^*)(t,\mathbf{x})\phi(t,\mathbf{x}), \phi(t,\mathbf{y})(\partial_0 f_q)(t,\mathbf{y}) - \pi(t,\mathbf{y}) f_q(t,\mathbf{y})] \\
&= -\int d^3x \int d^3y \, (f_k^*(t,\mathbf{x})(\partial_0 f_q)(t,\mathbf{y})[\pi(t,\mathbf{x}), \phi(t,\mathbf{y})] - 0 - 0 + (\partial_0 f_k^*)(t,\mathbf{x}) f_q(t,\mathbf{y})[\phi(t,\mathbf{x}), \pi(t,\mathbf{y})] \\
&= -\int d^3x \int d^3y \, (f_k^*(t,\mathbf{x})(\partial_0 f_q)(t,\mathbf{y})(-i)\delta(\mathbf{y}-\mathbf{x}) + (\partial_0 f_k^*)(t,\mathbf{x}) f_q(t,\mathbf{y}) i\delta(\mathbf{x}-\mathbf{y})) \\
&= i \int d^3y f_k^*(t,\mathbf{y})(\partial_0 f_q)(t,\mathbf{y}) - i \int d^3x (\partial_0 f_k^*)(t,\mathbf{x}) f_q(t,\mathbf{x}) \\
&= -\int d^3z f_q)(t,\mathbf{z}) i\overleftrightarrow{\partial_0} f_k^*)(t,\mathbf{z}) \\
&= \delta(\mathbf{q}-\mathbf{k}) = \delta(\mathbf{k}-\mathbf{q})
\end{aligned}
$$

We have used the definition of π and the assumed commutation relations for ϕ and π.

c) It suffices to discuss the claim $\phi(t,\mathbf{x})|0\rangle = |x\rangle$ because $\phi^\dagger(t,\mathbf{x}) = \phi(t,\mathbf{x})$. Define

$$
|\mathbf{p}\rangle := \sqrt{2\omega_{\mathbf{p}}} e^{i\omega_p t} a_{\mathbf{p}}^\dagger |0\rangle. \tag{11}
$$

Then

$$\begin{aligned}
\phi(t,\mathbf{x})|0\rangle &= \int \frac{d^3q}{\sqrt{(2\pi)^3 2\omega_{\mathbf{q}}}}\, a^\dagger_{\mathbf{q}} e^{-i(\mathbf{qx}-\omega_{\mathbf{q}}t)}|0\rangle \\
&= \int d^3k\, |\mathbf{k}\rangle\langle\mathbf{k}| \int \frac{d^3q}{\sqrt{(2\pi)^3 2\omega_{\mathbf{q}}}}\, a^\dagger_{\mathbf{q}} e^{-i(\mathbf{qx}-\omega_{\mathbf{q}}t)}|0\rangle \\
&= \int d^3k\, |\mathbf{k}\rangle\langle 0|\sqrt{2\omega_{\mathbf{p}}}e^{-i\omega_p t} a_{\mathbf{k}} \int \frac{d^3q}{\sqrt{(2\pi)^3 2\omega_{\mathbf{q}}}}\, a^\dagger_{\mathbf{q}} e^{-i(\mathbf{qx}-\omega_{\mathbf{q}}t)}|0\rangle \\
&= \int d^3k \int \frac{d^3q}{\sqrt{(2\pi)^3 2\omega_{\mathbf{q}}}} \sqrt{2\omega_{\mathbf{p}}} e^{i(\omega_p-\omega_k)t} e^{-i\mathbf{qx}}\, |\mathbf{k}\rangle\langle 0|a_{\mathbf{k}} a^\dagger_{\mathbf{q}}|0\rangle .
\end{aligned}$$

The observation

$$\langle 0|a_{\mathbf{k}} a^\dagger_{\mathbf{q}}|0\rangle = \langle 0|[a_{\mathbf{k}}, a^\dagger_{\mathbf{q}}]|0\rangle = \delta(\mathbf{k}-\mathbf{q}) \tag{12}$$

then leads to

$$\phi(t,\mathbf{x})|0\rangle = \frac{1}{(2\pi)^{3/2}} \int d^3k\, e^{-i\mathbf{qx}}|\mathbf{k}\rangle = |\mathbf{x}\rangle \tag{13}$$

d) Define

$$f_k(t,\mathbf{x}) := \frac{1}{\sqrt{(2\pi)^3 2\omega_{\mathbf{k}}}} e^{i(\mathbf{kx}-\omega_{\mathbf{k}}t)}, \tag{14}$$

such that

$$\phi(t,\mathbf{x}) = \int d^3k\, f_k(t,\mathbf{x}) a_{\mathbf{k}} + f_k^*(t,\mathbf{x}) a^\dagger_{\mathbf{k}}. \tag{15}$$

We are now computing the Hamiltonian

$$H = \frac{1}{2}\int d^3x\, \pi^2 + (\nabla\phi)^2 + m^2\phi^2 \tag{16}$$

by considering the contributions ϕ^2, $\dot\phi^2$ and $(\nabla\phi)^2$ separately:

$$\int d^3x\, \phi^2 = \int d^3x d^3k d^3q\, \left(f_k(t,\mathbf{x}) a_{\mathbf{k}} + f_k^*(t,\mathbf{x}) a^\dagger_{\mathbf{k}}\right)\left(f_q(t,\mathbf{x}) a_{\mathbf{q}} + f_q^*(t,\mathbf{x}) a^\dagger_{\mathbf{q}}\right). \tag{17}$$

The terms $f_k f_q a_{\mathbf{k}} a_{\mathbf{q}}$ and $f_k^* f_q^* a^\dagger_{\mathbf{k}} a^\dagger_{\mathbf{q}}$ would lead to time-dependent terms (which we do not have to consider in this exercise) in the following calculation. We thus set them to zero right now such that the formulas are less cumbersome. We thus get

$$\begin{aligned}
\int d^3x\, \phi^2 &\sim \int d^3x d^3k d^3q\, \left(f_k f_q^* a_{\mathbf{k}} a^\dagger_{\mathbf{q}} + f_k^* f_q a^\dagger_{\mathbf{k}} a_{\mathbf{q}}\right) \\
&= \int d^3x d^3k d^3q\, \frac{1}{(2\pi)^3}\frac{1}{\sqrt{2\omega_{\mathbf{k}} 2\omega_{\mathbf{q}}}} \left(e^{i(\mathbf{k}-\mathbf{q})\mathbf{x}} e^{i(-\omega_{\mathbf{k}}+\omega_{\mathbf{q}})t} a_{\mathbf{k}} a^\dagger_{\mathbf{q}} + e^{i(-\mathbf{k}+\mathbf{q})\mathbf{x}} e^{i(\omega_{\mathbf{k}}-\omega_{\mathbf{q}})t} a^\dagger_{\mathbf{k}} a_{\mathbf{q}}\right) \\
&= \int d^3k d^3q\, \frac{1}{\sqrt{2\omega_{\mathbf{k}} 2\omega_{\mathbf{q}}}} \left(\delta(\mathbf{k}-\mathbf{q}) e^{i(-\omega_{\mathbf{k}}+\omega_{\mathbf{q}})t} a_{\mathbf{k}} a^\dagger_{\mathbf{q}} + \delta(\mathbf{q}-\mathbf{k}) e^{i(\omega_{\mathbf{k}}-\omega_{\mathbf{q}})t} a^\dagger_{\mathbf{k}} a_{\mathbf{q}}\right) \\
&= \int d^3k\, \frac{1}{2\omega_{\mathbf{k}}} \left(a_{\mathbf{k}} a^\dagger_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a_{\mathbf{k}}\right)
\end{aligned}$$

using

$$\int d^3y\, e^{i\mathbf{yx}} = (2\pi)^3\delta(\mathbf{x}). \tag{18}$$

The starting point for the $\dot\phi^2$-contribution is

$$\int d^3x\, \dot\phi^2 = \int d^3x d^3k d^3q\, i\omega_{\mathbf{k}} \left(-f_k(t,\mathbf{x}) a_{\mathbf{k}} + f_k^*(t,\mathbf{x}) a^\dagger_{\mathbf{k}}\right) i\omega_{\mathbf{q}} \left(-f_q(t,\mathbf{x}) a_{\mathbf{q}} + f_q^*(t,\mathbf{x}) a^\dagger_{\mathbf{q}}\right). \tag{19}$$

Again we drop the same terms as before to get

$$
\begin{aligned}
\int d^3x\,\dot{\phi}^2 &\sim -\int d^3x d^3k d^3q\,\omega_{\mathbf{k}}\omega_{\mathbf{q}}\left(-f_k f_q^* a_{\mathbf{k}} a_{\mathbf{q}}^\dagger - f_k^* f_q a_{\mathbf{k}}^\dagger a_{\mathbf{q}}\right) \\
&= \int d^3x d^3k d^3q\,\frac{1}{(2\pi)^3}\frac{1}{\sqrt{2\omega_{\mathbf{k}}2\omega_{\mathbf{q}}}}\omega_{\mathbf{k}}\omega_{\mathbf{q}}\left(e^{i(\mathbf{k}-\mathbf{q})\mathbf{x}}e^{i(-\omega_{\mathbf{k}}+\omega_{\mathbf{q}})t}a_{\mathbf{k}}a_{\mathbf{q}}^\dagger + e^{i(-\mathbf{k}+\mathbf{q})\mathbf{x}}e^{i(\omega_{\mathbf{k}}-\omega_{\mathbf{q}})t}a_{\mathbf{k}}^\dagger a_{\mathbf{q}}\right) \\
&= \int d^3k d^3q\,\frac{1}{\sqrt{2\omega_{\mathbf{k}}2\omega_{\mathbf{q}}}}\omega_{\mathbf{k}}\omega_{\mathbf{q}}\left(\delta(\mathbf{k}-\mathbf{q})e^{i(-\omega_{\mathbf{k}}+\omega_{\mathbf{q}})t}a_{\mathbf{k}}a_{\mathbf{q}}^\dagger + \delta(\mathbf{q}-\mathbf{k})e^{i(\omega_{\mathbf{k}}-\omega_{\mathbf{q}})t}a_{\mathbf{k}}^\dagger a_{\mathbf{q}}\right) \\
&= \int d^3k\,\frac{1}{2}\omega_{\mathbf{k}}\left(a_{\mathbf{k}}a_{\mathbf{k}}^\dagger + a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right)
\end{aligned}
$$

The treatment of the $(\nabla\phi)^2$-contribution is absolutely similar. One ends up with

$$
\int d^3x\,(\nabla\phi)^2 = \int d^3k\,\frac{1}{2\omega_{\mathbf{k}}}\mathbf{k}^2\left(a_{\mathbf{k}}a_{\mathbf{k}}^\dagger + a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right) \tag{20}
$$

The combination of these results leads to (using $\omega_{\mathbf{k}}^2 = m^2 + \mathbf{k}^2$)

$$
\begin{aligned}
H &= \frac{1}{2}\int d^3x\,\pi^2 + (\nabla\phi)^2 + m^2\phi^2 \\
&\sim \frac{1}{2}\int d^3k\,\frac{1}{2\omega_{\mathbf{k}}}\left(m^2 + \omega_{\mathbf{k}}^2 + \mathbf{k}^2\right)\left(a_{\mathbf{k}}a_{\mathbf{k}}^\dagger + a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right) \\
&= \frac{1}{2}\int d^3k\,\omega_{\mathbf{k}}\left(a_{\mathbf{k}}a_{\mathbf{k}}^\dagger + a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right) \\
&= \frac{1}{2}\int d^3k\,\omega_{\mathbf{k}}\left(2a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + [a_{\mathbf{k}}, a_{\mathbf{k}}^\dagger]\right) \\
&= \int d^3k\,\omega_{\mathbf{k}}\left(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2}\delta(0)\right)
\end{aligned}
$$