Physics 563 (Quantum Field Theory 1) Fall 2009

Solution to: problem set 4, question 1

In a discretized Klein-Gordon theory, we have a quantum-mechanical system with generalized coordinates $\phi(t, n_1, n_2, n_3)$ and

$$L = \sum_{\mathbf{n}} a^3 \left[\frac{1}{2}\dot{\phi}^2 - \frac{1}{2} \sum_{j=1,2,3} (D_j\phi)^2 - \frac{m^2}{2}\phi^2 \right]. \tag{1}$$

Each of n_1, n_1, and n_3 is an integer, and we use periodic boundary conditions, with N points in each coordinate direction. To exhibit the connection with a continuum field theory we also write the field as $\phi(t, \mathbf{x})$, which means the same as $\phi(t, n_1, n_2, n_3)$ with $\mathbf{x}_{\mathbf{n}} = a(n_1, n_2, n_3)$. The finite-difference versions of derivatives are defined by

$$D_1\phi = \frac{\phi(t, n_1 + 1, n_2, n_3) \; - \; \phi(t, n_1, n_2, n_3)}{a}, \tag{2}$$

etc.

The equations of motion are the usual Euler Lagrange equations

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{\phi}(t, n_1, n_2, n_3)} \; - \; \frac{\partial L}{\partial \phi(t, n_1, n_2, n_3)} \\ &= a^3 \frac{\partial^2 \phi(t, n_1, n_2, n_3)}{\partial t^2} \; - \; \frac{\partial L}{\partial \phi(t, n_1, n_2, n_3)}. \end{aligned} \tag{3}$$

Differentiating the mass term in L gives $-m^2\phi$, but obtaining the derivative of the derivative term needs some care. Consider the terms involving $(D_1\phi)^2$. We need keep only the terms which involve $\phi(t, n_1, n_2, n_3)$; these arise from two terms in the Lagrangian:

$$\begin{aligned} &\frac{a^3}{2} \left[(D_1\phi(t, n_1, n_2, n_3))^2 + (D_1\phi(t, n_1 - 1, n_2, n_3))^2 \right] \\ &\qquad = \frac{a^3}{2} \left[\left(\frac{\phi(t, n_1 + 1, n_2, n_3) \; - \; \phi(t, n_1, n_2, n_3)}{a} \right)^2 \right. \\ &\qquad\qquad \left. + \left(\frac{\phi(t, n_1, n_2, n_3) \; - \; \phi(t, n_1 - 1, n_2, n_3)}{a} \right)^2 \right]. \end{aligned} \tag{4}$$

Differentiating with respect to $\phi(t, n_1, n_2, n_3)$ gives

$$-a^3 \; \frac{\phi(t, n_1 + 1, n_2, n_3) - 2\phi(t, n_1, n_2, n_3) + \phi(t, n_1 - 1, n_2, n_3)}{a^2}, \tag{5}$$

an object we call $-D_1^2\phi$, with D_1^2 providing a discrete approximation to the second derivative $\partial^2/\partial x_1^2$. Watch the signs carefully! (To see that the name and normalization are appropriate, apply D_1^2 to the function $f(n_1) = a^2 n_1^2 = x_1^2$.)

Then the equation of motion is

$$0 = \frac{\partial^2 \phi(t, n_1, n_2, n_3)}{\partial t^2} - D_1^2 \phi - D_2^2 \phi - D_3^2 \phi + m^2 \phi. \tag{6}$$

Any function can be written as a Fourier transform: a continuous Fourier transform on t, and discrete Fourier transforms on the spatial points. A single Fourier mode has the form $f(t, \mathbf{n}) = e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}}$. The spatial derivatives have the form

$$\begin{aligned} D_1^2 f(t, \mathbf{n}) &= \frac{f(t, n_1+1, n_2, n_3) - 2f(t, n_1, n_2, n_3) + f(t, n_1-1, n_2, n_3)}{a^2} \\ &= e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} \frac{e^{ik_1 a} - 2 + e^{-ik_1 a}}{a^2} \\ &= -e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} \frac{4}{a^2} \sin^2 \frac{k_1 a}{2}. \end{aligned} \tag{7}$$

Substituting into the equation of motion (6) and projecting onto each Fourier mode separately gives

$$\omega = \sqrt{m^2 + \sum_{j=1,2,3} \frac{4}{a^2} \sin^2 \frac{k_j a}{2}}. \tag{8}$$

There are also negative-frequency solutions, which we allow for by a separate term in the resulting expression for ϕ:

$$\phi = \sum_\alpha \left(\hat{a}_\alpha e^{-i\omega_\alpha t + i\mathbf{k}_\alpha \cdot \mathbf{x}} + \hat{a}_\alpha^\dagger e^{i\omega_\alpha t - i\mathbf{k}_\alpha \cdot \mathbf{x}} \right). \tag{9}$$

The coefficients $\hat{a}_\alpha^\dagger$ of the negative-frequency solutions are the hermitian conjugates of those of the positive-frequency solutions, in order that ϕ is hermitian.

Finally we impose periodic boundary conditions, so that $\phi(t, n_1, n_2, n_3) = \phi(t, n_1 + N, n_2, n_3)$, and similarly for the other two coordinate directions. This implies that

$$k_j a N = 2\pi \times \text{integer}, \tag{10}$$

so that the allowed modes can be written as

$$\mathbf{k} = \frac{2\pi}{aN} (j_1, j_2, j_3), \tag{11}$$

where the j_1. j_2, and j_3 are integers.