Lecture 4 Quantizing the Scalar Field Theory

We will start with the system in the discretised picture and use the results to deduce what the continuum procedure should be. To remind you we have a Hamiltonian

$$H = a^3 \sum_k H_k$$

$$= a^3 \sum_k \frac{1}{2}\pi_k^2 + K \sum_{\hat{\mu}} (\phi_{k+\hat{\mu}} - \phi_k)^2 + \frac{1}{2}\omega^2 \phi_k^2$$

where k runs over all vertices, $\hat{\mu}$ over all positive lattice directions x, y, z so $k+\hat{\mu}$ is a vertex adjacent to k in a positive direction. The commutators are

$$[\pi_k, \phi_\ell] = -i\hbar \frac{\delta_{k\ell}}{a^3}, \quad [\pi_k, \pi_\ell] = [\phi_k, \phi_\ell] = 0$$

Start with $K=0$. Then

$$H_k = \frac{1}{2}\pi_k^2 + \frac{1}{2}\omega^2 \phi_k^2$$

which is a standard SHO. To solve this problem we define annihilation and creation operators

$$a_k^+ = -i\sqrt{\frac{a^3}{2\omega}}\left(\pi_k + i\omega\phi_k\right)$$

$$a_k = i\sqrt{\frac{a^3}{2\omega}}\left(\pi_k - i\omega\phi_k\right).$$

$$\left[a_k^+, a_k\right] = \frac{a^3}{2\omega}\left[\pi_k + i\omega\phi_k, \pi_k - i\omega\phi_k\right]$$

$$= \frac{a^3}{2\omega}\cdot -2i\omega\cdot\left[\pi_k, \phi_k\right]$$

From now on we will drop $\hbar$, but not the $1/a^3$ in $[\pi_k, \phi_l]$!! So

$$\left[a_k^+, a_k\right] = \frac{a^3}{2\omega}\cdot -2i\omega\cdot -\frac{i}{a^3} = -1 \qquad \mp$$

Then

$$a_k^+ a_k = \frac{a^3}{2\omega}\left(\pi_k + i\omega\phi_k\right)\left(\pi_k - i\omega\phi_k\right)$$

$$= \frac{a^3}{2\omega}\left(\pi_k^2 + \omega^2\phi_k^2 - i\omega\left[\pi_k, \phi_k\right]\right).$$

$$a_k^+ a_k + a_k a_k^+ = \frac{a^3}{\omega}\left(\pi_k^2 + \omega^2\phi_k^2\right)$$

$$H_k = \frac{1}{2}\left(a_k^+ a_k + a_k a_k^+\right)\frac{\omega}{a^3}$$

$$= \left(a_k^+ a_k + \frac{1}{2}\right)\frac{\omega}{a^3}$$

Note that because of the commutator $\mp$ $a_k^+ a_k$ is simply the number operator ie it gives the number of excitation quanta in the oscillator k.

The vacuum state $|0\rangle$ is annihilated by a_k

$$a_k|0\rangle = 0$$

and energy eigenstates are

$$|n\rangle = (a_k^\dagger)^n|0\rangle$$

$$H_k|n\rangle = (n+\tfrac{1}{2})\frac{\omega}{a^3}$$

The energy eigenstates for the whole system can therefore be described in a basis

$$|n_1, n_2, n_3, \ldots n_k \ldots\rangle = |n_1\rangle|n_2\rangle \ldots |n_k\rangle \ldots$$

so n_k is the occupation number for the kth oscillator. Note that

$$H|n_1, n_2, \ldots\rangle = a^3 \sum_k (a_k^\dagger a_k + \tfrac{1}{2})\frac{\hbar\omega}{a^3}|n_1, n_2, \ldots\rangle$$

$$= \sum_k (n_k + \tfrac{1}{2})\hbar\omega|n_1, n_2, \ldots\rangle$$

The lowest energy state is the <u>vacuum state</u>

$$|0, 0, \ldots\rangle$$

There is a zero point energy that at this stage is not well defined for an infinite system. However the difference between the energy of an excited state and the energy of the ~~gs~~ vacuum state is well defined, we will call it E.

We interpret this model as describing a system where there are n_k particles of

$\hbar = 1$ mass/energy $(\hbar)\omega$ at site k so $E_k = n_k(\hbar)\omega$

So this formalism naturally accounts for varying particle number – but at the moment the particles cannot move!

What happens when $\kappa \neq 0$? We have

$$\phi_k = \frac{1}{\sqrt{2a^3\omega}}\left(a_k^+ + a_k\right)$$

so $\sum_{\hat{\mu}} \left(\phi_{k+\hat{\mu}} - \phi_k\right)^2$ contains terms such as

$$a^+_{k+\hat{\mu}}\, a_k$$

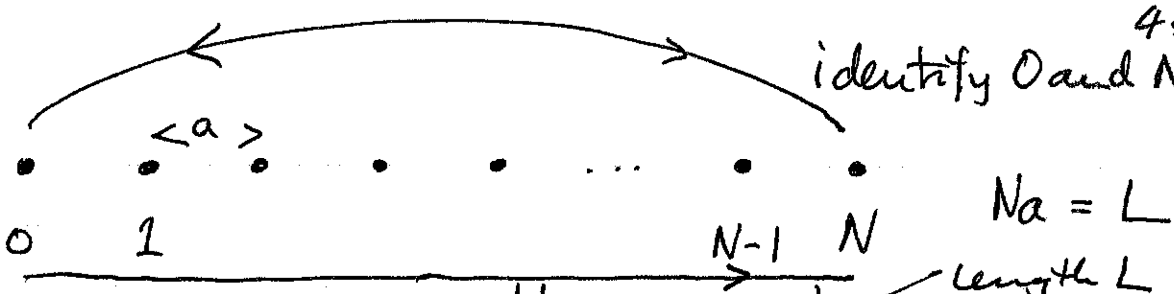
which decrease n_k by one, hence removing a particle from k, and increasing $n_{k+\hat{\mu}}$ by one hence creating a particle at $k + \hat{\mu}$. The particle has moved! Obviously we can't get far doing this piecemeal, how do we diagonalise H systematically?

The clue to doing this is that H is <u>translation invariant</u>. Its form is unchanged by shifting

$$\underline{x}_k \longrightarrow \underline{x}_k + a\left(s_x \hat{\underline{x}} + s_y \hat{\underline{y}} + s_z \hat{\underline{z}}\right)$$

$s_{x,y,z}$ all being integers. This implies that there is a <u>conserved lattice momentum</u> and therefore H would be diagonal in the basis of lattice momentum eigenstates.

It's easiest to work out how to do this on a finite lattice with periodic boundary conditions. We only need to do the detail in one dimension, the generalization is trivial.



We will assume N is odd for convenience.

$$x_k \in \mathcal{X} = \{ka \,;\, k = 0 \ldots N-1\}$$

$$x_N = x_0$$

so any function of x defined on $\mathcal{X}$ satisfies

$$f(x+Na) = f(x)$$

The Fourier (or momentum space) decomposition is

$$f(x) = C \sum_{p \in \mathcal{B}} \bar{f}(p)\, e^{ipx}$$

where we have to determine $\mathcal{B}$ and C is a real constant that we'll leave arbitrary for the moment.

$$f(x) = f(x+Na) = C \sum_{p \in \mathcal{B}} \bar{f}(p)\, e^{ip(x+Na)}$$

so $\quad pL = 2\pi l$

integer $l = -\frac{N-1}{2}, \ldots 0, \ldots \frac{N-1}{2}$

(so exactly N degrees of freedom again)

and $\mathcal{B} = \left\{ \frac{2\pi l}{L} \,;\, l = -\frac{N-1}{2}, \ldots 0, \ldots \frac{N-1}{2} \right\}$

Note that

$$f(x)^* = C \sum_{p \in \mathcal{B}} \bar{f}(p)^*\, e^{-ipx}$$

$$= C \sum_{p \in \mathcal{B}} \bar{f}(-p)^* e^{ipx}$$

so if $f(x)$ is real**

$$\bar{f}(-p)^* = \bar{f}(p)$$

or $$\bar{f}(-p) = \bar{f}(p)^*$$

These considerations extend immediately to (eg) 3 dimensions so $\underline{x} \in \mathcal{X}_3$ which is simply three copies of $\mathcal{X}$ – one for the x, y, z directions respectively and

$$f(\underline{x}) = C^3 \sum_{\underline{p} \in \mathcal{B}_3} \bar{f}(\underline{p}) e^{i \underline{p} \cdot \underline{x}}$$

where $\mathcal{B}_3$ is similarly three copies of $\mathcal{B}$. And

$$\bar{f}(-\underline{p}) = \bar{f}(\underline{p})^*$$

** Here we use the fact that $\{e^{ipx}, p \in \mathcal{B}\}$ span an N-dimensional space and linear independence.

We will need

$$\sum_{x\in X} f(x)^2 = C^2 \sum_{x\in X} \sum_{p\in B} \sum_{q\in B} \bar{f}(p)\,\bar{f}(q) \times e^{i(p+q)x}$$

Now

$$\sum_{x\in X} e^{i(p+q)x} = \sum_{k=0}^{N-1} e^{i(p+q)ak}$$

$$= \frac{1 - e^{i(p+q)aN}}{1 - e^{i(p+q)a}} = \frac{1-e^{i(p+q)L}}{1-e^{i(p+q)a}}$$

If $p+q \neq 0$ the numerator is zero and the denominator (remember that $p,q \in B$) non-zero so we get

$$= N\,\delta_{p,-q} \qquad \ddagger$$

and therefore

$$\sum_{x\in X} f(x)^2 = C^2 N \sum_{p\in B} \sum_{q\in B} \bar{f}(p)\,\bar{f}(q)\,\delta_{p,-q}$$

$$= C^2 N \sum_{p\in B} \bar{f}(p)\,\bar{f}(-p)$$

The converse of $\ddagger$ is

$$\frac{1}{N}\sum_{p\in B} e^{ip(x-x')} = \frac{1}{N}\sum_{l} e^{i 2\pi \frac{l}{Na}(k-k')a}$$

$$= \frac{1}{N}\sum_{l} e^{i 2\pi (k-k') l/N}$$

$$\left.\begin{aligned} &= 0 && \text{if } k\neq k' \\ &= 1 && \text{if } k=k' \end{aligned}\right\} = \delta_{x,x'}$$

There is of course also an inverse transform. Starting from

$$f(x) = C \sum_{p\in B} \tilde{f}(p)\, e^{ipx}$$

$$\sum_{x\in X} f(x) e^{-iqx} = C \sum_{p\in B} \tilde{f}(p) \sum_{x\in X} e^{ix(p-q)}$$

use ∓ on 4.6a $\quad = NC \sum_{p\in B} \tilde{f}(p)\, \delta_{p,q}$

so $\quad \tilde{f}(q) = \dfrac{1}{NC} \sum_{x\in X} f(x)\, e^{-iqx}$

We have now

$$H = a^3 \sum_{\underline{x} \in \chi_3} \left(\frac{1}{2} \pi(\underline{x})^2 + K \sum_{\hat{\mu}} \left(\phi(\underline{x} + a\hat{\underline{\mu}}) - \phi(\underline{x})\right)^2 + \frac{1}{2} \omega^2 \phi(\underline{x})^2 \right)$$

where $\hat{\underline{\mu}}$ is a unit vector in x, y, z directions. When we re-write in ~~the~~ momentum space we have to deal with

$$\phi(\underline{x} + a\hat{\underline{\mu}}) - \phi(\underline{x}) = C^3 \sum_{\underline{p} \in B_3} \bar{\phi}(\underline{p}) \left(e^{i\underline{p}\cdot(\underline{x} + a\hat{\underline{\mu}})} - e^{i\underline{p}\cdot\underline{x}} \right)$$

$$= C^3 \sum_{p \in B_3} \underbrace{(e^{i\underline{p}\cdot a\hat{\underline{\mu}}} - 1)\, \bar{\phi}(\underline{p})}_{\text{we can regard this as a modified } \bar{\phi}(\underline{p})}\, e^{i\underline{p}\cdot\underline{x}}$$

so we get

$$H = a^3 (C^2 N)^3 \sum_{\underline{p} \in B_3} \frac{1}{2} \bar{\pi}(-\underline{p}) \bar{\pi}(\underline{p}) + K \bar{\phi}(-\underline{p}) \bar{\phi}(\underline{p}) \sum_{\hat{\mu}} \left| e^{i\underline{p}\cdot a\hat{\underline{\mu}}} - 1 \right|^2 + \frac{1}{2} \bar{\phi}(-\underline{p}) \bar{\phi}(\underline{p})\, \omega^2$$

$$= a^3 (C^2 N)^3 \sum_{\underline{p} \in B_3} \frac{1}{2} \bar{\pi}^{+}(\underline{p}) \bar{\pi}(\underline{p}) + \frac{1}{2} E_{\underline{p}}^2 \bar{\phi}^{+}(\underline{p}) \bar{\phi}(\underline{p})$$

where $E_{\underline{p}}^2 = \omega^2 + 2K \sum_{i=1,2,3} 4 \sin^2 \frac{a p_i}{2}$

You can see that we have a collection of oscillators, one for each momentum mode $\underline{p}$ having angular frequency $E_{\underline{p}} = +\sqrt{\omega^2 + 8K \sum_{i=1,2,3} \sin^2 \frac{ap_i}{2}}$

To quantize it we need the commutators

$$[\tilde{\pi}(\underline{p}), \tilde{\phi}(\underline{q})] = \frac{1}{(NC)^6} \sum_{\underline{x} \in X_3} \sum_{\underline{y} \in X_3} e^{-i\underline{p}\cdot\underline{x}} e^{-i\underline{q}\cdot\underline{y}} \times [\pi(\underline{x}), \phi(\underline{y})]$$

$$= \frac{1}{(NC)^6} \times \frac{-i}{a^3} \sum_{\underline{x} \in X_3} e^{-i\underline{x}\cdot(\underline{p}+\underline{q})}$$

$$= \frac{1}{(NC)^6} \times \frac{-i}{a^3} \cdot N^3 \delta_{\underline{p}+\underline{q},0}$$

$$= \frac{-i}{(aNC^2)^3} \delta_{\underline{p}+\underline{q},0}$$

Now we see that the quantization problem is a copy of the $K=0$ case with the changes

1. The modes are labelled by momentum $\underline{p}$ (rather than location $\underline{k}$)
2. Instead of all modes having angular frequency ω the mode of momentum $\underline{p}$ has angular frequency $E_{\underline{p}} = +\sqrt{\omega^2 + 8K \sum_{i=1,2,3} \sin^2 \frac{ap_i}{2}}$
3. a is replaced by $aNC^2 = LC^2 = \bar{L}$

So, copying our previous calculation, we define

$$a_{\underline{p}} = i\sqrt{\frac{L^3}{2E_p}}\left(\bar{\pi}(\underline{p}) - iE_p\,\bar{\phi}(\underline{p})\right)$$

$$a_{\underline{p}}^+ = -i\sqrt{\frac{L^3}{2E_p}}\left(\bar{\pi}(-\underline{p}) + iE_p\,\bar{\phi}(-\underline{p})\right)$$

then

$$\left[a_{\underline{p}}^+, a_{\underline{q}}\right] = \frac{L^3}{2E_p}\, iE_p\left(-\left[\bar{\pi}(-\underline{p}), \bar{\phi}(\underline{q})\right] + \left[\bar{\phi}(-\underline{p}), \bar{\pi}(\underline{q})\right]\right)$$

$$= \frac{L^3 i}{2} \times -\frac{i}{L^3}\left(-\delta_{\underline{q}-\underline{p},0} \times 2\right)$$

$$= -\delta_{\underline{q}-\underline{p},0}$$

and

$$E_p\, a_{\underline{p}}^+ a_{\underline{p}} = \frac{L^3}{2}\left\{\bar{\pi}(-\underline{p})\bar{\pi}(\underline{p}) + E_p^2\,\bar{\phi}(-\underline{p})\bar{\phi}(\underline{p}) - iE_p\left(\bar{\pi}(-\underline{p})\bar{\phi}(\underline{p}) - \bar{\phi}(-\underline{p})\bar{\pi}(\underline{p})\right)\right\}$$

So

$$\sum_{\underline{p}\in B_3} E_p a_{\underline{p}}^+ a_{\underline{p}} = H - \frac{iL^3}{2}\sum_{\underline{p}\in B_3} E_p\left(\bar{\pi}(-\underline{p})\bar{\phi}(\underline{p}) - \bar{\phi}(\underline{p})\bar{\pi}(-\underline{p})\right)$$

in this term we have changed variables $\underline{p} \to -\underline{p}$ under the sum

$$= H - \frac{iL^3}{2}\sum_{\underline{p}\in B_3} E_p \cdot -\frac{i}{L^3}$$

$$= H - \sum_{\underline{p}\in B_3}\frac{E_p}{2}$$

The second term on the r.h.s. is the zero point energy. As we discussed earlier we will set the energy scale so that the vacuum state which is annihilated by any $a_{\underline{p}}$

$$a_{\underline{p}} |0\rangle = 0$$

has energy 0 ie

$$H|0\rangle = \sum_{\underline{p} \in B_3} E_{\underline{p}} a^{\dagger}_{\underline{p}} a_{\underline{p}} |0\rangle = 0$$

The vacuum state contains <u>no particles</u>

Excited states that are energy eigenstates contain $\{ n_{\underline{p}}$ particles of energy $E_{\underline{p}}, \ \underline{p} \in B_3 \}$

$$H \, | \{ n_{\underline{p}} ; \underline{p} \in B_3 \} \rangle = \left(\sum_{\underline{p} \in B_3} n_{\underline{p}} E_{\underline{p}} \right) \times | \{ n_{\underline{p}} ; \underline{p} \in B_3 \} \rangle$$

and $\displaystyle | \{ n_{\underline{p}} ; \underline{p} \in B_3 \} \rangle = \prod_{\underline{p} \in B_3} (a^{\dagger}_{\underline{p}})^{n_{\underline{p}}} |0\rangle$

(note this state is not normalized, we will deal with that later)

The energy of this state is always positive and there is a <u>state of lowest energy</u> ie $|0\rangle$. Thus the <u>physical requirement</u> that systems have ground states is implemented in this formalism and we have banished the negative energy problem.