Quantum Field Theory 1

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Part I

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Chapter 1

Discrete systems

1.1 One-dimensional harmonic crystal

Consider a simple one-dimensional model of a crystal where atoms of mass $m \equiv 1$ lie at rest on the x-axis, with equilibrium positions labelled by $n \in \mathbb{N}$ and equally spaced by a distance a.
Assuming these atoms are free to vibrate only in the x direction (longitudinal waves), and denoting the displacement of the atom at position n as η_n, one can write the Lagrangian for a *harmonic crystal* as:

$$L = \sum_n \left[\frac{1}{2}\dot{\eta}_n^2 - \frac{\lambda}{2} \left(\eta_n - \eta_{n-1}\right)^2 \right] \tag{1.1}$$

where λ is the spring constant. From the Lagrange equations, the classical equations of motions are:

$$\ddot{\eta}_n = \lambda \left(\eta_{n+1} - 2\eta_n + \eta_{n-1}\right) \tag{1.2}$$

The solutions can be written as complex travelling waves:

$$\eta_n(t) = e^{i(kn - \omega t)} \tag{1.3}$$

where the dispersion relation is:

$$\omega^2 = 2\lambda \left(1 - \cos k\right) \approx \lambda k^2 \tag{1.4}$$

Therefore, in the long-wavelength limit $k \ll 1$ waves propagate with velocity $c = \sqrt{\lambda}$. To determine the normal modes, there need to be boundary conditions: imposing boundary conditions:

$$\eta_{n+N} = \eta_n \qquad \Rightarrow \qquad k_m = \frac{2\pi m}{N} \, , \, m = 0, 1, \ldots, N-1 \tag{1.5}$$

The normal-mode expansion can then be written as:

$$\eta(t) = \sum_{m=0}^{N-1} \left[\mathcal{A}_m e^{i(k_m n - \omega_m t)} + \mathcal{A}^* e^{-i(k_m n - \omega_m t)} \right] \tag{1.6}$$

where the complex conjugate is added to ensure that the total displacement is real. The momentum canonically-conjucated to the displacement is defined as:

$$\pi_n := \frac{\partial L}{\partial \dot{\eta}_n} = \dot{\eta}_n \tag{1.7}$$

In quantum mechanics, η_n and Π_n become operators with canonical commutator $[\hat{\eta}_j, \hat{\pi}_k] = i\hbar\delta_{jk}$. Implementing time evolution with the *Heisenberg picture*[1]:

$$[\hat{\eta}_j(t), \hat{\pi}_k(t)] = i\hbar\delta_{jk} \tag{1.8}$$

The commutator of operators evaluated at different times requires solving the dynamics of the system. It is useful to introduce *annihilation* and *creation operators* [2]$\hat{a}(t)$ and $\hat{a}^\dagger(t)$, so that Eq. 1.6 becomes:

$$\hat{\eta}_n(t) = \sum_{m=0}^{N-1} \sqrt{\frac{\hbar}{2\omega_m}} \frac{1}{\sqrt{N}} \left[e^{i(k_m n - \omega_m t)}\hat{a}_m + e^{-i(k_m n - \omega_m t)}\hat{a}_m^\dagger\right] \tag{1.9}$$

where $[\hat{a}_j, \hat{a}_k^\dagger] = \delta_{jk}$ and the $N^{-1/2}$ ensures the normalization of normal modes. The proof of Eq. 1.8 follows from the finite Fourier series identity (sum of a geometric progression):

$$\sum_{m=0}^{N-1} e^{ik_m(n-n')} = N\delta_{nn'} \tag{1.10}$$

The Hamiltonian of the system can be written as:

$$\hat{\mathcal{H}} = \sum_n \left[\frac{1}{2}\hat{\pi}_n^2 + \frac{\lambda}{2}\left(\hat{\eta}_n - \hat{\eta}_{n-1}\right)^2\right] = \sum_{m=0}^{N-1} \hbar\omega_m \left(\hat{a}_m^\dagger \hat{a}_m + \frac{1}{2}\right) \tag{1.11}$$

Generalizing the harmonic oscillator operator algebra (proven unique by Von Neumann), one can construct the Hilbert space for the harmonic crystal as:

$$\hat{a}_m |0\rangle \quad \forall m = 0, 1, \ldots, N-1 \tag{1.12}$$

$$|n_0, n_1, \ldots, n_{N-1}\rangle = \prod_{m=0}^{N-1} \frac{(\hat{a}_m^\dagger)^{n_m}}{\sqrt{n_m!}} |0\rangle \tag{1.13}$$

These are normalized eigenstates of Eq. 1.1 with energy eigenvalues:

$$E_0 = \frac{1}{2}\sum_{m=0}^{N-1} \hbar\omega_m \tag{1.14}$$

$$E_{n_0, n_1, \ldots, n_{N-1}} = E_0 + \sum_{m=0}^{N-1} n_m \hbar\omega_m \tag{1.15}$$

This Hilbert space is called *Fock space* and the excited states *phonons*: these can be thought as "particles" and n_m is the number of phonons in the m^{th} normal mode.

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[1]Recall that $\hat{\mathcal{O}}(t) = e^{\frac{i}{\hbar}\hat{\mathcal{H}}t}\hat{\mathcal{O}}(0)e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}$ and $\frac{\mathrm{d}\hat{\mathcal{O}}}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{\mathcal{H}}, \hat{\mathcal{O}}]$.

[2]For a harmonic oscillator $\hat{\mathcal{H}} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega^2\hat{x}^2$, so $\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = \hat{p}(t)$ and $\frac{\mathrm{d}\hat{p}}{\mathrm{d}t} = -\omega^2\hat{x}(t)$ and the solution can be written as:

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2\omega}}\left[\hat{a}(t) + \hat{a}^\dagger(t)\right] \qquad \hat{p}(t) = -i\omega\sqrt{\frac{\hbar}{2\omega}}\left[\hat{a}(t) - \hat{a}^\dagger(t)\right]$$

Inverting these expressions one finds $[\hat{a}(t), \hat{a}^\dagger(t)] = 1$ and $\hat{\mathcal{H}} = \hbar\omega\left(\hat{a}^\dagger(t)\hat{a} + \frac{1}{2}\right)$. The time evolution $\hat{a}(t) = e^{-i\omega t}\hat{a}(0)$ ensures that $\hat{\mathcal{H}}$ is times-independent.