Quantentheorie II Übung 9

– Sample solutions –

SS 2021 Dr. H. Stöckinger-Kim, Prof. Dominik Stöckinger (IKTP)

2. **Linear chain:** $L = \sum_{n=1}^{N} \left(\frac{\dot{q}_n^2}{2} - \frac{\kappa}{2}(q_{n+1} - q_n)^2 \right)$.

(a) Euler-Lagrange equation: $\frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0$. We focus on the terms of the n-th oscillator

$$\begin{aligned}
L = &\frac{\dot{q}_1^2}{2} - \frac{\kappa}{2}(q_2 - q_1)^2 + \cdots \\
&+ \frac{\dot{q}_{n-1}^2}{2} - \frac{\kappa}{2}(q_n - q_{n-1})^2 + \frac{\dot{q}_n^2}{2} - \frac{\kappa}{2}(q_{n+1} - q_n)^2 \\
&+ \cdots + \frac{\dot{q}_N^2}{2} - \frac{\kappa}{2}(q_1 - q_N)^2,
\end{aligned} \tag{1}$$

from which we calculate

$$\frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{q}_n} = \ddot{q}_n, \tag{2}$$

$$\frac{\partial L}{\partial q_n} = \kappa(q_{n-1} - 2q_n + q_{n+1}), \tag{3}$$

$$\Longrightarrow \quad \frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{q}_n} - \frac{\partial L}{\partial q_n} = \ddot{q}_n - \kappa(q_{n-1} - 2q_n + q_{n+1}), \tag{4}$$

$$\therefore \quad \frac{d^2}{dt^2}q_n = \kappa(q_{n-1} - 2q_n + q_{n+1}). \tag{5}$$

(b) We apply the periodic boundary condition $q_{N+n} = q_n$ to the Ansatz $q_n(t) = e^{\pm i(\omega_k t - kan)}$ and obtain

$$\begin{aligned}
e^{i\omega_k t - ika(N+1)} &= e^{i\omega_k t - ika}e^{-ikaN} \\
&= e^{i\omega_k t - ika} \Longleftarrow \ (q_{N+1} = q_1), \\
\therefore \quad e^{-ikaN} &= 1 = e^{-2\pi i l}, \ \text{where } l = 1, 2, 3, \cdots
\end{aligned}$$

$$\therefore k = \frac{2\pi}{aN}l, \tag{6}$$

$$\Longrightarrow \quad |\vec{k}|_{\text{min.}} = \frac{2\pi}{aN} \quad (l = 1). \tag{7}$$

(c) Let $ka = 2\pi y + x$, where y is an integer and x is any number between $0 < x \le 2\pi$.

$$\begin{aligned}
q_n = e^{-i\omega_k t - i(2\pi y + x)n} &= e^{i\omega_k t - ixn} \Longleftarrow \ e^{-2\pi i y n} = 1, \\
\therefore \quad q_n|_{ka=x} = q_n|_{ka=x+2\pi y} &\Longrightarrow \text{We can restrict } k \text{ as } 0 < ka \le 2\pi \\
\Longrightarrow \ -\frac{\pi}{a} < k \le \frac{\pi}{a}.&
\end{aligned} \tag{8}$$

After applying Eq.(6) to Eq.(8) we obtain

$$-\frac{\pi}{a} < \frac{2\pi}{aN} l \leq \frac{\pi}{a}, \tag{9}$$

and the range of l is

$$-\frac{N}{2} < l \leq \frac{N}{2}. \tag{10}$$

For odd N, $l_{\max} = \frac{N}{2} - \frac{1}{2}$, and the possible integer l values are $l = 0, \pm 1, \pm 2, \cdots, \pm \frac{N-1}{2}$. We obtain

$$|\vec{k}|_{\max} = \frac{2\pi}{aN} m_{\max} = \frac{\pi}{aN}(N-1) = \frac{\pi}{a} - \frac{2\pi}{aN} \xrightarrow{L=.aN\to\infty} \frac{\pi}{a}. \tag{11}$$

From Eq.(10) we obtain N possible different k values.

(d) Apply the Ansatz $q_n(t) = e^{i\omega_k t - ikan}$ to the Euler-Lagrange equation Eq. (5):

$$\begin{aligned} -\omega_k^2 e^{i\omega_k t - ikan} &= \kappa(e^{i\omega_k t - ikan} e^{-ika} - 2e^{i\omega_k t - ikan} + e^{i\omega_k t - ikan} e^{ika}) \\ &= \kappa(e^{-ika} + e^{ika} - 2) e^{i\omega_k t - ikan}, \\ \Longrightarrow -\omega_k^2 &= 2\kappa(\cos ka - 1) = 2\kappa \sin^2 \frac{ka}{2} \end{aligned}$$

$$\therefore \text{ The dispersion relation is } \omega_k = 2\sqrt{\kappa}|\sin\frac{ka}{2}|. \tag{12}$$

(e) For small k (keeping everything else constant) we simply obtain the linear dispersion relation $\omega_k = \sqrt{\frac{\kappa}{m}}|k|a$. This linear dispersion corresponds to a so called Goldstone mode.

For fixed momentum k, the question allows several different kinds of limits with different physical interpretations. A particularly interesting one is obtianed by keeping the product aN constant (while $a \to 0$ and $N \to \infty$), which corresponds to constant total length of the linear chain. In this limit, $\omega_k \sim \sqrt{\kappa}|k|a$ and the speed of sound approaches $\frac{\omega_k}{k} = \frac{d\omega_k}{dk} = a\sqrt{\kappa}$.

(f) Canonical conjugate momenta p_n are

$$p_n = \frac{\partial L}{\partial \dot{q}_n} = \dot{q}_n, \tag{13}$$

and the Hamiltonian function is

$$\begin{aligned} H(q_n, p_n) &= \sum_{n=1}^{N} p_n \dot{q}_n - L(q_n, \dot{q}_n) = \sum_{n=1}^{N} p_n^2 - \sum_{n=1}^{N} \left(\frac{p_n^2}{2} - \frac{\kappa}{2}(q_{n+1} - q_n)^2 \right) \\ &= \sum_{n=1}^{N} \left(\frac{p_n^2}{2} + \frac{\kappa}{2}(q_{n+1} - q_n)^2 \right). \end{aligned} \tag{14}$$

(g) $\hat{q}_n$ and $\hat{p}_n$ are

$$\hat{q}_n(t) = \sum_k \sqrt{\frac{1}{2\omega_k N}} \left(\hat{a}_k e^{-i(\omega_k t - kan)} + \hat{a}_k^\dagger e^{i(\omega_k t - kan)} \right), \tag{15}$$

$$\hat{p}_n(t) = \dot{\hat{q}}_n(t) = -i \sum_k \sqrt{\frac{\omega_k}{2N}} \left(\hat{a}_k e^{-i(\omega_k t - kan)} - \hat{a}_k^\dagger e^{i(\omega_k t - kan)} \right). \tag{16}$$

The explicit calculation of the commutator $[\hat{q}_n, \hat{p}_m]$ is

$$
\begin{aligned}
[\hat{q}_n, \hat{p}_m] &= \frac{-i}{2N} \sum_{k,k'} \sqrt{\frac{\omega_{k'}}{\omega_k}} \Big([\hat{a}_k, \hat{a}_{k'}] e^{-i(\omega_k+\omega_{k'})t} e^{ia(kn+k'm)} \\
&\quad - [\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger] e^{i(\omega_k+\omega_{k'})t} e^{-ia(kn+k'm)} \\
&\quad - [\hat{a}_k, \hat{a}_{k'}^\dagger] e^{-i(\omega_k-\omega_{k'})t} e^{ia(kn-k'm)} \\
&\quad + [\hat{a}_k^\dagger, \hat{a}_{k'}] e^{i(\omega_k-\omega_{k'})t} e^{ia(kn-k'm)} \Big) \\
&= \frac{-i}{2N} \sum_{k,k'} \sqrt{\frac{\omega_{k'}}{\omega_k}} \left(-\delta_{k,k'} e^{-it(\omega_k-\omega_{k'})} e^{ia(kn-k'm)} - \delta_{k,k'} e^{i(\omega_k-\omega_{k'})t} e^{-ia(kn-k'm)} \right) \\
&\Longleftarrow \ [\hat{a}_k, \hat{a}_{k'}^\dagger] = \delta_{k,k'}, [\hat{a}_k, \hat{a}_{k'}] = [\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger] = 0 \\
&= \frac{i}{N} \sum_k \cos(ka(n-m)) \\
&= \frac{i}{N} \sum_{l=-\frac{N-1}{2}}^{\frac{N-1}{2}} \cos \frac{2\pi(n-m)}{N} l \Longleftarrow \ ka = \frac{2\pi}{N} l \\
&= \frac{i}{N} \sum_{l=-j}^{j} \cos \frac{2\pi(n-m)}{N} l \Longleftarrow \ N = 2j+1 \\
&= \begin{cases} i, & \text{for } n = m \\ 0, & \text{for } n \neq m \Longleftarrow \ 1 + 2\cos x + 2\cos 2x + \cdots + 2\cos nx = \frac{\sin\left((n+\frac{1}{2})x\right)}{\sin\frac{x}{2}} \end{cases} ,
\end{aligned} \tag{17}
$$

$$\therefore \quad [\hat{q}_n, \hat{p}_m] = i\delta_{nm} \tag{18}$$

(h) Verify

$$\hat{H}(\hat{q}_n, \hat{p}_n) = \sum \hat{p}_n \dot{\hat{q}}_n - L = \sum_{n=1}^{N} \frac{\hat{p}_n^2}{2} + \sum_{n=1}^{N} \frac{\kappa}{2} (\hat{q}_{n+1} - \hat{q}_n)^2 \tag{19}$$

$$\rightarrow \hat{H} = \sum_k \hat{a}_k^\dagger \hat{a}_k + \text{ constant.} \tag{20}$$

From the Ansatz we have

$$\hat{q}_n = \sum_k \sqrt{\frac{1}{2N\omega_k}} (\hat{a}_k e^{-i(\omega_k t - kan)} + \hat{a}_k^\dagger e^{i(\omega_k t - kan)}) \tag{21}$$

The canonical conjugate momenta are $p_n \equiv \frac{\partial L}{\partial \dot{q}_n} = \dot{q}_n$ and the operators are

$$\hat{p}_n = \dot{\hat{q}}_n = -i \sum_k \sqrt{\frac{\omega_k}{2N}} \left(\hat{a}_k e^{-i(\omega_k t - kan)} - \hat{a}_k^\dagger e^{i(\omega_k t - kan)} \right). \tag{22}$$

The first term of the Hamiltonian in Eq. (19) is

$$\begin{aligned}
\sum_n \frac{p_n^2}{2} = \frac{(-i)^2}{2} \sum_{k,k'} \sum_{n=1}^{N} \frac{\sqrt{\omega_k \omega_{k'}}}{2N} \Big(\\
&\hat{a}_k \hat{a}_{k'} e^{-i(\omega_k+\omega_{k'})t} e^{i(k+k')an} + \hat{a}_k^\dagger \hat{a}_{k'}^\dagger e^{i(\omega_k+\omega_{k'})t} e^{-i(k+k')an} \\
&- \hat{a}_k \hat{a}_{k'}^\dagger e^{-i(\omega_k-\omega_{k'})t} e^{i(k-k')an} - \hat{a}_k^\dagger \hat{a}_{k'} e^{i(\omega_k-\omega_{k'})t} e^{-i(k-k')an} \Big) \\
&= -\frac{1}{4} \sum_k \omega_k \Big(\hat{a}_k \hat{a}_{-k} e^{-2i\omega_k t} + \hat{a}_k^\dagger \hat{a}_{-k}^\dagger e^{2i\omega_k t} - \hat{a}_k \hat{a}_k^\dagger - \hat{a}_k^\dagger \hat{a}_k \Big). \qquad (23) \\
&\Longleftarrow \left(\sum_{n=1}^{N} e^{i(k-k')an} = N\delta_{k,k'} \right)
\end{aligned}$$

To calculate the second term in Eq.(19) we first simplify $\hat{q}_{n+1} - \hat{q}_n$ as

$$\begin{aligned}
\hat{q}_{n+1} - \hat{q}_n &= \sum_k \frac{1}{\sqrt{2N\omega_k}} \Big(\hat{a}_k e^{-i(\omega_k t - ka(n+1))} + \hat{a}_k^\dagger e^{i(\omega_k t - ka(n+1))} \\
&\qquad - \hat{a}_k e^{-i(\omega_k t - kan)} - \hat{a}_k^\dagger e^{i(\omega_k t - kan)} \Big) \\
&= \sum_k \frac{1}{\sqrt{2N\omega_k}} \Big(\hat{a}_k e^{-i(\omega_k t - kan)} (e^{ika} - 1) + \hat{a}_k^\dagger e^{i(\omega_k t - kan)} (e^{-ika} - 1) \Big) \qquad (24) \\
&\Longleftarrow \left(e^{-i(\omega_k t - ka(n+1))} = e^{-i(\omega_k t - kan)} e^{ika} \right).
\end{aligned}$$

The explicit calculation of the second term of Eq. (19) is

$$
\begin{aligned}
&\frac{\kappa}{2}\sum_n(\hat{q}_{n+1}-\hat{q}_n)^2\\
&=\frac{\kappa}{2}\sum_{k,k'}\sum_{n=1}^{N}\frac{1}{2N}\frac{1}{\sqrt{\omega_k\omega_{k'}}}\Big(\\
&\quad\hat{a}_k\hat{a}_{k'}e^{-i(\omega_k+\omega_{k'})t}e^{i(k+k')an}(e^{ika}-1)(e^{ik'a}-1)\\
&+\hat{a}_k^\dagger\hat{a}_{k'}^\dagger e^{i(\omega_k+\omega_{k'})t}e^{-i(k+k')an}(e^{-ika}-1)(e^{-ik'a}-1)\\
&+\hat{a}_k\hat{a}_{k'}^\dagger e^{-i(\omega_k-\omega_{k'})t}e^{i(k-k')an}(e^{ika}-1)(e^{-ik'a}-1)\\
&+\hat{a}_k^\dagger\hat{a}_{k'}e^{i(\omega_k-\omega_{k'})t}e^{-i(k-k')an}(e^{-ika}-1)(e^{ik'a}-1)\Big)\\
&=\frac{\kappa}{2}\sum_k\frac{1}{2\omega_k}\Big(\\
&\quad\hat{a}_k\hat{a}_{-k}e^{-2i\omega_k t}(e^{ika}-1)(e^{-ika}-1)+\hat{a}_k^\dagger\hat{a}_{-k}^\dagger e^{2i\omega_k t}(e^{ika}-1)(e^{-ika}-1)\\
&+\hat{a}_k\hat{a}_k^\dagger(e^{ika}-1)(e^{-ika}-1)+\hat{a}_k^\dagger\hat{a}_k(e^{ika}-1)(e^{-ika}-1)\Big)\\
&\Longleftarrow\left(\sum_{n=1}^{N}e^{i(k-k')an}=N\delta_{k,k'}\right)\\
&=\frac{1}{4}\sum_k\omega_k\left(\hat{a}_k\hat{a}_{-k}e^{-2i\omega_k t}+\hat{a}_k^\dagger\hat{a}_{-k}^\dagger e^{2i\omega_k t}+\hat{a}_k\hat{a}_k^\dagger+\hat{a}_k^\dagger\hat{a}_k\right)\\
&\Longleftarrow\left((e^{ika}-1)(e^{-ika}-1)=4\sin^2\left(\frac{ka}{2}\right),\omega_k^2=4\kappa\sin^2\left(\frac{ka}{2}\right)\right).
\end{aligned}
\tag{25}
$$

Using Eqs. (23) and (25) we rewrite Eq. (19) as

$$
\begin{aligned}
\hat{H}&=-\frac{1}{4}\sum_k\omega_k\left(\hat{a}_k\hat{a}_{-k}e^{-2i\omega_k t}+\hat{a}_k^\dagger\hat{a}_{-k}^\dagger e^{2i\omega_k t}-\hat{a}_k\hat{a}_k^\dagger-\hat{a}_k^\dagger\hat{a}_k\right)\\
&+\frac{1}{4}\sum_k\omega_k\left(\hat{a}_k\hat{a}_{-k}e^{-2i\omega_k t}+\hat{a}_k^\dagger\hat{a}_{-k}^\dagger e^{2i\omega_k t}+\hat{a}_k\hat{a}_k^\dagger+\hat{a}_k^\dagger\hat{a}_k\right)\\
&=\frac{1}{2}\sum_k\omega_k\left(\hat{a}_k\hat{a}_k^\dagger+\hat{a}_k^\dagger\hat{a}_k\right)\\
&=\sum_k\omega_k\hat{a}_k^\dagger\hat{a}_k+\text{ constant}\Longleftarrow[\hat{a}_k,\hat{a}_{k'}^\dagger]=\delta_{k,k'},\frac{1}{2}\sum_k\omega_k=\text{constant}.
\end{aligned}
\tag{26}
$$