Quantentheorie II Übung 9

Besprechung: 2021WE25 (KW25)

SS 2021 Prof. Dominik Stöckinger (IKTP)

1. **Questions**

   (a) Explain the interpretation of the operators $a^\dagger_{\vec{p}}$ and $\hat{\Psi}^\dagger(\vec{x})$ in the context of a non-relativistic Fock space.

   (b) What was the relationship between these two kinds of operators in the case of the lecture (non-relativistic case)?

   (c) What is the Lagrangian in the lecture whose canonical quantization reproduces the above operators and their (anti-)commutation relations?

   (d) Write down the Lagrangian and the Hamiltonian for the hydrogen atom (as given in QM1) and for a 1-dimensional harmonic oscillator.

   (e) Give an example of a key relationship which should be satisfied in relativistic quantum mechanics.

2. **From Lagrangian to Hamiltonian:** in the canonical formalism the canonical conjugate momentum for a given L is defined as $p_i \equiv \frac{\partial L}{\partial \dot{q}_i}$ and the Hamiltonian (function) is $H(q,p) = \sum_i p_i \dot{q}_i - L(q,\dot{q})$. Write the canonical conjugate momentum and Hamiltonian (function) for each L below.

   (a) The 1-dimensional simple harmonic oscillator: $L = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}\kappa^2 q^2$, where κ is a constant.

   (b) $L = \frac{\alpha}{2}\dot{q}^2 q^2$

   (c) $L = (\alpha\dot{q} + \beta q)^2$

   (d) A particle with charge Q in a 4-potential: $L = \frac{1}{2}m\dot{\vec{q}}^2 + Q\dot{\vec{q}} \cdot \vec{A}(\vec{q}) - Q\phi(\vec{q})$

3. **Linear chain:** we consider a 1-dimensional chain of N connected oscillators with mass $m = 1$. Its Lagrangian is

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

   The oscillators sit on a lattice with lattice distance a. q_n satisfy the periodic boundary condition $q_{n+N} = q_n$, and N is an odd number.

   (a) Verify the Euler-Lagrange equation

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

   (b) Use the Ansatz $q_n(t) = e^{\pm i(\omega_k t - kna)}$ for Eq. (2). What are the values of k allowed by the boundary condition? Show that there exists a minimum non-vanishing value of $|k|$.

(c) Show that the range of $|k|$ can be restricted as $-\pi < ka \leq \pi$ without losing generality (1. Brillouin-Zone). How many physically different values of k do we obtain? What is the largest $|k|$?

(d) Write the dispersion relation ω_k of the solution obtained by using the Ansatz.

(e) What is the behavior of ω_k when $k \to 0$? Discuss the behavior of ω_k for fixed k when $a \to 0$ and $N \to \infty$! The solution corresponds to sound waves. What is the speed of sound?

(f) Write the canonical conjugate momenta p_n and the Hamiltonian (function) $H(p, q)$

$$p_n \equiv \frac{\partial L}{\partial \dot{q}_n}, \qquad H(p,q) = \sum_n p_n \dot{q}_n - L(q, \dot{q}). \tag{3}$$

(g) Now we turn to canonical quantization. We introduce operators $\hat{q}_n$ and $\hat{p}_n$ which correspond to the variables q_n and p_n respectively, and assume that the operators satisfy the commutation relations

$$[\hat{q}_n, \hat{p}_m] = i\delta_{nm}, \quad [\hat{q}_n, \hat{q}_m] = 0, \quad [\hat{p}_n, \hat{p}_m] = 0, \tag{4}$$

We use the Ansatz

$$\hat{q}_n(t) = \sum_k \sqrt{\frac{1}{2\omega_k N m}} \left(\hat{a}_k e^{-i(\omega_k t - kan)} + \hat{a}_k^\dagger e^{i(\omega_k t - kan)} \right). \tag{5}$$

What are the commutation relations that $\hat{a}_k$ and ${a_k}^\dagger$ should satisfy in order that $\hat{q}$ and $\hat{p}$ can fulfill the assumptions in Eq. (4)?

The range of summation in Eq. (5) is $k = 0, \pm\frac{2\pi}{Na}, \cdots, \pm\frac{\pi(N-1)}{Na}$.

(h) Show that the Hamiltonian (operator) can be written as

$$\hat{H} = \sum_k \omega_k {\hat{a}_p}^\dagger \hat{a}_k + \text{ constant}. \tag{6}$$

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(b) What was the relationship between these two kinds of operators in the case of the lecture (non-relativistic case)?

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(d) Write down the Lagrangian and the Hamiltonian for the hydrogen atom (as given in QM1) and for a 1-dimensional harmonic oscillator.

(e) Give an example of a key relationship which should be satisfied in relativistic quantum mechanics.

a) $a_{\vec{p}}^{\dagger}|0\rangle = |\vec{p}\rangle$ Impuls EZ $\quad \Psi^{\dagger}(\vec{x})|0\rangle = a_{\vec{x}}^{\dagger}|0\rangle = |\vec{x}\rangle$ Orts EZ

b)

$$|\vec{x}\rangle = \int d^3p \; |p\rangle \underbrace{\langle p|x\rangle}_{\underbrace{e^{-ipx}\frac{1}{(2\pi)^{3/2}}}_{\text{Ebene Welle}}}$$

(#) $$\Psi^{\dagger}(\vec{x}) = \int \frac{d^3p}{(2\pi)^{3/2}} \, a_{\vec{p}}^{\dagger} e^{-ipx}$$

Feldoperator (nicht Kausal)

c) $$\mathcal{L} = i\Psi^* \dot{\Psi} - \frac{1}{2m}(\nabla\Psi)^2$$

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi(\partial^\mu\phi)^+ - \frac{1}{2}m^2\phi^2$$ nicht rel.

$$[\Psi(\vec{x}), \Psi^{\dagger}(\vec{y})] = \delta^{(3)}(\vec{x}-\vec{y})$$

2. Quant.

d) $$\mathcal{L} = \frac{m}{2}\dot{q}^2 - \frac{m\omega^2}{2}q^2$$

$$H = -\frac{\nabla^2}{2\mu} - \frac{\alpha}{r} \qquad \mu = \frac{m_e M}{(m_e+M)} \approx m_e$$

e) Kausalität

$$[\Psi(x), \Psi^{\dagger}(y)] = 0 \qquad (x-y)^2 < 0 \quad \text{raumartig}$$

nicht erfüllt (#)

3. **Linear chain:** we consider a 1-dimensional chain of N connected oscillators with mass $m = 1$. Its Lagrangian is

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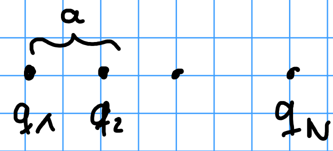

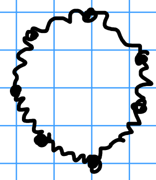

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0$$

a) $$L = \sum_{n=1}^{N} \underbrace{\left(\frac{1}{2} \dot{q}_n^2 - \frac{K}{2} (q_{n+1} - 2q_{n+1} q_n + q_n) \right)}_{L_n}$$

$$\frac{\partial L_n}{\partial \dot{q}_n} = \dot{q}_n \, m$$

$$\frac{\partial L_n}{\partial q_n} = -\frac{K}{2} \left(-2q_{n+1} + 2q_n \right) = K(q_{n+1} - q_n)$$

$$\frac{\partial L_{n-1}}{\partial q_n} = -\frac{K}{2} \frac{\partial}{\partial q_n} \left(q_n^2 - 2q_n q_{n-1} + q_{n-1}^2 \right)$$
$$= K(q_{n-1} - q_n)$$

$$\frac{\partial L}{\partial q_n} = \underline{K(q_{n+1} + q_{n-1} - 2q_n)} = \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_n} = \underline{\ddot{q}_n}$$

b) $q_n(t) = e^{\pm i(\omega_K t - Kna)}$

RB: $q_{n+N} = q_n$

$$e^{\pm i(\cancel{\omega_K t})} e^{\pm i(-K(n+N)a)} = e^{\cancel{\pm i \omega_K t}} e^{\pm i(-Kna)}$$
$$e^{\pm i(-KNa)} = 1$$

$e^{\pm ix} = 1 \Leftrightarrow x = 2\pi n \quad n \in \mathbb{Z}$

$KNa = 2\pi m \quad m \in \mathbb{Z}$

$$\Rightarrow |K| = \frac{2\pi}{Na} m \xrightarrow[m=1]{\min} |K_{min}| = \frac{2\pi}{Na}$$

IR cutoff. durch N endlich

(c) Show that the range of $|k|$ can be restricted as $-\pi < ka \lesssim \pi$ without losing generality (1. Brillouin-Zone). How many physically different values of k do we obtain? What is the largest $|k|$?

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$N \hat{=}$ ungerade

c) $ka = 2\pi y + x \qquad y$ integer $\qquad 0 \leq x \leq 2\pi$

$$q_n = e^{\pm i\omega_k t} e^{\pm(-i(2\pi y + x) n)} = e^{\pm i\omega_k t} e^{\pm(-ixn)}$$

$$q_n(t)\big|_{ka = x} = q_n(t)\big|_{ka = 2\pi y + x}$$

$x = 0 \quad y = 1 \quad \longrightarrow \quad 0 < ka \leq 2\pi$

$\Leftrightarrow \quad -\pi < ka \leq \pi$

$\hookrightarrow \quad -\frac{\pi}{a} < k \leq \frac{\pi}{a}$

$|k_{max}| = \frac{\pi}{a}$

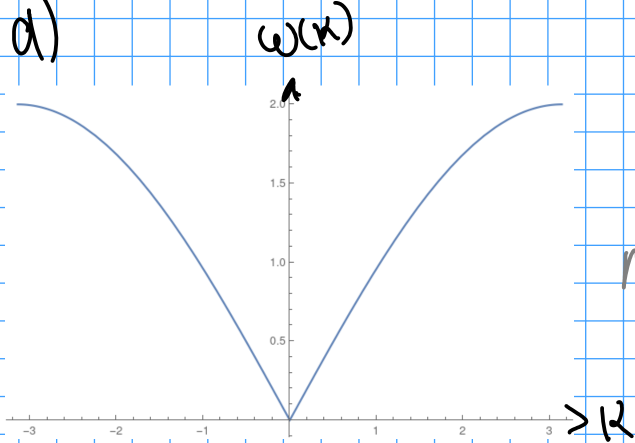
$= \frac{2\pi}{Na} m = \frac{\pi}{a} \quad \Rightarrow \quad m = \frac{N}{2} \quad \lightning$

$\Rightarrow$ UV cutoff
min. a

$\Rightarrow N$ versch. Werte $\qquad k = 0, \pm \underbrace{\frac{2\pi}{Na}}_{m=1}, \ldots, \pm \frac{2\pi}{Na} \frac{N-1}{2}$

$$1 + \frac{N-1}{2} + \frac{N-1}{2} = N$$

d)



$$q_n = e^{\pm i(\omega_k t - kna)}$$

$$m\ddot{q}_n = K(q_{n+1} + q_{n-1} - 2q_n)$$

$\oplus \quad \ominus$

$$\underbrace{-m\omega_k^2}_{= (\pm i\omega_k)^2 m} = K(e^{\pm ika} + e^{\mp ika} - 2)$$

$$= K\, 2\cos(ka) - 2$$

$$\omega_K = \sqrt{\frac{2K}{m}\left(1-\cos(Ka)\right)} = 2\sqrt{\frac{K}{m}}\left|\sin\left(\frac{Ka}{2}\right)\right|$$

$$\cos x = \cos^2\left(\frac{x}{2}\right) - \sin^2\left(\frac{x}{2}\right)$$

$$1 - \cos x = 1 - \cos^2 + \sin^2 = \underbrace{1 - \cos^2 - \sin^2}_{= \sin^2\left(\frac{x}{2}\right)} + \overbrace{\sin^2 + \sin^2}^{0}$$

d) • $K \to 0$ $\quad \omega(K) = \sqrt{\frac{2K}{m}}\,\frac{|K|a}{2}$ linear!

• Schallwellenlimes $a \to 0$ $N \to \infty$ fixed K

$Na = \text{const}$

fixed $K = \frac{2\pi}{Na} m \Rightarrow m = \text{const}.$

$\sim \sin\left(\frac{Ka}{2}\right) = \sin\left(\frac{2\pi}{Na} m \frac{a}{2}\right) = \sin\left(\frac{\pi m}{N}\right)$ $\rightsquigarrow$ das gleiche

$\to N \to \infty$

$\Rightarrow$ lin. Dispersion

$\hat{=}$ Schallgeschw.

(f) Write the canonical conjugate momenta p_n and the Hamiltonian (function) $H(p,q)$

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$\Rightarrow$ Kausalität

$$\overset{\phi}{\hat{q}_n}(t) = \sum_k \sqrt{\frac{1}{2\omega_k N m}} \left(\hat{a}_k e^{-i(\omega_k t - kan)} + \hat{a}_k^\dagger e^{i(\omega_k t - kan)} \right). \tag{5}$$

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$\psi = \int d^3p \, a_p^+ e^{-ipx}$

$a^+ \rightsquigarrow$ Phonon

$\Rightarrow$ Boson

f) $p_n = \frac{\partial \mathcal{L}}{\partial \dot{q}_n} = \dot{q}_n \qquad H = \sum_n \dot{q}_n^2 - \frac{1}{2}\dot{q}_n^2 + \frac{K}{2}(q_{n+1} - q_n)^2$

$= \sum_n \frac{1}{2}\dot{q}_n^2 + \frac{K}{2}(q_{n+1} - q_n)^2 = T + V$

g) $[q_n(t), q_m(t)] = 0$

$= \sum_{kk'} \frac{1}{2mN} \sqrt{\frac{1}{\omega_k \omega_{k'}}} \Big(\cancel{[a_k a_{k'} - a_{k'} a_k]} \cdot e^{\cdots}$

$+ \underbrace{[a_k a_{k'}^+ - a_{k'}^+ a_k]}^{\delta_{kk'}} e^{-i(\omega_k - \omega_{k'})t + ia(kn - k'm)}$

$+ \overbrace{[a_k^+ a_{k'} - a_{k'} a_k^+]}^{-\delta_{kk'}} e^{i(\omega_k - \omega_{k'})t - ia(k'm - kn)}$

$+ \cancel{[a_k^+ a_{k'}^+ - a_{k'}^+ a_k^+]} e^{\cdots} \Big)$

Annahme: Boson $\qquad \bullet \; \omega_k = \omega_{-k}$

$= \sum_k \frac{1}{2mN} \frac{1}{\omega_k} \left(e^{ia(kn - km)} - e^{-ia(km - kn)} \right)$

$= \sum_k \frac{1}{2mN} \underbrace{\frac{1}{\omega_k}}_{\text{symm.}} 2i \underbrace{\sin}_{\text{antisymm.}}(ak(n-m)) \overset{!}{=} 0$

N ungerade $\quad k = 0, \pm 1 \ldots \pm \ldots \Rightarrow$ Summe symmetrisch

$$[q_n, p_m] = \sum_{kk'} \frac{-i}{2N} \sqrt{\frac{\omega_{k'}}{\omega_k}} \left\{ \delta_{kk'} e^{\cdots} + \delta_{kk'} \right\}$$

$$= \frac{i}{N} \sum_k \cos\left(ka(n-m)\right) = i\,\delta_{nm}$$

$n=m \Rightarrow$ offensichtlich

$n \neq m$

Fourier δ-Relationen

$$\cos(\ldots) = \mathrm{Re}\left(\sum_p e^{iap(n-m)}\right) = N\,\delta_{nm}$$

$$\sum_{n=1}^{N} e^{i(k-k')an} = N\,\delta_{kk'} \Longrightarrow h)$$

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Nr 2)

a) $\mathcal{L} = \frac{1}{2} m \dot{q}^2 - \frac{1}{2} k^2 q^2$

$p = \frac{\partial \mathcal{L}}{\partial \dot{q}} = m \dot{q}$ $\quad \dot{q} = \frac{p}{m}$

$H = p \frac{p}{m} - \frac{1}{2} m \left(\frac{p}{m}\right)^2 + \frac{1}{2} k^2 q^2 = \frac{p^2}{2m} + \frac{1}{2} k^2 q^2$

a) $\mathcal{L} = \frac{\alpha}{2} \dot{q}^2 q^2$

$p = \frac{\partial \mathcal{L}}{\partial \dot{q}} = \alpha \dot{q} q^2$ $\quad \dot{q} = \frac{p}{\alpha q^2}$

$H = \frac{p^2}{\alpha q^2} - \frac{p^2}{2 \alpha q^2} = \frac{p^2}{2 \alpha q^2}$

c) $\mathcal{L} = (\alpha \dot{q} + \beta q)^2$

$p = \frac{\partial \mathcal{L}}{\partial \dot{q}} = 2\alpha (\alpha \dot{q} + \beta q)$ $\quad \dot{q} = \frac{p}{2\alpha^2} - \frac{\beta q}{\alpha}$

$H = \frac{p^2}{2\alpha^2} - \frac{p \beta q}{\alpha} - \left(\frac{p}{2\alpha} - \beta q + \beta q\right)^2 = \frac{p^2}{4\alpha^2} - \frac{p \beta q}{\alpha}$

d) $\mathcal{L} = \frac{1}{2} m \dot{q}^2 + Q \dot{q} A(q) - Q \,\phi(q)$

$p = \frac{\partial \mathcal{L}}{\partial \dot{q}} = m \dot{q} + Q A(q)$ $\quad \dot{q} = \frac{p - Q A(q)}{m}$

$$H = \frac{p^2}{m} - \frac{p\,Q\,A(q)}{m} - \frac{1}{2}m\left(\frac{p - Q\,A(q)}{m}\right)^2 + Q\left(\frac{p - Q\,A(q)}{m}\right)A(q) + Q\,\phi(q)$$

$$= \frac{1}{2m}\cdot\left(p - Q\,A(q)\right)^2 + Q\,\phi(q)$$