II. Canonical quantization of fields

II.1 Quantization of the one dimensional harmonic chain

remember section I. 3

$$L = \sum_{i=0}^{N-1} \left(\frac{m}{2} \dot{q}_i^2 - \frac{k}{2} (q_{i+1} - q_i)^2 \right)$$

canonical momenta $\qquad p_i = m\dot{q}_i$

$$H = \sum_{i=0}^{N-1} \left(\frac{1}{2m} p_i^2 + \frac{k}{2} (q_{i+1} - q_i)^2 \right)$$

One way of quantizing would be to replace $q_i, p_i \to \vec{q}_i, \vec{p}_i$ with the standard commutation relations and then to perform the continuum limit. We will do this in a different way and first consider the continuum limit

$$L = \frac{1}{2} \int_0^L dz \left[\frac{1}{v^2} \left(\frac{\partial q(z,t)}{\partial t} \right)^2 - \left(\frac{\partial q(z,t)}{\partial z} \right)^2 \right] \qquad v^2 = \frac{\kappa}{\mu}$$

The Lagrange equations read

$$\frac{1}{v^2} \frac{\partial^2 q}{\partial t^2} - \frac{\partial^2 q}{\partial z^2} = 0$$

which can be solved in a finite length L with PBC:

$$q_n(z,t) \sim e^{\pm i(k_n z - \omega_n t)}$$

where $\quad k_n = \frac{2\pi n}{L} \qquad n = 0, \pm 1, \pm 2$

$$\omega_n^2 = k_n^2 v^2 \qquad \omega_n \equiv v|k_n|$$

normalized complex valued solutions

$$\phi_n(z,t) = \frac{1}{\sqrt{L}} e^{i(k_n z - \omega_n t)}$$

orthonormality

$$\int_0^L dz\, \phi_n^*(z,t)\,\phi_m(z,t) = \delta_{nm}$$

decomposition of $q(z,t)$ into $\phi_n(z,t)$ $\qquad c_n = c_n^*$

$$q(z,t) = \sum_{n=-\infty}^{\infty} c_n \left(a_n(0)\,\phi_n(z,t) + a_n^*(0)\,\phi_n^*(z,t) \right)$$

$$\equiv \sum_{n=-\infty}^{\infty} \frac{c_n}{\sqrt{L}} \left(a_n(t)\, e^{i k_n z} + a_n^*(t)\, e^{-i k_n z} \right)$$

with

$$a_n(t) = a_n(0)\, e^{-i\omega_n t}$$

substitution into Lagrange equations shows

$$\ddot{a}_n + \omega_n^2 a_n = 0 \qquad \hat{=} \text{ harmonic oscillator}$$

likewise one finds for the Hamiltonian after some calculations

$$H = \sum_{n=-\infty}^{\infty} c_n^2 \frac{2\omega_n^2}{v^2} a_n^*(t)\, a_n(t)$$

lets choose $\qquad c_n \equiv \dfrac{v}{\sqrt{2\omega_n}}$

then

$$H = \sum_{n=-\infty}^{\infty} \omega_n\, a_n^*(t)\, a_n(t) \qquad \omega_n = \frac{2\pi v}{L}|n|$$

which is identical to a sum of harmonic oscillators with frequencies ω_n, which can be rewritten as

$$H = \frac{1}{2} \sum_{n=-\infty}^{\infty} \left[p_n^2(t) + \omega_n^2 x_n^2(t) \right]$$

where $\qquad x_n(t) = \dfrac{1}{\sqrt{2\omega_n}} \left(a_n(t) + a_n^*(t) \right)$

$$p_n(t) = -i\sqrt{\frac{\omega_n}{2}} \left(a_n(t) - a_n^*(t) \right)$$

and $m=1$. The harmonic oscillator can be quantized as in standard quantum mechanics

$$\{x_n, x_m\}_p = \{p_n, p_m\}_p = 0 \qquad \{x_n, p_m\}_p = \delta_{nm}$$

$$\hookrightarrow [\hat{x}_n, \hat{x}_m] = [\hat{p}_n, \hat{p}_m] = 0 \qquad \hookrightarrow [\hat{x}_n, \hat{p}_m] = i\,\delta_{nm}$$

This is equivalent to

$$\boxed{[\hat{a}_n, \hat{a}_m] = [\hat{a}_n^+, \hat{a}_m^+] = 0 \qquad [\hat{a}_n, \hat{a}_m^+] = \delta_{nm}}$$

We will show now that this quantization is equivalent to

$$\boxed{\begin{aligned}&[\hat{\varphi}(z,t),\hat{\varphi}(z',t)] = [\hat{\pi}(z,t),\hat{\pi}(z',t)] = 0\\ &[\hat{\varphi}(z,t),\hat{\pi}(z',t)] = i\,\delta(z-z') \quad \text{on } (0,L]\end{aligned}}$$

<u>proof:</u> $\pi(z,t) = \dfrac{\partial \mathcal{L}}{\partial \dot{\varphi}(z,t)} = \dfrac{1}{v^2}\dot{\varphi}(z,t)$

$$= \frac{1}{v}\sum_n \frac{1}{\sqrt{2\omega_n L}}\left(-i\omega_n a_n(t) e^{ik_n z} + i\omega_n a_n^*(t) e^{-ik_n z}\right)$$

$$\Rightarrow \quad [\hat{\varphi}(z,t),\hat{\pi}(z',t)] = \frac{i}{2L}\sum_{n,m}\sqrt{\frac{\omega_n}{\omega_m}}$$

$$\Big\{ \underbrace{[\hat{a}_m,\hat{a}_n^+]}_{=\delta_{mn}} e^{i(k_m z - k_n z')} e^{-i(\omega_m-\omega_n)t}$$

$$- \underbrace{[\hat{a}_m^+,\hat{a}_n]}_{=-\delta_{mn}} e^{-i(k_m z - k_n z')} e^{i(\omega_m-\omega_n)t}\Big\}$$

$$= \frac{i}{L}\sum_n e^{ik_n(z-z')} = \frac{i}{L}\sum_n e^{i\frac{2\pi}{L}n(z-z')}$$

$$= i\,\delta(z-z') \quad \text{on } (0,L] \qquad \square$$

These results will now be generalized.

II.2 fundamental commutator relations of fields

canonical quantization

$$\{A(z,t), B(z',t)\}_P$$

bosons $\swarrow$ $\searrow$ fermions

bosons	fermions
$-i\left[\hat{A}(z,t), \hat{B}(z',t)\right]$	$-i\left\{\hat{A}(z,t), \hat{B}(z',t)\right\}$
commutator	anti-commutator
scalar fields, tensor fields	scalar fields, spinor fields

We will see later that for certain types of fields we have to use anti-commutator relations for the quantization.

We postulate the rules of quantum theory:

(i) the physical state of the field is described by a vector in Hilbert space $\mathcal{H}$ or generalizations thereof

(ii) the physical quantities, i.e. the fields are linear operators in $\mathcal{H}$

(iii) physical observables are self-adjoint operators

remark: complex valued fields such as the Schrödinger or Dirac fields do not correspond to self-adjoint operators and are thus no observables. Only combinations such as $\psi^\dagger\psi$ (Schrödinger) or $\bar{\psi}\psi$ (Dirac) are self-adjoint and thus observables.

(iv) measurement of an observable leads to a projection of the state to the eigenspace corresponding to the measurement outcome; the probability to find a measurement result is given by the scalar product of the initial state with the corresponding eigenstates

(v) the time evolution is described by a unitary transformation $\hat{U}(t)$ with the generator being the Hamiltonian

$$\hat{U}(t) = e^{-i\hat{H}t}$$

$$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle$$

or $$\hat{\phi}(\vec{r},t) = \hat{U}^{-1}(t)\,\hat{\phi}(\vec{r},0)\,\hat{U}(t)$$

$$\Rightarrow \quad \boxed{i\frac{\partial\hat{\phi}(\vec{r},t)}{dt} = [\hat{\phi}(\vec{r},t),\hat{H}]}$$

always commutator!

which is the equivalent of

$$\frac{\partial}{\partial t}\phi(\vec{r},t) = \{\phi(\vec{r},t),H\}_P$$

II.3 Quantization of the non-relativistic Schrödinger-field and many-body quantum mechanics

classical Lagrange density

$$\mathcal{L} = \frac{1}{2}\psi^* i \overrightarrow{\partial_t} \psi - \frac{1}{2}\psi^* i \overleftarrow{\partial_t}\psi - \frac{1}{2m}(\vec{\nabla}\psi^*)(\vec{\nabla}\psi)$$

Euler-Lagrange equations = Schrödinger equation

$$i\partial_t \psi = -\frac{1}{2m}\vec{\nabla}^2\psi$$

canonical momentum

$$\pi^* = \frac{\partial \mathcal{L}}{\partial(\partial_t \psi)} = \frac{i}{2}\psi^* \qquad \pi = \frac{\partial \mathcal{L}}{\partial(\partial_t \psi^*)} = -\frac{i}{2}\psi$$

problem: fields are their own canonical momenta

solution: canonical trafo (add total time derivative)

$$\mathcal{L} = i\psi^*\partial_t\psi - \frac{1}{2m}(\vec{\nabla}\psi^*)(\vec{\nabla}\psi)$$

$\Rightarrow$ only $\pi^* = i\psi^*$ exists

quantization (for bosons)

$$\boxed{\begin{gathered}\left[\hat{\psi}(\vec{r},t), \hat{\psi}(\vec{r}',t)\right] = \left[\hat{\psi}^+(\vec{r},t), \hat{\psi}^+(\vec{r}',t)\right] = 0 \\ \left[\hat{\psi}(\vec{r},t), \hat{\psi}^+(\vec{r}',t)\right] = \delta(\vec{r}-\vec{r}')\end{gathered}}$$

Hamiltonian

$$\boxed{\hat{H} = \int d^3r \; \hat{\Psi}^+(\vec{r},t)\left(-\frac{1}{2m}\vec{\nabla}^2\right)\hat{\Psi}(\vec{r},t)}$$

the Heisenberg equation of motion can be obtained from

$$[\hat{\Psi}(\vec{r},t), \hat{H}] =$$

$$= \int d^3r' \underbrace{[\hat{\Psi}(\vec{r},t), \hat{\Psi}^+(\vec{r}',t)]}_{\delta(\vec{r}-\vec{r}')} \left(-\frac{1}{2m}\vec{\nabla}'^2\right)\hat{\Psi}(\vec{r}',t)$$

$$= -\frac{1}{2m}\vec{\nabla}^2\hat{\Psi}(\vec{r},t)$$

which has the same form as the "classical" Schrödinger equation

$$i\partial_t \hat{\Psi}(\vec{r},t) = [\hat{\Psi}(\vec{r},t), \hat{H}] = -\frac{1}{2m}\vec{\nabla}^2\hat{\Psi}(\vec{r},t) \quad \checkmark$$

It is interesting to note, that the Schrödinger field equation also follows if we assume fermionic quantization

$$\boxed{\begin{aligned} \{\hat{\Psi}(\vec{r},t), \hat{\Psi}(\vec{r}',t)\} &= \{\hat{\Psi}^+(\vec{r},t), \hat{\Psi}^+(\vec{r}',t)\} = 0 \\ \{\hat{\Psi}(\vec{r},t), \hat{\Psi}^+(\vec{r}',t)\} &= \delta(\vec{r}-\vec{r}') \end{aligned}}$$

proof: $[\hat{\Psi}(\vec{r},t), \hat{H}]$

$$= \int d^3r' \; \hat{\Psi}(\vec{r})\hat{\Psi}^+(\vec{r}')\left(-\frac{1}{2m}\vec{\nabla}'^2\right)\hat{\Psi}(\vec{r}') \; -$$

$$- \int d^3r' \, \hat{\psi}^+(\vec{r}')\left(-\frac{1}{2m}\vec{\nabla}'^2\right) \hat{\psi}(\vec{r}')\,\hat{\psi}(\vec{r})$$

with $\hat{\psi}(\vec{r})\hat{\psi}^+(\vec{r}') = \delta(\vec{r}-\vec{r}') - \hat{\psi}^+(\vec{r}')\hat{\psi}(\vec{r})$

and $\hat{\psi}(\vec{r}')\hat{\psi}(\vec{r}) = -\hat{\psi}(\vec{r})\hat{\psi}(\vec{r}')$

one finds

$$[\hat{\psi}(\vec{r},t), \hat{H}] = -\frac{1}{2m}\vec{\nabla}^2\hat{\psi}(\vec{r}) \qquad \square$$

$\Rightarrow$ The Schrödinger field can be quantized either according bosonic or fermionic quantization rules.

normal mode decomposition

Similarly to the linear harmonic chain we will now try to find a decomposition into normal modes.

Let us consider a cubic box of length L and periodic boundary conditions. We know that the classical Schrödinger equation has the following normalized eigensolutions

$$\phi_n(\vec{r},t) = \frac{1}{\sqrt{L^3}}\, e^{i(\vec{k}_n\cdot\vec{r} - \omega_n t)}$$

where $\vec{k}_n = \frac{2\pi}{L}(n_x, n_y, n_z)$ and $\omega_n = \frac{|\vec{k}_n|^2}{2m}$

$n_x, n_y, n_z = 0, \pm 1, \pm 2, \ldots$

decomposition of field operator

$$\hat{\psi}(\bar{r},t) = \begin{cases} \sum_n \hat{a}_n \phi_n(\bar{r}) e^{-i\omega_n t} & \text{boson case} \\ \sum_n \hat{c}_n \phi_n(\bar{r}) e^{-i\omega_n t} & \text{fermion case} \end{cases}$$

substitution into field commutation / anti-commutation rules yields

$$\boxed{[\hat{a}_n, \hat{a}_m] = [\hat{a}_n^+, \hat{a}_m^+] = 0 \qquad [\hat{a}_n, \hat{a}_m^+] = \delta_{nm}}$$

$$\boxed{\{\hat{c}_n, \hat{c}_m\} = \{\hat{c}_n^+, \hat{c}_m^+\} = 0 \qquad \{\hat{c}_n, \hat{c}_m^+\} = \delta_{nm}}$$

The Hamiltonian can be written in terms of these operators as

$$\hat{H} = \int d^3r\, \hat{\psi}^+(\bar{r},t)\left(-\frac{1}{2m}\vec{\nabla}^2\right)\hat{\psi}(\bar{r},t) = \int d^3r\, \hat{\psi}^+(\bar{r},t)\, i\partial_t\, \hat{\psi}(\bar{r},t)$$

$$= \int d^3r \sum_{n,m} \hat{a}_n^+ e^{i\omega_n t} \phi_n^*(\bar{r})\, i\omega_m \hat{a}_m e^{-i\omega_m t} \phi_m(\bar{r})$$

with the orthogonality relation one finds $(\varepsilon_n = \omega_n)$

$$\boxed{\hat{H} = \sum_n \varepsilon_n \hat{a}_n^+ \hat{a}_n} \quad \text{or} \quad \boxed{\hat{H} = \sum_n \varepsilon_n \hat{c}_n^+ \hat{c}_n}$$

In both cases $\hat{H}$ is positiv definit.

eigenstates can be written as $\boxed{|\ldots, m_{j-1}, m_j, m_{j+1}, \ldots\rangle}$

where for

bosonic fields $\quad m_k = 0, 1, 2, \ldots$

fermionic fields $\quad m_n = 0, 1$

The m_k are eigenvalues of $\hat{a}_n^+ \hat{a}_k$ or $\hat{c}_n^+ \hat{c}_k$ and must be interpreted as <u>particle numbers</u> in the mode $\phi_n(\bar{r})$. The state $|0,0,0,\ldots\rangle$ is called <u>particle vacuum.</u>

$\hat{a}_n^+, \hat{c}_n^+$	particle creation operator in mode $\phi_n(\bar{r})$
$\hat{a}_n, \hat{c}_n$	particle annihilation operator in mode $\phi_n(\bar{r})$

We will see that those properties carry over to other field theories.

The anti-commutation relation for Fermions $\{\hat{c}_n^+, \hat{c}_n^+\} = 0$ represents the <u>Pauli-principle</u>

$$\boxed{\hat{c}_n^{+\,2} = 0}$$

$\nexists$ 2 Fermions in the same mode $\phi_n(\bar{r})$ (the same single-particle state)

conservation of particle number in Schrödinger theory

$$\hat N \equiv \int d^3r\ \hat\psi^+ \hat\psi$$

$$= \int d^3r \sum_{n,m} \hat a_n^+(t)\, \hat a_m(t)\ \underbrace{\phi_n^*(\vec r)\,\phi_m(\vec r)}_{\hookrightarrow\ \delta_{nm}}$$

$$= \sum_n \hat a_n^+ \hat a_n \qquad \text{(similarly for } \hat c_n, \hat c_m^+ \text{)}$$

lets consider time evolution

$$i\frac{d}{dt}\hat N = [\hat N, \hat H] = \int d^3r \int d^3r'\ \hat\psi^+(r)\hat\psi(r)\hat\psi^+(\vec r')\left(-\frac{1}{2m}\Delta'\right)\hat\psi(r')$$

$$-\int d^3r \int d^3r'\ \hat\psi^+(\vec r')\left(-\frac{1}{2m}\Delta'\right)\hat\psi(\vec r')\,\hat\psi^+(\vec r)\hat\psi(\vec r)$$

$$= \int d^3r \int d^3r' \pm\left(\hat\psi^+(\vec r')\cancel{\hat\psi^+(\vec r)}\hat\psi(\vec r) + \cancel{\delta(r-r')}\hat\psi(r')\right)\left(-\frac{1}{2m}\Delta'\right)\hat\psi(r')$$

$$-\int d^3r \int d^3r'\ \hat\psi^+(\vec r')\left(-\frac{1}{2m}\Delta'\right)\left(\hat\psi^+(\vec r)\cancel{\hat\psi(\vec r)}\hat\psi(\vec r') + \cancel{\delta(r-r')}\hat\psi(r')\right)$$

$= 0$ for bosonic and fermionic field

$$\boxed{\text{The total number of particles of the non-interacting Schrödinger field is a constant of motion. Particles cannot be created or annihilated}}$$

Observation shows that this is also true for interacting Schrödinger fields.

One recognizes that the Hamiltonian has the structure

$$\hat{H} = \int d^3r \; \hat{\Psi}^+(\vec{r}) \, h_D(r) \, \hat{\Psi}(\vec{r})$$

where $h_D(\vec{r}) = -\frac{1}{2m}\vec{\nabla}^2$ is the single-particle Hamilton operator in position representation. (differential Op.)
In general one finds

<u>single-particle operator</u>

$$\boxed{\hat{O}_1 = \int d^3r \; \hat{\Psi}^+(\vec{r}) \, O_D(r) \hat{\Psi}(\vec{r})}$$

other example:

$$\hat{\vec{r}} = \int d^3r \; \hat{\Psi}^+(\vec{r}) \, \vec{r} \, \hat{\Psi}(\vec{r})$$ center of mass <u>position</u>

$$\hat{\vec{p}} = \int d^3r \; \hat{\Psi}^+(\vec{r}) (-i\vec{\nabla}) \hat{\Psi}(\vec{r})$$ <u>momentum</u>

likewise one can introduce <u>two-particle operators</u>

$$\boxed{\hat{O}_2 = \int d^3r \int d^3r' \; \hat{\Psi}^+(\vec{r}) \hat{\Psi}^+(\vec{r}\,') \, O_D(\vec{r},\vec{r}\,') \, \hat{\Psi}(\vec{r}\,') \hat{\Psi}(\vec{r})}$$

etc. All of these Operators commute with the total particle number

$$[\hat{O}_1, \hat{N}] = [\hat{O}_2, \hat{N}] = 0$$

Schrödinger field with interactions

The Hamilton operator of interacting Schrödinger-particles has the generic form

$$\hat{H} = \int d^3r \; \hat{\psi}^+(\vec{r})\, h_0(\vec{r})\, \hat{\psi}(\vec{r})$$

$$+ \int d^3r \int d^3r' \; \hat{\psi}^+(\vec{r})\, \hat{\psi}^+(\vec{r}\,')\, V_2(\vec{r},\vec{r}\,')\, \hat{\psi}(\vec{r}\,')\, \hat{\psi}(\vec{r})$$

$$+ \int d^3r \int d^3r' \int d^3r'' \; \hat{\psi}^+(\vec{r})\, \hat{\psi}^+(\vec{r}\,')\, \hat{\psi}^+(\vec{r}\,'')\, V_3(\vec{r},\vec{r}\,',\vec{r}\,'')\, \hat{\psi}(\vec{r}\,'')\, \hat{\psi}(\vec{r}\,')\, \hat{\psi}(\vec{r})$$

$$+ \dots$$

where $V_2(\vec{r},\vec{r}\,')$, $V_3(\vec{r},\vec{r}\,',\vec{r}\,'')$ is the two-particle and three-particle interaction potential and $h_0(\vec{r}) = -\frac{1}{2m}\Delta + V_1(\vec{r})$ contains next to the kinetic energy also an external potential $V_1(\vec{r})$. Note that the structure of $\hat{H}$ is such that the total number of particles is conserved.

A consequence of the conservation of particle number is the <u>complete equivalence</u> of the non-relativistic Schrödinger field theory <u>to the N-particle quantum mechanics</u>

<u>N-particle wavefunction</u>

$$\boxed{\phi_N(\vec{r}_1, \vec{r}_2, \dots \vec{r}_N, t) \equiv \langle 0 |\, \hat{\psi}(\vec{r}_1,t)\, \hat{\psi}(\vec{r}_2,t) \dots \hat{\psi}(\vec{r}_N,t)\, | \phi \rangle}$$

$$[\hat{\psi}(\vec{r}_i), \hat{\psi}(\vec{r}_k)] = 0 \Rightarrow$$

$$\phi(\vec{r}_1, \dots, \vec{r}_i, \dots, \vec{r}_k, \dots) = \phi(\vec{r}_1, \dots, \vec{r}_k, \dots, \vec{r}_i, \dots)$$

total symmetry of N-particle wavefunction for bosonic field

$$\{\hat{\psi}(\vec{r}_i), \hat{\psi}(\vec{r}_k)\} = 0 \Rightarrow$$

$$\phi(\vec{r}_1, \dots, \vec{r}_i, \dots \vec{r}_k \dots) = -\phi(\vec{r}_1, \dots \vec{r}_k \dots \vec{r}_i \dots)$$

total anti-symmetry of N-particle wave-function for fermionic field

Since $\hat{N}$ is conserved the state vector of the field can always be represented in terms of the N-particle wavefunction if N is the number of particles present at some initial time

$$\boxed{|\phi(t)\rangle = \frac{1}{\sqrt{N!}} \int d^3r_1 \dots \int d^3r_N \, \phi_N(\vec{r}_1, \dots \vec{r}_N, t) \, \hat{\psi}^+(\vec{r}_1) \dots \hat{\psi}^+(\vec{r}_N) |0\rangle}$$

This establishes a relation between the quantum theory of the Schrödinger field and many-body quantum mechanics.