2.2 Quantum mechanics and first quantization

2.2.1 Reminder: State vectors and operators in Hilbert space

Let us briefly recall the main ideas of quantum theory. The essence of quantum mechanics or "first" quantization is to replace functions by operators, starting from the coordinate and momentum (here we use the momentum representation),

$$\begin{aligned} \mathbf{r} &\rightarrow \hat{\mathbf{r}} = \mathbf{r}, \\ \mathbf{p} &\rightarrow \hat{\mathbf{p}} = \frac{\hbar}{i}\frac{\partial}{\partial \mathbf{r}}, \end{aligned}$$

where the last equalities refer to the coordinate representation. These operators are hermitean, $\hat{\mathbf{r}}^\dagger = \hat{\mathbf{r}}$ and $\hat{\mathbf{p}}^\dagger = \hat{\mathbf{p}}$, and do not commute

$$[\hat{x}_i, \hat{p}_j] = i\hbar\,\delta_{ij}, \tag{2.26}$$

which means that coordinate and momentum (the same components) cannot be measured simultaneously. The minimal uncertainty of such a simultaneous measurement is given by the Heisenberg relation

$$\Delta\hat{x}_i \Delta\hat{p}_i \geq \frac{\hbar}{2}, \tag{2.27}$$

where the standard deviation ("uncertainty") of an operator $\hat{A}$ is defined as

$$\Delta\hat{A} = \sqrt{\left\langle \left(\hat{A} - \langle\hat{A}\rangle\right)^2 \right\rangle}, \tag{2.28}$$

and the average is computed in a given state $|\psi\rangle$, i.e. $\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle$. The general formulation of quantum mechanics describes an arbitrary quantum system in terms of abstract states $|\psi\rangle$ that belong to a Hilbert space (Dirac's notation), and operators act on this state returning another Hilbert space state, $\hat{A}|\psi\rangle = |\phi\rangle$.

The central quantity of classical mechanics – the hamilton function – retains its functional dependence on coordinate and momentum in quantum mechanics as well (correspondence principle) but becomes an operator depending on operators, $H(\mathbf{r}, \mathbf{p}) \rightarrow \hat{H}(\hat{\mathbf{r}}, \hat{\mathbf{p}})$. The classical equations of motion – Hamilton's equations or Newton's equation (2.4) – are now replaced by a partial differential equation for the Hamilton operator, the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle. \tag{2.29}$$

Stationary properties are governed by the stationary Schrödinger equation that follows from the ansatz[6]

$$\begin{aligned} |\psi(t)\rangle &= e^{-\frac{i}{\hbar}\hat{H}t}|\psi\rangle\,, \\ \hat{H}|\psi\rangle &= E|\psi\rangle\,. \end{aligned} \tag{2.30}$$

The latter is an eigenvalue equation for the Hamilton operator with the eigenfunctions $|\psi\rangle$ and corresponding eigenvalues E.

2.2.2 Probabilistic character of "First" quantization. Comparison to experiments

Experiments in quantum mechanics never directly yield the wave function or the probability distribution. Individual (random) realizations of possible configurations and their dynamics.

Examples:

1. double slit experiment with electrons of Tonomura

2. photons on a photo plate or CCD detector,

3. many-body dynamics in ultracold atom experiments in optical lattices

Possible configurations are particularly evident in the case of fermionic atoms (assuming spin $s = 1/2$, for simplicity) in optical lattices. Due to the Pauli principle each lattice site can be occupied only by zero, one or two atoms – in the latter case they have to have different spin projections. If an initial configuration of atoms is excited (e.g. by a confinement quench), a dynamical evolution will start. This will, of course, not be described by the time-dependent Schrödinger equation for the many-atom wave function! This equation only describes the *average dynamics* that follow from averaging over the dynamics that start from many independent realizations. This has been very successful but, on the other hand, reproduces only part of the information. For example, it completely misses the fluctuations of the numbers of atoms around the average.[7]

"First" quantization is evident in the case of particle motion in a confining potential $U(\mathbf{r})$, such as an oscillator potential: classical bounded motion transforms, in quantum mechanics, into a set of eigenstates $|\psi_n\rangle$ (that are localized as well) that exist only for a sequence of discrete (quantized) energies E_n. This example is discussed more in detail below.

[6]Here we assume a time-independent hamiltonian.

[7]This section is not complete yet.

2.3 The linear harmonic oscillator and the ladder operators

Let us now recall the simplest example of quantum mechanics: one particle in a one-dimensional harmonic potential $U(x) = \frac{m}{2}\omega^2 x^2$, i.e. in Eq. (2.1), $N = 1$ and the interaction potentials vanish. We will use this example to introduce the basic idea of "second quantization". In writing the potential $U(x)$ we switched to the coordinate representation where states $|\psi_n\rangle$ are represented by functions of the coordinate, $\psi_n(x)$. At the end we will return to the abstract notation in terms of Dirac states.

2.3.1 One-dimensional harmonic oscillator

The stationary properties of the harmonic oscillator follow from the stationary Schrödinger equation (2.30) which now becomes, in coordinate representation

$$\hat{H}(\hat{x},\hat{p})\psi_n(x) = \left\{\frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2\right\}\psi_n(x) = E_n\psi_n(x), \tag{2.31}$$

where $\hat{x} = x$ and $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$.

Dimensionless variables. We may bring the Hamilton operator to a more symmetric form by introducing the dimensionless coordinate $\xi = x/x_0$ with the length scale $x_0 = [\hbar/m\omega]^{1/2}$, whereas energies will be measured in units of $\hbar\omega$. Then we can replace $\frac{d}{dx} = \frac{1}{x_0}\frac{d}{d\xi}$ and obtain

$$\frac{\hat{H}}{\hbar\omega} = \frac{1}{2}\left\{-\frac{\partial^2}{\partial\xi^2} + \xi^2\right\}. \tag{2.32}$$

Ladder operators. This quadratic form can be rewritten in terms of a product of two first order operators $a, a^\dagger$, the "ladder operators" (we skip the "hat"),

$$a = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial\xi} + \xi\right), \tag{2.33}$$

$$a^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial\xi} + \xi\right). \tag{2.34}$$

Indeed, computing the product

$$\begin{aligned}\hat{N} &= a^\dagger a = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial\xi} + \xi\right)\frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial\xi} + \xi\right) \\ &= \frac{1}{2}\left\{-\frac{\partial^2}{\partial\xi^2} + \xi^2 - 1\right\},\end{aligned} \tag{2.35}$$

the hamiltonian (2.32) can be written as

$$\frac{\hat{H}}{\hbar\omega} = \hat{N} + \frac{1}{2}. \tag{2.36}$$

It is obvious from (2.36) that $\hat{N}$ commutes with the hamiltonian,

$$[\hat{H}, \hat{N}] = 0, \tag{2.37}$$

and thus the two have common eigenstates. This way we have transformed the hamiltonian from a function of the two non-commuting hermitean operators $\hat{x}$ and $\hat{p}$ into a function of the two operators a and $a^\dagger$ which are also non-commuting[8], but not hermitean, instead they are the hermitean conjugate of each other,

$$[a, a^\dagger] = 1, \tag{2.38}$$
$$(a)^\dagger = a^\dagger, \tag{2.39}$$

which is easily verified.

Computing the energy spectrum from the ladder operators. The advantage of the ladder operators is that they allow for a straightforward computation of the energy spectrum of $\hat{H}$, using only the properties (2.35) and (2.38), without need to solve the Schrödinger equation, i.e. avoiding explicit computation of the eigenfunctions $\psi_n(\xi)$ [9]. This allows us to return to a representation-independent notation for the eigenstates, $\psi_n \to |n\rangle$. The only thing we require is that these states are complete and orthonormal, $\hat{1} = \sum_n |n\rangle\langle n|$ and $\langle n|n'\rangle = \delta_{n,n'}$.

Now, acting with $\hat{N}$ on an eigenstate, using Eq. (2.36), we obtain

$$\hat{N}|n\rangle = a^\dagger a\,|n\rangle = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)|n\rangle = n|n\rangle, \quad \forall n, \tag{2.40}$$
$$n = \frac{E_n}{\hbar\omega} - \frac{1}{2},$$

where the last line relates the eigenvalues of $\hat{N}$ and $\hat{H}$ that correspond to the common eigenstate $|n\rangle$. Let us now introduce two new states that are created by the action of the ladder operators,

$$a|n\rangle = |\tilde{n}\rangle,$$
$$a^\dagger|n\rangle = |\bar{n}\rangle,$$

[8]The appearance of the standard commutator indicates that these operators describe bosonic excitations.

[9]We will use the previous notation ψ, which means that the normalization is $x_0 \int d\xi |\psi(\xi)|^2 = 1$

where this action is easily computed. In fact, multiplying Eq. (2.40) from the left by a, we obtain

$$aa^\dagger |\tilde{n}\rangle = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)|\tilde{n}\rangle.$$

Using the commutation relation (2.38) this expression becomes

$$a^\dagger a |\tilde{n}\rangle = \left(\frac{E_n}{\hbar\omega} - \frac{3}{2}\right)|\tilde{n}\rangle = (n-1)|\tilde{n}\rangle,$$

which means the state $|\tilde{n}\rangle$ is an eigenstate of $\hat{N}$ [and, therefore, of $\hat{H}$] and has an energy lower than $|n\rangle$ by $\hbar\omega$, whereas the eigenvalue of $\hat{N}$ is $\tilde{n} = n-1$. Thus, the action of the operator a is to switch from an eigenstate with eigenvalue n to one with eigenvalue $n-1$.

Determination of the ground state. Obviously, this is impossible for the ground state, i.e. when a acts on $|0\rangle$, so we have to require

$$|\tilde{0}\rangle = a|0\rangle \equiv 0. \tag{2.41}$$

When we use this result in Eq. (2.40) for $n = 0$, the l.h.s. is zero with the consequence that the term in parantheses must vanish. This immediately leads to the well-known result for the ground state energy: $E_0 = \hbar\omega/2$, corresponding to the eigenvalue 0 of $\hat{N}$.

Computation of the excited states. From this we now obtain the energy spectrum of the excited states: acting with $a^\dagger$ from the left on Eq. (2.40) and using the commutation relation (2.38), we obtain

$$\hat{N}|\bar{n}\rangle = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2} + 1\right)|\bar{n}\rangle = \bar{n}|\bar{n}\rangle.$$

Thus, $\bar{n}$ is again an eigenstate of $\hat{N}$ and $\hat{H}$. Further, if the eigenstate $|n\rangle$ has an energy E_n, cf. Eq. (2.40), then $\bar{n}$ has an energy $E_n + \hbar\omega$, whereas the associated eigenvalue of $\hat{N}$ is $\bar{n} = n + 1$. Starting from the ground state and acting repeatedly with $a^\dagger$ we construct the whole spectrum, E_n, and may express all eigenfunctions via ψ_0:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots \tag{2.42}$$

$$|n\rangle = C_n \left(a^\dagger\right)^n |0\rangle. \tag{2.43}$$

$$C_n = \frac{1}{\sqrt{n!}}, \tag{2.44}$$

Abbildung 2.1: **Left**: oscillator potential and energy spectrum. The action of the operators a and $a^\dagger$ is illustrated. **Right**: alternative interpretation: the operators transform between "many-particle" states containing different number of elementary excitations.

where the normalization constant C_n will be verified from the properties of $a^\dagger$ below. The above result shows that the eigenvalue of the operator $\hat{N}$ is just the quantum number n associated with the eigenstate $|n\rangle$.

Re-interpretation as creation and annihilation operators. In other words, since $|n\rangle$ is obtained by applying $a^\dagger$ to the groundstate function n times or by "n-fold excitation", the operator $\hat{N}$ is the number operator counting the number of excitations (above the ground state). Therefore, if we are not interested in the analytical details of the eigenstates we may use the operator $\hat{N}$ to count the number of excitations "contained" in the system. For this reason, the common notion for the operator a ($a^\dagger$) is "annihilation" ("creation") operator of an excitation. For an illustration, see Fig. 2.3.1.

From the eigenvalue problem of $\hat{N}$, Eq. (2.40) we may also obtain the explicit action of the two operators a and $a^\dagger$. Since the operator a transforms a state into one with quantum number n lower by 1 we have

$$a|n\rangle = \sqrt{n}|n-1\rangle, \qquad n = 0, 1, 2, \ldots \tag{2.45}$$

where the prefactor may be understood as an ansatz[10]. The correctness is proven by deriving, from Eq. (2.45), the action of $a^\dagger$ and then verifying that we recover the eigenvalue problem of $\hat{N}$, Eq. (2.40). The action of the creation operator is readily obtained using the property (2.39):

$$\begin{aligned} a^\dagger|n\rangle &= \sum_{\bar{n}} |\bar{n}\rangle\langle\bar{n}|a^\dagger|n\rangle = \sum_{\bar{n}} |\bar{n}\rangle\, a[\langle\bar{n}|]\,|n\rangle \\ &= \sum_{\bar{n}} |\bar{n}\rangle\,\sqrt{\bar{n}}\,\langle\bar{n}-1\,|n\rangle = \sqrt{n+1}\,|n+1\rangle. \end{aligned} \tag{2.46}$$

Inserting these explicit results for a and $a^\dagger$ into Eq. (2.40), we immediately verify the consistency of the choice (2.45). Obviously the oscillator eigenstates $|n\rangle$ are no eigenstates of the creation and annihilation operators [11].

[10] This expression is valid also for $n = 0$ where the prefactor assures that application of a to the ground state does not lead to a contradiction.

[11] A particular case are Glauber states (coherent states) that are a special superposition of the oscillator states which are the eigenstate of the operator a.

Problems:

1. Calculate the explicit form of the ground state wave function by using Eq. (2.41).
2. Show that the matrix elements of $a^\dagger$ are given by $\langle n+1|a^\dagger|n\rangle = \sqrt{n+1}$, where $n = 0, 1, \ldots$, and are zero otherwise.
3. Show that the matrix elements of a are given by $\langle n-1|a|n\rangle = \sqrt{n}$, where $n = 0, 1, \ldots$, and are zero otherwise.
4. Proof relation (2.44).

2.3.2 Generalization to several uncoupled oscillators

The previous results are directly generalized to a three-dimensional harmonic oscillator with frequencies $\omega_i, i = 1, 2, 3$, which is described by the hamiltonian

$$\hat{H} = \sum_{i=1}^{3} \hat{H}(\hat{x}_i, \hat{p}_i), \tag{2.47}$$

which is the sum of three one-dimensional hamiltonians (2.31) with the potential energy $U(x_1, x_2, x_3) = \frac{m}{2}(\omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2)$. Since $[p_i, x_k] \sim \delta_{k,i}$ all three hamiltonians commute and have joint eigenfunction (product states). The problem reduces to a superposition of three independent one-dimensional oscillators. Thus we may introduce ladder operators for each component independently as in the 1d case before,

$$a_i = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial \xi_i} + \xi_i\right), \tag{2.48}$$

$$a_i^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial \xi_i} + \xi_i\right), \quad [a_i, a_k^\dagger] = \delta_{i,k}. \tag{2.49}$$

Thus the hamiltonian and its eigenfunctions and eigenvalues can be written as

$$\begin{aligned} \hat{H} &= \sum_{i=1}^{3} \hbar\omega_i \left(a_i^\dagger a_i + \frac{1}{2}\right) \\ a_i|0\rangle &= 0, \quad i = 1, 2, 3 \\ \psi_{n_1,n_2,n_3} = |n_1 n_2 n_3\rangle &= \frac{1}{\sqrt{n_1! n_2! n_3!}} (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} (a_3^\dagger)^{n_3} |0\rangle \\ E &= \sum_{i=1}^{3} \hbar\omega_i \left(n_i + \frac{1}{2}\right). \end{aligned} \tag{2.50}$$

Abbildung 2.2: Illustration of the one-dimensional chain with nearest neighbor interaction. The chain is made infinite by connecting particle $N+1$ with particle 1 (periodic boundary conditions).

Here $|0\rangle \equiv |000\rangle = |0\rangle|0\rangle|0\rangle$ denotes the ground state and a general state $|n_1 n_2 n_3\rangle = |n_1\rangle|n_2\rangle|n_3\rangle$ contains n_i elementary excitations in direction i, created by n_i times applying operator $a_i^\dagger$ to the ground state.

Finally, we may consider a more general situation of any number M of coupled independent linear oscillators and generalize all results by replacing the dimension $3 \to M$.

2.4 Generalization to interacting particles. Normal modes

The previous examples of independent linear harmonic oscillators are of course the simplest situations which, however, are of limited interest. In most problems of many-particle physics the interaction between the particles which was neglected so far, is of crucial importance. We now discuss how to apply the formalism of the creation and annihilation operators to interacting systems.

2.4.1 One-dimensional chain and its normal modes

We consider the simplest case of an interacting many-particle system: N identical classical particles arranged in a linear chain and interacting with their left and right neighbor via springs with constant k.[12], see Fig. 2.2.

This is the simplest model of interacting particles because each particle is assumed to be fixed around a certain position x_i in space around which it can perform oscillations with the displacement q_i and the associated momentum p_i.[13] Then the hamiltonian (2.1) becomes

$$H(p,q) = \sum_{j=1}^{N} \left\{ \frac{p_j^2}{2m} + \frac{k}{2}\left(q_j - q_{j+1}\right)^2 \right\}. \tag{2.51}$$

[12]Here we follow the discussion of Huang [Hua98].

[13]Such "lattice" models are very popular in theoretical physics because they allow to study many-body effects in the most simple way. Examples include the Ising model, the Anderson model or the Hubbard model of condensed matter physics.

Abbildung 2.3: Dispersion of the normal modes, Eq. (2.55), of the $1d$ chain with periodic boundary conditions.

Applying Hamilton's equations we obtain the system of equations of motion (2.4)

$$m\ddot{q}_j = k\left(q_{j+1} - 2q_j + q_{j-1}\right), \qquad j = 1 \ldots N \tag{2.52}$$

which have to be supplemented with boundary and initial conditions. In the following we consider a macroscopic system and will not be interested in effects of the left and right boundary. This can be achieved by using "periodic" boundary conditions, i.e. periodically repeating the system according to $q_{j+N}(t) = q_j(t)$ for all j [for solutions for the case of a finite system, see Problem 5]. We start with looking for particular (real) solutions of the following form[14]

$$q_j(t) = e^{i(-\omega t + jl)} + c.c., \tag{2.53}$$

which, inserted into the equation of motion, yield for any j

$$-m\omega^2\left(q_j + q_j^*\right) = k\left(e^{il} - 2 + e^{-il}\right)\left(q_j + q_j^*\right), \tag{2.54}$$

resulting in the following relation between ω and k (dispersion relation)[15]:

$$\omega^2(l) = \omega_0^2 \sin^2\frac{l}{2}, \qquad \omega_0^2 = 4\frac{k}{m}. \tag{2.55}$$

Here ω_0 is just the eigenfrequency of a spring with constant k, and the prefactor 2 arises from the fact that each particle interacts with two neighbors. While the condition (2.55) is independent of the amplitudes q_j^0, i.e. of the initial conditions, we still need to account for the boundary (periodicity) condition. Inserting it into the solution (2.53) gives the following condition for l, independently of ω: $l \to l_n = \frac{n}{N}2\pi$, where $n = 0, \pm1, \pm2, \cdots \pm\frac{N}{2}$. Thus there exists a discrete spectrum of N frequencies of modes which can propagate along the chain (we have to exclude $n = 0$ since this corresponds to a time-independent trivial constant displacement),

$$\omega_n^2 = 4\frac{k}{m}\sin^2\frac{n\pi}{N}, \quad n = \pm1, \pm2, \cdots \pm\frac{N}{2}. \tag{2.56}$$

This spectrum is shown in Fig. 2.3. These N solutions are the complete set of

[14] In principle, we could use a prefactor $q_j^0 = q^0$ different from one, but by rescaling of q it can always be eliminated. The key is that the amplitudes of all particles are strictly coupled.

[15] We use the relation $1 - \cos x = 2\sin^2\frac{x}{2}$.

normal modes of the system (2.51), corresponding to its N degrees of freedom. These are *collective modes* in which all particles participate – all oscillate with the same frequency but with a well-defined phase which depends on the particle number. These normal modes are waves running along the chain with a phase velocity[16] $c_n \sim \omega_n/l_n$.

Due to the completeness of the system of normal modes, we can expand any excitation of particle j and the corresponding momentum, $p_j(t) = m\dot{q}_j(t)$, into a superposition of normal mode contributions ($n \neq 0$)

$$q_j(t) = \frac{1}{\sqrt{N}} \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} Q_n^0 \, e^{i\left(-\omega_n t + 2\pi \frac{n}{N} j\right)} = \frac{1}{\sqrt{N}} \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} e^{-i\omega_n t} Q_n(j)\,, \quad (2.57)$$

$$p_j(t) = \frac{1}{\sqrt{N}} \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} P_n^0 \, e^{i\left(-\omega_n t + 2\pi \frac{n}{N} j\right)} = \frac{1}{\sqrt{N}} \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} e^{-i\omega_n t} P_n(j), \quad (2.58)$$

where $P_n^0 = -im\omega_n Q_n^0$. Note that the complex conjugate contribution to mode n is contained in the sum (term $-n$). Also, $q_j(t)$ and $p_j(t)$ are real functions. By computing the complex conjugate q_j^* and equating the result to q_j we obtain the conditions $(Q_n^0)^* = Q_{-n}^0$ and $\omega_{-n} = -\omega_{-n}$. Analogously we obtain for the momenta $(P_n^0)^* = P_{-n}^0$. To make the notation more compact we introduced the N-dimensional complex vectors $\vec{Q}_n$ and $\vec{P}_n$ with the component j being equal to $Q_n(j) = Q_n^0 e^{i2\pi nj/N}$ and $P_n(j) = P_n^0 e^{i2\pi nj/N}$. One readily proofs[17] that these vectors form an orthogonal system by computing the scalar product (see problem 5)

$$\vec{Q}_n \vec{Q}_m = Q_n^0 Q_m^0 \sum_{j=1}^{N} e^{i2\pi \frac{n+m}{N} j} = N Q_n^0 Q_m^0 \delta_{n,-m}. \quad (2.59)$$

Using this property it is now straightforward to compute the hamilton function in normal mode representation. Consider first the momentum contribution,

$$\sum_{j=1}^{N} p_j^2(t) = \frac{1}{N} \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} \sum_{m=-\frac{N}{2}}^{\frac{N}{2}} \vec{P}_n \vec{P}_m \, e^{-i(\omega_n + \omega_m)t}, \quad (2.60)$$

where the sum over j has been "absorbed" in the scalar product. Using now

[16] The actual phase velocity is ω_n/k_n, where the wave number $k_n = l_n/a$ involves a length scale a which does not appear in the present discrete model.

[17] See problem 5

the orthogonality condition (2.59) we immediately simplify

$$\sum_{j=1}^{N} p_j^2(t) = \sum_n |P_n^0|^2. \tag{2.61}$$

Analogously, we compute the potential energy

$$\begin{aligned} U &= \frac{k}{2}\sum_{j=1}^{N}[q_j(t)-q_{j+1}(t)]^2 = \frac{k}{2N}\sum_{n=-\frac{N}{2}}^{\frac{N}{2}}\sum_{m=-\frac{N}{2}}^{\frac{N}{2}} e^{-i(\omega_n+\omega_m)t} \\ &\quad \times \sum_{j=1}^{N} Q_n^0 Q_m^0 \left\{e^{i2\pi\frac{n}{N}j} - e^{i2\pi\frac{n}{N}(j+1)}\right\}\left\{e^{i2\pi\frac{m}{N}j} - e^{i2\pi\frac{m}{N}(j+1)}\right\}. \end{aligned}$$

The sum over j can again be simplified, using the orthogonality condition (2.59), which allows to replace m by $-n$,

$$\begin{aligned} &\frac{1}{N}\sum_{j=1}^{N} Q_n^0 Q_m^0 \left\{e^{i2\pi\frac{n}{N}j} - e^{i2\pi\frac{n}{N}(j+1)}\right\}\left\{e^{i2\pi\frac{m}{N}j} - e^{i2\pi\frac{m}{N}(j+1)}\right\} = \\ &= \left(1-e^{i2\pi\frac{n}{N}}\right)\left(1-e^{i2\pi\frac{m}{N}}\right)\vec{Q}_n\vec{Q}_m = \\ &= 2\left[1-\cos\frac{2\pi n}{N}\right]\delta_{n,-m}Q_n^0Q_m^0 = 4\frac{\omega_n^2}{\omega_0^2}\delta_{n,-m}|Q_n^0|^2, \end{aligned}$$

where we have used Eq. (2.55) and the relation $1-\cos x = 2\sin^2\frac{x}{2}$. This yields for the potential energy

$$U = \frac{k}{2}\sum_n \frac{m\omega_n^2}{k}$$

and for the total hamilton function

$$H(P,Q) = \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} \left\{\frac{1}{2m}|P_n^0|^2 + \frac{m}{2}\omega_n^2|Q_n^0|^2\right\}. \tag{2.62}$$

Problem 5: Prove the orthogonality relation (2.59).

2.4.2 Quantization of the $1d$ chain

We now quantize the interacting system (2.51) by replacing coordinates and momenta of all particles by hermitean operators

$$\begin{aligned} (q_i,p_i) &\rightarrow (\hat{q}_i,\hat{p}_i), \qquad i=1,\dots N, \\ \text{with}\quad \hat{q}_i^\dagger &= \hat{q}_i, \quad \hat{p}_i^\dagger = \hat{p}_i, \quad [\hat{q}_i,\hat{p}_j] = i\hbar\delta_{ij}. \end{aligned} \tag{2.63}$$

The Hamilton function (2.51) now becomes an operator of the same functional form (correspondence principle),

$$\hat{H}(\hat{p},\hat{q}) = \sum_{j=1}^{N} \left\{ \frac{\hat{p}_j^2}{2m} + \frac{k}{2}\left(\hat{q}_j - \hat{q}_{j+1}\right)^2 \right\},$$

and we still use the periodic boundary conditions $\hat{q}_{N+i} = \hat{q}_i$. The normal modes of the classical system remain normal modes in the quantum case as well, only the amplitudes Q_n^0 and P_n^0 become operators

$$\hat{q}_j(t) = \frac{1}{\sqrt{N}} \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} e^{-i\omega_n t}\hat{Q}_n(j) \tag{2.64}$$

$$p_j(t) = \frac{1}{\sqrt{N}} \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} e^{-i\omega_n t}\hat{P}_n(j), \tag{2.65}$$

where $\hat{Q}_n(j) = \hat{Q}_n^0 \exp\{i2\pi nj/N\}$, $\hat{P}_n(j) = \hat{P}_n^0 \exp\{i2\pi nj/N\}$ and $\hat{P}_n^0 = -im\omega_n \hat{Q}_n^0$.

What remains is to impose the necessary restrictions on the operators $\hat{Q}_n^0$ and $\hat{P}_n^0$ such that they guarantee the properties (2.63). One readily verifies that hermiticity of the operators is fulfilled if $(\hat{Q}^0)_n^\dagger = \hat{Q}_{-n}^0$, $(\hat{P}^0)_n^\dagger = \hat{P}_{-n}^0$ and $\omega_{-n} = -\omega_n$. Next, consider the commutator of $\hat{q}_i$ and $\hat{p}_j$ and use the normal mode representations (2.64, 2.65),

$$[\hat{q}_k, \hat{p}_j] = \frac{1}{N} \sum_n \sum_m [\hat{Q}_n^0, \hat{P}_m^0] e^{-i(\omega_n+\omega_m)t} e^{i\frac{2\pi}{N}(kn+jm)}. \tag{2.66}$$

A sufficient condition for this expression to be equal $i\hbar\delta_{k,j}$ is evidently $[\hat{Q}_n^0, \hat{P}_m^0] = i\hbar\delta_{n,-m}$ which is verified separately for the cases $k = j$ and $k \neq j$. In other words, the normal mode operators obey the commutation relation

$$\left[\hat{Q}_n^0, (\hat{P}_m^0)^\dagger\right] = i\hbar\delta_{n,m}, \tag{2.67}$$

and the hamiltonian becomes, in normal mode representation,

$$\hat{H}(\hat{P},\hat{Q}) = \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} \left\{ \frac{1}{2m}|\hat{P}_n^0|^2 + \frac{m}{2}\omega_n^2 |\hat{Q}_n^0|^2 \right\}. \tag{2.68}$$

This is a superposition of N independent linear harmonic oscillators with the frequencies ω_n given by Eq. (2.56). Applying the results for the superposition

of oscillators, Sec. 2.3.2, we readily can perform the second quantization by defining dimensionless coordinates, $\xi_n = \sqrt{\frac{m\omega_n}{\hbar}} Q_n,\ n = -\frac{N}{2}, \ldots \frac{N}{2},\ n \neq 0$, and introducing the creation and annihilation operators,

$$a_n = \frac{1}{\sqrt{2}} \left(\frac{\partial}{\partial \xi_n} + \xi_n \right), \tag{2.69}$$

$$a_n^\dagger = \frac{1}{\sqrt{2}} \left(-\frac{\partial}{\partial \xi_n} + \xi_n \right), \quad [a_n, a_k^\dagger] = \delta_{n,k}. \tag{2.70}$$

Thus the hamiltonian and its eigenfunctions and eigenvalues can be written as

$$\begin{aligned} \hat{H} &= \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} \hbar\omega_n \left(a_n^\dagger a_n + \frac{1}{2} \right) \\ a_n|0\rangle &= 0, \quad n = -\frac{N}{2}, \ldots \frac{N}{2} \\ \psi_{m_1,\ldots m_N} = |m_1 \ldots m_N\rangle &= \frac{1}{\sqrt{m_1! \ldots m_N!}} \left(a^\dagger_{-\frac{N}{2}} \right)^{m_1} \ldots \left(a^\dagger_{\frac{N}{2}} \right)^{m_N} |0\rangle \\ E &= \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} \hbar\omega_n \left(m_n + \frac{1}{2} \right). \end{aligned}$$

Here $|0\rangle \equiv |0 \ldots 0\rangle = |0\rangle \ldots |0\rangle$ [N factors] denotes the ground state and a general state $|m_{-N/2} \ldots m_{N/2}\rangle = |m_{-N/2}\rangle \ldots |m_{N/2}\rangle$ contains m_n elementary excitations of the normal mode n, created by m_n times applying operator $a_n^\dagger$ to the ground state.

Problem 6: The commutation relation (2.67) which was derived to satisfy the commutation relations of coordinates and momenta is that of bosons. This result was independent of whether the particles in the chain are fermions or bosons. Discuss this seeming contradiction.

2.4.3 Generalization to arbitrary interaction

Of course, the simple $1d$ chain is a model with a limited range of applicability. A real system of N interacting particles in $1d$ will be more difficult, at least by three issues: first, the pair interaction potential V may have any form. Second, the interaction, in general, involves not only nearest neighbors, and third, the effect of the full $3d$ geometry may be relevant. We, therefore, now return to

the general $3d$ system of N classical particles (2.1) with the total potential energy[18]

$$U_{\rm tot}(q) = \sum_{i=1}^{N} U(\mathbf{r}_i) + \sum_{1\le i<j\le N} V(\mathbf{r}_i - \mathbf{r}_j), \tag{2.71}$$

leading to Newton's equations

$$m\ddot{\mathbf{r}}_i = -\frac{\partial}{\partial \mathbf{r}_i} U_{\rm tot}(q), \qquad i = 1, \dots N. \tag{2.72}$$

Let us consider stationary solutions, where the time derivatives on the l.h.s. vanish. The system will then be in a stationary state "s" corresponding to a minimum $q_s^{(0)}$ of $U_{\rm tot}$ of depth $U_s^{(0)} = U_{\rm tot}(q_s^{(0)})$ [the classical ground state corresponds to the deepest minimum].

Taylor expansion around the stationary state. In the case of weak excitations from the minimum, $q = q_s^{(0)} + \xi$, with $|\xi| \ll q_s^{(0)}$, the potential energy can be expanded in a Taylor series[19]

$$U_{\rm tot}(q) = U_s^{(0)} + \frac{\partial}{\partial q} U_{\rm tot}(q = q_s^{(0)})\xi + \frac{1}{2}\xi^T \mathcal{H}^{(s)} \xi + ... \tag{2.73}$$

where all first derivatives are zero, and we limit ourselves to the second order (harmonic approximation). Here we introduced the $3N \times 3N$ Hesse matrix $\mathcal{H}_{ij}^{(s)} = \frac{\partial^2}{\partial x_i \partial x_j} U_{\rm tot}(q = q_s^{(0)})$, where $x_i, x_j = x_1, y_1, \dots z_N$, and ξ^T is the transposed vector (row) of ξ. Thus, for weak excitations, the potential energy change $\Delta U_{\rm tot} = U_{\rm tot}(q) - U_s^{(0)}$ is reduced to an expression which is quadratic in the displacements ξ, i.e. we are dealing with a system of coupled harmonic oscillators[20]

Diagonalization of the hamiltonian. We can easily transform this to a system of uncoupled oscillators by diagonalizing the Hesse matrix which can be achieved by solving the eigenvalue problem (we take the mass out for dimensional reasons)

$$\lambda_n m Q_n = \mathcal{H} Q_n, \qquad n = 1, \dots 3N. \tag{2.74}$$

Since $\mathcal{H}$ is real, symmetric and positive definite[21] the eigenvalues are real and positive corresponding to the normal mode frequencies $\omega_n = \sqrt{\lambda_n}$. An example

[18] Here we follow the discussion of Ref. [HKL$^+$09]

[19] Recall that q, $q_s^{(0)}$ and ξ are $3N$-dimensional vectors in configuration space.

[20] Strictly speaking, from the $3N$ degrees of freedom, up to three [depending on the symmetry of U] may correspond to rotations of the whole system (around one of the three coordinate axes, these are center of mass excitations which do not change the particle distance), and the remaining are oscillations.

[21] $q_s^{(0)}$ corresponds to a mininmum, so the local curvature of $U_{\rm tot}$ is positive in all directions

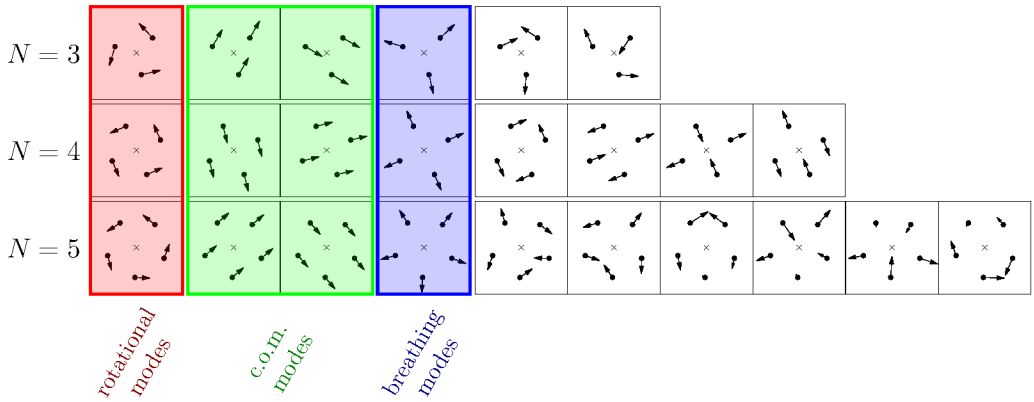

Abbildung 2.4: All normal modes of two-dimensional harmonically confined Coulomb systems with $N = 3, 4, 5$ particles. The dots picture the particles within the ground-state configuration, and the arrows show the direction and amplitude of the oscillatory motion (eigenvectors). The N-independent modes, i.e., the rotational modes, the modes of center-of-mass oscillation (com), and the breathing modes are highlighted. From Ref. [HKL+09].

of the normal modes of small two-dimensional clusters of charged particles in a harmonic confinement of frequency ω is shown in Fig. 2.4. There are three modes that are present for all particle numbers: first, the rotation of the entire system which does not require excitation energy due to the rotational symmetry of the system ($\omega_n = 0$). Second, the center of mass oscillation of all particles ("sloshing mode", frequency $\omega_n = \omega$). Third is the uniform isotropic expansion/contraction of all particle ("breathing mode") that has a frequency $\omega_n = \sqrt{3}\,\omega$, in the case of Coulomb interaction[22]. The complete set of $2N$ eigenmodes is sketched in the figure.

Furthermore, as a result of the diagonalization, the $3N$-dimensional eigenvectors form a complete orthogonal system $\{Q_n\}$ with the scalar product $Q_n Q_m \equiv \sum_{i=1}^{3N} Q_n(i) Q_m(i) \sim \delta_{m,n}$ which means that any excitation can be expanded into a superposition of the eigenvectors (normal modes),

$$q(t) = q_s^{(0)} + \sum_{n=1}^{3N} c_n(t) Q_n. \tag{2.75}$$

The expansion coefficients $c_n(t)$ (scalar functions) are the normal coordinates. Their equation of motion is readily obtained by inserting a Taylor expansion

[22] An interesting feature of the breathing mode is that its frequency is sensitive to the pair interaction [HFL+08], as well as to quantum and spin effects [BBHB09]. This makes it a sensitive diagnostic of interacting quantum systems, e.g. [MOA+13].

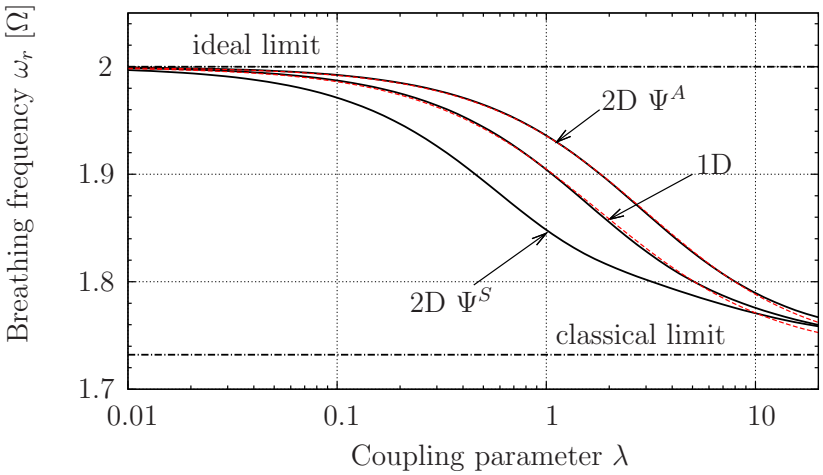

Abbildung 2.5: Frequency of the breathing mode of $N = 2$ particles in a harmonic trap for varying interaction strength $\lambda = \frac{q^2}{4\pi\epsilon_0 l_0}\frac{1}{\hbar\omega}$, with $l_0^2 = \hbar/(m\omega)$. The results for electrons with the same (A, anti-symmetric coordinate wave function) and opposite (S, symmetric coordinate wave function) spin projections are shown and compared to the 1D case. From Ref. [BBHB09].

of the gradient of $U_{\rm tot}$ [analogous to (2.73)] into (2.72),

$$0 = m\ddot{q} + \frac{\partial U_{\rm tot}}{\partial q} = m\ddot{q} + \mathcal{H}\cdot\xi, \tag{2.76}$$

and, using Eq. (2.75) for $\ddot{q}$ and eliminating $\mathcal{H}$ with the help of (2.74),

$$0 = m\sum_{n=1}^{3N}\left\{\ddot{c}_n(t) + c_n(t)\omega_n^2\right\}Q_n. \tag{2.77}$$

Due to the orthogonality of the Q_n which are non-zero, the solution of this equation implies that the terms in the parantheses vanish simultaneously for every n, leading to an equation for a harmonic oscillator with the solution

$$c_n(t) = A_n\cos\{\omega_n t + B_n\}, \qquad n = 1,\ldots 3N, \tag{2.78}$$

where the coefficients A_n and B_n depend on the initial conditions. Thus, the normal coordinates behave as independent linear $1d$ harmonic oscillators.

In analogy to the coordinates, also the particle momenta, corresponding to some excitation $q(t)$, can be expanded in terms of normal modes by using $p(t) = m\dot{q}(t)$. Using the result for $c_n(t)$, Eq. (2.78), we have the following

general expansion

$$q(t) - q_s^{(0)} = \sum_{n=1}^{3N} A_n \cos\{\omega_n t + B_n\} Q_n \equiv \sum_{n=1}^{3N} Q_n(t) \tag{2.79}$$

$$p(t) = \sum_{n=1}^{3N} A_n \sin\{\omega_n t + B_n\} P_n \equiv \sum_{n=1}^{3N} P_n(t), \tag{2.80}$$

where the momentum amplitude vector is $P_n = -m\omega_n Q_n$. Finally, we can transform the Hamilton function into normal mode representation, using the harmonic expansion (2.73) of the potential energy

$$H(p,q) = \frac{p^2}{2m} + U_{\rm tot}(q) = U_s^{(0)} + \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} \xi^T(i)\mathcal{H}_{ij}^{(s)}\xi(j). \tag{2.81}$$

Eliminating the Hesse matrix with the help of (2.74) and inserting the expansions (2.79) and (2.80) we obtain

$$\begin{aligned} H(p,q) - U_s^{(0)} &= \sum_{n=1}^{3N}\sum_{n'=1}^{3N} \left\{ \frac{P_n(t)P_{n'}(t)}{2m} + \frac{m}{2}\omega_n^2 \delta_{n,n'} Q_n(t) Q_{n'}(t) \right\} \\ &= \sum_{n=1}^{3N} \left\{ \frac{P_n^2(t)}{2m} + \frac{m}{2}\omega_n^2 Q_n^2(t) \right\} \equiv H(P,Q), \end{aligned} \tag{2.82}$$

where, in the last line, the orthogonality of the eigenvectors has been used.

Thus we have succeeded to diagonalize the hamiltonian of the N-particle system with arbitrary interaction. Assuming weak excitations from a stationary state the hamiltonian can be written as a superposition of $3N$ normal modes. This means, we can again apply the results from the case of uncoupled harmonic oscillators, Sec. 2.3.2, and immediately perform the "first" and "second" quantization.

2.4.4 Quantization of the strongly coupled N-particle system

For the first quantization we have to replace the normal mode coordinates and momenta by operators,

$$\begin{aligned} Q_n(t) &\rightarrow \hat{Q}_n(t) = A_n \cos\{\omega_n t + B_n\}\hat{Q}_n \\ P_n(t) &\rightarrow \hat{P}_n(t) = A_n \sin\{\omega_n t + B_n\}\hat{P}_n, \end{aligned} \tag{2.83}$$

leaving the time-dependence of the classical system unchanged. Further we have to make sure that the standard commutation relations are fulfilled, i.e. $[\hat{Q}_n, \hat{P}_m] = i\hbar\delta_{n,m}$. This should follow from the commutation relations of the original particle coordinates and momenta, $[x_{i\alpha}, p_{j\beta}] = i\hbar\delta_{i,j}\delta_{\alpha,\beta}$, where $\alpha, \beta = 1, 2, 3$ and $i, j = 1, \ldots N$, see Problem 7. Then, the Hamilton operator becomes, in normal mode representation

$$\hat{H}(\hat{P}, \hat{Q}) = \sum_{n=1}^{3N} \left\{ \frac{\hat{P}_n^2(t)}{2m} + \frac{m}{2}\omega_n^2 \hat{Q}_n^2(t) \right\}, \tag{2.84}$$

which allows us to directly introduce the creation and annihilation operators by introducing $\xi_n = \sqrt{\frac{m\omega_n}{\hbar}}\hat{Q}_n,\ n = 1, \ldots 3N)$

$$a_n = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial\xi_n} + \xi_n\right), \tag{2.85}$$

$$a_n^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial\xi_n} + \xi_n\right), \quad [a_n, a_k^\dagger] = \delta_{n,k}. \tag{2.86}$$

Thus the hamiltonian and its eigenfunctions and eigenvalues can be written as

$$\begin{aligned} \hat{H} &= \sum_{n=1}^{3N} \hbar\omega_n \left(a_n^\dagger a_n + \frac{1}{2}\right) \\ a_n|0\rangle &= 0, \quad n = 1, \ldots 3N \\ \psi_{n_1,\ldots n_{3N}} = |n_1 \ldots n_{3N}\rangle &= \frac{1}{\sqrt{n_1! \ldots n_{3N}!}} (a_1^\dagger)^{n_1} \ldots (a_{3N}^\dagger)^{n_{3N}} |0\rangle \\ E &= \sum_{n=1}^{3N} \hbar\omega_n \left(n_n + \frac{1}{2}\right). \end{aligned}$$

Here $|0\rangle \equiv |0 \ldots 0\rangle = |0\rangle \ldots |0\rangle$ [$3N$ factors] denotes the ground state and a general state $|n_1 \ldots n_{3N}\rangle = |n_1\rangle \ldots |n_{3N}\rangle$ contains n_n elementary excitations of the normal mode n, created by n_n times applying operator $a_n^\dagger$ to the ground state.

The expansion of the potential energy around its local minimum is, of course, possible only if kinetic energy is small. The extreme case is that of strong particle localization such as in a crystal. In a quantum system this is possible only at low density. An example is crystallization of electrons in quantum dots at low temperature. This was investigated with quantum Monte Carlo simulations by A. Filinov et al. in Refs. [FBL01, FLB00]. An analysis of normal modes and anharmonic corrections to the Taylor expansion of the potential energy was performed by K. Balzer *et al.* in Ref. [BNBF06].

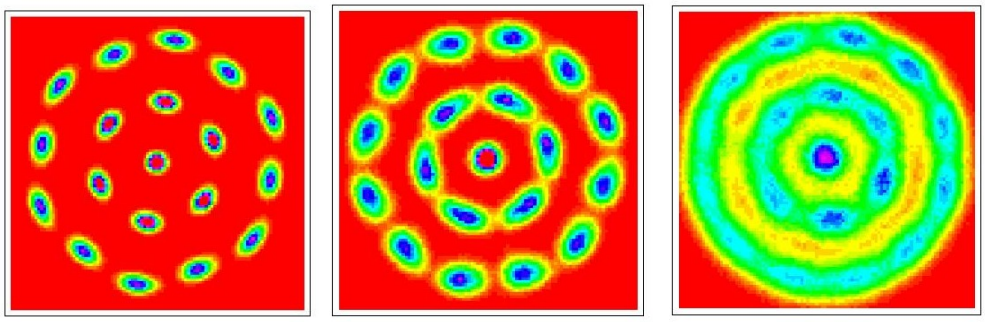

Abbildung 2.6: Probability density of $N = 19$ quantum electrons in a 2D harmonic trap. The coupling strength λ decreases from left to right, correspondingly the electron overlap increases. Path integral Monte Carlo simulations. From Ref. [FBL01], see also the discussion in Physical Review Focus, 19.4. 2001.

In summary, in finding the normal modes of the interacting N-particle system the description is reduced to a superposition of independent contributions from $3N$ degrees of freedom. Depending on the system dimensionality, these include (for a three-dimsional system) 3 translations of the center of mass and 3 rotations of the system as a whole around the coordinate axes. The remaining normal modes correspond to excitations where the particle distances change. Due to the stability of the stationary state with respect to weak excitations, these relative excitations are harmonic oscillations which have been quantized. In other words, we have $3N - 6$ phonon modes associated with the corresponding creation and annihilation operators and energy quanta. The frequencies of the modes are determined by the local curvature of the total potential energy (the diagonal elements of the Hesse matrix).

Problem 7: Prove the commutation relation $[\hat{Q}_n, \hat{P}_m] = i\hbar\delta_{n,m}$.
Problem 8: Apply the concept of the eigenvalue problem of the Hesse matrix to the solution of the normal modes of the $1d$ chain. Rederive the normal mode representation of the hamiltonian and check if the time dependencies vanish.

2.5 Continuous systems

2.5.1 Continuum limit of $1d$ chain

So far we have considered discrete systems containing N point particles. If the number of particles grows and their spacing becomes small we will eventually reach a continuous system – the $1d$ chain becomes a $1d$ string. We start with assigning particle i a coordinate $x_j = ja$ where $j = 0, \dots N$, a is the constant interparticle distance and the total length of the system is $l = Na$, see Fig.

We again consider a macroscopic system which is now periodically repeated after length l, i.e. points $x = 0$ and $x = l$ are identical[23]. In the discrete system we have an equally spaced distribution of masses m of point particles with a linear mass density $\rho = m/a$. The interaction between the masses is characterized by an elastic tension $\sigma = \kappa a$ where we relabeled the spring constant by κ. The continuum limit is now performed by simulataneously increasing the particle number and reducing a but requiring that the density and the tension remain unchanged,

$$\begin{aligned} a, m &\longrightarrow 0 \\ N, \kappa &\longrightarrow \infty \\ l, \rho, \sigma &= \text{const.} \end{aligned}$$

We now consider the central quantity, the displacement of the individual particles $q_i(t)$ which now transforms into a continuous displacement field $q(x,t)$. Further, with the continuum limit, differences become derivatives and the sum over the particles is replaced by an integral according to

$$\begin{aligned} q_j(t) &\longrightarrow q(x,t) \\ q_{j+1} - q_j &\longrightarrow a\frac{\partial q}{\partial x} \\ \sum_j &\longrightarrow \frac{1}{a}\int_0^l dx. \end{aligned}$$

Instead of the Hamilton function (2.51) we now consider the Lagrange function which is the difference of kinetic and potential energy, $L = T - V$,

[23] Thus we have formally introduced $N + 1$ lattice points but only N are different.

Abbildung 2.7: Illustration of the minimal action principle: the physical equation of motion corresponds to the tractory $q(x,t)$ which minimizes the action, Eq. (2.89) at fixed initial and final points $(t_i, 0)$ and (t_f, l).

which in the continuum limit transforms to

$$\begin{aligned} L(q,\dot{q}) &= \sum_{j=1}^{N} \left\{ \frac{m}{2} \left(\dot{q}_j\right)^2 - \frac{\kappa}{2} \left(q_j - q_{j+1}\right)^2 \right\} \\ &\longrightarrow \frac{1}{2} \int_0^l dx \left\{ \rho \left(\frac{\partial q(x,t)}{\partial t} \right)^2 - \sigma \left(\frac{\partial q(x,t)}{\partial x} \right)^2 \right\} \end{aligned} \tag{2.87}$$

The advantage of using the Lagrange function which now is a functional of the displacement field, $L = L[q(x,t)]$, is that there exists a very general method of finding the corresponding equations of motion – the minimal action principle.

2.5.2 Equation of motion of the $1d$ string

We now define the one-dimensional Lagrange density $\mathcal{L}$

$$L = \int_0^l dx\, \mathcal{L}[\dot{q}(x,t), q'(x,t)], \tag{2.88}$$

where Eq. (2.87) shows that Lagrange density of the spring depends only on two fields – the time derivative $\dot{q}$ and space derivative q' of the displacement field. The action is defined as the time integral of the Lagrange function between a fixed initial time t_i and final time t_f

$$S = \int_{t_i}^{t_f} dt L = \int_{t_i}^{t_f} dt \int_0^l dx\, \mathcal{L}[\dot{q}(x,t), q'(x,t)]. \tag{2.89}$$

The equation of motion of the $1d$ string follows from minimizing the action with respect to the independent variables of $\mathcal{L}$ [this "minimal action principle" has been discussed in detail in Chapter 1, Sec. 1.1], for illustration, see Fig. 2.7,

$$\begin{aligned} 0 = \delta S &= \int_{t_i}^{t_f} dt \int_0^l dx \left\{ \frac{\delta \mathcal{L}}{\delta \dot{q}} \delta \dot{q} + \frac{\delta \mathcal{L}}{\delta q'} \delta q' \right\} \\ &= \int_{t_i}^{t_f} dt \int_0^l dx \left\{ \rho \dot{q}\, \delta \dot{q} - \sigma q'\, \delta q' \right\}. \end{aligned} \tag{2.90}$$

We now change the order of differentiation and variation, $\delta\dot{q} = \frac{\partial}{\partial t}\delta q$ and $\delta q' = \frac{\partial}{\partial x}\delta q$ and perform partial integrations with respect to t in the first term and x in the second term of (2.90)

$$0 = -\int_{t_i}^{t_f} dt \int_0^l dx \, \{\rho\ddot{q} - \sigma q''\} \, \delta q, \tag{2.91}$$

where the boundary values vanish because one requires that the variation $\delta q(x,t)$ are zero at the border of the integration region, $\delta q(0,t) = \delta q(l,t) \equiv 0$. Since this equation has to be fulfilled for any fluctuation $\delta q(x,t)$ the term in the parantheses has to vanish which yields the equation of motion of the $1d$ string

$$\frac{\partial^2 q(x,t)}{\partial t^2} - c^2 \frac{\partial^2 q(x,t)}{\partial x^2} = 0, \quad \text{with} \quad c = \sqrt{\frac{\sigma}{\rho}} = a\sqrt{\frac{\kappa}{m}}. \tag{2.92}$$

This is a linear wave equation for the displacement field, and we introduced the phase velocity, i.e. the sound speed c. The solution of this equation can be written as

$$q(x,t) = q_0 e^{i(kx-\omega t)} + c.c., \tag{2.93}$$

which, inserted into Eq. (2.92), yields the dispersion relation

$$\omega(k) = c \cdot k, \tag{2.94}$$

i.e., the displacement of the string performs a wave motion with linear dispersion – we observe an acoustic wave where the wave number k is continuous.

It is now interesting to compare this result with the behavior of the original discrete $N-$particle system. There the oscillation frequencies ω_n were given by Eq. (2.56), and the wave numbers are discrete[24] $k_n = 2\pi n/Na$ with $n = \pm 1, \cdots \pm N/2$, and the maximum wave number is $k_{max} = \pi/a$. Obviously, the discrete system does not have a linear dispersion, but we may consider the small k limit and expand the sin to first order:

$$\omega_n^2 \approx 4\frac{\kappa}{m}\left(\frac{\pi n}{N}\right)^2 = 4\frac{c^2}{a^2}\left(\frac{ak_n}{2}\right)^2 = ck_n, \tag{2.95}$$

i.e. for small k the discrete system has exactly the same dispersion as the continuous system. The comparison with the discrete system also gives a hint at the existence of an upper limit for the wave number in the continuous system. In fact, k cannot be larger than π/a_{min} where a_{min} is the minimal distance of neighboring particles in the "continuous medium". The two dispersions are shown in Fig. 2.8.

[24]The wave number follows from the mode numbers l_n by dividing by a

Abbildung 2.8: Dispersion of the normal modes of the discrete $1D$ chain and of the associated continuous system – the $1D$ string. The dispersions agree for small k up to a $k_{max=\pi/a}$.

One may, of course, ask whether a continuum model has its own right of existence, without being a limit of a discrete system. In other words, this would correspond to a system with an infinite particle number and, correspondingly, an infinite number M of normal modes. While we have not yet discussed how to quantize continuum systems it is immediately clear that there should be problems if the number of modes is unlimited. In fact, the total energy contains a zero point contribution for each mode which, with M going to infinity, will diverge. This problem does not occur for any realistic system because the particle number is always finite (though, possibly large). But a pure continuum model will be only physically relevant if such divergencies are avoided. The solution is found by co-called "renormalization" procedures where a maximum k-value (a cut-off) is introduced. This maybe not easy to derive for any specific field theory, however, based on the information from discrete systems, such a cut-off can always be motivated by choosing a physically relevant particle number, as we have seen in this chapter.

Thus we have succeeded to perform the continuum limit of the $1d$ chain – the $1d$ string and derive and solve its equation of motion. The solution is a continuum of acoustic waves which are the normal modes of the medium which replace the discrete normal modes of the linear chain. Now the question remains how to perform a quantization of the continuous system, how to introduce creation and annihilation operators. To this end we have to develop a more general formalism which is called canonical quatization and which will be discussed in the next chapter.

2.6 Solutions of Problems

1. A simple equation for ψ_0 is readily obtained by inserting the definition of a into Eq. (2.41),

$$0 = \psi_0'(\xi) + \xi\psi_0(\xi), \tag{2.96}$$

with the solution $\psi_0(\xi) = C_0 e^{-\xi^2/2}$, where C_0 follows from the normalization $x_0 \int_{-\infty}^{\infty} d\xi \psi_0^2 = 1$, with the result $C_0 = (\pi^{1/2}/x_0)^{-1/2}$, where the phase is arbitrary and chosen to be zero.

2. Proof: Using $\langle\psi|a^\dagger = a|\psi\rangle$ and Eq. (2.44), direct computation yields

$$\left\langle \psi_{n+1}|a^\dagger|\psi_n\right\rangle = \frac{1}{\sqrt{n!(n+1)!}} \left\langle \psi_0|a^{n+1}a^\dagger(a^\dagger)^n|\psi_0\right\rangle .$$

The final result $\sqrt{n+1}$ is obtained by induction, starting with $n = 0$.

3. This problem reduces to the previous one by applying hermitean conjugation

$$\langle\psi_{n-1}|a|\psi_n\rangle = \left\langle \psi_n|a^\dagger|\psi_{n-1}\right\rangle^* = \sqrt{n}$$

Kapitel 3

Fermions and bosons

We now turn to the quantum statistical description of many-particle systems. The indistinguishability of microparticles leads to a number of far-reaching consequences for the behavior of particle ensembles. Among them are the symmetry properties of the wave function. As we will see there exist only two different symmetries leading to either Bose or Fermi-Dirac statistics.

Consider a single nonrelativistic quantum particle described by the hamiltonian $\hat{h}$. The stationary eigenvalue problem is given by the Schrödinger equation

$$\hat{h}|\phi_i\rangle = \epsilon_i|\phi_i\rangle, \qquad i = 1, 2, \dots , \tag{3.1}$$

where the eigenvalues of the hamiltonian are ordered, $\epsilon_1 < \epsilon_2 < \epsilon_3 \dots$. The associated single-particle orbitals ϕ_i form a complete orthonormal set of states in the single-particle Hilbert space[1]

$$\begin{aligned} \langle\phi_i|\phi_j\rangle &= \delta_{i,j}, \\ \sum_{i=1}^{\infty} |\phi_i\rangle\langle\phi_i| &= 1. \end{aligned} \tag{3.2}$$

3.1 Spin statistics theorem

We now consider the quantum mechanical state $|\Psi\rangle$ of N identical particles which is characterized by a set of N quantum numbers[2] $j_1, j_2, ..., j_N$, meaning that particle i is in single-particle state $|\phi_{j_i}\rangle$. The states $|\Psi\rangle$ are elements of the N-particle Hilbert space which we define as the direct product of single-particle

[1] The eigenvalues are assumed to be non-degenerate. Also, the extension to the case of a continuous basis is straightforward.

[2] The quantum numbers comprise all orbital and spin quantum numbers of a single particle.

Abbildung 3.1: Example of the occupation of single-particle orbitals by 3 particles. Exchange of identical particles (right) cannot change the measurable physical properties, such as the occupation probability.

Hilbert spaces, $\mathcal{H}_N = \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \dots$ (N factors), and are eigenstates of the total hamiltonian $\hat{H}$,

$$\hat{H}|\Psi_{\{j\}}\rangle = E_{\{j\}}|\Psi_{\{j\}}\rangle, \qquad \{j\} = \{j_1, j_2, \dots\}\,. \tag{3.3}$$

The explicit structure of the $N-$particle states is not important now and will be discussed later[3].

Since the particles are assumed indistinguishable it is clear that all physical observables cannot depend upon which of the particles occupies which single particle state, as long as all occupied orbitals, i.e. the set j, remain unchainged. In other words, exchanging two particles k and l (exchanging their orbitals, $j_k \leftrightarrow j_l$) in the state $|\Psi\rangle$ may not change the probability density, cf. Fig. 3.1. The mathematical formulation of this statement is based on the permutation operator P_{kl} with the action

$$\begin{aligned} P_{kl}|\Psi_{\{j\}}\rangle &= P_{kl}|\Psi_{j_1,\dots,j_k,\dots j_l,\dots,j_N}\rangle = \\ &= |\Psi_{j_1,\dots,j_l,\dots j_k,\dots,j_N}\rangle \equiv |\Psi'_{\{j\}}\rangle, \qquad \forall k,l = 1,\dots N, \end{aligned} \tag{3.4}$$

where we have to require

$$\langle\Psi'_{\{j\}}|\Psi'_{\{j\}}\rangle = \langle\Psi_{\{j\}}|\Psi_{\{j\}}\rangle. \tag{3.5}$$

Indistinguishability of particles requires $P_{kl}\hat{H} = \hat{H}$ and $[P_{kl}, \hat{H}] = 0$, i.e. P_{kl} and $\hat{H}$ have common eigenstates. This means P_{kl} obeys the eigenvalue problem

$$P_{kl}|\Psi_{\{j\}}\rangle = \lambda_{kl}|\Psi_{\{j\}}\rangle = |\Psi'_{\{j\}}\rangle. \tag{3.6}$$

[3]Recall that, in this section, we assume that the particles do not interact with each other. The generalization to interacting particles will be discussed in Sec. 3.2.5.

Obviously, $P_{kl}^\dagger = P_{kl}$, so the eigenvalue λ_{kl} is real. Then, from Eqs. (3.5) and (3.6) immediately follows

$$\lambda_{kl}^2 = \lambda^2 = 1, \qquad \forall k, l = 1, \ldots N, \tag{3.7}$$

with the two possible solutions: $\lambda = 1$ and $\lambda = -1$. From Eq. (3.6) it follows that, for $\lambda = 1$, the wave function $|\Psi\rangle$ is symmetric under particle exchange whereas, for $\lambda = -1$, it changes sign (i.e., it is "anti-symmetric").

This result was obtained for an arbitrary pair of particles, so we may expect that it is straightforwardly extended to systems with more than two particles. Experience shows that, in nature, there exist only two classes of microparticles – one which has a totally symmetric wave function with respect to exchange of any particle pair whereas, for the other, the wave function is antisymmetric. The first case describes particles with Bose-Einstein statistics ("bosons") and the second, particles obeying Fermi-Dirac statistics ("fermions")[4].

The one-to-one correspondence of (anti-)symmetric states with bosons (fermions) is the content of the spin-statistics theorem. It was first proven by Fierz [Fie39] and Pauli [Pau40] within relativistic quantum field theory. Requirements include 1.) Lorentz invariance and relativistic causality, 2.) positivity of the energies of all particles and 3.) positive definiteness of the norm of all states.

3.2 Symmetric and antisymmetric N-particle wave functions

We now explicitly construct the N-particle wave function of a system of many fermions or bosons.

Case of $N = 2$. For two particles occupying the orbitals $|\phi_{j_1}\rangle$ and $|\phi_{j_2}\rangle$, respectively, there are two possible wave functions: $|\Psi_{j_1,j_2}\rangle$ and $|\Psi_{j_2,j_1}\rangle$ which follow from one another by applying the permutation operator P_{12}. Since both wave functions represent the same physical state it is reasonable to eliminate this ambiguity by constructing a new wave function as a suitable linear combination of the two,

$$|\Psi_{j_1,j_2}\rangle^\pm \;=\; C_{12}\left\{|\Psi_{j_1,j_2}\rangle + A_{12}P_{12}|\Psi_{j_1,j_2}\rangle\right\}, \tag{3.8}$$

with an arbitrary complex coefficient A_{12}. Using the eigenvalue property of the permutation operator, Eq. (3.6), we require that this wave function has the

[4]Fictitious systems with mixed statistics have been investigated by various authors, e.g. [MG64, MG65] and obey "parastatistics". For a text book discussion, see Ref. [Sch08], p. 6.

proper symmetry,

$$P_{12}|\Psi_{j_1,j_2}\rangle^{\pm} = \pm|\Psi_{j_1,j_2}\rangle^{\pm}\,, \tag{3.9}$$

which follows from the linearity of $|\Psi\rangle^{\pm}$ in the eigenstates of P. The explicit form of the coefficients in Eq. (3.8) is obtained by acting on this equation with the permutation operator and equating this to $\pm|\Psi_{j_1,j_2}\rangle^{\pm}$, according to Eq. (3.9), and using $P_{12}^2 = \hat{1}$,

$$\begin{aligned} P_{12}|\Psi_{j_1,j_2}\rangle^{\pm} &= C_{12}\left\{|\Psi_{j_2,j_1}\rangle + A_{12}P_{12}^2|\Psi_{j_1,j_2}\rangle\right\} = \\ &= C_{12}\left\{\pm A_{12}|\Psi_{j_2,j_1}\rangle \pm |\Psi_{j_1,j_2}\rangle\right\}, \end{aligned}$$

which leads to the requirement $A_{12} = \lambda$, whereas normalization of $|\Psi_{j_1,j_2}\rangle^{\pm}$ yields $C_{12} = 1/\sqrt{2}$. The final result is

$$\boxed{|\Psi_{j_1,j_2}\rangle^{\pm} = \frac{1}{\sqrt{2}}\left\{|\Psi_{j_1,j_2}\rangle \pm P_{12}|\Psi_{j_1,j_2}\rangle\right\} \equiv \Lambda_{12}^{\pm}|\Psi_{j_1,j_2}\rangle} \tag{3.10}$$

where,

$$\Lambda_{12}^{\pm} = \frac{1}{\sqrt{2}}\{1 \pm P_{12}\}, \tag{3.11}$$

denotes the (anti-)symmetrization operator of two particles which is a linear combination of the identity operator and the pair permutation operator.

Case of $N = 3$. The extension of this result to 3 fermions or bosons is straightforward. For 3 particles $(1,2,3)$ there exist $6 = 3!$ permutations: three pair permutations, $(2,1,3), (3,2,1), (1,3,2)$, that are obtained by acting with the permutation operators P_{12}, P_{13}, P_{23}, respectively on the initial configuration. Further, there are two permutations involving all three particles, i.e. $(3,1,2)$ and $(2,3,1)$, which are obtained by applying the operators $P_{13}P_{12}$ and $P_{23}P_{12}$, respectively. Thus, the three-particle (anti-)symmetrization operator has the form

$$\Lambda_{123}^{\pm} = \frac{1}{\sqrt{3!}}\{1 \pm P_{12} \pm P_{13} \pm P_{23} + P_{13}P_{12} + P_{23}P_{12}\}, \tag{3.12}$$

where we took into account the necessary sign change in the case of fermions resulting for any pair permutation.

General case. This result is generalized to N particles where there exists a total of $N!$ permutations, according to[5]

$$|\Psi_{\{j\}}\rangle^{\pm} = \Lambda_{1\ldots N}^{\pm}|\Psi_{\{j\}}\rangle, \tag{3.13}$$

[5]This result applies only to fermions. For bosons the prefactor has to be corrected, cf. Eq. (3.25).

with the definition of the (anti-)symmetrization operator of N particles,

$$\boxed{\Lambda^{\pm}_{1\ldots N} = \frac{1}{\sqrt{N!}} \sum_{P \epsilon S_N} \mathrm{sign}(P) \hat{P}} \tag{3.14}$$

where the sum is over all possible permutations $\hat{P}$ which are elements of the permutation group S_N. Each permutation P has the parity, $\mathrm{sign}(P) = (\pm 1)^{N_p}$, which is equal to the number N_p of successive pair permuations into which $\hat{P}$ can be decomposed (cf. the example $N = 3$ above). Below we will construct the (anti-)symmetric state $|\Psi_{\{j\}}\rangle^{\pm}$ explicitly. But before this we consider an alternative and very efficient notation which is based on the occupation number formalism.

The properties of the (anti-)symmetrization operators $\Lambda^{\pm}_{1\ldots N}$ are analyzed in Problem 1, see Sec. 3.9.

3.2.1 Occupation number representation

The original N-particle state $|\Psi_{\{j\}}\rangle$ contained clear information about which particle occupies which state. Of course, this information is unphysical, as it is in conflict with the indistinguishability of particles. With the construction of the symmetric or anti-symmetric N-particle state, $|\Psi_{\{j\}}\rangle^{\pm}$, this information about the identity of particles is eliminated, and the only information which is retained is *how many particles*, n_p, occupy the single-particle orbital $|\phi_p\rangle$. We thus may use a different notation for the state $|\Psi_{\{j\}}\rangle^{\pm}$ in terms of the *occupation numbers* n_p of the single-particle orbitals,

$$|\Psi_{\{j\}}\rangle^{\pm} = |n_1 n_2 \ldots\rangle \equiv |\{n\}\rangle, \qquad n_p = 0, 1, 2, \ldots, \qquad p = 1, 2, \ldots \tag{3.15}$$

Here $\{n\}$ denotes the total set of occupation numbers of all single-particle orbitals. Since this is the complete information about the N-particle system, these states form a complete system that is orthonormal by construction of the (anti-)symmetrization operators,

$$\begin{aligned} \langle\{n\}|\{n'\}\rangle &= \delta_{\{n\},\{n'\}} \equiv \delta_{n_1,n'_1}\delta_{n_2,n'_2}\ldots \\ \sum_{\{n\}} |\{n\}\rangle\langle\{n\}| &= 1. \end{aligned} \tag{3.16}$$

The attractive feature of this representation is that it is equally applicable to fermions and bosons. The only difference between the two lies in the allowed values of the occupation numbers, as we will see in the next two sections.

3.2.2 Fock space

In Sec. 3.1 we have introduced the N-particle Hilbert space $\mathcal{H}_N$. In the following we will need either totally symmetric or totally anti-symmetric states which form the sub-spaces $\mathcal{H}_N^+$ and $\mathcal{H}_N^-$ of the Hilbert space. Furthermore, below we will develop the formalism of second quantization by defining creation and annihilation operators acting on symmetric or anti-symmetric states. Obviously, the action of these operators will give rise to a state with $N+1$ or $N-1$ particles. Thus, we have to introduce, in addition, a more general space containing states with different particle numbers: We define the symmetric (anti-symmetric) *Fock space* $\mathcal{F}^\pm$ as the direct sum of symmetric (anti-symmetric) Hilbert spaces $\mathcal{H}_N^\pm$ with particle numbers $N = 0, 1, 2, \ldots$,

$$\begin{aligned} \mathcal{F}^+ &= \mathcal{H}_0 \cup \mathcal{H}_1^+ \cup \mathcal{H}_2^+ \cup \ldots, \\ \mathcal{F}^- &= \mathcal{H}_0 \cup \mathcal{H}_1^- \cup \mathcal{H}_2^- \cup \ldots. \end{aligned} \tag{3.17}$$

Here, we included the *vacuum state* $|0\rangle = |0, 0, \ldots\rangle$ which is the state without particles which belongs to both Fock spaces.

3.2.3 Non-interacting many-fermion wave function

Pauli principle: Let us return to the case of two particles, Eq. (3.10), and consider the case $j_1 = j_2$. Due to the minus sign in front of P_{12}, we immediately conclude that $|\Psi_{j_1,j_1}\rangle^- \equiv 0$. This state is not normalizable and thus cannot be physically realized. In other words, two fermions cannot occupy the same single-particle orbital – this is the *Pauli principle* stating that two fermions cannot occupy an identical single-particle quantum state, which has far-reaching consequences for the behavior of fermions.

We now construct the explicit form of the anti-symmetric wave function. This is particularly simple if the particles are non-interacting. Then, the total hamiltonian is additive[6],

$$\hat{H} = \sum_{i=1}^{N} \hat{h}_i, \tag{3.18}$$

and all hamiltonians commute, $[\hat{h}_i, \hat{h}_j] = 0$, for all i and j. Then all particles have common eigenstates, and the total wave function (prior to anti-symmetrization) has the form of a product

$$\boxed{|\Psi_{\{j\}}\rangle = |\Psi_{j_1,j_2,\ldots j_N}\rangle = |\phi_{j_1}(1)\rangle |\phi_{j_2}(2)\rangle \ldots |\phi_{j_N}(N)\rangle}$$

[6]This is an example of an observable of single-particle type which will be discussed more in detail in Sec. 3.3.1.