Kapitel 2

Introduction to second quantization

Now we turn to a different approach of treating quantum N-particle systems. Instead of first constructing a classical field theory with two canonically conjugate fields, that are being quantized, in a second step, we now proceed differently. We will start from a quantum mechanical description of the state of many particles which is first symmetrized (anti-symmetrized), for the case of bosons (fermions). We then switch to occupation number representation for which the quantization is rather trivial, based on the introduction of creation and annihilation operators. This scheme will be realized for fermions and bosons in chapter 3.

But before that, it is very instructive to consider the analogous many-body problem in the limit of classical particles and to perform a "second quantization in phase space". This is achieved by introducing the microscopic phase space density which is due to Klimontovich, cf. Eq. (2.13) below. We will observe that this quantity obeys an equation of motion that is completely analogous to the equations of motion of the field operators of fermions and bosons that will be derived in Sec. 5.2. This allows for valuable insights into the common statistical concepts of second quantization.

2.1 Second quantization in phase space

2.1.1 Classical dynamics in terms of point particles

We consider systems of a large number N of identical particles which interact via pair potentials V and may be subject to an external field U. The system

is described by the Hamilton function

$$\boxed{H(p,q) = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i=1}^{N} U(\mathbf{r}_i) + \sum_{1\le i<j\le N} V(\mathbf{r}_i - \mathbf{r}_j)} \tag{2.1}$$

where p and q are $3N$-dimensional vectors of all particle momenta and coordinates, $p \equiv \{\mathbf{p}_1, \mathbf{p}_2, \dots \mathbf{p}_N\}$ and $q \equiv \{\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_N\}$. Examples of the external potentials U are the electrostatic potential of a capacitor, the potential of an atomic nucleus or the potential an electron feels at a solid surface. In general, the potential is time-dependent. The interaction potentials V can arise from gravitational fields, from the Coulomb interaction of charged particles, the magnetic interaction of currents and so on. From the hamiltonian (2.1) the equations of motion follow by applying Hamilton's equations[1],

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = \frac{p_i}{m}, \tag{2.2}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = -\frac{\partial U}{\partial q_i} - \sum_{j\neq i} \frac{\partial V}{\partial q_i}, \tag{2.3}$$

which is to be understood as two systems of $3N$ scalar equations for $x_1, y_1, \dots z_N$ and $p_{x1}, p_{y1}, \dots p_{zN}$ where $\partial/\partial q \equiv \{\partial/\partial \mathbf{r}_1, \dots \partial/\partial \mathbf{r}_N\}$, and the latter equalities are obtained by inserting the hamiltonian (2.1). The system (2.3) is nothing but Newton's equations containing the forces arising from the gradient of the external potential and the gradient of all pair interaction potentials involving the given particle, i.e. for any particle $i = 1 \dots N$

$$\dot{\mathbf{p}}_i = -\frac{\partial U(\mathbf{r}_1, \dots \mathbf{r}_N)}{\partial \mathbf{r}_i} - \sum_{j\neq i} \frac{\partial V(\mathbf{r}_i - \mathbf{r}_j)}{\partial \mathbf{r}_i}. \tag{2.4}$$

Consider, as an example, a system of identical charged particles with charge e_i which may be subject to an external electrostatic potential ϕ_{ext} and interact with each other via the Coulomb potential $V_c = \frac{e_i e_j}{|\mathbf{r}_i - \mathbf{r}_j|}$. Then Newton's equation (2.4) for particle i contains, on the r.h.s., the gradients of the potential $U = e_i \phi_{ext}$ and of the $N-1$ Coulomb potentials involving all other particles.

$$\dot{\mathbf{p}}_i = -\frac{\partial e_i \phi_{\text{ext}}(\mathbf{r}_i)}{\partial \mathbf{r}_i} - \sum_{j\neq i} \frac{\partial}{\partial \mathbf{r}_i} \frac{e_i e_j}{|\mathbf{r}_i - \mathbf{r}_j|}, \tag{2.5}$$

[1] Generalized equations of motion can, of course, also be obtained for non-Hamiltonian (dissipative) systems

2.1.2 Point particles coupled via classical fields

An alternative way of writing Eq. (2.5) is to describe the particle interaction not by all pair interactions but to compute the total electric field, $\mathbf{E}(\mathbf{r},t)$, all particles produce in the whole space. The force particle "i" experiences is then just the Lorentz force, $e_i\mathbf{E}$, which is minus the gradient of the total electrostatic potential ϕ which is readily identified from the r.h.s. of Eq. (2.5)

$$\dot{\mathbf{p}}_i = e_i\mathbf{E}(\mathbf{r}_i,t) = -e_i\frac{\partial\phi(\mathbf{r},t)}{\partial\mathbf{r}}\bigg|_{\mathbf{r}=\mathbf{r}_i}, \tag{2.6}$$

$$\phi(\mathbf{r},t) = \phi_{ext}(\mathbf{r}) + \sum_{j=1}^{N}\frac{e_j}{|\mathbf{r}-\mathbf{r}_j(t)|}. \tag{2.7}$$

In this case we explicitly know the form of the potential (2.7) but we can also rewrite this in terms of the Poisson equation which is solved by the potential (2.7)

$$\Delta\phi(\mathbf{r},t) = -4\pi\sum_{j=1}^{N}e_j\delta[\mathbf{r}-\mathbf{r}_j(t)] = -4\pi\rho(\mathbf{r},t). \tag{2.8}$$

The potential ϕ contains the external potential and the potentials induced by all particles at a given space point $\mathbf{r}$ at time t. When computing the force on a given particle i, the potential has to be taken at $\mathbf{r} = \mathbf{r}_i(t)$, and the contribution of particle "i" to the sum over the particles in Eqs. (2.7, 2.8) has to be excluded (to avoid selfinteraction). Also, on the r.h.s. we have introduced the charge density ρ of the system of N point particles.

Considering the formal structure of Eq. (2.6) we notice that the Coulomb forces between discrete particles have been completely eliminated in favor of a space-dependent function – the electric field. Obviously, this description is readily generalized to the case of time-dependent external potentials and magnetic fields which yields a coupled set of Newton's and Maxwell's equations,

$$\dot{\mathbf{p}}_i = e_i\left\{\mathbf{E}(\mathbf{r}_i,t) + \frac{1}{c}\mathbf{v}_i\times\mathbf{B}(\mathbf{r}_i,t)\right\}, \tag{2.9}$$

$$\mathrm{div}\mathbf{E}(\mathbf{r},t) = 4\pi\rho(\mathbf{r},t), \quad \nabla\times\mathbf{E}(\mathbf{r},t) = -\frac{1}{c}\frac{\partial\mathbf{B}(\mathbf{r},t)}{\partial t}, \tag{2.10}$$

$$\mathrm{div}\mathbf{B}(\mathbf{r},t) = 0, \quad \nabla\times\mathbf{B}(\mathbf{r},t) = \frac{4\pi}{c}\mathbf{j}(\mathbf{r},t) + \frac{1}{c}\frac{\partial\mathbf{E}(\mathbf{r},t)}{\partial t}, \tag{2.11}$$

where we introduced the current density j which, for a system of point particles, is given by $\mathbf{j}(\mathbf{r},t) = \sum_{j=1}^{N}e_j\mathbf{v}_j(t)\delta[\mathbf{r}-\mathbf{r}_j(t)]$. Charge and current density are

determined by the instantaneous phase space trajectories $\{q(t), p(t)\}$ of all particles.

The two sets of equations (2.6, 2.8) and (2.9, 2.10, 2.11) form closed systems coupling the dynamics of classical charged point particles and a classical electromagnetic field. This coupling occurs, in the particle equation–via the Lorentz force–and, in the field equations–via the charge and current density. The classical description, therefore, requires knowledge of the N discrete particle trajectories $\{q(t), p(t)\}$ and the dynamics of the two continuous vector fields, $\mathbf{E}(\mathbf{r}, t), \mathbf{B}(\mathbf{r}, t)$.

Using the electric and magnetic fields, we may rewrite the Hamilton function (2.1) corresponding to the full system (2.6, 2.10, 2.11)

$$\boxed{H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i=1}^{N} U(\mathbf{r}_i) + \frac{1}{8\pi} \int d^3r \left\{ \mathbf{E}^2(\mathbf{r}, t) + \mathbf{B}^2(\mathbf{r}, t) \right\}} \tag{2.12}$$

where the integral contains the energy of the electromagnetic field familiar from standard electrodynamics.

2.1.3 Classical dynamics via particle and Maxwell fields

We have now found two alternative descriptions of the dynamics of interacting point charges:

1. via the system (2.5), involving only discrete point particles, and
2. via the system (2.9, 2.10, 2.11) which gives a hybrid description in which the particles are discrete but the fields (or the particle interaction) continuous.

One may ask if there is third form which contains only continuous field-type quantities. This would require to represent also the particles by fields, also in the classical case. This is, indeed possible, as we show in this section.

In fact, the right hand sides of Maxwell's equations already do contain (formally) continuous quantities, ρ and $\mathbf{j}$, representing the particles. However, they contain (via the delta functions) only the particle coordinates. It is, therefore, tempting to consider a symmetric, with respect to q and p, quantity – the microscopic phase space density which was introduced by Yuri Klimontovich in the 1950s [Kli57]

$$\boxed{N(\mathbf{r}, \mathbf{p}, t) = \sum_{i=1}^{N} \delta[\mathbf{r} - \mathbf{r}_i(t)] \delta[\mathbf{p} - \mathbf{p}_i(t)] \equiv \sum_{i=1}^{N} \delta[x - x_i(t)]} \tag{2.13}$$

where we introduced the short notations $x \equiv \{\mathbf{r}, \mathbf{p}\}$ and $x_i(t) \equiv \{\mathbf{r}_i(t), \mathbf{p}_i(t)\}$.[2] The function N is related to the particle density $n(\mathbf{r}, t)$, and it obeys a normalization condition,

$$\int d^3p\, N(\mathbf{r}, \mathbf{p}, t) = n(\mathbf{r}, t), \tag{2.14}$$

$$\int d^6x\, N(\mathbf{r}, \mathbf{p}, t) = N(t). \tag{2.15}$$

Comment: the quantum statistical expression of $N(\mathbf{r}, \mathbf{p}, t)$ is the single-particle density operator, $\hat{n}_{ij}(t) = \hat{c}_i^\dagger(t)\hat{c}_j(t)$ which we will introduce in chapter 3.

Equation of motion for N: If there are no particle sources or sinks, $N(t)$ =const, and there exists a local conservation law, $\frac{d}{dt}N = 0$. From this we obtain the equation of motion of $N(\mathbf{r}, \mathbf{p}, t)$:

$$\frac{dN(\mathbf{r}, \mathbf{p}, t)}{dt} = \frac{\partial N(\mathbf{r}, \mathbf{p}, t)}{\partial t} + \sum_{i=1}^{N} \delta[\mathbf{p} - \mathbf{p}_i(t)] \frac{\partial}{\partial \mathbf{r}} \delta[\mathbf{r} - \mathbf{r}_i(t)] \frac{\partial \mathbf{r}_i}{\partial t} + \sum_{i=1}^{N} \delta[\mathbf{r} - \mathbf{r}_i(t)] \frac{\partial}{\partial \mathbf{p}} \delta[\mathbf{p} - \mathbf{p}_i(t)] \frac{\partial \mathbf{p}_i}{\partial t}.$$

Using Newton's equations (2.5) the time derivatives can be computed after which the delta functions allow us to replace $\mathbf{r}_i \to \mathbf{r}$ and $\mathbf{p}_i \to \mathbf{p}$ which can be taken out of the sum. As a result we obtain[3]

$$\left\{ \frac{\partial}{\partial t} + \mathbf{v}\frac{\partial}{\partial \mathbf{r}} + e\left[\mathbf{E}(\mathbf{r}, t) + \frac{1}{c}\mathbf{v} \times \mathbf{B}(\mathbf{r}, t) \right] \frac{\partial}{\partial \mathbf{p}} \right\} N(\mathbf{r}, \mathbf{p}, t) = 0. \tag{2.16}$$

Thus we have obtained a field description of the particles via the function N and eliminated (formally) all discrete particle information. The remarkable property of this equation is that it has the same form as the equation of a single particle subject to an external electromagnetic field. Nevertheless this equation describes a system of N interacting particles where all interactions are "hidden" in the fields $\mathbf{E}$ and $\mathbf{B}$ which are the total fields – external plus induced fields. This single-particle-type behavior is called mean field dynamics, so Eq. (2.16) is exactly of the form of a mean field equation.

[2]Note that for a vector $\mathbf{y} = \{y_1, y_2, y_3\}$, $\delta[\mathbf{y}] \equiv \delta[y_1]\delta[y_2]\delta[y_3]$, so N contains a product of six scalar delta functions.

[3]To simplify the notation, in the following we consider a one-component system with identical charges, $e_1 = \ldots e_N = e$. An extension to multi-component systems is straightforwardly done by introducing a separate function N_a, for each component.

The field N also replaces the charge and current density in Maxwell's equations (2.10, 2.11) via the relations [cf. Eq. (2.14)]

$$\rho(\mathbf{r},t) = e\int d^3p\, N(\mathbf{r},\mathbf{p},t), \tag{2.17}$$

$$\mathbf{j}(\mathbf{r},t) = e\int d^3p\, \mathbf{v}N(\mathbf{r},\mathbf{p},t). \tag{2.18}$$

Example: unmagnetized system of Coulomb interacting particles: A particularly simple form is obtained in the absence of a magnetic field, in the case of particles interacting by Coulomb potentials, cf. Eqs. (2.6, 2.7) above. Then, we may use the solution of Poisson's equation, expressing ρ via $N(\mathbf{r},\mathbf{p},t)$,

$$\begin{aligned}\phi(\mathbf{r},t) &= \phi_{\rm ext}(\mathbf{r},t) + \int d\mathbf{r}'\,\frac{\rho(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|} \\ &= \phi_{\rm ext}(\mathbf{r},t) + \int d\mathbf{r}'\int d\mathbf{p}'\,\frac{eN(\mathbf{r}',\mathbf{p}',t)}{|\mathbf{r}-\mathbf{r}'|}.\end{aligned} \tag{2.19}$$

With this expression the electrostatic field has been eliminated, and the particle dynamics (2.16) become a closed equation for $N(\mathbf{r},\mathbf{p},t)$:

$$\boxed{\left\{\frac{\partial}{\partial t} + \mathbf{v}\frac{\partial}{\partial \mathbf{r}} - e\frac{\partial}{\partial \mathbf{r}}\left[\phi_{\rm ext} + \int d^6x'\,\frac{eN(\mathbf{r}',\mathbf{p}',t)}{|\mathbf{r}-\mathbf{r}'|}\right]\frac{\partial}{\partial \mathbf{p}}\right\}N(\mathbf{r},\mathbf{p},t) = 0} \tag{2.20}$$

Using the phase space density, all observables of the system can be expressed in terms of fields. For example, the hamilton function now becomes

$$\begin{aligned}H &= \int d^6x\,\frac{\mathbf{p}^2}{2m}N(\mathbf{r},\mathbf{p},t) + \int d^6x\,U(\mathbf{r})N(\mathbf{r},\mathbf{p},t) + \\ &\quad + \frac{1}{8\pi}\int d^3r\left\{\mathbf{E}^2(\mathbf{r},t) + \mathbf{B}^2(\mathbf{r},t)\right\}.\end{aligned} \tag{2.21}$$

We underline that this is an exact equation (as long as a classical description is valid) – no assumptions with respect to the interactions have been made. It is fully equivalent to Newton's equations (2.6). The discrete nature of the particles has now vanished – it is hidden in the highly singular phase space field N. As Newton's equation, Eq. (2.20) allows for an exact solution of the particle dynamics, once the initial conditions are precisely known.

2.1.4 Discussion: ensemble averages, fluctuations, quantum effects

The possibility to find an exact solution for the dynamics is, of course, restricted to few particles. In contrast, if our goal is to describe the behavior of a macroscopic particle ensemble, any particular initial condition, and the resulting dynamics have to be regarded as random. However, we will be interested in statistically reliable predictions, so we need to average over a certain statistical ensemble, e.g. over all possible initial conditions. An ensemble average of N yields directly the single-particle phase space distribution $\langle N(\mathbf{r},\mathbf{p},t)\rangle = nf(\mathbf{r},\mathbf{p},t)$, where n denotes the mean density, and Eq. (2.20) immediately turns into an equation for the distribution function f, i.e. a kinetic equation.

Fluctuations of the phase space density. It is easy to see that application of such an ensemble average does not lead to a closed equation for $f(\mathbf{r},\mathbf{p},t)$. This is because Eq. (2.20) contains a product of two N functions for which, of course, $\langle NN\rangle \neq \langle N\rangle\langle N\rangle$. Instead one has to introduce the fluctuations δN, by writing $N = nf + \delta N$. Then one obtains (we omit the arguments)

$$\langle N\cdot N\rangle = n^2\, f\cdot f + \langle \delta N\cdot \delta N\rangle. \tag{2.22}$$

The last term appears additionally in the ensemble averaged version of Eq. (2.20) and gives rise to collision and correlation effects,

$$\left\{\frac{\partial}{\partial t} + \mathbf{v}\frac{\partial}{\partial \mathbf{r}} - e\frac{\partial}{\partial \mathbf{r}}\left[\phi_{\rm ext} + \int d^6x'\,\frac{enf(\mathbf{r}',\mathbf{p}',t)}{|\mathbf{r}-\mathbf{r}'|}\right]\frac{\partial}{\partial \mathbf{p}}\right\} f(\mathbf{r},\mathbf{p},t) = \\ = \frac{e^2}{n}\int d^6x'\,\left[\frac{\partial}{\partial \mathbf{r}}\frac{1}{|\mathbf{r}-\mathbf{r}'|}\right]\frac{\partial}{\partial \mathbf{p}}\,\langle \delta N(\mathbf{r}',\mathbf{p}',t)\delta N(\mathbf{r},\mathbf{p},t)\rangle\ . \tag{2.23}$$

This is a kinetic equation for the one-particle phase space distribution function f and has the same form as the Boltzmann equation. The only difference is that the collision term on the r.h.s. is formulated differently, in terms of a correlation function of fluctuations of N.

Field fluctuations. In a similar manner, also the fields have to be decomposed into an average and a fluctuating part,

$$\mathbf{E}(\mathbf{r},t) = \langle \mathbf{E}(\mathbf{r},t)\rangle + \delta\mathbf{E}(\mathbf{r},t)$$
$$\mathbf{B}(\mathbf{r},t) = \langle \mathbf{B}(\mathbf{r},t)\rangle + \delta\mathbf{B}(\mathbf{r},t)\,.$$

This expansion has to be inserted into Maxwell's equations. Obviously, the expectation values of the fields then obey equations that are driven by the

expectation values of the charge density and the charge current density, respectively, which follows from the linearity of Maxwell's equations. On the other hand, the fluctuations, δN, will give rise to fluctuations of the charge and current densities, $\delta\rho$ and $\delta\mathbf{j}$,

$$\rho(\mathbf{r},t)+\delta\rho(\mathbf{r},t) = e\int d^3p\,\{nf(\mathbf{r},\mathbf{p},t)+\delta N(\mathbf{r},\mathbf{p},t)\}\,, \tag{2.24}$$

$$\mathbf{j}(\mathbf{r},t)+\delta\mathbf{j}(\mathbf{r},t) = e\int d^3p\,\mathbf{v}\,\{nf(\mathbf{r},\mathbf{p},t)+\delta N(\mathbf{r},\mathbf{p},t)\}\,. \tag{2.25}$$

These fluctuating particle contributions will give rise, via Maxwell's equations, to fluctuating electric and magnetic field contributions. Similarly, in the electrostatic case, the fluctuation δN creates a fluctuation of the induced potential, $\delta\phi$. In addition, the correlation functions $\langle\delta N\delta N\rangle$ allow one to compute density-density and current-current correlation functions, $\langle\delta\rho\,\delta\rho\rangle$, $\langle\delta\mathbf{j}\,\delta\mathbf{j}\rangle$ that are closely related to important transport quantities such as st dynamic structure factor, the diffusion coefficient or the conductivity, e.g. [HDV$^+$20]. Finally, the correlation functions of the phase space density give also access to the correlation functions of the electric field, $\langle\delta\mathbf{E}\,\delta\mathbf{E}\rangle$ that are important in experiments including light-scattering, or in random media or in the cases of turbulence.

Emergence of a hierarchy of equations. Obviously, the equation of motion for the distribution function, Eq. (2.23), is not closed as it involves an unknown quantity $\langle\delta N\cdot\delta N\rangle$. This correlation function obeys its own equation of motion which is straightforwardly derived from the equation[4] of N. This equation is, again, not closed but involves the correlation function of three fluctuations, $\langle\delta N\cdot\delta N\cdot\delta N\rangle$. This means, an entire hierarchy of equations is obtained. To solve it, approximations are necessary. This will be discussed in more detail for the quantum case in Sec. 5.2.

The hierarchy of fluctuations is similar to the hierarchy of reduced distribution functions (or, in quantum mechanics, reduced density operators) – the BBGKY-hierarchy which is the subject of Sec. 6.3. The use of the phase space density N and the concept of fluctuations as starting point for the derivation of a kinetic theory of gases and plasmas has been successfully demonstrated by Klimontovich, for details see his text books [Kli75, Kli80].

With Eqs. (2.16) and (2.20) we have realized the third picture of coupled particle-electromagnetic field dynamics – in terms of the particle field, N,

[4]One first derives an equation for δN by subtracting the equations for N and nf. We will return to this point in the context of the equations for the field operators of quantum systems in Sec. 5.2

and the electric and magnetic fields. While we have concentrated on charged particles and Coulomb interaction, the approach may be equally applied to other interactions, e.g. electrons interacting with lattice vibrations of a solid described by the displacement field, see Sec. 2.5.1. Thus the basis for a classical field theory has been achieved.

Quantum effects. Of course, the formalism outlined so far is based on classical physics, i.e. on Newton's equations for point particles, and Maxwell's equations for the electromagnetic field. No quantum effects appear, neither in the description of the particles nor the EM field. The classical picture has been questioned only at the end of the 19th century where the experiments on black body radiation could not be correctly explained by Maxwell's theory of the electromagnetic field. The classical expression for the field energy of an electromagnetic wave which only depends on the field amplitudes $\mathbf{E}_0, \mathbf{B}_0$ and, therefore, is a continuous function, cf. hamiltonian (2.21), did not reproduce the measured spectral energy density. The solution which was found by Max Planck indicated that the field energy cannot depend on the field amplitudes alone. The energy exchange between electromagnetic field and matter is even entirely independent of $\mathbf{E}_0, \mathbf{B}_0$, instead it depends on the frequency ω of the wave. Thus the total energy of an electromagnetic wave of frequency ω is an integer multiple, $N = 0, 1, 2, \ldots$ of an elementary energy, $W_{\text{field}}(\omega) = N\hbar\omega$, where $\hbar$ is Planck's constant, i.e. the energy is quantized. For the ("canonical") quantization of the electromagnetic field, we refer to Chapter 1.

What Planck had discovered in 1900 was the quantization of the electromagnetic field [5]. This concept is very different from the quantum mechanical description of the electron dynamics from which it is, therefore, clearly distinguished by the now common notion of "second quantization". Interestingly, however, the "first quantization" of the motion of microparticles was introduced only a quarter century later when quantum mechanics was discovered.

Problem 1: Perform the ensemble average of Eqs. (2.16) and (2.20) and find an explicit expression for the additional term arising from the correlation function of the fluctuations.

[5] Planck himself, initially, regarded the introduction of the energy quantum $\hbar\omega$ only as a formal mathematical trick to derive the known spectral distribution (Planck or Bose function) and did not question the validity of Maxwell's field theory. Only half a century later, when field quantization was systematically derived, the coexistence of the concepts of energy quanta and electromagnetic waves became fully understandable, see Sec. 1.5.

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 these 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].

Problems:

[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.

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 operators

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

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

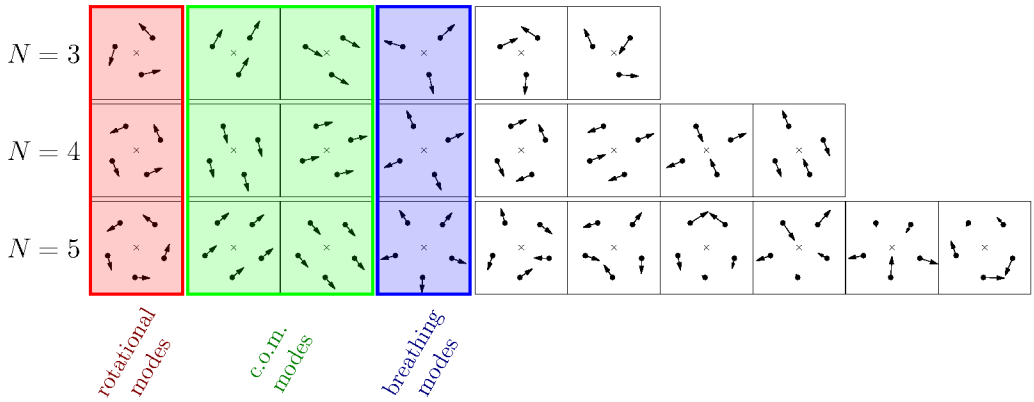

Abbildung 2.4: All normal modes of two-dimensional harmonically confined Coulomb systems with $N = 3, 4, 5$ particles. The dots picture the particles within the ground-state configuration, and the arrows show the direction and amplitude of the oscillatory motion (eigenvectors). The N-independent modes, 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].

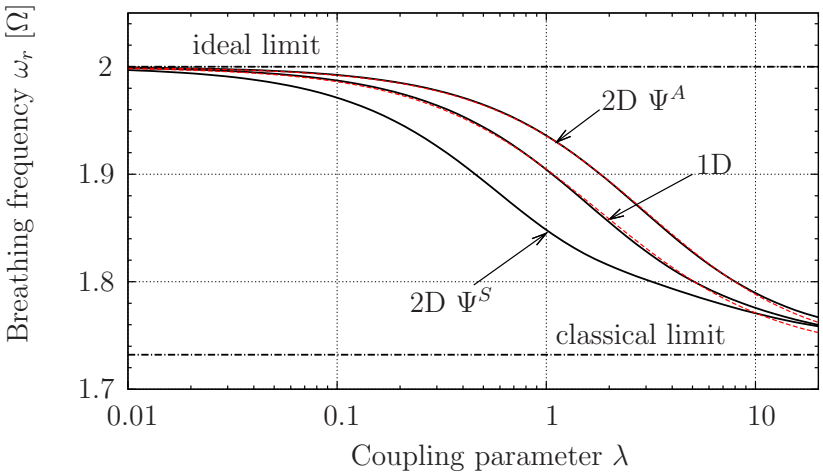

Abbildung 2.5: Frequency of the breathing mode of $N = 2$ particles in a harmonic trap for varying interaction strength $\lambda = \frac{q^2}{4\pi\epsilon_0 l_0}\frac{1}{\hbar\omega}$, with $l_0^2 = \hbar/(m\omega)$. The results for electrons with the same (A, anti-symmetric coordinate wave function) 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].

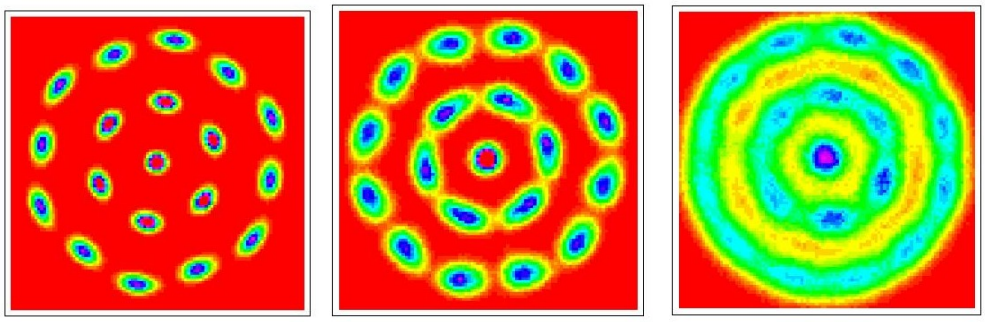

Abbildung 2.6: Probability density of $N = 19$ quantum electrons in a 2D harmonic trap. The coupling strength λ decreases from left to right, correspondingly the electron overlap increases. Path integral Monte Carlo simulations. From Ref. [FBL01], see also the discussion in Physical Review Focus, 19.4.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

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