## Advanced quantum mechanics (20104301)

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Chapter 8: Lattice models and strongly correlated systems

## Contents

8 Lattice models and strongly correlated systems ..... 5
8.1 Lattice models and spin chains ..... 6
8.2 XY Model as a paradigmatic exactly solvable model ..... 7
8.2.1 Jordan-Wigner transformation ..... 7
8.2.2 XY model as a fermionic model ..... 9
8.2.3 Spectrum and ground state ..... 10
8.2.4 Criticality and quantum phase transitions ..... 11
8.3 Structure of non interacting bosons and fermions ..... 13
8.3.1 Coordinate transformations ..... 13
8.3.2 Covariance matrices ..... 15

## Chapter 8

## Lattice models and strongly correlated systems

In the following we would like to turn towards lattice models. Those are very important models in physics as they describe many systems in solid state physics, like the structure of crystals, that determines the graph $G=(V, E)$. There are many kinds of lattices, in different dimensions, the simple chain in $1 D$ being the easiest case. Lattices are described by graphs, bonds and sites, where quantum particles sit at each site. There is a natural metric $\operatorname{dist}(j, k)$, which describes the minimal number of bonds one has to cross to get from site $j$ to site $k$, the graph theoretical distance.

An important class of examples is constitutes by one-dimensional chains with sites $1, \ldots, n$, where on each site sits a quantum degree of freedom, like a spin with Hilbert space $\mathbb{C}^{2}$, or a bosonic degree of freedom $\mathcal{H}=L^{2}(\mathbb{R})$, or a fermion with spin, and the distance is of course just $\operatorname{dist}(j, k)=|j-k|$. Interactions in such systems are usually local: that is, not all particles interact with all others but only with their nearest neighbours or next nearest neighbours. The Hamiltonian of a local chain with nearest neighbour interaction takes the following form.

## Hamiltonian of local chain:

$$
\begin{equation*}
H=\sum_{j=1}^{n} h_{j, j+1} \tag{8.1}
\end{equation*}
$$

where site $n+1$ is again the first site (periodic boundary conditions).

Strictly speaking, the summands are

$$
\begin{equation*}
\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes h_{j, j+1} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \tag{8.2}
\end{equation*}
$$

but the sites on which the Hamiltonian only acts in a trivial manner are usually neglected; $h_{j, j+1}$ acts (non trivially) only on site $j$ and $j+1$. They are of the form

$$
\begin{equation*}
h_{j, j+1}=u_{j}+v_{j, j+1} \tag{8.3}
\end{equation*}
$$

where $u_{j}$ is the onsite term and $v_{j, j+1}$ is the interaction between sites.
We will have a look at some examples. Non interacting models that relate to fermions by virtue of the Jordan-Wigner transformations, the XY-model, quantum criticality and even strongly correlated systems.

### 8.1 Lattice models and spin chains

The subsequent list summarizes some paradigmatic models of this kind that are frequently discussed in the literature.

- The harmonic chain is described by

$$
\begin{equation*}
H=\frac{1}{2} \sum_{i, j \in L}\left(p_{i} P_{i, j} p_{j}+x_{i} X_{i, j} x_{j}\right) \tag{8.4}
\end{equation*}
$$

where $X, P \in \mathbb{R}^{n \times n}$ are real, symmetric and positive matrices, which determine the coupling. The operators $\left\{x_{i}\right\}$ and $\left\{p_{i}\right\}$ fulfill canonical commutation relations

$$
\begin{equation*}
\left[x_{j}, p_{k}\right]=i \delta_{j, k} \tag{8.5}
\end{equation*}
$$

The Hamiltonian in terms of bosonic operators $b_{j}=\left(x_{j}+i p_{j}\right) / \sqrt{2}$ for $i=$ $1, \ldots, n$ reads

$$
\begin{equation*}
H=\frac{1}{2} \sum_{i, j}\left(b_{i}^{\dagger} A_{i, j} b_{j}+b_{i} A_{i, j} b_{j}^{\dagger}+b_{i} B_{i, j} b_{j}+b_{i}^{\dagger} B_{i, j} b_{j}^{\dagger}\right) \tag{8.6}
\end{equation*}
$$

where

$$
\begin{equation*}
A=(X+P) / 2, B=(X-P) / 2 \tag{8.7}
\end{equation*}
$$

This model, e.g., captures lattice vibrations in solid bodies or discrete versions of free fields in quantum field theory. It is a non interacting model, as the Hamiltonian is quadratic in bosonic operators. If the interaction is translational invariant, $A$ and $B$ are circulant matrices. Also, if there is only nearest neighbour interaction, $A$ and $B$ are nonzero only at the diagonal and first off diagonals.

- Fermionic chain:

$$
\begin{equation*}
H=\frac{1}{2} \sum_{i, j=1}^{n}\left(f_{i}^{\dagger} A_{i, j} f_{j}-f_{i} A_{i, j} f_{j}^{\dagger}+f_{i} B_{i, j} f_{j}-f_{i}^{\dagger} B_{i, j} f_{j}^{\dagger}\right) \tag{8.8}
\end{equation*}
$$

For this Hamiltonian to be Hermitian

$$
\begin{equation*}
A^{T}=A, B^{T}=-B \tag{8.9}
\end{equation*}
$$

has to hold. Now $x_{j}=\left(f_{j}^{\dagger}+f_{j}\right) / \sqrt{2}$ and $p_{j}=i\left(f_{j}^{\dagger}-f_{j}\right) / \sqrt{2}$ are not position and momentum operators but Majorana fermions. The energy gap between ground and first excited state is the smallest non zero singular value of $A+B$

- XY-chain: spin chains of that kind are important models. At each site sits a $\mathbb{C}^{2}$ spin. The most popular and exactly solvable model is the XY-chain with a transverse magnetic field. The corresponding Hamiltonian reads

$$
\begin{equation*}
H=-\frac{1}{2} \sum_{i=1}^{n}\left(\frac{1+\gamma}{4} X_{i} X_{i+1}+\frac{1-\gamma}{4} Y_{i} Y_{i+1}\right)-\frac{\lambda}{2} \sum_{i=1}^{n} Z_{i} \tag{8.10}
\end{equation*}
$$

where $\langle i, j\rangle$ denotes summation over nearest neighbours. $\gamma$ is some weird parameter, $\lambda$ the extern magnetic field. We are coming back to that model later.

- The Heisenberg model: is another important spin model and can be described by

$$
\begin{equation*}
H=-\frac{1}{2} \sum_{i=1}^{n}\left(X_{i} X_{i+1}+Y_{i} Y_{i+1}+Z_{i} Z_{i+1}\right)-\frac{\lambda}{2} \sum_{i=1}^{n} Z_{i} \tag{8.11}
\end{equation*}
$$

which is not a free model anymore.

- Obviously, this is only the tip of the iceberg, and there are lots of further models of a similar type.


### 8.2 XY Model as a paradigmatic exactly solvable model

The XY model is the easiest model that shows critical behaviour, quantum phase transitions, scaling properties and degenerate ground states, while still being easily solvable. The central insight is, that even though being a spin chain, the model can be translated to free fermions.

### 8.2.1 Jordan-Wigner transformation

The corresponding transformation is the Jordan-Wigner transformation (Jordan-Wigner transformation ), which states that a system of

- $n$ fermionic modes and
- $n$ spins
are isomorphic to each other. In second quantization a state of fermions in $n$ modes reads

$$
\begin{equation*}
\left|N_{1}, \ldots, N_{n}\right\rangle=\left(f_{1}^{\dagger}\right)^{N_{1}} \ldots\left(f_{n}^{\dagger}\right)^{N_{n}}|\varnothing\rangle \tag{8.12}
\end{equation*}
$$

with $N_{k} \in\{0,1\}$ for all $k$. This is nothing but a state vector in $\left(\mathbb{C}^{2}\right)^{\otimes n}$, which looks just like a chain of $n$ spins, where each can be either up (0) or down (1).

The only difficulty is to represent the spin operators $\left(O_{j}\right)$ by fermionic operators $\left(f_{j}\right)$. Fermionic operators anti-commute, whereas local spin operators do not. The key question to be solved, hence, is to find way to make sure that

$$
\begin{equation*}
\langle\varnothing| f_{N}^{M_{n}} \ldots f_{1}^{M_{1}}\left(f_{j}^{\dagger} f_{j}\right)\left(f_{1}^{\dagger}\right)^{N_{1}} \ldots\left(f_{n}^{\dagger}\right)^{N_{n}}|\emptyset\rangle=\left\langle M_{1}, \ldots, M_{n}\right| O_{j}\left|N_{1}, \ldots, N_{n}\right\rangle \tag{8.13}
\end{equation*}
$$

## 8CHAPTER 8. LATTICE MODELS AND STRONGLY CORRELATED SYSTEMS

holds? The answer is that spin operators are not locally represented. And the specific transformation at the heart of this is given by the Jordan-Wigner transformation, which is actually less of a transformation than a representation.

Jordan-Wigner transformation: Systems of $n$ fermionic modes are isomorphic to a system of $n$ spins. For a fixed order of fermionic modes one can transform operators like

$$
\begin{align*}
f_{j}^{\dagger} & =\left(\prod_{k=1}^{j-1} Z_{j}\right) \sigma_{j}^{-}  \tag{8.14}\\
f_{j} & =\left(\prod_{k=1}^{j-1} Z_{j}\right) \sigma_{j}^{+} \tag{8.15}
\end{align*}
$$

and inversely

$$
\begin{array}{r}
Z_{j}=1-2 f_{j}^{\dagger} f_{j} \\
\sigma_{j}^{+}=\prod_{k=1}^{j-1}\left(1-2 f_{k}^{\dagger} f_{k}\right) f_{j}, \\
\sigma_{j}^{-}=\prod_{k=1}^{j-1}\left(1-2 f_{k}^{\dagger} f_{k}\right) f_{j}^{\dagger} . \tag{8.18}
\end{array}
$$

Here, as always

$$
\begin{align*}
\sigma_{j}^{-} & =\left(X_{j}-i Y_{j}\right) / 2  \tag{8.19}\\
\sigma_{j}^{+} & =\left(X_{j}+i Y_{j}\right) / 2 \tag{8.20}
\end{align*}
$$

Some remarks are in order at this point.

- Again, a core insight is that the Jordan-Wigner transformation is non local, and necessarily so. Fermionic modes that have support only on few fermionic modes can have support on almost the whole lattice in terms of spin operators. This is a consequence of the anti-commutation-relation-problem mentioned above.
- Consequently the order of fermionic modes plays a role as the spin operator on site $j$ contains all fermionic modes to the left of $j$. As such, we have to fix the order in the beginning.
- Physical operators are only those, which do not depend on the order. See the first example below.

Two examples of operators under Jordan-Wigner transformation :

$$
\begin{equation*}
f_{j}^{\dagger} f_{j}=\left(1-Z_{j}\right) / 2 \tag{8.21}
\end{equation*}
$$

for all $j$. So the number operator on mode $j$ becomes the Pauli- $Z$ operator in spin representation. Also the non local string canceled out (because $Z_{j}^{2}=\mathbb{1}$ ), and it is thus a physical operator. Say, for $s>0$

$$
\begin{equation*}
f_{j}^{\dagger} f_{j+s}=\sigma_{j}^{-}\left(\prod_{l=j+1}^{j+s-1} Z_{l}\right) \sigma_{j+s}^{+} \tag{8.22}
\end{equation*}
$$

Evidently $f_{j}^{\dagger} f_{j+s}$ are not mapped to $Z_{j} Z_{j+s}$, as one might have expected, but there is still a string between $j$ and $j+s$. Hence the operator could have support on many sites, which is a problem in the theoretical characterization of fermions as most models depend on some locality of interactions. In the following, we will look at an example, where this problem does not occur.

### 8.2.2 XY model as a fermionic model

Consider the XY model again, a chain of spins with nearest neighbour interaction. Choosing the order such that nearest neighbours are always on neighbouring sites, one gets a non interacting local fermionic model:

XY model as non interacting fermionic model: A Jordan-Wigner transformation of the XY model gives a non interacting fermionic model of the form indicated in Eq.8.8. With

$$
\begin{align*}
A_{i, i} & =\lambda,  \tag{8.23}\\
A_{i, j} & =-1 / 2, \text { if }|i-j|=1  \tag{8.24}\\
B_{i, j} & =-B_{j, i}=\frac{\gamma}{2}, \text { if }|i-j|=1 \tag{8.25}
\end{align*}
$$

and else $A_{j, k}=B_{j, k}=0$. This corresponds to a non interacting fermionic chain Hamiltonian with nearest neighbour interaction, with $A$ and $B$ being circulant matrices.

We chose periodic boundary conditions, which means site $n+1$ is site 1 again. We get:

$$
\begin{align*}
H & =-\frac{1}{2} \sum_{i=1}^{n}\left(f_{i}^{\dagger} f_{i+1}+h . c .\right) \\
& +\frac{\gamma}{4} \sum_{i=1}^{n}\left(f_{i} f_{i+1}+h . c .\right)+\frac{\lambda}{2} \sum_{j=1}^{n} f_{j}^{\dagger} f_{j} \tag{8.26}
\end{align*}
$$

and in the isotropic case of $\gamma=0$ simply

$$
\begin{equation*}
H=-\frac{1}{2} \sum_{i=1}^{n}\left(f_{i}^{\dagger} f_{i+1}+h . c .\right)+\frac{\lambda}{2} \sum_{j=1}^{n} f_{j}^{\dagger} f_{j} . \tag{8.27}
\end{equation*}
$$

The case $\gamma=0$ is (not very intuitively) called XX model. No strings occur, so the model is indeed local.

### 8.2.3 Spectrum and ground state

Let us be specific and take the value $\gamma=0$ to be concise in what follows. We introduce a new set of fermionic operators $\left\{a_{1}, \ldots, a_{n}\right\}$, that are Fourier transforms of the old fermionic operators and retain anti-commutation relation

$$
\begin{equation*}
a_{k}=\frac{1}{n^{1 / 2}} \sum_{j=1}^{n} f_{j} e^{-i 2 \pi k j / n} \tag{8.28}
\end{equation*}
$$

for $k=1, \ldots, n$. The operation that maps the old set to the new one is indeed unitary

$$
\begin{equation*}
\left(a_{1}, \ldots, a_{n}\right)^{T}=U\left(f_{1}, \ldots, f_{n}\right)^{T} \tag{8.29}
\end{equation*}
$$

with $U \in U(n)$. The transformed Hamiltonian reads

$$
\begin{equation*}
H=\sum_{k=1}^{n} \Lambda_{k} a_{k}^{\dagger} a_{k} \tag{8.30}
\end{equation*}
$$

with the following spectrum.

## Spectrum of the XX model:

$$
\begin{equation*}
\Lambda_{k}=\frac{\lambda}{2}-\frac{1}{2} \cos \left(\frac{2 \pi k}{n}\right) \tag{8.31}
\end{equation*}
$$

In the limit $n \rightarrow \infty$ and with periodic boundary conditions one may also write

$$
\begin{equation*}
\Lambda_{\phi}=\frac{\lambda}{2}-\frac{1}{2} \cos \phi \tag{8.32}
\end{equation*}
$$

with $\pi \in[0,2 \pi)$, by replacing $2 \pi k / n$ with $\phi$.

The discussion of this spectrum is easy but nevertheless shows rich behaviour.

- if $\lambda<-1$ then, for all $k$

$$
\begin{equation*}
\Lambda_{k} \geq 0 \tag{8.33}
\end{equation*}
$$

so the ground state is the fermionic vacuum $|\varnothing\rangle$ for which

$$
\begin{equation*}
f_{k}|\varnothing\rangle=0 \text { for all } k \tag{8.34}
\end{equation*}
$$

mapped back to spins, the ground state is

$$
\begin{equation*}
|\mathrm{GS}\rangle=|0,0, \ldots, 0\rangle \tag{8.35}
\end{equation*}
$$

a product state of fermions, all pointing in the same direction.

- Similarly for $\lambda>1$ and all $k$ one gets

$$
\begin{equation*}
\Lambda_{k} \leq 0 \tag{8.36}
\end{equation*}
$$

and the ground state of the XX model in spin representation reads

$$
\begin{equation*}
|\mathrm{GS}\rangle=|1,1, \ldots, 1\rangle \tag{8.37}
\end{equation*}
$$

Those two phases are called ferromagnetic phases. It is highly plausible, that for a sufficiently strong magnetic field $(|\lambda|>1)$ all spins align to it. The only surprise value might be, that there is no correlation whatsoever and the ground state is a proper product state.

- It remains the case $\lambda \in(-1,1)$. Since there is a shift of sign in the Hamiltonian one has to consider two cases for the ground state. One is:

$$
\begin{equation*}
f_{k}|\mathrm{GS}\rangle=0 \text { for all } k \text { for which } \Lambda_{k}>0 \tag{8.38}
\end{equation*}
$$

And the other one:

$$
\begin{equation*}
f_{k}^{\dagger}|\mathrm{GS}\rangle=0 \quad \text { for all } k \text { for which } \Lambda_{k} \leq 0 \tag{8.39}
\end{equation*}
$$

We define the Fermi level as

$$
\begin{equation*}
k_{c}=\left\lfloor\frac{n}{2 \pi} \arccos \left(\frac{\lambda}{2}\right)\right\rfloor \tag{8.40}
\end{equation*}
$$

It is easy to see that

$$
\lambda_{k} \begin{cases}<0, & \text { for } k_{c} \leq k \leq 0 \text { or } n-1 \geq k \geq b-k_{c}  \tag{8.41}\\ \geq 0, & \text { else }\end{cases}
$$

(Here $\lfloor x\rfloor$ denotes the floor function, which gives the largest integer that is smaller than $x$.) So the ground state is the one, where the system is filled up to the Fermi level. The ground state energy is

$$
\begin{equation*}
\sum_{k} \Lambda_{k} \theta\left(-\Lambda_{k}\right) \tag{8.42}
\end{equation*}
$$

### 8.2.4 Criticality and quantum phase transitions

There can be said a lot about critical systems but we will only discuss the ideas by taking the above example (XX chain). Consider again the energy spectrum

$$
\begin{equation*}
\Lambda_{\phi}=\frac{\lambda}{2}-\frac{1}{2} \cos \phi \tag{8.43}
\end{equation*}
$$

with $\phi \in[0,2 \pi)$.

- If $|\lambda|>1$, the spectrum has no zeros: as explained above, this leads to all spins pointing either up or down (ferromagnetic phases). The first excited state is the one, where one fermion is taken out. To do so, the energy

$$
\begin{equation*}
\Delta E:=\min \left\{\Lambda_{\phi}: \phi \in[0,2 \pi)\right\} \tag{8.44}
\end{equation*}
$$

is needed. And in that case

$$
\begin{equation*}
\Delta E>0 \tag{8.45}
\end{equation*}
$$

therefor there is a nonzero energy gap between the ground state and first excited state. Such phases are called critical or gapped phases. In general, gapped phases are those that have a nonzero energy gap between its ground state(s) and its first excited state in the thermodynamic limit.

- In contrast, for $\lambda \in(-1,1)$, there are zeros. So

$$
\begin{equation*}
\Delta E=0 \tag{8.46}
\end{equation*}
$$

A system in that phase is at a critical point. In the thermodynamic limit, to go to an excited state costs arbitrarily little energy.

Whether or not there is an energy gap makes a huge difference on physical grounds.
If there is one, one can show, that the ground state always exhibits some locality. correlations decay exponentially in distance. For any observable $O_{j}$ that has support on $j$ alone, and $O_{i}$ that has support on $i$ alone, one has

$$
\begin{align*}
\left|\left\langle O_{i} O_{j}\right\rangle-\left\langle O_{i}\right\rangle\left\langle O_{j}\right\rangle\right| & \left.=\left|\langle\mathrm{GS}| O_{i} O_{j}\right| \mathrm{GS}\right\rangle-\langle\mathrm{GS}| O_{i}|\mathrm{GS}\rangle\langle\mathrm{GS}| O_{j}|\mathrm{GS}\rangle \mid \\
& \sim e^{-|i-j| / \xi}, \tag{8.47}
\end{align*}
$$

for an appropriate correlation length

$$
\begin{equation*}
\xi>0 \tag{8.48}
\end{equation*}
$$

So if one measures at two sites, far enough from each other, the results will be uncorrelated. That this holds was "known" for many years. Maybe surprisingly, it was first properly proven with rigorous methods only in 2004, with methods referred to as Lieb-Robinson theorems, bounds to group velocities in general lattice models (and then using an ingenious trick of an integral in the complex plane).

The situation changes radically for critical models. Correlations do not decay exponentially anymore, but following power laws. In fact. there is no length scale anymore and the correlation function (Eq. 8.47) decays only algebraically. The ground state will in a sense that can be made precise look the same on all scales. The field of conformal field theory captures such physical systems that follow such scaling laws at critical points.

The theory of universality studies what happens close to critical points $\lambda_{c}$ (in our case $\left|\lambda_{c}\right|=1$ ). One finds

$$
\begin{equation*}
\xi \sim\left|\lambda-\lambda_{c}\right|^{-\nu} \tag{8.49}
\end{equation*}
$$

with $\nu \in \mathbb{R}$ being some critical exponent. And for the energy gap

$$
\begin{equation*}
\Delta E \sim\left|\lambda-\lambda_{c}\right|^{s} \tag{8.50}
\end{equation*}
$$

with another critical exponent $s$. The universality hypothesis (which is a hypothesis since is has not been proven yet) states that there are only finitely many critical exponents possible in nature, which is quite surprising. Models with different critical exponents are collected in different universality classes. In our XX model we find that

$$
\begin{equation*}
\Delta E=|\lambda-1| \tag{8.51}
\end{equation*}
$$

so the critical exponent $s=1$ and

$$
\begin{equation*}
\xi=\frac{1}{(\lambda-1)^{1 / 2}} \tag{8.52}
\end{equation*}
$$

so the critical exponent $\nu=1 / 2$.
Let us take the opportunity to be at this point a bit more precise about quantum phase transitions in the first place.

- The family of Hamiltonians

$$
\begin{equation*}
H(g)=H_{0}+g H_{1}, \tag{8.53}
\end{equation*}
$$

where $g \in \mathbb{R}$ is some parameter (like a magnetic field strength) shows quantum phase transition if there are non analyticities in the ground state energy for some $g=g_{c}$.

- One classifies quantum phase transitions of first and second order, where first order quantum phase transitions are indicated by kinks in the ground state energy and second order quantum phase transitions by a smooth energy but kinks in the first derivative. The XX model is an example of such a second order quantum phase transition.


### 8.3 Structure of non interacting bosons and fermions

It should be clear by now, that non interacting models play an important role in physics, either exactly or at least in good approximation. Let's have some general words on such systems again.

### 8.3.1 Coordinate transformations

Let us at this point go more into detail what we precisely mean by linearly transforming one set of bosonic or fermionic coordinates into a new one. We consider bosonic $\left(b_{1}, \ldots, b_{n}\right)$ or fermionic $\left(f_{1}, \ldots, f_{n}\right)$ annihilation operators that commute or anticommute. From those we can define

$$
\begin{align*}
x_{j} & =\left(a_{j}^{\dagger}+a_{j}\right) / \sqrt{2}  \tag{8.54}\\
p_{j} & =i\left(a_{j}^{\dagger}+a_{j}\right) / \sqrt{2} \tag{8.55}
\end{align*}
$$

where $a_{j}=b_{j}, f_{j}$ are the position and momentum operators, or the Majorana fermions, respectively. So how can we transform them linearly, respecting the relevant commutation or anti-commutation relations?

Symplectic transformations for bosons: The allowed linear transformations from one set of canonical coordinates $\left(x_{1}, \ldots, x_{n}, p_{1}, \ldots, p_{n}\right)$ to a new such set that satisfies the canonical commutation relations give rise to the so-called symplecic transformations

$$
\begin{equation*}
\left(x_{1}, \ldots, x_{n}, p_{1}, \ldots, p_{n}\right) \mapsto S\left(x_{1}, \ldots, x_{n}, p_{1}, \ldots, p_{n}\right) \tag{8.56}
\end{equation*}
$$

They satify

$$
\begin{equation*}
S \sigma S^{T}=\sigma \tag{8.57}
\end{equation*}
$$

where $\sigma$ is a matrix that embodies the canonical commutation relations (again choosing $\hbar=1$ ) as

$$
\sigma=\left[\begin{array}{cc}
0 & \mathbb{1}  \tag{8.58}\\
-\mathbb{1} & 0
\end{array}\right]
$$

These transformations form a group, the real symplectic group $S \in S p(2 n, \mathbb{R})$.

Some remarks are again in order here ${ }^{1}$

- It is not difficult to see that those are precisely the linear transformations that respect the canonical commutation relations.
- $\sigma$ has the given form, since positions of one mode of course commute with the momentum of another mode. There is only an entry in $\sigma$ if a position coordinate of one mode comes together with a momentum coordinate of the very same mode.
- The same structure is encountered in classical statistical mechanics.

An important special case we have already encountered before: The case in which the positions and momenta are all rotated orthogonally in the same fashion. Such transformations are always symplectic. Formally, this means that

$$
\begin{equation*}
O \oplus O \in S p(2 n, \mathbb{R}) \tag{8.59}
\end{equation*}
$$

for all $O \in O(n)$, where the latter denotes the real orthogonal group (the real unitary transformations). This is no surprise: If we rotate momenta and positions in the same way, then the commutation relations are preserved. ${ }^{2}$ If should be clear that all transformations that we have encountered as "Bogoliobov transformationens" are included in this group, and are special cases of such symplectic transformations.

[^0]the maximum compact subgroup of $S p(2 n, \mathbb{R})$. Such transformations are tremendously important in qauntum optics, as they are those that can be generated with passive optical elements such as beam splitters, mirrors, and phase shifters. Sometimes, a bit of group theory can be helpful.

An important insight is that with such symplectic transformations, one can diagonalize strictly positive matrices. This is different from the "diagonalization" with unitary transformations, but to the same effect. This insight is at the heart of notions of decoupling harmonic chains, in normal mode decomposition. In condensed matter physics and in quantum optics, this is very important. The statement goes as follows.

Williamson theorem: Every strictly positive $2 n \times 2 n$-Matrix $M$ can be brought into a diagonal form under symplectic transformations,

$$
\begin{equation*}
S M S^{T}=\operatorname{diag}\left(d_{1}, d_{1}, d_{2}, d_{2}, \ldots, d_{n}, d_{n}\right) \tag{8.61}
\end{equation*}
$$

where $\left\{d_{j}\right\}$ are the positive square roots of the eigenvalues of $-\sigma M \sigma M$. The are called symplectic eigenvalues.

While the core statement is difficult to show, the latter statement is rather easy. Note also that the symplectic eigenvalues are in general different from the ordinary eigenvalues. How, now, can we transform fermionic operators? Well, in a somewhat similar fashion.

Linear coordinate transformations for fermions: The allowed transformations that linearly map $\left(x_{1}, \ldots, x_{n}, p_{1}, \ldots, p_{n}\right)$ into a new set of Majorana fermions, are transformations of the form

$$
\begin{equation*}
\left(x_{1}, \ldots, x_{n}, p_{1}, \ldots, p_{n}\right) \mapsto O\left(x_{1}, \ldots, x_{n}, p_{1}, \ldots, p_{n}\right) \tag{8.62}
\end{equation*}
$$

with $O \in O(2 n)$.

Interestingly, the operations $O \oplus O$ with orthogonal $O \in S O(n)$ are contained in both groups. In fact, in many practical settings, one can treat bosons and fermions in an analogous fashion.

### 8.3.2 Covariance matrices

Non-interacting systems have another interesting property: Its ground states as well as its thermal states are Gaussian states which are perfectly defined by means of their first and second moments (for fermions actually only the second moments). The first moments

$$
\begin{equation*}
m_{j}=\operatorname{tr}\left[\rho r_{j}\right] \tag{8.63}
\end{equation*}
$$

are simply the expectation values of

$$
\begin{equation*}
\left(r_{1}, \ldots, r_{2 n}\right)=\left(x_{1}, \ldots, x_{n}, p_{1}, \ldots, p_{n}\right) \tag{8.64}
\end{equation*}
$$

Again, for fermions, they are all zero. For bosons, they are often also zero: What is more, one can often shift systems in phase space to make them zero. The second moments can be embodied in covariance matrices.

Bosonic covariance matrices: The second moments of a bosonic state with vanishing first moments can be embodied in the $2 n \times 2 n$ symmetric covariance matrix with entries

$$
\begin{equation*}
\gamma_{j, k}=\operatorname{tr}\left[\rho\left(r_{j} r_{k}+r_{k} r_{j}\right)\right] . \tag{8.65}
\end{equation*}
$$

It is not only positive, but satisfies with

$$
\begin{equation*}
\gamma+i \sigma \geq 0 \tag{8.66}
\end{equation*}
$$

the Heisenberg uncertainty principle.

The latter, of course, also implies that $\gamma=\gamma^{T}$. Maybe in this form, the uncertainty principle it is a bit in disguise. But a moment of thought reveals that this is the right form. Using the above Williamson theorem, one can treat each mode separately. For each such mode, we then have

$$
\gamma+i \sigma=\left[\begin{array}{cc}
2\left\langle x^{2}\right\rangle & \langle x p\rangle+\langle p x\rangle  \tag{8.67}\\
\langle x p\rangle+\langle p x\rangle & 2\left\langle p^{2}\right\rangle
\end{array}\right]+i\left[\begin{array}{cc}
0 & 1 \\
-1 & 0
\end{array}\right] \geq 0
$$

which is the common form of the uncertainty principle. Based on such covariance matrices, one can compute all properties one can dream of, in particular quantities such as entropies. Fermonic covariance matrices are defined as follows.

Fermionic covariance matrices: The $2 n \times 2 n$ anti-symmetric fermionic covariance matrices $\gamma=-\gamma^{T}$ are defined as

$$
\begin{equation*}
\gamma_{j, k}=2 i \operatorname{tr}\left[\rho r_{j} r_{k}\right]-i \delta_{j, k} \tag{8.68}
\end{equation*}
$$

It satisfies

$$
\begin{equation*}
i \gamma \leq \mathbb{1} \tag{8.69}
\end{equation*}
$$

Similar to bosons, one can "decouple fermions", in a way that reminds of the normal mode decomposition. Simple as this may look, it is at the basis of a huge body of material in condensed matter physics.

Normal form of fermionic covariance matrices: Every fermionic covariance matrix $\gamma \in \mathbb{R}^{2 n \times 2 n}$ can be broght into the form

$$
O \gamma O^{T}=\bigoplus_{j=1}^{n}\left[\begin{array}{cc}
0 & d_{j}  \tag{8.70}\\
-d_{j} & 0
\end{array}\right]
$$

with a suitable $O \in S O(2 n)$, where now $d_{j} \in[0,1]$.

Again, say, tight binding models can be solved in this form. The above fermionic Bogoliubov transformations are all special cases of this more general formalism.


[^0]:    ${ }^{1}$ If $S \in S p(2 n, \mathbb{R})$, then also $S^{-1} \in S p(2 n, \mathbb{R})$ and $S^{T} \in S p(2 n, \mathbb{R})$.
    ${ }^{2}$ These transformations constitute a reducible representation of $O(n)$, which in turn is a subgroup of $K(2 n)$,

    $$
    \begin{equation*}
    K(2 n)=S p(2 n, \mathbb{R}) \cap O(2 n) \tag{8.60}
    \end{equation*}
    $$

