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## Chapter 10

# Atoms, molecules, open and complex quantum systems

At this point, we are now done with the main part of the course, introducing the formalism of quantum theory and its consequences. At this point, we should feel familiar with the basic equations and should be able to solve simple but interesting problems. Needless to say, this is the point where things become really interesting – but a lot of that we have to shift to the next course. Still, we would like to use the remaining time to get at least an impression of further aspects of quantum theory. These topics will not be mentioned in the exam, in any case.

### 10.1 Open quantum systems

A good starting point of this is the insight that every (quantum) system is to some extent open. Of course, every system will always be coupled to some extent to an environment, no matter how much we try to isolate this. Clearly, a balanced picture of quantum theory would be somewhat incomplete without at least a brief glimpse at how one can treat this only situation that is actually relevant in practice.

#### 10.1.1 Reduced system dynamics

The Schroedinger equation that we have encountered earlier is the equation that governs the evolution of closed quantum systems. How about open systems then? At first, it seems not entirely obvious of how to alter the Schroedinger equation; some ad hoc ansatz would easily lead to baroque non-linear equations of motion, ones that easily violate causality.

The key insight is that open systems are ones interacting with an environment, and the evolution of a system of salient interest is then captured by look-

ing at the evolution of the reduced state belonging to this system. Let us be more specific:

- Let us denote our system of interest with  $S$ . It has a Hilbert space  $\mathcal{H}_S$ , the free evolution is governed by a Hamiltonian  $H_S$ .
- Then there is its environment  $E$ . It is equipped with a Hilbert space  $\mathcal{H}_E$ , and its free evolution in turn is specified by a Hamiltonian  $H_E$ . The environment includes all the degrees of freedom one is not particularly interested in; it could be surrounding modes, field modes, some background degrees of freedom that incorporate some notion of “quantum noise”. Usually, the dimension of this environment is quite large.
- Then there is an interaction Hamiltonian  $H_I$ .

Of course, there are two tensor factors here, one for the system  $S$  and one for the environment  $E$ . Let us emphasize this fact in a box:

**Hamiltonian of an open quantum system:** The total Hamiltonian of an open system  $S$  surrounded by its environment  $E$  is of the form

$$H = H_S \otimes \mathbb{1} + \mathbb{1} \otimes H_E + H_I. \quad (10.1)$$

How is the evolution then described? Well, we do not need any new equations any more, we have already discussed all relevant fundamental equations: The joint system of system  $S$  and environment  $E$  is a closed system, so follows the Schrodinger equation. So if the Hamiltonians are not time-dependent, which we will assume throughout this chapter, we have for the state, the density operator, at time  $t \geq t_0$ ,

$$\rho(t) = U(t, t_0)\rho(t_0)U(t, t_0)^\dagger, \quad (10.2)$$

where

$$U(t, t_0) = e^{-i(t-t_0)H/\hbar}. \quad (10.3)$$

This is no news to us. This is the equation of motion of the density operator on

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E, \quad (10.4)$$

so the Hilbert space of the total system.

Usually, one assumes the system and its environment to be uncorrelated initially. This is often a natural and physical assumption. After all, the correlations build up in time through the interaction. (Sometimes, it is rather done as a simplifying assumption, however, with little physical justification. One has to be a bit careful, therefore. But let us not be overly cautious here.) Such an *uncorrelated or product initial condition* corresponds to

$$\rho(t_0) = \rho_S(t_0) \otimes \rho_E(t_0). \quad (10.5)$$

So what is the state of the system  $S$ ? It is the reduced state to the system  $S$ :

**Reduced system dynamics:** The state of the system  $S$  at time  $t \geq t_0$  is given by the partial trace

$$\begin{aligned}\rho_S(t) &= \text{tr}_E(\rho(t)) \\ &= \text{tr}_E\left(U(t, t_0)(\rho_S(t_0) \otimes \rho_E(t_0))U(t, t_0)^\dagger\right).\end{aligned}\quad (10.6)$$

The interaction changes the dynamics profoundly; it is in fact quite different usually from basic Schroedinger dynamics (which is included in this picture in the absence of interaction, so for  $H_I = 0$ ).

### 10.1.2 Decoherence

In particular, we are already aware of the fact that reduced states of pure entangled states are not necessarily pure. This means that even if we start off in a totally pure state, at later times the state of the system can – and usually will – be mixed to some extent. In yet other words, states of a system can look after a while as if one had a classically probabilistic situation. This effect is called *decoherence*: Via the interaction with an environment, objects lose to some extent their quantum features and classical features emerge.

Let us be a bit more specific and let us consider an example to see how this happens. We will take the simplest possible system and a quite simple environment. Let us assume that  $S$  is a spin-1/2 system with Hilbert space  $\mathbb{C}^2$ . Let us take

$$H_S = 0, \quad H_E = 0, \quad (10.7)$$

so we abstract from the free evolution of the system and its environment,  $H = H_I$ . The interaction Hamiltonian is taken to be

$$H_I = \sigma_x \otimes \sigma_x \quad (10.8)$$

Here the environment “measures” whether the system is in  $|0\rangle\langle 0|$  or  $|1\rangle\langle 1|$ , respectively. Let us take

$$\rho_E(t_0) = |0\rangle\langle 0| \quad (10.9)$$

to be the initial state of the environment. Let us now consider two scenarios:

- In the first scenario the system is initially in

$$\rho_S(t_0) = |+\rangle\langle +|, \quad (10.10)$$

where, again as usual,  $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ . Then there will be no time evolution,

$$\rho(t) = |+\rangle\langle +| \otimes |0\rangle\langle 0| = \rho(t_0) = \rho_S(t_0) \otimes \rho_E(t_0). \quad (10.11)$$

for all times  $t \geq t_0$ . This is no surprise, as  $|+\rangle$  is an eigenvector of  $\sigma_x$ .

- The second scenario is that the system starts off in

$$\rho_S(t_0) = |0\rangle\langle 0|. \quad (10.12)$$

Now the initial state no longer commutes with the Hamiltonian, so there will be some time evolution. It is also very easy to compute the state at later times: It is easy to compute  $U(t, t_0) = e^{-i(t-t_0)H/\hbar}$ , and for

$$t - t_0 = \pi\hbar/4, \quad (10.13)$$

it is quite straightforward to find that

$$\rho_S(t) = \frac{1}{2}\mathbb{1} = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|). \quad (10.14)$$

That is to say, the state of the system  $S$  is no longer pure, but in fact maximally mixed.

This is a common feature of open quantum systems: States which start off pure can become entangled with their environment, and hence the reduced state becomes mixed: In slightly vague terms, we can say the following:

**Decoherence:** Decoherence is the process of states becoming mixed and superpositions to decay into mixtures due to the coupling with an environment.

Often, decoherence has the effect that there is little energy dissipation to the environment, but still, superpositions associated with state vectors  $\alpha|0\rangle + \beta|1\rangle$  with  $\alpha, \beta \in \mathbb{C}$  with  $|\alpha|^2 + |\beta|^2 = 1$  decay into

$$\rho_S(t) = |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1|. \quad (10.15)$$

Since superpositions are usually responsible for encountering “coherent dynamics” and interference, decoherence is accompanied by a loss of the capability of exhibiting such coherent effects and by the emergence of rather “classical dynamics”.

Indeed, the process of decoherence plays an important role in understanding why we see so few genuine quantum effects in our everyday experiences: Chairs, for example, rarely occur in superpositions between two different places. In fact, we would not even know how that would look like! The crude form of the argument goes as follows: Even if one could prepare a chair in a superposition between two different positions, this superposition would quickly decay into a mixture of two alternative places. And then it would rather look like a probabilistic process for all practical purposes, which is something we are well familiar with.

### 10.1.3 Quantum channels

Let us push this a bit further. This is really more advanced, so do not worry too much if you think this is somewhat too much. We have so far encountered a number of operations in quantum theory: We are well familiar with

- (a) Schroedinger dynamics,
- (b) measurement,
- (c) partial traces and
- (d) additions of systems using tensor products.

In fact, in open system dynamics we have included each of these operations, except from measurement:

- We (d) append a system (namely the one of the environment),
- then (a) apply Schroedinger dynamics, namely let the system  $S$  and the environment  $E$  evolve,
- and (c) finally look at the reduced state, so perform a partial trace.

Obviously, at the end of all this, there is again a quantum state. This is a manifestation of the rather obvious fact that states are mapped onto states in any operation allowed by quantum mechanics. This is also true for quantum measurements: Again, the state obtained immediately after a measurement is again a state. So any of these operations we could capture as a map of the form

$$\rho \mapsto T(\rho), \quad (10.16)$$

where  $T$  “does something to the state”. This map must be a so-called positive linear map. This is a map that maps positive operators (initial states) onto positive operators (final states). This must be the case, since we know that all density operators have non-negative eigenvalues, and are hence positive operators.

So two related questions arise:

1. What is the most general operation we can achieve by concatenating ingredients (a-d) of the above list? Presumably, this is a difficult classification problem?
2. Then, is every positive map allowed by the formalism of quantum mechanics, meaning, can one for every positive map find a procedure with elements from (a-d) such that the concatenation realizes this map.

The answer to the second question is: Not quite, we need something slightly more. We need a map that is what is called *completely positive*: This means that

$$T \otimes \mathbb{1} \quad (10.17)$$

must be positive, so must map states onto states. You must be joking, you might be tempted to say: the  $\mathbb{1}$  operation does nothing to the system it acts on, it is simply the identity operation. This is correct, but the input to this map could be entangled and does not have to be a product! So remarkably, to ask for Eq. (10.17) to be positive is something stronger than to ask for  $T$  to be positive.

The good news is then that every operation in quantum mechanics is completely positive, and conversely, any completely positive map can be realized by a sequence of operations from (a-d). Such operations are also called quantum channels.

**Quantum channels:** The most general evolution in quantum theory is that of a quantum channel

$$\rho \mapsto T(\rho), \quad (10.18)$$

where  $T$  is a completely positive map. This can always be written in the form

$$\rho \mapsto \sum_j A_j \rho A_j^\dagger, \quad (10.19)$$

with suitable operators  $\{A_j\}$ .

Open system dynamics gives rise to such quantum channels. So does Schroedinger evolution: Then we only have a single term in the sum, and

$$A_j = U(t, t_0), \quad (10.20)$$

the time evolution operator. For measurements, the  $A_j$  become the projections  $\pi_j$  that we encountered earlier. Even if this may look a bit complicated at the moment, this is a convenient way of looking at operations in quantum mechanics. But let us leave it at that.

#### 10.1.4 Markovian evolution and exponential decay

We end this subsection by looking at open quantum systems that are weakly coupled to their environment. This is a common situation: In the lab, one looks at coherent quantum dynamics. Still, there is a small influence of the environment that one cannot quite neglect. This often means that the systems' dynamics is only weakly disturbed by the environment. If this dynamics is "forgetful", so in a sense the noise only ever depends on the situation at a given time but not at the entire past (this can be made precise), then one calls the dynamics Markovian. The evolution equation – then called a *master equation* – is then of the following form:

**Markovian quantum noise:** The most general

$$\begin{aligned} \frac{\partial}{\partial t} \rho_S(t) &= -i[H_S, \rho_S(t)] \\ &+ \frac{1}{2} \sum_j \left( L_j^\dagger L_j \rho_S(t) + \rho_S(t) L_j^\dagger L_j - 2L_j \rho_S(t) L_j^\dagger \right). \end{aligned} \quad (10.21)$$

Here  $H_S$  is the Hamiltonian of the open system as such and the  $\{L_j\}$  are called *Lindblad operators*. They reflect the weak open system dynamics.



The first term

$$\frac{\partial}{\partial t}\rho_S(t) = -i[H_S, \rho_S(t)] \quad (10.22)$$

would just be the Schroedinger equation alone. But this is disturbed by the environment in the way described above, with the not necessarily Hermitian Lindblad operators capturing the influence of the environment. Such master equations are frequently encountered in quantum optics, atomic physics and condensed matter physics, for the obvious reasons that weakly open systems are ubiquitous in physics. In this picture, one still implicitly thinks of an environment  $E$ , needless to say, but this is no longer made explicit in the description: It is an evolution equation of the reduced state of the system alone.

Let us have a look at an example. Let us have a look at a simple harmonic oscillator which is weakly coupled to the environment in the following way: We take

$$H_S = \hbar\omega \left( a^\dagger a + \frac{1}{2} \right), \quad (10.23)$$

as well as a single Lindblad operator

$$L = \sqrt{c}a. \quad (10.24)$$

with some constant  $c > 0$ . This situation describes a single mode – for example the motional degree of freedom of an atom – weakly coupled to many other modes, say, of a radiation field surrounding the atom. How does the dynamics

$$\frac{\partial}{\partial t}\rho_S(t) = -i[H_S, \rho_S(t)] + \frac{1}{2} (L^\dagger L \rho_S(t) + \rho_S(t) L^\dagger L - 2L \rho_S(t) L^\dagger).$$

manifest itself? A calculation shows that if we say, start in

$$\rho_S(t_0) = |1\rangle\langle 1|, \quad (10.25)$$

so the motion is initially in the situation of “having one motional quanta excited” (so is in the first excited state of the harmonic oscillator), then the long time dynamics reads

$$\rho_S(t) = e^{-c(t-t_0)}|1\rangle\langle 1| + (1 - e^{-c(t-t_0)})|0\rangle\langle 0|. \quad (10.26)$$

That is to say, there is an exponential decay of the system into its ground state, due to the coupling with the environment. This happens with a rate  $c$ . Asymptotically,

$$\lim_{t \rightarrow \infty} \rho_S(t) = |0\rangle\langle 0|. \quad (10.27)$$

So for long times, the system will be in the ground state and will stay there – it has decayed exponentially.

How is this compatible with our view of quantum dynamics being governed by the Schroedinger evolution of the system and its environment? Well, this is perfectly compatible: The system  $S$  interacts with the environment, and

the excitation initially present in the system will be diluted to the many degrees of freedom of the environment. In the limit of a very large number of environment degrees of freedom, the excitation will never come back. This mechanism – in a slightly more sophisticated form – is at the basis of every exponential decay in quantum theory, in particular phenomena such as the famous alpha-decay.

## 10.2 Atoms and molecules

From now on more elliptic: There simply is neither time nor space to cover meaningfully the interesting but complex description of systems with several degrees of freedom, as they are encountered in the study of atoms and molecules, and even more so in the study of systems of condensed matter physics. We will leave it at a number of remarks, therefore.

### 10.2.1 Alkali atoms

To start with, we have discussed in great detail the hydrogen atom. But in fact, by doing that, we have done something slightly more general: In our discussion of the hydrogen atom, when considering the Coulomb potential, we can write

$$V(r) = -\frac{e_0 Z}{r}, \quad (10.28)$$

for a nucleus that now has  $1 < Z \in \mathbb{N}$ . All we have said is still valid, except that the entire problem is rescaled by the factor. So the energy levels now become the following:

**Energy levels of Alkali atoms:** We have for  $n = 1, 2, \dots$ ,

$$E_n = -\frac{mZ^2 e_0^4}{2\hbar^2} \frac{1}{n^2}. \quad (10.29)$$

So we still have the same  $1/n^2$  dependence, merely a change in the energy by the factor  $Z^2$ . This is the situation of electrons in Alkali atoms.

### 10.2.2 Helium atom

Of course, we will not get away so easily in the next simplest atom, the Helium atom. There is no way we can properly treat the Helium atom in this course, hence only an impression.

## 10.3 Complex quantum systems

So far, we have discussed quantum systems with few degrees of freedom only: Mostly one or two. Quite obviously, one often encounters the situation of having many degrees of freedom: after all, macroscopic bodies are consisting of  $10^{23}$  and way more constituents. To describe such quantum many-body systems is not easy at all. To add insult to injury, the constituents are usually also interacting, resulting in a fairly complicated situation. Quantum systems with such many degrees of freedom as usually encountered in the context of condensed matter systems are sometimes referred to as being complex quantum systems (although the term is used in several different ways).

### 10.3.1 Quantum many-body systems and condensed matter

It is far beyond the scope of the course to give an introduction to a quantum description of condensed matter physics: This is a large science in its own right, and even a single course would not be sufficient to give a comprehensive overview. Here, therefore, we will rather have a glimpse at what this is all about, using the methods that we have acquired so far. In fact, we will have a look at a single type of example, one that resembles the situation of interacting electrons in a solid body. This solid will have a lattice structure that is given, and the degree of freedom of the electrons can often to a good approximation be described by a spin degree of freedom sitting at a lattice site. More generally, such a situation gives rise to the concept of a lattice model.

**Lattice models:** Let  $G$  be some given lattice, with physical degrees of freedom being associated with the vertices of the lattice. This could be a spin degree of freedom associated with  $\mathcal{H} = \mathbb{C}^2$  or a harmonic oscillator  $\mathcal{H} = L^2(\mathbb{R})$ . A  $k$ -local Hamiltonian of a lattice model is a Hamiltonian of the form

$$H = \sum_j H_j, \quad (10.30)$$

where  $H_j$  is supported only on  $k$  different sites. Usually,  $k = 2$  and interactions are between nearest-neighbors only.

This is a common situation: Not everybody feels everybody in the lattice. But single degrees of freedom directly feel their nearest neighbors in the lattice. The situation is still very complex, as indirectly every constituent can not be treated separately from any other constituent in the lattice.

**Ground state:** The ground state of a model is the one that has the smallest energy, so is associated with the normalized state vector  $|\psi\rangle$  that minimizes

$$\langle\psi|H|\psi\rangle. \quad (10.31)$$

This is the state the system will be in at zero temperature.

### 10.3.2 Bose-Hubbard-Modell

We will now discuss some properties of a prominent example of this type: The Bose-Hubbard model. Its fermionic analogue, the Hubbard model, is even more prominent, where the fermionic degrees of freedom are associated with electronic ones. This goes beyond the scope of our course, however. We can understand the basics of its bosonic variant, however. Here, the single degrees of freedom are simple harmonic oscillators, as we have already encountered them in the course.

Such a situation can interestingly be created in the lab: By letting laser light counter-propagate, one can realize an optical standing wave. If one cools down single atoms, they feel a Stark shift, and they would like to sit in the potential minima of the laser light. Hence, they form a kind of “egg carton”, where the carton is the lattice and the eggs the single atoms. This is quite remarkable: In this way, one can simulate a condensed-matter system under controlled conditions in the lab. Let us now have a look how the resulting Hamiltonian looks like. What we call “bosons” here are the excitations of the harmonic oscillator. So  $|0\rangle$  reflects no boson at all,  $|1\rangle$  one boson, and  $|k\rangle$   $k$  bosons at a site.

**Hamiltonian of the Bose-Hubbard model:** In one dimension, we have for  $N$  lattice sites

$$H = -J \sum_{j=1}^N (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j) + \frac{U}{2} \sum_{j=1}^N n_j(n_j - 1) - \mu \sum_{j=1}^N n_j, \quad (10.32)$$

where

$$n_j = b_j^\dagger b_j. \quad (10.33)$$

The index  $j$  denotes individual sites here, so  $b_j$  is the annihilation operator of the  $j$ -th harmonic oscillator sitting at lattice site  $j$ .

Let us carefully interpret each term.

- Each term

$$b_j^\dagger b_{j+1} \quad (10.34)$$

gives rise to a tunneling, a hopping of a boson. A boson tunnels through the potential barrier and emerges at a neighboring site. Formally argued,  $b_{j+1}$  annihilates a boson at site  $j + 1$  and  $b_j^\dagger$  creates a new one at site  $j$ . The rate of this process is governed by the prefactor  $J$ .

- On each site, there can be many bosons – surely more than one. They will then interact. This is reflected by the interaction term

$$n_j(n_j - 1). \quad (10.35)$$

Again, we have a prefactor  $U > 0$  that governs the strength of this interaction.

- Finally,  $\mu$  is what is called a chemical potential. For practical purposes, this is just some offset potential of the harmonic oscillator.

This model is an interesting model of strongly correlated atoms and has many if not most features that condensed matter quantum many-body systems have. In particular, it exhibits what is called a second order quantum phase transition. Let us first define what a phase transition is. This is a phase transition that is not driven by temperature: It occurs at zero temperature! Let us properly define what a phase transition is.

**Quantum phase transition:** For a family of Hamiltonians,

$$H(g) = H_0 + gV \quad (10.36)$$

one encounters a quantum phase transition at some point  $g_0$  if the ground state energy,

$$\min \langle \psi | H(g) | \psi \rangle \quad (10.37)$$

is non-analytic in  $g_0$ .

There are in fact two phases, where  $U$  takes the role of  $g$  and the other values  $J$  and  $\mu$  are held fixed.

- One is called the *superfluid phase*. This is a phase that is delocalized: The ground state vector will be highly entangled over large regions of the lattice.
- The other phase is the Mott insulator. In the deep Mott phase, the ground state is very simple: Its state vector is a product vector

$$|\psi\rangle = |k, k, \dots, k\rangle. \quad (10.38)$$

That is to say, in such a situation we have exactly  $k$  bosons sitting there per lattice site, and no correlations and entanglement whatsoever.

### 10.3.3 Mean field theory

Unfortunately, this model is too difficult to be treated exactly. This is not only a problem of our course, but it is indeed not analytically solvable. There are strong methods to numerically solve it up to machine precision, however, and this is an exciting type of research in its own right. This is beyond the scope of this course, however. It is clear where the difficulty is: Even if we could describe few sites exactly, the dimension of the Hilbert space grows exponentially with the system size, rendering naive approaches doomed to failure.

A simple theory, however, already gives qualitatively the correct phase diagram. In high dimensions, this is even for good reasons a good ansatz. The main idea is rooted in the fact that one can describe the influence of the neighbors by a mean classical influence, in a mean field fashion. We define the so-called *superfluid parameter*

$$\psi = \langle b_j^\dagger \rangle = \langle b_j \rangle. \quad (10.39)$$

Since we assume the system to be translationally invariant, this number will indeed not depend on  $j$ . It takes the role of an *order parameter* in the sense of the theory of phase transitions. The ad hoc replacement of mean field theory is to replace the Hamiltonian for neighbors  $i, j$  by

$$\begin{aligned} b_i^\dagger b_j &= \langle b_i^\dagger \rangle b_j + b_i^\dagger \langle b_j \rangle - \langle b_i^\dagger \rangle \langle b_j \rangle \\ &= \psi(b_i^\dagger + b_i) - \psi^2. \end{aligned} \quad (10.40)$$

This is a meaningful, but uncontrolled approximation. In this way, we get the Hamiltonian

$$H_{\text{MF}} = -J2\psi \sum_j (b_j + b_j^\dagger) + 2J\psi^2 N \frac{U}{2} \sum_j n_j(n_j - 1) - \mu \sum_j n_j. \quad (10.41)$$

Here  $N$  is the total number of bosons. That is to say, for this Hamiltonian, we have again the simple form of product terms. For a given  $\psi$  the model is simple to solve: The ground state is just again a product state. Let us choose different units to simplify the situation somewhat:

$$\bar{U} = U/(2J), \quad \bar{\mu} = \mu/(2J). \quad (10.42)$$

In these units, we get for each lattice site

$$H_{\text{MF},j} = -\psi(b_j + b_j^\dagger) + \psi^2 + \frac{\bar{U}}{2} n_j(n_j - 1) - \bar{\mu} \sum_j n_j. \quad (10.43)$$

We can also suppress the index  $j$ , as we have to solve the same problem at each site anyway.

In the so-called Landau theory of phase transitions one progresses as follows: We write

$$H_{\text{MF}} = H_{\text{MF}}^{(0)} + \psi V, \quad (10.44)$$

where now

$$H_{\text{MF}}^{(0)} = \frac{\bar{U}}{2} n_j (n_j - 1) - \bar{\mu} \sum_j n_j + \psi^2, \quad (10.45)$$

$$V = -(b_j + b_j^\dagger). \quad (10.46)$$

If we denote the energy of the unperturbed operator with exactly  $k$  particles by  $E_k^{(0)}$  then the ground state energy of the Hamiltonian is

$$E^{(0)} = \min_k E_k^{(0)}. \quad (10.47)$$

In this way, we find

$$E_k^{(0)} = \begin{cases} 0 & \text{if } \bar{\mu} < 0, \\ \bar{U}k(k-1) - \bar{\mu}k & \text{if } \bar{U}(k-1) < \bar{\mu} < \bar{U}k. \end{cases} \quad (10.48)$$

This is the unperturbed energy. The next term we get in perturbation theory as we learned it earlier in this course. We get in second order the expression

$$E_k^{(2)} = \psi^2 \sum_{n \neq k} \frac{|\langle \psi_k | V | \psi_n \rangle|^2}{E_k^{(0)} - E_n^{(0)}} \quad (10.49)$$

where  $|\psi_n\rangle$  is the unperturbed state vector with exactly  $n$  particles. Therefore

$$E_k^{(2)} = \frac{k}{\bar{U}(k-1) - \bar{\mu}} + \frac{k+1}{\bar{\mu} - \bar{U}k}. \quad (10.50)$$

In the Landau theory of phase transitions of second order, one writes the ground state energies hence in powers of  $\psi$  as follows:

**Energy function in Landau theory:** In orders of  $\psi$  we have

$$E_k(\psi) = a_0 + a_2 \psi^2 + O(\psi^4). \quad (10.51)$$

We now minimize this expression as a function of  $\psi$ . It is clear that if

- $a_2 > 0$ , then also  $\psi = 0$ . In turn,
- $\psi \neq 0$  for  $a_2 < 0$ .

Therefore,  $a_2 = 0$  denotes a phase transition. The solutions of

$$a_2 = \frac{k}{\bar{U}(k-1) - \bar{\mu}} + \frac{k+1}{\bar{\mu} - \bar{U}k} + 1 = 0 \quad (10.52)$$

give

$$\mu_{\pm} = \frac{1}{2}(\bar{U}(2k-1) - 1) \pm \frac{1}{2}(\bar{U}^2 - 2\bar{U}(2k+1) + 1)^{1/2}, \quad (10.53)$$

where  $\pm$  are the upper and lower halves of the Mott lobe. We hence have found a way of determining the phase boundaries of the Bose-Hubbard model. Of course, this is only an approximate method, in that we have neglected one of the main features of quantum many-body systems: intricate quantum correlations between the constituents. Still, it gives rise to a fairly good approximation (and what is more, mean field theory can be made entirely rigorously).