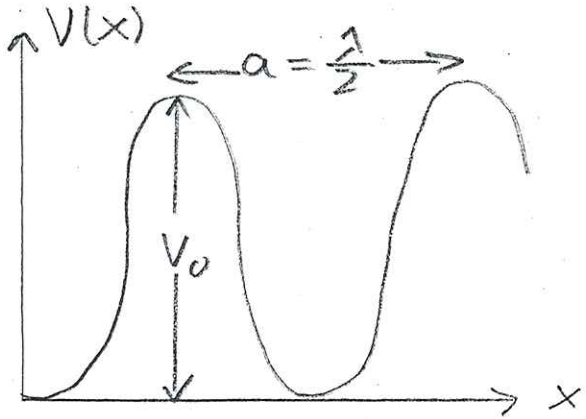
## 1. Phenomenology:

An optical lattice represents a periodic potential which is generated by a certain arrangement of laser fields. Usually, one considers a cubic optical lattice which is generated by three orthogonally aligned pairs of lasers. Thereby each laser pair generates a standing electromagnetic wave. Bosons in such an optical lattice feel a periodic potential due to the Stark effect which is of the form

$$V(\vec{x}) = V_0 \sum_{k=1}^{3} \sin^2\left(\frac{\pi}{a} x_k\right) \qquad (1)$$




Here the lattice constant $a = \lambda/2$ is given by the wave length of the laser light and $V_0$ denotes the laser strength. The absorption or the emission of a photon due to the Stark effect leads to the recoil energy

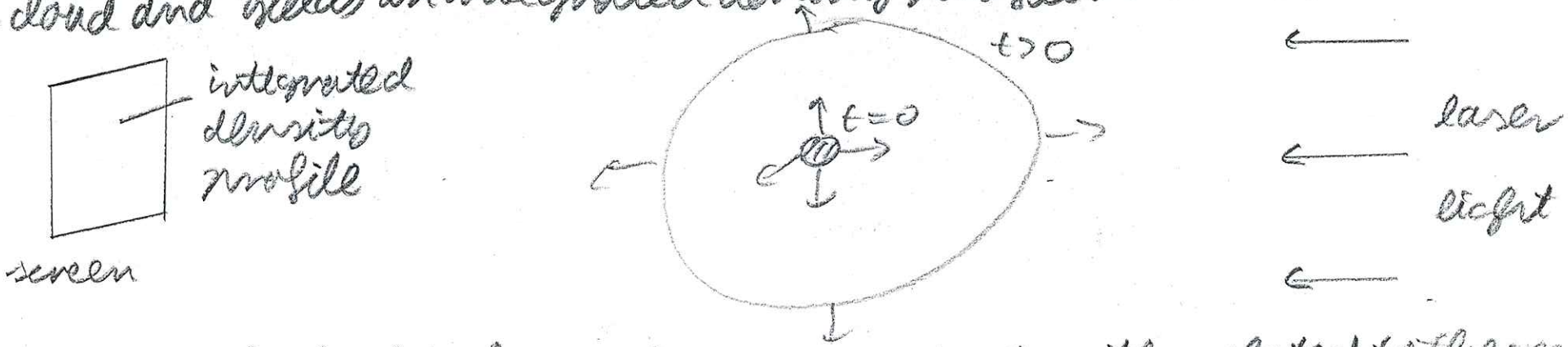
$$E_R = \frac{\hbar^2 \pi^2}{2 M a^2} \qquad (2)$$

In a typical experiment the wave length is $\lambda = 1030\,nm$, thus the lattice constant is $a = 515\,nm$, yielding for $^{87}Rb$ atoms the recoil energy $E_R = 1{,}43 \cdot 10^{-30}\,J$ as the characteristic energy scale of the system. All energies as, for instance the laser strength $V_0$, are measured in units of the recoil energy.

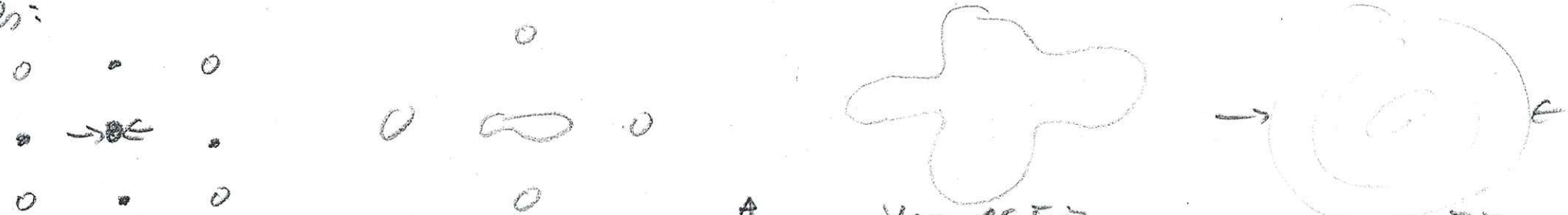
Experimentally, an additional magnetic trap is used which generates a harmonic potential. This yields an effective distortion of the minima of (1) in such a way that only the potential minima in the center are oc-

cupied by bosons. Thus, the additional harmonic potential has the purpose to confine the system. For the sake of simplicity we will neglect in the following the additional magnetic trap and restrict ourselves to study the properties of a homogeneous Bose gas in an optical lattice.

Basically, this system is too small to be directly observed. Therefore, one switches off both the magnetic potential and the optical lattice, so that the cloud expands. From the side an additional laser shines through the expanding cloud and yields an integrated density profile on a screen:




Such a time-of-flight absorption picture is directly related to the momentum distribution of bosons in the trap when the potentials are switched off. Different potential depths $V_0$ yield different absorption pictures:



$V_0 = 8 E_R$ small lattice depth superfluid phase

$V_0 = 14 E_R$

$V_0 = 16 E_R$ quantum phase transition at around $V_0 = 15 E_R$

$V_0 = 30 E_R$ large lattice depth Mott insulator phase

A small lattice depth yields a small uncertainty of momenta, thus the spatial uncertainty is huge. This means that the bosons are coherently delocalised over the whole lattice, forming a superfluid. The characteristic length scale is given by the oscillator length of the overall harmonic trap. In the opposite case of a large lattice depth the resulting uncertainty of momenta is huge, which corresponds to a small spatial uncertainty. This means that the bosons are localised in one of the respective minima and can no longer tunnel to the neighboring minima, forming a Mott insulator. The characteristic length scale is now given by the oscillator length of one potential minimum.

The location of the quantum phase transition can be more precisely determined from slightly tilting the optical lattice. The Mott insulator phase is characterised by gapped excitations, thus a slight tilt does not lead to a motion of the bosons. Contrary to that the superfluid phase is characterised by a gapless Goldstone mode, thus a slight tilt initiates a motion of the bosons.

## 2. Bose-Hubbard Hamiltonian:

Starting point for the description of bosons in an optical lattice in the grand-canonical ensemble is the following second-quantised Hamiltonian:

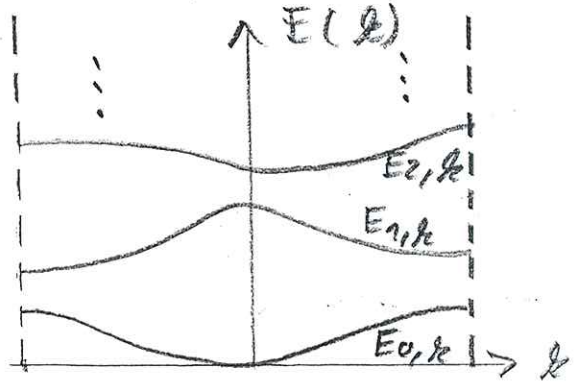
$$\hat{H} = \int d^3x \left\{ \hat{\psi}^+(\vec{x}) \left[ -\frac{\hbar^2}{2m}\Delta + V(\vec{x}) - \tilde{\mu} \right] \hat{\psi}(\vec{x}) + \frac{g}{2} \hat{\psi}^+(\vec{x}) \hat{\psi}^+(\vec{x}) \hat{\psi}(\vec{x}) \hat{\psi}(\vec{x}) \right\} \tag{3}$$

Here $\hat{\psi}^+(\vec{x})$, $\hat{\psi}(\vec{x})$ denote the standard field operators which create or annihilate a boson at space point $\vec{x}$:

$$[\hat{\psi}(\vec{x}), \hat{\psi}(\vec{x}')]_- = [\hat{\psi}^+(\vec{x}), \hat{\psi}^+(\vec{x}')]_- = 0, \quad [\hat{\psi}(\vec{x}), \hat{\psi}^+(\vec{x}')]_- = \delta(\vec{x} - \vec{x}') \tag{4}$$

In the following we will expand the field operators with respect to a basis which is defined from solving the corresponding one-particle problem:

$$\left\{ -\frac{\hbar^2}{2m}\Delta + V(\vec{x}) \right\} \phi_{n,\vec{k}}(\vec{x}) = E_{n,\vec{k}}\, \phi_{n,\vec{k}}(\vec{x}) \tag{5}$$




Here $\vec{k}$ denotes wave vectors within the first Brillouin zone and $n$ enumerates the respective Bloch bands. Due to the Bloch theorem the Bloch waves

$$\phi_{n,\vec{k}}(\vec{x}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\vec{x}}\, u_{n,\vec{k}}(\vec{x}) \tag{6}$$

are plane waves with amplitudes $u_{n,\vec{k}}(\vec{x})$ which inherit the symmetry of the optical lattice. They fulfill the orthonormality

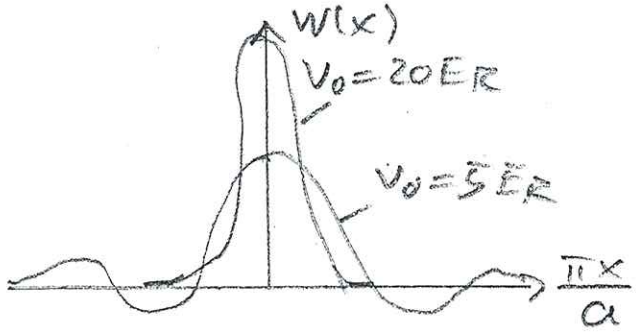
$$\int d^3x\, \phi^*_{n,\vec{k}}(\vec{x})\, \phi_{n',\vec{k}'}(\vec{x}) = \delta_{n,n'}\, \delta_{\vec{k},\vec{k}'} \tag{7}$$

and the completeness relation

$$\sum_n \sum_{\vec{k}} \phi^*_{n,\vec{k}}(\vec{x})\, \phi_{n,\vec{k}}(\vec{x}') = \delta(\vec{x} - \vec{x}') \tag{8}$$

superimposing Bloch waves, which are localised in momentum space, yields Wannier functions

$$w_n(\vec{x}-\vec{x}_i) = \frac{1}{\sqrt{N_s}} \sum_{\vec{k}} e^{-i\vec{k}\vec{x}_i} \phi_{n,\vec{k}}(\vec{x}) \qquad (9)$$




which are localised in space. Also the Wannier functions fulfill the orthonormality

$$\int d^3x\, w_n^*(\vec{x}-\vec{x}_i)\, w_{n'}(\vec{x}-\vec{x}_{i'}) = \delta_{n,n'}\,\delta_{i,i'} \qquad (10)$$

and the completeness relation

$$\sum_n \sum_i w_n^*(\vec{x}-\vec{x}_i)\, w_n(\vec{x}'-\vec{x}_i) = \delta(\vec{x}-\vec{x}') \qquad (11)$$

For low enough temperatures we can assume that only the lowest Bloch band is filled. Thus, the field operators can be expanded in the corresponding one-particle Wannier functions $w_0(\vec{x}-\vec{x}_i)$ which have the property of being localised at site $i$:

$$\hat{\psi}(\vec{x}) = \sum_i \hat{a}_i\, w_0(\vec{x}-\vec{x}_i), \qquad \hat{\psi}^+(\vec{x}) = \sum_i \hat{a}_i^+\, w_0^*(\vec{x}-\vec{x}_i) \qquad (12)$$

The expansion operators $\hat{a}_i^+, \hat{a}_i$ then fulfill the canonical commutator relations

$$[\hat{a}_i, \hat{a}_{i'}]_- = [\hat{a}_i^+, \hat{a}_{i'}^+]_- = 0, \quad [\hat{a}_i, \hat{a}_{i'}^+]_- = \delta_{i,i'} \qquad (13)$$

Therefore, they describe the process of creating or annihilitating a boson in a Wannier state of the lowest Bloch band which is localised at site $i$. Inserting (12) in (3) and considering only the dominant terms yields the single-band Bose-Hubbard-Hamiltonian

$$\hat{H}_{BH} = -J \sum_{\langle i,j\rangle} \hat{a}_i^+ \hat{a}_j + \sum_i \left\{ \frac{U}{2} \hat{n}_i(\hat{n}_i - 1) - \mu \hat{n}_i \right\}; \quad \hat{n}_i = \hat{a}_i^+ \hat{a}_i \qquad (14)$$

The original chemical potential $\tilde{\mu}$ becomes shifted:

$$\mu = \tilde{\mu} + \int d^3x \, w_0^*(\vec{x}-\vec{x}_i) \left\{ -\frac{\hbar^2}{2m}\Delta + V(\vec{x}) \right\} w_0(\vec{x}-\vec{x}_i) \tag{15}$$

The first term in (14) describes the tunneling of a boson between two neighbouring sites $i$ and $j$. Its energy scale is characterized by the tunneling or hopping matrix element

$$J = -\int d^3x \, w_0^*(\vec{x}-\vec{x}_i) \left\{ -\frac{\hbar^2}{2m}\Delta + V(\vec{x}) \right\} w_0(\vec{x}-\vec{x}_j) \tag{16}$$

If $J$ is large enough then it is energetically favourable that the bosons tunnel from one lattice site to another. The second term in (14) describes the repulsive on-site interaction between bosons at one single site. If there are $n$ bosons at a certain site, then there exist, indeed, $n(n-1)/2$ different possibilities for a two-particle interaction. Its energy scale is set by the on-site energy

$$U = g \int d^3x \, |w_0(\vec{x}-\vec{x}_i)|^4 \tag{17}$$

where the coupling strength

$$g = \frac{4\pi\hbar^2}{M} a_s \tag{18}$$

is related to the s-wave scattering length $a_s$. If $U$ is large enough, then it is energetically unfavourable that many bosons stay in one and the same lattice site. Thus, the physical properties of the Bose-Hubbard model depend on the size of both energy scales $J$ and $U$. They strongly change with varying lattice depth $V_0$. Whereas $J$ decreases exponentially with increasing $V_0$, $U$ increases algebraically

$$J = E_R \frac{4}{\sqrt{\pi}} \left(\frac{V_0}{E_R}\right)^{\frac{3}{4}} e^{-2\sqrt{\frac{V_0}{E_R}}} \tag{19}$$

$$U = E_R \sqrt{8\pi} \left(\frac{V_0}{E_R}\right)^{\frac{3}{4}} \frac{a_s}{a} \tag{20}$$

## 3. Mean-Field Hamiltonian:

We observe from the Bose-Hubbard-Hamiltonian (14) that the interaction term is local and diagonal in the occupation number representation. In contrast to that the hopping term in (14) is non-local, as it couples neighbouring lattice sites and non-diagonal in the occupation number representation. Therefore, the Bose-Hubbard Hamiltonian (14) is not analytically solvable and one has to resort to an approximative treatment.

Within the mean-field approach the non-local Bose-Hubbard Hamiltonian (14) is approximated by a local one. To this end we assume that the creation and annihilation operators in the hopping term are decomposed into their thermal expectation and small fluctuations around them:

$$\hat{a}_i = \langle \hat{a}_i \rangle + \delta \hat{a}_i \,, \quad \hat{a}_i^+ = \langle \hat{a}_i^+ \rangle + \delta \hat{a}_i^+ \tag{21}$$

Neglecting contributions which are quadratic in the small fluctuations

$$0 \approx \delta \hat{a}_i^+ \delta \hat{a}_j = (\hat{a}_i^+ - \langle \hat{a}_i^+ \rangle)(\hat{a}_j - \langle \hat{a}_j \rangle) \tag{22}$$

we obtain the following approximation

$$\hat{a}_i^+ \hat{a}_j \approx \langle \hat{a}_i^+ \rangle \hat{a}_j + \hat{a}_i^+ \langle \hat{a}_j \rangle - \langle \hat{a}_i^+ \rangle \langle \hat{a}_j \rangle \tag{23}$$

Due to translational invariance we expect that the thermal expectations $\langle \hat{a}_i^+ \rangle$, $\langle \hat{a}_i \rangle$ do not depend on the site $i$. This defines the Landau order parameter

$$\psi^* = \langle \hat{a}_i^+ \rangle \,, \quad \psi = \langle \hat{a}_i \rangle \tag{24}$$

Inserting the mean-field approximation (23) with (24) into the Bose-Hubbard-Hamiltonian (14) yields

$$H_{MF} = \sum_i \{ -zJ(\psi^* \hat{a}_i + \hat{a}_i^+ \psi - \psi^* \psi) + \frac{U}{2} \hat{n}_i(\hat{n}_i - 1) - \mu \hat{n}_i \} \tag{25}$$

here $z = 6$ denotes the coordination number of a three-dimensional cubic lattice.

Now we show that the Landau order parameters defined by (24) correspond to an extremisation of the grand-canonical free energy

$$F_{MF} = -\frac{1}{\beta} \ln Z_{MF} \tag{26}$$

To this end we define the grand-canonical partition function

$$Z_{MF} = \mathrm{Tr}\, e^{-\beta \hat{H}_{MF}} \tag{27}$$

where the trace is suitably defined with the occupation number basis

$$\mathrm{Tr}\, \bullet = \sum_i \sum_{n_i=0}^{\infty} \langle \ldots, n_i, \ldots | \bullet | \ldots, n_i, \ldots \rangle \tag{28}$$

At first the extremisation of (26) yields with (27)

$$\frac{\partial F_{MF}}{\partial \psi^*} = \frac{-1}{\beta} \frac{1}{Z_{MF}} \mathrm{Tr} \left\{ \frac{\partial}{\partial \psi^*} e^{-\beta \hat{H}_{MF}} \right\} = 0 \tag{29}$$

As the operators $\hat{H}_{MF}$ and $\partial \hat{H}_{MF} / \partial \psi^* = -z J \sum_i (\hat{a}_i - \psi)$ do not commute, we have

$$\frac{\partial}{\partial \psi^*} e^{-\beta \hat{H}_{MF}} \neq -\beta \frac{\partial \hat{H}_{MF}}{\partial \psi^*} e^{-\beta \hat{H}_{MF}} \tag{30}$$

but one can show that with the trace we obtain

$$\mathrm{Tr} \left\{ \frac{\partial}{\partial \psi^*} e^{-\beta \hat{H}_{MF}} \right\} = -\beta\, \mathrm{Tr} \left\{ \frac{\partial \hat{H}_{MF}}{\partial \psi^*} e^{-\beta \hat{H}_{MF}} \right\} \tag{31}$$

Thus, we conclude

$$\frac{1}{Z_{MF}} \mathrm{Tr} \left\{ \frac{\partial \hat{H}_{MF}}{\partial \psi^*} e^{-\beta \hat{H}_{MF}} \right\} = \frac{-zJ}{Z_{MF}} \sum_i \mathrm{Tr} \left\{ (\hat{a}_i - \psi) e^{-\beta \hat{H}_{MF}} \right\} \stackrel{!}{=} 0 \tag{32}$$

due to the definition of the thermal expectation value

$$\langle \bullet \rangle = \frac{1}{Z_{MF}} \mathrm{Tr} \left\{ \bullet\, e^{-\beta \hat{H}_{MF}} \right\} \tag{33}$$

Condition (32) reduces to

$$\sum_i \left( \langle \hat{a}_i \rangle - \psi \right) = 0 \tag{34}$$

Due to translational invariance the thermal expectation value $\langle \hat{a}_i \rangle$ does not depend on the site $i$, so (34) simplifies further

$$N_s \left( \langle \hat{a}_i \rangle - \psi \right) = 0 \tag{35}$$

where $N_s$ denotes the number of lattice sites. Thus, (35) coincides with the self-consistency condition (24).

We remark that the mean-field Hamiltonian (25) is local. Therefore, we can restrict ourselves without loss of generality to study a single site $i$ and omit the site index in the following. With this we end up with the single-site mean-field Hamiltonian

$$\hat{H} = -zJ \left( \psi^* \hat{a} + \hat{a}^+ \psi - \psi^* \psi \right) + \frac{U}{2} \hat{n}(\hat{n}-1) - \mu \hat{n} \, ; \; \hat{n} = \hat{a}^+ \hat{a} \tag{36}$$

It decomposes naturally according to

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \tag{37}$$

where the first term is diagonal in the occupation number representation and therefore can be solved exactly

$$\hat{H}_0 = \frac{U}{2} \hat{n}(\hat{n}-1) - \mu \hat{n} \tag{38}$$

whereas the second term is non-diagonal in the occupation number representation and has therefore to be treated perturbatively:

$$\hat{H}_1 = -zJ \left( \psi^* \hat{a} + \hat{a}^+ \psi - \psi^* \psi \right) \tag{39}$$

## 4. Dirac Interaction Picture:

Hamiltonian: $\hat{H}(\tau) = \hat{H}_0 + \hat{H}_1(\tau)$

**Schrödinger picture:**

$$-\hbar \frac{\partial}{\partial \tau} \hat{O} = 0$$

$$-\hbar \frac{\partial}{\partial \tau} |\psi(\tau)\rangle = \hat{H}(\tau)|\psi(\tau)\rangle$$

$$|\psi(\tau)\rangle = \hat{U}(\tau,\tau_0)|\psi(\tau_0)\rangle$$

$$\hat{U}(\tau,\tau_0) = \hat{T}\, e^{-\frac{1}{\hbar}\int_{\tau_0}^{\tau} d\tau' \hat{H}(\tau')}$$

$$= 1 + \sum_{n=1}^{\infty} \frac{1}{n!}\left(\frac{-1}{\hbar}\right)^n \int_{\tau_0}^{\tau} d\tau_1 \cdots \int_{\tau_0}^{\tau} d\tau_n \cdot \hat{T}\left[\hat{H}(\tau_1)\hat{H}(\tau_2)\cdots\hat{H}(\tau_n)\right]$$

$$\hat{O}_D(\tau) = e^{\frac{1}{\hbar}\hat{H}_0\tau}\, \hat{O}\, e^{-\frac{1}{\hbar}\hat{H}_0\tau}$$

$$|\psi_D(\tau)\rangle = e^{\frac{1}{\hbar}\hat{H}_0\tau}|\psi\rangle$$

$$\hat{U}_D(\tau,\tau_0) = e^{\frac{1}{\hbar}\hat{H}_0\tau}\, \hat{U}(\tau,\tau_0)\, e^{-\frac{1}{\hbar}\hat{H}_0\tau_0} \quad (40)$$

**Dirac interaction picture:**

$$-\hbar \frac{\partial}{\partial \tau} \hat{O}_D(\tau) = \left[\hat{O}_D(\tau), \hat{H}_{0D}(\tau)\right]_-$$

$$-\hbar \frac{\partial}{\partial \tau} |\psi_D(\tau)\rangle = \hat{H}_{1D}(\tau)|\psi_D(\tau)\rangle$$

$$|\psi_D(\tau)\rangle = \hat{U}_D(\tau,\tau_0)|\psi_D(\tau_0)\rangle$$

$$\hat{U}_D(\tau,\tau_0) = \hat{T}\, e^{-\frac{1}{\hbar}\int_{\tau_0}^{\tau} d\tau' \hat{H}_{1D}(\tau')} \quad (41)$$

$$= 1 + \sum_{n=1}^{\infty} \frac{1}{n!}\left(\frac{-1}{\hbar}\right)^n \int_{\tau_0}^{\tau} d\tau_1 \int_{\tau_0}^{\tau} d\tau_2 \cdots \int_{\tau_0}^{\tau} d\tau_n \cdot \hat{T}\left[\hat{H}_{1D}(\tau_1)\hat{H}_{1D}(\tau_2)\cdots\hat{H}_{1D}(\tau_n)\right] \quad (42)$$

## 5. Partition Function:

Definition of partition function in Schrödinger picture:

$$Z = \mathrm{Tr}\left\{ \hat{U}(\hbar\beta, 0) \right\} \tag{43}$$

Now we switch over to Dirac interaction picture via the manipulation

$$Z = \mathrm{Tr}\left\{ e^{-\beta \hat{H}_0} e^{\frac{1}{\hbar}\hat{H}_0 \hbar\beta} \hat{U}(\hbar\beta, 0)\, e^{-\frac{1}{\hbar}\hat{H}_0 \cdot 0} \right\} \overset{(40)}{=} \mathrm{Tr}\left\{ e^{-\beta \hat{H}_0} \hat{U}_D(\hbar\beta, 0) \right\} \tag{44}$$

with the unperturbed partition function

$$Z^{(0)} = \mathrm{Tr}\, e^{-\beta \hat{H}_0} \tag{45}$$

and the expectation value with respect to the unperturbed hamiltonian

$$\langle \cdot \rangle^{(0)} = \frac{1}{Z^{(0)}} \mathrm{Tr}\left\{ e^{-\beta \hat{H}_0} \cdot \right\} \tag{46}$$

we can rewrite (44) according to

$$Z = Z^{(0)} \langle \hat{U}_D(\hbar\beta, 0) \rangle^{(0)} \tag{47}$$

For general considerations we insert (41) in (47)

$$Z = Z^{(0)} \left\langle \hat{T}\, e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau' \hat{H}_{1D}(\tau')} \right\rangle^{(0)} \tag{48}$$

For practical considerations it is more useful to insert (42) in (47):

$$Z = Z^{(0)} \left\{ 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{-1}{\hbar}\right)^n \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \cdots \int_0^{\hbar\beta} d\tau_n \left\langle \hat{T}\left[ \hat{H}_{1D}(\tau_1) \hat{H}_{1D}(\tau_2) \cdots \hat{H}_{1D}(\tau_n) \right] \right\rangle^{(0)} \right. \tag{49}$$

## 6. Quantum Phase Diagram:

Now we come back to the decomposition (37)–(39) of the mean-field Hamiltonian and treat the term (39), which is non-diagonal in the occupation number representation, as being small. This is justified in the vicinity of the quantum phase transition as there the order parameter $\psi$ is expected to be small. Thus, we transform (39) to the Dirac interaction picture

$$\hat{H}_{1D}(\tau) = -z J \left\{ \psi^* \hat{a}_D(\tau) + \hat{a}_D^+(\tau) \psi - \psi^* \psi \right\} \tag{50}$$

and use (49) to evaluate the partition function perturbatively. With this we obtain the free energy

$$F = -\frac{1}{\beta} \ln Z \tag{51}$$

a Landau expansion with respect to the order parameter $\psi$

$$F = a_0(T) + a_2(T)|\psi|^2 + a_4(T)|\psi|^4 + \dots \tag{52}$$

Note that only those terms appear in (52) which reflect the global $U(1)$-symmetry of the mean-field Hamiltonian (36). The first two Landau coefficients in (52) read explicitly

$$a_0(T) = -\frac{1}{\beta} \ln \sum_{n=0}^{\infty} e^{-\beta E_n} \tag{53}$$

$$a_2(T) = z J - z^2 J^2 \frac{\sum_{n=0}^{\infty} \frac{U+\mu}{(\mu - Un)[U(n-1)-\mu]} e^{-\beta E_n}}{\sum_{n=0}^{\infty} e^{-\beta E_n}} \tag{54}$$

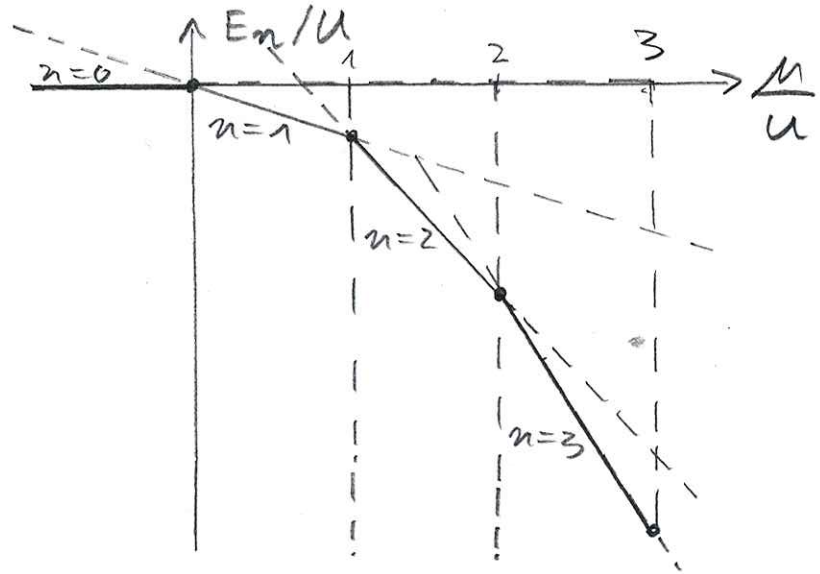
with the eigenvalues

$$E_n = \frac{U}{2} n(n-1) - \mu n \tag{55}$$

of the unperturbed Hamiltonian.

At first we discuss the zero-temperature limit. In case of $T \downarrow 0$ the Landau coefficient (53) converges to the ground-state energy of the Mott phase which is characterised by the condition $\psi = 0$:

$$a_0(T=0) = \min_n E_n \qquad (56)$$




A graphical evaluation of (56) yields the result

$$a_0(T=0) = E_n \text{ with } n-1 < \frac{\mu}{U} < n \qquad (57)$$

Thus, the Mott phase is characterised by a fixed number $n$ of bosons per lattice site, whereas the chemical potential can vary within a finite interval. Correspondingly we obtain from (54)

$$a_2(T=0) = z\,]-z^2[\,^2 \frac{U+\mu}{(\mu-Un)[U(n-1)-\mu]} \qquad (58)$$

so the Landau expansion converges for $T \downarrow 0$ to

$$E = a_0(T=0) + a_2(T=0)\,\psi^*\psi + a_4(T=0)\,\psi^{*2}\psi^2 + \dots \qquad (59)$$

The Landau order parameter is fixed by extremizing the ground-state energy:

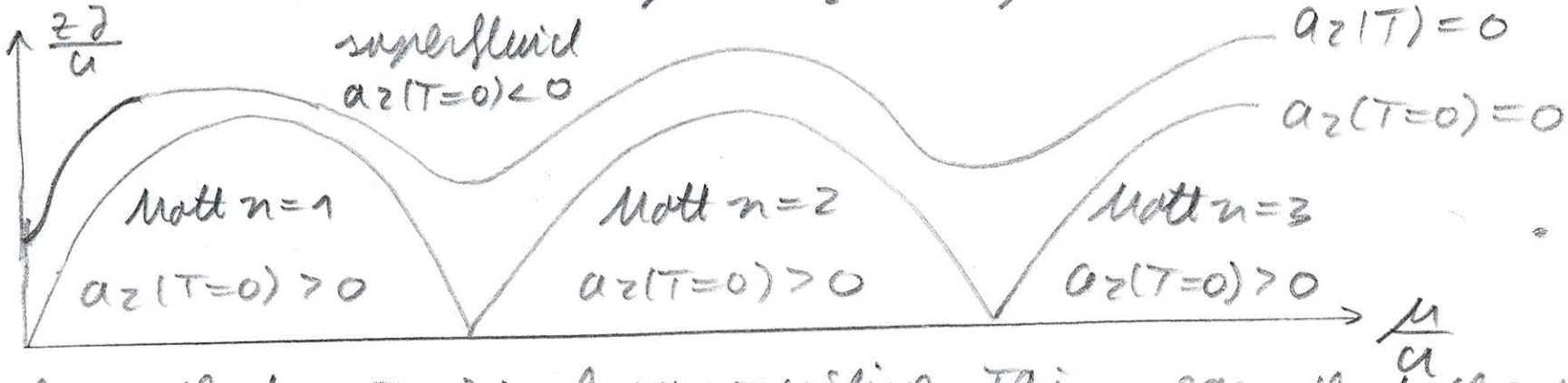
$$\frac{\partial E}{\partial \psi^*} = \psi \cdot \{ a_2(T=0) + 2a_4(T=0)\,\psi^*\psi + \dots \} = 0 \qquad (60)$$

This algebraic equation has two possible solutions:

- $\psi = 0 \;\hat{=}\;$ Mott phase
- $\psi \neq 0 \;\hat{=}\;$ superfluid phase $\Rightarrow \psi^*\psi = -\dfrac{a_2(T=0)}{2a_4(T=0)}$ (61)

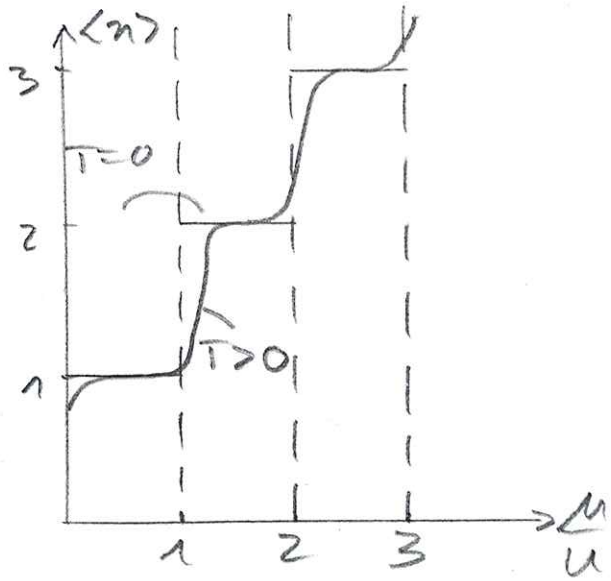
We read off from (61) that the phase boundary follows from the vanishing of the second Landau coefficient:

$$a_2(T=0)=0 \overset{(58)}{\Longrightarrow} zJ = z^2 J^2 \frac{U+\mu}{(\mu-Un)\left[U(n-1)-\mu\right]} \qquad (62)$$




It can be shown that $a_4(T=0)$ is always positive. This means that the superfluid phase occurs for $a_2(T=0)<0$ and the Mott phase is characterised by $a_2(T=0)>0$. Furthermore, we conclude from $a_4(T=0)>0$ that the phase transition between Mott insulator and superfluid is of second order.

At finite temperatures the condition $a_4(T)>0$ remains, so that we still have a second-order phase transition. However, the sharp distinction between the Mott lobes diminishes. In particular, the Mott phase is no longer characterised by an integer number of bosons per lattice site. Thermal fluctuations destroy quantum coherence. Therefore, the region of the superfluid phase decreases in the phase diagram, whereas the region of the Mott phase increases.



## 7. Ginzburg-Landau Theory:

Consider as a concrete example the Bose-Hubbard Hamiltonian as the unperturbed Hamiltonian

$$\hat{H}_0 \equiv \hat{H}_{BH} = -J \sum_{\langle i,j \rangle} \hat{a}_i^+ \hat{a}_j + \sum_i \left\{ \frac{U}{2} \hat{n}_i(\hat{n}_i - 1) - \mu \hat{n}_i \right\} ; \hat{n}_i = \hat{a}_i^+ \hat{a}_i \quad (62)$$

The perturbative part of the Hamiltonian is chosen to be given by artificial source terms in order to break artificially U(1) symmetry

$$\hat{H}_1(\tau) \equiv \hat{H}_S(\tau) = \sum_i \left\{ j_i(\tau) \hat{a}_i^+ + j_i^*(\tau) \hat{a}_i \right\} \quad (63)$$

Switching to the Dirac interaction picture yields

$$\hat{H}_{1D}(\tau) = \sum_i \left\{ j_i(\tau) \hat{a}_{iD}^+(\tau) + j_i^*(\tau) \hat{a}_{iD}(\tau) \right\} \quad (64)$$

With this the partition function (48) becomes a generating functional

$$Z[j^*, j] = Z^{(0)} \left\langle \hat{T} \exp\left\{ -\frac{1}{\hbar} \sum_i \int_0^{\hbar\beta} d\tau \left[ j_i(\tau) \hat{a}_{iD}^+(\tau) + j_i^*(\tau) \hat{a}_{iD}(\tau) \right] \right\} \right\rangle^{(0)} \quad (65)$$

Successive functional derivatives with respect to the currents would yield Green functions of the unperturbed system. Here we do not work out further this source formalism, but consider instead the free energy which also becomes a generating functional

$$F[j^*, j] = -\frac{1}{\beta} \ln Z[j^*, j] \quad (66)$$

In view of a possible symmetry-breaking we have to investigate whether the expectation value of the creation and annihilation operator turn out to be non-zero in the thermodynamic limit:

$$\psi_i(\tau) = \hbar\beta \frac{\delta F[j^*, j]}{\delta j_i^*(\tau)} \xrightarrow{j^*, j \to 0} \langle \hat{a}_{iD}(\tau) \rangle^{(0)}, \quad \psi_i^*(\tau) = \hbar\beta \frac{\delta F[j^*, j]}{\delta j_i(\tau)} \xrightarrow{j^*, j \to 0} \langle \hat{a}_{iD}^+(\tau) \rangle^{(0)} \quad (67)$$

We use (67) as a motivation to perform a functional Legendre transformation and define the effective action according to

$$\Gamma[\psi^*,\psi] = \mathcal{F}[j^*,j] - \frac{1}{\hbar\beta}\sum_i \int_0^{\hbar\beta} d\tau \left\{ j_i^*(\tau)\psi_i(\tau) + \psi_i^*(\tau) j_i(\tau) \right\} \tag{68}$$

The Legendre identities complementary to (67) read

$$\frac{\delta\Gamma[\psi^*,\psi]}{\delta\psi_i^*(\tau)} = -\frac{1}{\hbar\beta} j_i(\tau), \quad \frac{\delta\Gamma[\psi^*,\psi]}{\delta\psi_i(\tau)} = -\frac{1}{\hbar\beta} j_i^*(\tau) \tag{69}$$

In the physical limit of a vanishing current (69) reduces to

$$\frac{\delta\Gamma[\psi^*,\psi]}{\delta\psi_i^*(\tau)} = 0 = \frac{\delta\Gamma[\psi^*,\psi]}{\delta\psi_i(\tau)} \tag{70}$$

Thus, the order parameter is determined from extremising the effective action:

- static case:

$$\psi_i(\tau) = \psi_{eq} \begin{cases} = 0 \,; & \text{Mott phase} \\ \neq 0 \,; & \text{superfluid phase} \end{cases} \tag{71}$$

Studying the limit $\psi_{eq} \to 0$ yields the boundary for the quantum phase transition.

- dynamic case:

$$\psi_i(\tau) = \psi_{eq} + \delta\psi_i(\tau) \tag{72}$$

A linearisation in $\delta\psi_i(\tau)$ yields excitation modes both in the Mott and in the superfluid phase.

Furthermore, we conclude from (68) that evaluating the effective action at the equilibrium order parameter yields the physical free energy.

$$\mathcal{F} = \mathcal{F}[j^*=0, j=0] = \Gamma[\psi_{eq}^*, \psi_{eq}]$$

## 8. Finite-Temperature Perturbation Theory:

Now we decompose the total Hamiltonian

$$\hat{H}(\tau) = \hat{H}_{BH} + \hat{H}_S(\tau) \tag{73}$$

in a different way. We consider the solvable part, which is diagonal in the occupation number representation, as the unperturbed part:

$$\hat{H}_0 = \sum_i \left\{ \frac{U}{2} \hat{n}_i(\hat{n}_i - 1) - \mu \hat{n}_i \right\} ; \quad \hat{n}_i = \hat{a}_i^+ \hat{a}_i \tag{74}$$

The remaining part of the Hamiltonian

$$\hat{H}_1(\tau) = -\sum_{i,j} J_{ij} \hat{a}_i^+ \hat{a}_j + \sum_i \left\{ j_i^*(\tau) \hat{a}_i + \hat{a}_i^+ j_i(\tau) \right\} \tag{75}$$

where the hopping matrix

$$J_{ij} = \begin{cases} J & ; \quad i, j \text{ nearest neighbours} \\ 0 & ; \quad \text{otherwise} \end{cases} \tag{76}$$

can be considered as being small due to the following reasons:

- Near the quantum phase boundary the symmetry-breaking currents are expected to be small.
- The quantum phase transition occurs in $D = 3$ dimensions for small $J$.
- For large spatial dimension $D$ the hopping parameter $J$ is rescaled according to

$$J = \frac{\tilde{J}}{2D} \tag{77}$$

where $\tilde{J}$ is considered to be constant in the limit $D \to \infty$

Therefore, we determine the partition function perturbatively by using the series expansion (49). In zeroth order we evaluate the trace in (45) with respect to the basis of the occupation number representation

$$\mathrm{Tr}\, \bullet = \left\{ \prod_i \sum_{n_i=0}^{\infty} \right\} \left\{ \prod_i \langle n_i | \right\} \bullet \left\{ \prod_i | n_i \rangle \right\} \tag{78}$$

which yields the result

$$Z^{(0)} = z^{N_s} \quad , \quad z = \sum_{n=0}^{\infty} e^{-\beta E_n} \tag{79}$$

with the number of lattice sites $N_s$ and the on-site energy eigenvalues of the unperturbed system from (55). Higher orders in the perturbative expansion (49) lead to expectation values which are Green functions of the unperturbed system of the type

$$G^{(0)}_n(\tau'_1, i'_1; \dots; \tau'_n, i'_n | \tau_1, i_1; \dots; \tau_n, i_n) = \langle \hat{T}[\hat{a}^+_{i'_1 D}(\tau'_1)\hat{a}_{i_1 D}(\tau_1) \cdots \hat{a}^+_{i'_n D}(\tau'_n)\hat{a}_{i_n D}(\tau_n)] \rangle^{(0)} \tag{80}$$

Note that we have defined only those Green functions where the number of creation and annihilation operators coincide, otherwise they would vanish. Furthermore, we remark that the order of the Bose operators in (80) is irrelevant due to the presence of the time-ordering operator.

It is now crucial that the Green functions (80) can not be calculated as usual via the Wick theorem as the unperturbed Hamiltonian (74) is obviously not quadratic in the creation and annihilation operators. Instead we can use the observation that the unperturbed Hamiltonian (74) is local. According to Metzner, Vollhardt et al. the Green functions are then also local and can be decomposed in terms of cumulants

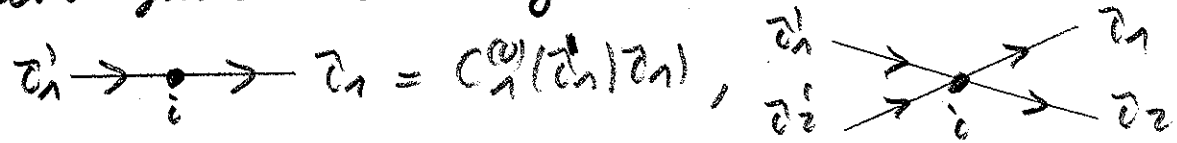
$$G^{(0)}_1(\tau'_1, i'_1 | \tau_1, i_1) = \delta_{i'_1 i_1} \, C^{(0)}_1(\tau'_1 | \tau_1) \tag{81}$$

$$\begin{aligned} G^{(0)}_1(\tau'_1, i'_1; \tau'_2, i'_2 | \tau_1, i_1; \tau_2, i_2) &= \delta_{i_1, i_2} \delta_{i'_1, i'_2} \delta_{i_1, i'_1} C^{(0)}_2(\tau'_1, \tau'_2 | \tau_1, \tau_2) \\ &+ \delta_{i_1, i'_1} \delta_{i_2, i'_2} C^{(0)}_1(\tau'_1 | \tau_1) C^{(0)}_1(\tau'_2 | \tau_2) + \delta_{i_1, i'_2} \delta_{i_2, i'_1} C^{(0)}_1(\tau'_1 | \tau_2) C^{(0)}_1(\tau'_2 | \tau_1) \end{aligned} \tag{82}$$

Here we do not work out that the cumulants can be defined by some generating functional.

Thus, we result in a corresponding perturbative expansion for the free energy (51). The respective perturbative contributions can be depicted graphically according to the following diagrammatic rules:

- we denote an $n$-point cumulant $C_n^{(0)}$ at a lattice site by a vertex with $n$ entering and $n$ leaving lines with imaginary time arguments:



(83)

- The hopping matrix element is symbolized by a line connecting two vertices

(84)

- The currents are depicted by crosses

(85)

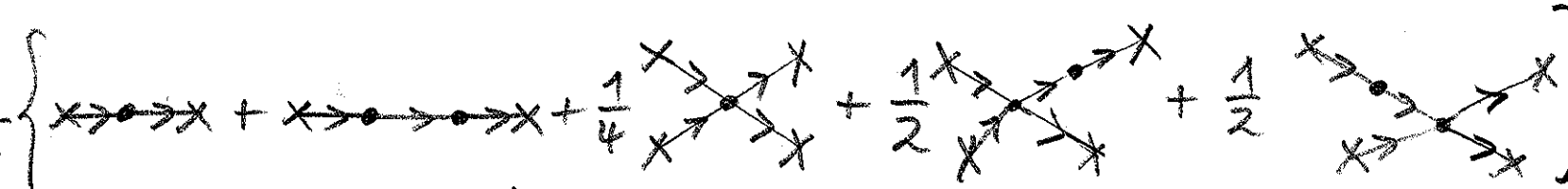
With these diagrammatic elements the connected vacuum diagrams contributing to the free energy in $n$th order in $J$ read as follows:

- Draw all possible combination of currents and vertices with $n$ entering and $n$ leaving lines.
- Connect them in all possible ways and assign imaginary-time variables, currents and hopping elements to the lines.
- Sum over all site indices over all lattice sites and integrate all imaginary time variables from 0 to $\beta\hbar$.

We note that we have to sum over all site indices over the whole lattice no matter whether two sites in a diagram coincide or not. Furthermore, we remark that each diagram is accompanied with a weight which is the inverse of the symmetry factor. The latter can be calculated by counting

the permutations of the imaginary-time variables and vertex indices which do not change the topological structure of the diagram. In first hopping order we obtain the following connected vacuum diagrams for the free energy:

$$\mathcal{F}[j^*, j] = \mathcal{F}^{(0)} - \frac{1}{\beta}\Bigg\{$$



$$\Bigg\} \quad (86)$$

The explicit expression of (86) reads:

$$\mathcal{F}[j^*, j] = \mathcal{F}^{(0)} - \frac{1}{\beta}\Bigg\{ \sum_i \frac{1}{\hbar^2}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2\, j_i(\tau_1)\, C_1^{(0)}(\tau_1|\tau_2)\, j_i^*(\tau_2)$$

$$+ \sum_i \frac{1}{4\hbar^4}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \int_0^{\hbar\beta} d\tau_4\, j_i(\tau_1)\, j_i(\tau_2)\, C_2^{(0)}(\tau_1,\tau_2|\tau_3,\tau_4)\, j_i^*(\tau_3)\, j_i^*(\tau_4)$$

$$+ \sum_i \sum_j \frac{1}{\hbar^3}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3\, j_i(\tau_1)\, C_1^{(0)}(\tau_1|\tau_3)\, \delta_{ij}\, C_1^{(0)}(\tau_3,\tau_2)\, j_j^*(\tau_2)$$

$$+ \sum_i \sum_j \frac{1}{2\hbar^5}\int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \int_0^{\hbar\beta} d\tau_3 \int_0^{\hbar\beta} d\tau_4 \int_0^{\hbar\beta} d\tau_5\, \delta_{ij}\Big[ j_i(\tau_1)\, j_i(\tau_2)\, C_2^{(0)}(\tau_1,\tau_2|\tau_5,\tau_4)\, C_1^{(0)}(\tau_5|\tau_3)$$

$$\cdot\, j_j^*(\tau_3)\, j_i^*(\tau_4) + j_i(\tau_1)\, j_j(\tau_2)\, C_2^{(0)}(\tau_1,\tau_5|\tau_3,\tau_4)\, j_i^*(\tau_3)\, j_i^*(\tau_4)\Big]\Bigg\} \quad (87)$$

The functional Legendre transformation can now be performed either graphically or analytically. The graphical consequence of the functional Legendre transformation is that all one-particle reducible diagrams in (86) are removed so that effective action only consists of one-particle irreducible vacuum diagrams. The analytical result reads with $\hbar = 1$

$$\Gamma[\psi^*, \psi] = \mathcal{F}^{(0)} + \frac{1}{\beta}\sum_i \Bigg\{ \sum_m \frac{\psi_i(w_m)\,\psi_i^*(w_m)}{C_1^{(0)}(w_m)} - \sum_j \delta_{ij}\, \psi_i(w_m)\, \psi_j^*(w_m)$$

$$- \sum_{\substack{m_1, m_2 \\ m_3, m_4}} \frac{C_2^{(0)}(w_{m_1}, w_{m_2}|w_{m_3}, w_{m_4})}{4\, C_1^{(0)}(w_{m_1})\, C_1^{(0)}(w_{m_2})\, C_1^{(0)}(w_{m_3})\, C_1^{(0)}(w_{m_4})}\, \psi_i(w_{m_1})\, \psi_i(w_{m_2})\, \psi_i^*(w_{m_3})\, \psi_i^*(w_{m_4})\Bigg\} \quad (88)$$

where the Matsubara frequencies are given by

$$\omega_m = \frac{2\pi}{\beta} m \tag{89}$$

and the Matsubara transformation is defined by

$$\psi_i(\omega_m) = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau \; e^{i\omega_m \tau} \psi_i(\tau) \tag{90}$$

Furthermore $\Gamma^{(0)}_1(\omega_m)$, $\Gamma^{(0)}_2(\omega_{m_1}, \omega_{m_2} | \omega_{m_3}, \omega_{m_4})$ are the respective Matsubara transformed of (80) and (81). Extremization of (88) yields the equation of motion for the order parameter

$$\frac{\delta \Gamma[\psi^*, \psi]}{\delta \psi_i(\omega_m)} = 0, \quad \frac{\delta \Gamma[\psi^*, \psi]}{\delta \psi_i^*(\omega_m)} = 0 \tag{91}$$

Both static and dynamic solutions of (91) are of interest.

1. Static Case:

A solution of (91) which does not depend on space and time represents the equilibrium solution:

$$\left.\frac{\delta \Gamma[\psi^*, \psi]}{\delta \psi_i(\omega_m)}\right|_{\substack{\psi_i^*(\omega_m) = \sqrt{\beta}\, \psi^*_{eq} \delta_{m,0} \\ \psi_i(\omega_m) = \sqrt{\beta}\, \psi_{eq} \delta_{m,0}}} = 0, \quad \left.\frac{\delta \Gamma[\psi^*, \psi]}{\delta \psi_i^*(\omega_m)}\right|_{\substack{\psi_i^*(\omega_m) = \sqrt{\beta}\, \psi^*_{eq} \delta_{m,0} \\ \psi_i(\omega_m) = \sqrt{\beta}\, \psi_{eq} \delta_{m,0}}} = 0 \tag{92}$$

2. Dynamic Case:

In the dynamic case we solve (91) for small deviations from the equilibrium solution:

$$\psi_i(\omega_m) = \sqrt{\beta}\, \psi_{eq} \delta_{m,0} + \delta\psi_i(\omega_m), \quad \psi_i^*(\omega_m) = \sqrt{\beta}\, \psi^*_{eq} \delta_{m,0} + \delta\psi_i^*(\omega_m) \tag{93}$$

Inserting (93) in (91) and a linearization in the deviations $\delta\psi_i(\omega_m)$, $\delta\psi_i^*(\omega_m)$ yields a homogeneous set of equations:

$$\sum_i \sum_{m'} \begin{bmatrix} \dfrac{\delta^2 \Gamma}{\delta \psi_i(\omega_m)\, \delta \psi_{i'}(\omega_{m'})} & \dfrac{\delta^2 \Gamma}{\delta \psi_i(\omega_m)\, \delta \psi_{i'}^*(\omega_{m'})} \\ \dfrac{\delta^2 \Gamma}{\delta \psi_i^*(\omega_m)\, \delta \psi_{i'}(\omega_{m'})} & \dfrac{\delta^2 \Gamma}{\delta \psi_i^*(\omega_m)\, \delta \psi_{i'}^*(\omega_{m'})} \end{bmatrix}_{\substack{\psi_i^*(\omega_m) = \sqrt{\beta}\, \psi_{eq}^* \delta_{m,0} \\ \psi_i(\omega_m) = \sqrt{\beta}\, \psi_{eq} \delta_{m,0}}} \begin{bmatrix} \delta \psi_{i'}(\omega_{m'}) \\ \delta \psi_{i'}^*(\omega_{m'}) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad (94)$$

The vanishing of the determinant of (94) yields the excitation spectra in both the hot and the superfluid phase.