JAGIELLONIAN UNIVERSITY MARIAN SMOLUCHOWSKI INSTITUTE OF PHYSICS

Dynamics of a quantum phase transition in systems of cold atoms

by

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under supervision of prof. dr hab. Jacek Dziarmaga.

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Abstract

Ultracold atomic gases in optical lattices are a very intensively researched today from both theoretical and experimental perspective. These systems may serve as quantum simulators of the many-body physics. If the atoms are bosons, the system is modelled by the Bose-Hubbard Hamiltonian. This thesis considers quenches in this model, i.e. transitions driven by a change of one of the parameters of the model. A quench may lead from one phase to another or keep the system in a single phase only. If the phase is gapless or there is a gapless critical point on the way of the quench, the system gets excited. This thesis comprises theoretical research of the excitations with the use of the impulse-adiabatic scenario (Kibble-Zurek mechanism) and derives scaling laws for the decay of the excitations. The results are in agreement with the previous theoretical works and with the experiment. To My Parents

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Preface

This thesis presents the author's doctoral research and its results on the dynamics of the transitions in the systems of ultracold bosonic gases in the field of an optical lattice. These systems are modelled by the Bose-Hubbard Hamiltonian. The thesis presents the results on the transition from the Mott insulator to the superfluid phases as well as a transition restricted to the entirely gapless phase. Such a transition, which takes place in finite time and results in excitations in the system, is hereafter called a *quench*.

The main structural unit of this thesis is a Section. Sections have a continuous numbering throughout the whole thesis, and Chapters are meant to group the Sections with like content together, for clarity.

This thesis tries to maintain a clear separation between the description of the existing results, which can be found in the literature and the results which come from the original research. Therefore, the structure of this thesis is as follows: Sections 1 through 7 (Chapter 1) contain the description of the physics existing prior to the author's research, introduce the necessary tools and models, review the relevant literature and present the problems which are elaborated thereafter.

Sections 8 through 21 present the author's research regarding the linear quench from the Mott insulator to the superfluid phase in one, two and three dimensions: Sections 8 to 13 present the application of the impulse-adiabatic scenario (a variant of Kibble-Zurek mechanism) and Sections 14 and 15 discuss the correlations in the system after a quench and the resulting domains and vortices. In Sections 16 to 21, we show the mechanism that leads to the trapping of the winding number in one-dimensional periodic chain after a linear quench. It turns out, that the variance of the random walk of phase decreases, causing the overall net winding number to freeze. These results were published in the scientific journals in the following papers:

- 1. J. Dziarmaga, M. Tylutki, and W. H. Zurek, Phys. Rev. B 84, 094528 (2011).
- 2. J. Dziarmaga, M. Tylutki, and W. H. Zurek, Phys. Rev. B 86, 144521 (2012).
- M. Tylutki, J. Dziarmaga, and W. H. Zurek, J. Phys.: Conf. Ser. 414, 012029 (2013).

The last Chapter (Sections 22 to 25) discusses the calculations that are somewhat different from the preceding results, in that we consider a quench entirely in a gapless phase in one dimension. The low-energy physics of this phase is modelled with the Luttinger liquid. We derive the scaling exponents of the excitation energy for a smooth transition and we compare it with a piecewise linear ramp. This research was published in

4. J. Dziarmaga and M. Tylutki, Phys. Rev. B 84, 214522 (2011).

Although in this thesis we avoided frequent use of abbreviations, some nevertheless appear:

- **BEC** Bose-Einstein condensation,
- BH Bose-Hubbard (Hamiltonian, model),
- **BKT** Berezinski-Kosterlitz-Thouless (transition),
- LL Luttinger liquid,
- 1,2 or 3 D one, two or three dimensions.

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Chapter 1

Introduction

1 Quantum Phase Transitions

Phase transitions have always been at the centre of experimental and theoretical research in modern physics. They allow for access to the physics underlying complex systems. Moreover, the real world virtually never allows us to study isolated physical phenomena, but confronts us with complex systems with complicated interactions among their ingredients and their environment, and often present in bulk and in finite temperature. In this way, thermodynamics was often accompanying discoveries of fundamental laws of physics. An example could be the early days of quantum mechanics with an explanation of black-body radiation given by Planck, which we now understand in terms of quantum statistics [1, 2].

Similarly, the research of the Bose-Einstein condensation (BEC), with its fairly recent experimental realization [3, 4], together with the discovery and theoretical description of superfluidity and superconductivity, where the concepts of statistical physics play a crucial role, allowed for a macroscopic manifestation of quantum phenomena [1, 2, 5, 6, 7].

Phase transition is a phenomenon where a continuous change of one parameter of a physical system through its critical value causes the qualitative change of physical properties of the system in question. The physical quantity that characterizes the system may have a discontinuity or non-analyticity at the critical value of that control parameter. In case of the continuous phase transition (i.e. no latent heat), in the vicinity of the critical parameter the fluctuations in the system become arbitrarily large and at the critical point the system has no length scale.

In classical terms, phase transitions are possible only in non-zero temperature, where there are statistical fluctuations in the system. The notion of temperature requires the division of the physical world into two realms: the system in question and its environment, which is much larger than the system. The unknown evolution of the environment turns the deterministic evolution of the classical system into a probabilistic one; the environment is a heat reservoir for the system and asserts constant temperature. The energy exchange between the system and the reservoir is allowed. In the same manner, the reservoir can admit exchange of matter (particles) and a quantity called the chemical potential, μ , is thereby set.

The theoretical description of phase transitions assumes the so called thermodynamic limit, where the size of the system goes to infinity, while the density of matter and the density of energy are kept finite. This gives rise to non-analyticities in critical points and diverging correlation lengths. These divergences would be otherwise impossible. Thus experimental conditions, where matter is in large but finite amount, smooth out all the divergences and allow the theory to describe the realistic situations only approximately. Nevertheless, since the number of atoms in typical setting is of the order of Avogadro's number, $N_A \sim 10^{23}$, the theory of phase transitions provides an excellent description of experiment, provided the temperature is sufficiently high.

The advent of quantum mechanics, however, allowed for a new type of phase transitions (see [8, 9, 10] for reviews). If there is a quantum operator that represents a Hamiltonian of a certain system, and this operator depends on some externally controllable parameter g:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}(g) ,$$
 (1.1)

then it is possible that, when g varies, the spectrum of \mathcal{H} undergoes an abrupt, qualitative change at one or more values of g. Here, we are mostly interested in the ground state of \mathcal{H} , that is the eigenvector of \mathcal{H} to its lowest eigenvalue. The ground state as a function of g may be non-analytic at some critical value $g = g_c$. This is again only possible in infinite systems; the finite size systems will have an analytic behaviour.

In contrast to a classical phase transition, a quantum phase transition is not an effect of statistical property of a complex system. We do not have to introduce the statistical ensemble and thus the notion of temperature is not necessary. In case of quantum phase transitions we say, that quantum phase transitions are in zero temperature, as they pertain to the Hamiltonian itself and not to a statistical ensemble. This does not exclude the possibility of investigating phase transitions of quantum systems in finite temperature, where both quantum and statistical behaviour are taken into account.

The quantum phase transitions are mostly studied in lattice Hamiltonians that describe spin chains or other systems of interest in condensed matter physics. Such Hamiltonians have their degrees of freedom on a lattice. The paradigmatic example is the Ising model, which describes spins interacting via nearest neighbour interactions and subject to external field, which tries to align the spins in a transverse direction. Another important lattice model is the Hubbard model, which arises in condensed matter physics in a tight-binding approximation and describes electrons in a field of a crystal lattice [8, 9]. Its bosonic counterpart is the Bose-Hubbard model, discussed in Section 3. The main focus of this thesis is a quantum phase transition that occurs in this model.

2 Ultracold atomic gases in optical lattices

The aforesaid Bose-Hubbard (BH) model can be realized experimentally via cold atomic gases in optical lattices [11, 12, 9, 10]. This is a key fact that makes study of cold atomic gases in optical lattices so interesting. The experimental results provide exact solutions to Bose-Hubbard Hamiltonian, regardless whether they are attainable through numerical simulation or not. Thank to this property, we can think of systems of cold atoms as a *quantum simulator* for condensed matter. The cold atomic system evolves the Bose-Hubbard model and provides an answer to a question that might be relevant, for example, in solid state physics. This is an approach to a more general problem of *quantum computation* - an area very intensively researched today. There, it is believed, that evolution of quantum systems can provide solutions to certain computational problems, often too complex to be solved by conventional, classical algorithms.

One of the most characteristic features of the Bose-Hubbard model is the presence of two phases: the Mott insulator phase, where there is a constant number of atoms at each lattice site, and the superfluid phase, which is characterized with correlations of the wave function's phase across the system, see the intuitive presentation in Fig. 2.1. Moreover, in the presence of a disorder, there is a third phase - a Bose glass, which is not discussed in this thesis. Theoretical proposals of the phase diagram for the Bose-Hubbard model go back to the seminal papers by Fisher *et al.* [13] and Jaksch *et al.* [14]. Nevertheless, the experimental realization of the Mott insulator to superfluid phase transition came about much later and was done by Greiner *et al.* [15, 16]. The experimental realization of the Bose-Hubbard model in [17] and in [18].

In one dimension, the physics is often completely different to the physics of higher dimensions. This is even more pronounced in quantum physics, where many bosonic or fermionic systems in one dimension have the low-energy behaviour of the quantum Luttinger liquid (LL) [19, 20, 21]. The Hamiltonian of the Luttinger liquid is quadratic in its variables and has only two parameters: the speed of sound, c, and the parameter K. The ultracold atoms can also be described in terms of the Luttinger liquid, as long as the low-energy behaviour is considered. The example is a free Bose gas [22], where the parameters of the gas: boson's mass m, density ρ , and compressibility κ relate to the parameters of the Luttinger liquid in the following way:

$$K = \sqrt{\frac{\kappa m}{\rho^3}} , \quad c = \sqrt{\frac{\kappa}{\rho m}} , \qquad (2.1)$$



Figure 2.1: The intuitive picture of an optical lattice with the atoms in its field. The laser field creates a potential with periodic wells separated by barriers of an adjustable height. If the barrier is high enough, the system is in the Mott insulator phase (left), where the atoms are uniformly distributed over the lattice, i.e. there is a constant number of atoms at each site. Contrary, if the potential barrier is lowered, the density of atoms is no longer uniform, but there is a correlation in the phase of the atomic wave function between different sites. This phase is a superfluid (right).

with $\hbar = 1$, see [22]. Also, the Luttinger liquid applies to bosons in a field of an optical lattice [23]. For the bosons interacting through contact interactions we can apply the Luttinger liquid description as well [9, 10, 24, 25]. The relation between the parameters reads as

$$K = 1 + \frac{4}{\gamma}$$
, $c = v_{\rm F}(1 - \frac{4}{\gamma})$. (2.2)

In (2.2)

$$\gamma = \frac{mg}{\hbar^2 \rho} \tag{2.3}$$

is the strength of the interaction, g is the strength of the contact interaction and ρ is the linear density of particles. When $\gamma \to \infty$, we obtain the Tonks-Girardeau gas [26, 27], the experimental realization of which was done by Kinoshita *et al.* [28]. Other low dimensional problems are also researched, such as the solitons in thermal equilibrium in the Lieb-Liniger model [29] or the equilibrium statistical properties of condensates, as in [30].

The systems in finite temperature are also investigated [31], as well as the processes of thermalization and equilibration [32, 33]. Another area of interest is related to the dipolar interaction in the optical lattices and condensates [34, 35]. Dipolar interactions in the spinor condensate leads, for example, to the realization of the Einstein-de Haas effect [35].

3 Bose-Hubbard model

The Bose-Hubbard model, already mentioned in the introduction,

$$\mathcal{H}_{\rm BH} = -J \sum_{\langle i,j \rangle} (a_i^{\dagger} a_j + a_j^{\dagger} a_i) + \frac{U}{2} \sum_i n_i (n_i - 1) + \sum_i V_i a_i^{\dagger} a_i - \mu \sum_i n_i , \qquad (3.1)$$

describes cold bosonic atoms in the field of an optical lattice. It is one of the most widely studied lattice models. The operators a_i and a_i^{\dagger} are the boson annihilation and creation operators respectively, and they obey the standard commutation relations,

$$[a_i, a_j^{\dagger}] = \delta_{ij} \ . \tag{3.2}$$

The particle number operator n_i at site *i* is defined in the usual way: $n_i = a_i^{\dagger}a_i$. The second (interaction) term is then often written as: $\sum_i n_i(n_i - 1) = \sum_i a_i^{\dagger}a_i^{\dagger}a_ia_i$. The parameter *J* multiplies the term responsible for hopping of atoms between neighbouring sites (kinetic energy in other words) and *U* is the magnitude of the repulsive interaction between the atoms at the same site. In case of $V_i \equiv 0$, one of them sets the energy scale for the system, so there is one dimensionless parameter $\frac{J}{U}$ which is responsible for the relative strength of the kinetic (tunnelling) term compared to the interaction term. The third term, $\sum_i V_i a_i^{\dagger}a_i$, represents a possible interaction with an external potential (such as a trap) and for some part of this thesis will be set to zero.

There is also the chemical potential μ in the model, which multiplies the total atom number operator $\sum_i n_i$. It can be regarded as a constraint on the model, asserting that the average total atom number should be constant. Therefore, we have two distinct dimensionless parameters of the model: $\frac{J}{U}$ and $\frac{\mu}{U}$, which define the space of different possible phases (phase diagram).

We start with the investigation of the limits of the model, a common approach to the analysis of models with complex behaviour.

Mott insulator phase. When the interaction dominates over the hopping term, i.e.

$$\frac{J}{U} \ll 1 , \qquad (3.3)$$

our Hamiltonian simplifies significantly. It comprises the interaction and the chemical potential terms only, and they do not couple different sites. This means they are already diagonal in the Fock basis. Thus, solving for the ground state reduces to a simple minimization problem and the ground state has the following form:

$$|\cdots n_0 \cdots n_0 \cdots \rangle$$
, (3.4)

where there is a constant number of atoms n_0 at each site. In other words, there is a uniform atom density. The integer value n_0 depends on the chemical potential and is equal to the closest non-negative integer to $\frac{\mu}{U} + \frac{1}{2}$, unless $\frac{\mu}{U}$ is integer itself.

Since the energy spectrum is a polynomial in non-negative integers, it must be discrete. Therefore, the first excited state above the ground state is finite amount of energy apart and there is energy gap $\Delta = E_1 - E_0$ that separates these states. Hence the name of the phase: *Mott insulator*.

Superfluid phase. In the opposite limit,

$$\frac{J}{U} \gg 1 , \qquad (3.5)$$

the Hamiltonian reduces to

$$\mathcal{H}_{SF} = -J \sum_{\langle i,j \rangle} (a_i^{\dagger} a_j + a_j^{\dagger} a_i) . \qquad (3.6)$$

It can be diagonalized in the Fourier space. Let us consider one dimension for the sake of simplicity. If we perform a discrete Fourier transform on the annihilation and creation operators:

$$a_s = \frac{1}{\sqrt{L}} \sum_{k=0}^{L-1} a_k e^{-2\pi i \frac{ks}{L}} , \qquad a_s^{\dagger} = \frac{1}{\sqrt{L}} \sum_{k=0}^{L-1} a_k^{\dagger} e^{2\pi i \frac{ks}{L}} , \qquad (3.7)$$

where L is the number of sites, we get a diagonal form of the Hamiltonian:

$$\mathcal{H}_{\rm SF} = -2J \sum_{k=0}^{L-1} a_k^{\dagger} a_k \cos \frac{2\pi k}{L} .$$
 (3.8)

The spectrum of the Hamiltonian is continuous and there is no energy gap, i.e. $\Delta = 0$. This phase is called a *superfluid*. The ground state of \mathcal{H}_{SF} is

$$|\mathrm{SF}\rangle \propto \left(a_{k=0}^{\dagger}\right)^{n}|0\rangle , \qquad (3.9)$$

where $|0\rangle$ is the Fock vacuum state, the state with no particles.

Clearly, there must be a boundary in the μ -J plane, which separates these two phases. Crossing the boundary from one side to the other would cause the energy gap Δ to vanish or appear. In the phase diagram, the Mott insulator phase forms *lobes*, where each lobe is characterised by a unique integer atom density, [8, 11, 12, 13, 15], see Fig. 3.1(a).



(a) The phase diagram of the Bose-Hubbard (b) The figure shows the phase diagram in one lations between different sites.

model. The blue lobes for small value of J/U dimension. Here, the gapless phase is effecare Mott insulators with a distinct value of con- tively a Luttinger liquid. The transition from stant atom density. The lobes are surrounded the Mott insulator to the Luttinger liquid is of a by the superfluid phase characterized by corre- commensurate-to-incommensurate type (K = 1)except for the tips of the lobes, where $K = \frac{1}{2}$, and the transition is the Berezinskii-Kosterlitz-Thouless transition [13, 23]. The red line shows the possible quench trajectory, one that we study in the last Chapter of this thesis.

Figure 3.1: The phase diagram of the Bose-Hubbard model.

Berezinskii-Kosterlitz-Thouless transition 4

The continuous phase transitions involve symmetry breaking of the order parameter, therefore leading from the ordered to the disordered phase or vice versa. However, due to the Mermin-Wagner-Hohenberg theorem [36, 5, 8], there cannot be a long-range order in low-dimensional systems (one and two dimensions). Nevertheless, in two dimensions, there can be a Berezinskii-Kosterlitz-Thouless (BKT) transition to a low-temperature phase, where the correlation function of the order parameter decays algebraically (powerlaw behaviour). A paradigmatic example of such a system is the two-dimensional XY model.

The BKT transition is characterised by the suppression of the vortex formation in the low-temperature phase. In high-temperature phase, on the other hand, the bound vortex-antivortex pairs dissolve. The BKT transition temperature is determined by the competing minimization of energy and entropy in the free energy F = E - TS. The BKT transition is also present in the two-dimensional fluid of bosons [36].

Due to the correspondence between the partition functions of (d+1)-dimensional classical systems and their *d*-dimensional quantum counterparts, there is a BKT transition in the one-dimensional Bose-Hubbard model. In contrast to the generic commensurate-to-incommensurate transition between the Mott insulator phase and the Luttinger liquid phase (which corresponds to the Luttinger parameter K = 1), at the tips of the Mott insulator lobes, there is a BKT transition, where the average atom density remains unaltered (and $K = \frac{1}{2}$).

5 Formulation of the problem

In Section 2 it was mentioned, that manipulation of ultracold atoms in optical lattices allows for simulation of quantum many-body systems driven by time-dependent Hamiltonian. In a typical experiment, the system is prepared in the ground state for one value of the control parameter and, afterwards, this parameter is varied, either continuously or by an abrupt, sudden change. Thus, the system is driven in time from the initial state to the final one in a process that we hereafter call a *quench* (for historical reasons [37, 38] and in order to be consistent with the existing literature).

The idea of the adiabatic computation is to prepare the system in a ground state of the initial Hamiltonian, and subsequently drive it adiabatically to the ground state of the final Hamiltonian. The ground state of the initial Hamiltonian is supposed to be simple, whereas the ground state of the final Hamiltonian does not necessarily have to be simple and should be interesting from the point of view of the simulated problem. Unfortunately, if the quench crosses a critical point, where the system is gapless, or if the system is quenched through a gapless phase, the adiabatic state preparation is likely to fail [9, 39]. The system gets excited and the excitation energy is supposed to decay algebraically with the rate of the quench [37, 38, 40], see Section 6.

In the first part of the thesis we consider a linear quench across a quantum phase transition, from the Mott insulator phase to the superfluid:

$$J(t) = \frac{t}{\tau_Q} , \qquad (5.1)$$

where τ_Q is called the *quench time* and sets the rate of the quench. The choice of the linear quench is rather generic; any smooth function can be linearised in the vicinity of the critical point. We investigate the excitation energy in Sections 8 to 13, where we apply the impulse-adiabatic approximation to the description of the transition. We generalize the theory suggested for one dimension in [41] and we find that the the excitation energy has a power-law behaviour also in two and three dimensions [42, 43],

according to the impulse-adiabatic scenario. The power turns out to be equal to 1/3, in agreement with the experiment of [18].

In Sections 16 through 21, we focus our attention on the one-dimensional periodic lattice, where we also study the linear quench (5.1). In this part of the thesis we focus, however, on the winding number and we find, that for quenches slow enough the Kibble-Zurek scenario ceases to hold, and the winding number no longer decays algebraically (as in [41]), but saturates [44].

In the simulation of the Bose-Hubbard model (3.1) we use the truncated Wigner method (described in Section 7), which we implement with the use of the *split-step method*, see Appendix A.

In the last part of the thesis we study quench in an entirely gapless phase in one dimension: a Luttinger liquid. The trajectory of the quench is schematically depicted in Fig. 3.1(b) with the red line. We derive the dynamical exponents for the scaling of the density of excitations and the excitation energy for the smooth quench and we compare it with the piecewise linear ramp, which excites the system beyond the Luttinger liquid description, see [45].

6 Kibble-Zurek mechanism

This Section provides a brief review of the Kibble-Zurek mechanism. This mechanism was first proposed in a cosmological context by Kibble, [46], and then was further generalized by Zurek for continuous phase transition [37, 38, 40]. For quantum generalization of the Kibble-Zurek mechanism see [47, 48, 49, 50]. In the subsequent presentation, we follow the derivation in Ref. [9].

6.1 Classical Kibble-Zurek mechanism

A classical continuous phase transition is induced by a change of temperature T across its critical value T_c . Continuous phase transitions are characterized by the change of the order parameter - a quantity whose value uniquely characterizes each of the phases. In many phase transitions, when the system is at temperature above T_c , it is in a symmetric phase, where the order parameter is zero, and the phase has a symmetry of the defining Hamiltonian. When the temperature is lowered below T_c , this symmetry becomes spontaneously broken, and the order parameter acquires a non-zero value. In the ideal equilibrium case, in which the transition through T_c is adiabatic, the value of the order parameter in the low-temperature phase should be everywhere constant and the phase should be uniform in space. However, when the transition is driven at a finite pace, there is a limited time for the information about the value of the order parameter to spread across the system. As a result, the system after the phase transition consists of domains with the spontaneously broken phase, where in each domain the value of the order parameter is constant, but varies from domain to domain. The average size of a domain depends on the rate of the transition, and the faster the transition is, the smaller the domains are and thus in bigger quantity.

In the subsequent calculations, ε is the relative, dimensionless distance from the critical point,

$$\varepsilon = \frac{T - T_c}{T_c} \ . \tag{6.1}$$

The correlation length ξ grows algebraically as the temperature approaches T_c , as does the relaxation time τ ,

$$\xi \sim |\varepsilon|^{-\nu} , \quad \tau \sim \xi^z .$$
 (6.2)

The above equations define the exponents ν and z. At the critical point the correlations become infinite and the system has no scale.

When the system is far from the critical point (either above T_c or below), the relaxation rate is very large compared to the relative transition rate,

transition rate =
$$\left| \frac{1}{\varepsilon} \frac{d\varepsilon}{dt} \right|$$
, (6.3)

and the system has ample time to equilibrate and adjust its correlation length to its equilibrium value. Therefore, the evolution is adiabatic. Close to T_c , on the other hand, the situation is opposite. The pace of the transition is much larger than the relaxation rate and the correlations cannot catch up with changing T. In the intermediate stage, the mechanism of the dynamics of a phase transition is, in principle, very complicated. However, a lot can be predicted with a simple approximation, called the *adiabaticimpulse-adiabatic* approximation. When the transition rate is larger than the relaxation rate, we model the evolution as impulse and when the relaxation is faster, we assume the evolution to be adiabatic. At $\hat{\varepsilon}$, when the two rates are comparable, the system crosses over from one regime to the other. Therefore, as the system is cooled down, the evolution is adiabatic up to $\hat{\varepsilon}$. There, the correlation length becomes frozen until the next crossover at $-\hat{\varepsilon}$, where the evolution becomes adiabatic again. The adiabaticimpulse-adiabatic approximation is depicted in Fig. 6.1.

We assume the change of $\varepsilon(t)$ to be linear in time,

$$\varepsilon(t) \approx -\frac{t}{\tau_Q} , \qquad (6.4)$$

which is a generic choice: any smooth function can be linearised in the vicinity of a given point. The impulse-adiabatic crossover takes place when

$$\left|\frac{1}{\varepsilon}\frac{d\varepsilon}{dt}\right| \sim \tau^{-1} , \qquad (6.5)$$



Figure 6.1: Impulse-adiabatic approximation is the key ingredient of the Kibble-Zurek mechanism. The complex dynamics of a transition across a critical point is approximated by three regimes: the adiabatic evolution when the relative pace of the transition (red line) is much lower than the relaxation rate (blue line), the impulse evolution across the critical point, when the transition rate exceeds the relaxation rate and the second adiabatic regime, when the reaction of the system is again much faster than the transition.

where τ^{-1} is a relaxation rate. Therefore,

$$\frac{1}{\hat{t}} \sim \tau^{-1} \tag{6.6}$$

and since

$$\hat{\varepsilon} \sim \frac{\tau}{\tau_Q} \sim \frac{\hat{\varepsilon}^{-\nu z}}{\tau_Q} ,$$
 (6.7)

we get the scaling of $\hat{\varepsilon}$ with the quench rate

$$\hat{\varepsilon} \sim \tau_Q^{-\frac{1}{1+\nu z}} \,. \tag{6.8}$$

6.2 Quantum Kibble-Zurek mechanism

A similar reasoning can be repeated for the quantum phase transitions, where one varies the parameters in the Hamiltonian instead of changing the temperature. Hence, the dimensionless distance form the critical point is

$$\varepsilon = \frac{J - J_c}{J_c} , \qquad (6.9)$$

where J is the control parameter of the Hamiltonian. The correlation length (and the healing length) and the reaction time scale algebraically again,

$$\tau \sim |\varepsilon|^{-\nu z}, \quad \xi \sim |\varepsilon|^{-\nu}, \quad (6.10)$$

respectively. When the system is driven and parameters of the Hamiltonian change, the ground state for one value of ε becomes an excited state for a subsequent value of ε . When the system is far from the critical point, the evolution is adiabatic, which means, that the state of the system follows the ground state of the changing Hamiltonian. When the system is close to the critical point, the state of the system does not have enough time to adjust to the changing ε .

In the quantum context, the entire evolution can again be divided into three regimes: the adiabatic regime, the impulse regime, where the state of the system is frozen, and the adiabatic regime again. The relaxation time of the system is an inverse of the energy gap (from dimensional analysis),

$$\tau \simeq \Delta^{-1} , \qquad (6.11)$$

and therefore

$$\Delta \sim |\varepsilon|^{\nu z} . \tag{6.12}$$

Similarly to the classical case, the impulse-adiabatic crossover takes place when the relaxation rate and transition rate are equal

$$\left|\frac{1}{\varepsilon}\frac{d\varepsilon}{dt}\right| \sim \frac{1}{\tau} \simeq \Delta \sim |\hat{\varepsilon}|^{\nu z} .$$
(6.13)

This gives

$$\frac{1}{\hat{t}} = \frac{1}{\tau_Q \hat{\varepsilon}} \sim \hat{\varepsilon}^{\nu z} \tag{6.14}$$

and the scaling of $\hat{\varepsilon}$ can be determined

$$\hat{\varepsilon} \sim \tau_Q^{-\frac{1}{1+\nu z}} . \tag{6.15}$$

Both in the classical case and in the quantum case, the derived exponents are the same, despite different physics beyond these equations. This allows to determine the scaling for $\hat{\xi}$ as

$$\hat{\xi} \sim \tau_Q^{\frac{\nu}{1+\nu z}} . \tag{6.16}$$

Since the evolution between $\hat{\varepsilon}$ and $-\hat{\varepsilon}$ is impulse, the value of the correlation length ξ is determined by its value at $\hat{\varepsilon}$, i.e. by $\hat{\xi}$. This sets, in turn, the length scale for the domains as a function of the quench rate. Furthermore, for large τ_Q , the expectation value of an operator at the state at $\hat{\varepsilon}$ is proportional to the power of the only length scale

 $\hat{\xi}$, and therefore depends algebraically on the quench rate τ_Q . An important example would be the density of quasiparticle excitations, which should scale like

$$n_{\rm ex} \sim \hat{\xi}^{-d} \sim \tau_Q^{-\frac{d\nu}{1+\nu z}} , \qquad (6.17)$$

where d is the dimension of the system [9].

7 Truncated Wigner approximation

A general quantum state, including mixed states, is represented by the density operator $\hat{\rho}$. Mixed states represent a statistical mixture of various quantum states with different probabilities. In classical physics, on the other hand, statistical systems are represented by the probability distribution over the available phase space. In analogy to the classical systems, a quantum state $\hat{\rho}$ may also be represented as a quasi-probability distribution over the phase space (q, p) of the system. One of such formulations is provided by the Wigner distribution, W(q, p), defined as

$$W(q,p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx \, \langle q + \frac{1}{2}x | \hat{\rho} | q - \frac{1}{2}x \rangle \, e^{\frac{i}{\hbar}px} \,, \tag{7.1}$$

where $|q \pm \frac{1}{2}x\rangle$ are the eigenstates of the position operator [51, 52]. The Wigner distribution may assume negative values and thereby is not a probability distribution. The negative values of W(q, p) indicate the presence of quantum interference and thus are indicators of how close or how far the given system is from the classical one. The Wigner function allows for calculation of operator averages; it can also be employed to computer simulations of quantum systems.

Therefore, the idea behind the Truncated Wigner approximation is to replace the full quantum dynamics of the original model by a classical evolution of a statistical ensemble. In case of the Bose-Hubbard model (3.1), we represent the system by a classical field on a lattice, ϕ_s , which evolves in time. The quantum dynamics is represented by the evolution of a whole ensemble of fields ϕ_s ; the quantum expectation values become statistical averages over this ensemble, and the initial Wigner distribution is the initial distribution over the ensemble. Truncated Wigner method was used to study dynamics of a quantum phase transition, for example, in [53, 54]. For alternative approaches not using the truncated Wigner method, see [55, 56, 57, 58, 59, 60, 61, 62, 63, 64].

7.1 Gross-Pitaevskii equation

For large values of density n, i.e. when $n \gg 1$, we choose the units of the model (3.1) in which the interaction U becomes the inverse of the atom density, $U = \frac{1}{n}$. Then the

 \mathcal{H}_{BH} becomes

$$\mathcal{H}_{\rm BH} = -J \sum_{\langle \mathbf{s}, \mathbf{r} \rangle} (a_{\mathbf{s}}^{\dagger} a_{\mathbf{r}} + a_{\mathbf{r}}^{\dagger} a_{\mathbf{s}}) + \frac{1}{2n} \sum_{\mathbf{s}} a_{\mathbf{s}}^{\dagger} a_{\mathbf{s}}^{\dagger} a_{\mathbf{s}} a_{\mathbf{s}} + \sum_{\mathbf{s}} V_{\mathbf{s}} a_{\mathbf{s}}^{\dagger} a_{\mathbf{s}} - \mu \sum_{\mathbf{s}} a_{\mathbf{s}}^{\dagger} a_{\mathbf{s}} .$$
(7.2)

We can now replace the annihilation operators $a_{\mathbf{s}}$ by a complex field $\phi_{\mathbf{s}}$,

$$a_{\mathbf{s}} \approx \sqrt{n} \phi_{\mathbf{s}} , \quad a_{\mathbf{s}}^{\dagger} \approx \sqrt{n} \phi_{\mathbf{s}}^{\star} , \qquad (7.3)$$

with the normalization condition

$$\sum_{\mathbf{s}} |\phi_{\mathbf{s}}|^2 = L^D , \qquad (7.4)$$

where L is the size of each of lattice D dimensions, and L^D is the volume of the lattice (number of sites). With this identification, we can express the original Hamiltonian \mathcal{H}_{BH} in the language of the field ϕ_s . The Hamiltonian \mathcal{H}_{BH} (7.2) becomes an energy functional

$$E_{\rm GP}[\phi_{\mathbf{s}},\phi_{\mathbf{s}}^{\star}] = J(t)\sum_{\mathbf{s}} \nabla\phi_{\mathbf{s}}^{\star} \cdot \nabla\phi_{\mathbf{s}} + \frac{1}{2}\sum_{\mathbf{s}} \left(\phi_{\mathbf{s}}^{\star}\phi_{\mathbf{s}} - 1\right)^{2} + \sum_{\mathbf{s}} V_{\mathbf{s}}\phi_{\mathbf{s}}^{\star}\phi_{\mathbf{s}} , \qquad (7.5)$$

up to the choice of the chemical potential $\mu = 1$ and an irrelevant, additive constant. The discrete differentiation operator ∇ is defined as

$$\nabla_{\alpha}\phi_{\mathbf{s}} = \phi_{\mathbf{s}+\mathbf{e}_{\alpha}} - \phi_{\mathbf{s}} , \qquad (7.6)$$

where $\{\mathbf{e}_{\alpha}\}$ form a basis of unit vectors in all lattice directions. Using the identification (7.3), the quantum evolution equations (Heisenberg equations) of the original model (7.2) reduce to an evolution equation for $\phi_{\mathbf{s}}$, which is the discrete Gross-Pitaevskii equation (GPE):

$$i\partial_t \phi_{\mathbf{s}} = -J(t)\nabla^2 \phi_{\mathbf{s}} + (\phi_{\mathbf{s}}^* \phi_{\mathbf{s}} - 1)\phi_{\mathbf{s}} + V_{\mathbf{s}} \phi_{\mathbf{s}} , \qquad (7.7)$$

where the chemical potential $\mu = 1$. For the details of the truncated Wigner approximation see [65, 66, 67, 68, 69, 70, 71, 72, 73]. Here, ∇^2 is the *D*-dimensional formal discrete Laplacian which reads as

$$\nabla^2 \phi_{\mathbf{s}} = \sum_{\alpha=1}^{D} \left(\phi_{\mathbf{s}+\mathbf{e}_{\alpha}} - 2\phi_{\mathbf{s}} + \phi_{\mathbf{s}-\mathbf{e}_{\alpha}} \right) \ . \tag{7.8}$$

The variation of the energy $E_{\rm GP}$ with respect to either $\phi_{\rm s}^{\star}$ or $\phi_{\rm s}$ gives the equation of motion (7.7):

$$i\partial_t \phi_{\mathbf{s}} = \frac{\delta}{\delta \phi_{\mathbf{s}}^{\star}} E_{\rm GP}[\phi_{\mathbf{s}}, \phi_{\mathbf{s}}^{\star}]$$
(7.9)

or its complex conjugate respectively.

Quantum expectation values are estimated by averages over stochastic realizations of ϕ_s . Each realization has different random initial conditions coming from a Wigner distribution of the initial state. In the case of the Mott state (3.4), $|\cdots n_0 \cdots n_0 \cdots \rangle$, we have

$$\phi_{\mathbf{s}}(0) = e^{i\theta_{\mathbf{s}}(0)} , \qquad (7.10)$$

with independent random initial phases $\theta_{\mathbf{s}}(0)$ uniformly distributed over the interval $(-\pi, \pi]$. This reflects an uncertainty relation between the phase and particle number, where a well defined atom density in the Mott state gives rise to a totally random phase $\theta_{\mathbf{s}}$. Moreover, such a choice for the initial conditions, where $|\phi_{\mathbf{s}}(0)|^2 = 1$, justifies our choice for the value of the chemical potential, $\mu = 1$.

In the thermodynamic limit, where the density n is large, $n \gg 1$, the quantum phase transition from the Mott insulator to the superfluid is at

$$J_{\rm cr} \approx \frac{1}{n^2} \ . \tag{7.11}$$

The expressions for the observable kinetic and potential energy take the form

$$\langle E_{\rm kin} \rangle = J \sum_{\rm s} \langle \nabla \phi_{\rm s}^{\star} \cdot \nabla \phi_{\rm s} \rangle , \qquad (7.12)$$

$$\langle E_{\text{pot}} \rangle = \frac{1}{2} \sum_{\mathbf{s}} \left\langle \left(\phi_{\mathbf{s}}^{\star} \phi_{\mathbf{s}} - 1 \right)^2 \right\rangle + \sum_{\mathbf{s}} \left\langle V_{\mathbf{s}} \phi_{\mathbf{s}}^{\star} \phi_{\mathbf{s}} \right\rangle .$$
 (7.13)

The total energy is a sum of the above terms:

$$\langle E \rangle = \langle E_{\rm kin} \rangle + \langle E_{\rm pot} \rangle .$$
 (7.14)

Hereafter, the bracket $\langle \cdot \rangle$ denotes the statistical average over the ensemble of configurations of the field ϕ_s .

7.2 Ground state

In order to calculate the excitation energy for a certain configuration at a some value of J(t), one has to know the ground state energy of the system. For a given, fixed $J = J_0$, the ground state configuration $\phi_{\mathbf{s}}^{\text{GS}}$ obeys

$$\frac{\delta}{\delta\phi_{\mathbf{s}}^{\star}} E_{\mathrm{GP}}[\phi_{\mathbf{s}}, \phi_{\mathbf{s}}^{\star}] \bigg|_{\phi=\phi^{\mathrm{GS}}} = -J_0 \nabla^2 \phi_{\mathbf{s}}^{\mathrm{GS}} + \left(\phi_{\mathbf{s}}^{\mathrm{GS}} \phi_{\mathbf{s}}^{\mathrm{GS}} - 1\right) \phi_{\mathbf{s}}^{\mathrm{GS}} + V_{\mathbf{s}} \phi_{\mathbf{s}}^{\mathrm{GS}} = 0 , \qquad (7.15)$$

where we assumed $|\phi_0(0)|^2 = 1$ in the centre, see Section 13. Numerically, the solution to the above equation can be computed through an evolution of a non-unitary equation

$$\partial_t \phi_{\mathbf{s}} = -\frac{\delta}{\delta \phi_{\mathbf{s}}^{\star}} E_{\mathrm{GP}}[\phi_{\mathbf{s}}, \phi_{\mathbf{s}}^{\star}]$$
(7.16)

for a time long enough, that the field configuration reaches its stationary state, for which the left hand side of Eq. (7.16) vanishes.

In case of $V_{\rm s} \equiv 0$, the configuration which minimizes the total energy is a constant field $\phi_{\rm s} \equiv 1$. For this configuration, the energy E = 0. We can therefore consider the kinetic and potential energies separately and the formulae (7.12) and (7.13) already give the excitation energies above the ground state. This is not true, however, if $V_{\rm s} \neq 0$, the case which is also studied in this thesis.

CHAPTER 2

Excitations in a non-adiabatic quench

8 Josephson regime

In the introduction, it was mentioned, that the excitation energy is a measure of a nonadiabaticity of a transition. Moreover, the excitation energy should decay algebraically with the decreasing transition rate. In the subsequent Sections we study the excitation energy as a function of τ_Q in the linear quench (5.1). We perform the numerical simulations and test the impulse-adiabatic scenario.

8.1 Josephson equations

We begin, however, with the regime, where the tunnelling coefficient is small, $J \ll 1$. This regime is known as the Josephson regime. There, the fluctuations of the density are small, $|\phi_{\rm s}| \approx 1$, and we can write the field as

$$\phi_{\mathbf{s}} = (1 + f_{\mathbf{s}})e^{i\theta_{\mathbf{s}}} , \qquad (8.1)$$

where $f_{\rm s}$ is a small correction. In this approximation, the Gross-Pitaevskii equation (7.7), turns into a set of two equations for $f_{\rm s}$ and $\theta_{\rm s}$, which in turn can be rewritten in terms of $\theta_{\rm s}$ only, i.e. as the Josephson equations:

$$\partial_t^2 \theta_{\mathbf{s}} = 2J(t) \sum_{\alpha=1}^D \left\{ \sin(\theta_{\mathbf{s}+\mathbf{e}_\alpha} - \theta_{\mathbf{s}}) + \sin(\theta_{\mathbf{s}-\mathbf{e}_\alpha} - \theta_{\mathbf{s}}) \right\} .$$
(8.2)

Equation (8.2) can be conveniently shortened as

$$\partial_t^2 \theta_{\mathbf{s}} = 2J(t) \sum_{\mathbf{r}\,\mathrm{n.n.s}} \sin(\theta_{\mathbf{r}} - \theta_{\mathbf{s}}) , \qquad (8.3)$$

where the sum is over \mathbf{r} 's that are the neighbouring sites of the site \mathbf{s} (so called *nearest neighbours* of \mathbf{s}).

The initial conditions inherited from the Gross-Pitaevskii equation (7.7) become here again random phases $\theta_{s} \equiv 0$ and vanishing $f_{s} \equiv 0$, which translate to vanishing velocities of θ_{s} :

$$\left. \frac{d\theta_{\mathbf{s}}}{dt} \right|_{t=0} = 0 \ . \tag{8.4}$$

The expressions for energies (7.12) and (7.13) become

$$E_{\rm kin} = J(t) \sum_{\rm s} \nabla \phi_{\rm s}^{\star} \cdot \nabla \phi_{\rm s}$$
$$= J(t) \sum_{\rm s} (\phi_{\rm s}^{\star} \phi_{\rm s} \nabla \theta_{\rm s} \cdot \nabla \theta_{\rm s} + \mathcal{O}(f_{\rm s}, \nabla f_{\rm s})) \simeq J(t) \sum_{\rm s} \nabla \theta_{\rm s} \cdot \nabla \theta_{\rm s} , \qquad (8.5)$$

$$E_{\text{pot}} = \frac{1}{2} \sum_{\mathbf{s}} \left(|\phi_{\mathbf{s}}|^2 - 1 \right)^2 = \frac{1}{2} \sum_{\mathbf{s}} \left(2f_{\mathbf{s}} + \mathcal{O}(f_{\mathbf{s}}^2) \right)^2 \simeq 2 \sum_{\mathbf{s}} f_{\mathbf{s}}^2 .$$
(8.6)

8.2 Josephson Hamiltonian

We can calculate the Josephson Hamiltonian \mathcal{H}_J by integrating the Hamilton equations, if we observe that we can identify the conjugate momentum to the coordinate θ_s as

$$p_{\mathbf{s}} = \theta_{\mathbf{s}} \ . \tag{8.7}$$

Then, the Josephson equation is the Hamilton equation,

$$\dot{p}_{\mathbf{s}} = -\frac{\partial \mathcal{H}_{\mathbf{J}}}{\partial \theta_{\mathbf{s}}} = 2J(t) \sum_{\alpha=1}^{D} \left\{ \sin(\theta_{\mathbf{s}+\mathbf{e}_{\alpha}} - \theta_{\mathbf{s}}) + \sin(\theta_{\mathbf{s}-\mathbf{e}_{\alpha}} - \theta_{\mathbf{s}}) \right\} , \qquad (8.8)$$

and by integration we can obtain the formula for the Hamiltonian:

$$\mathcal{H}_{\mathrm{J}} = \sum_{\mathbf{s}} \frac{p_{\mathbf{s}}^2}{2} + \sum_{\mathbf{s}} \sum_{\alpha=1}^{D} 2J \left\{ 1 - \cos(\theta_{\mathbf{s}+\mathbf{e}_{\alpha}} - \theta_{\mathbf{s}}) \right\} .$$
(8.9)

9 Thermalization in the Josephson regime

9.1 Thermalization

If we consider the evolution of the Josephson equations with constant non-zero J, which corresponds to a sudden quench (i.e. when the tunnelling parameter J instantaneously jumps from J = 0 to its final value at time t = 0), then the J coefficient can be absorbed into a new timelike variable

$$u = \sqrt{J} t , \qquad (9.1)$$

with $\partial_t^2 = J \partial_u^2$, which gives

$$\partial_u^2 \theta_{\mathbf{s}} = 2 \sum_{\mathbf{r}\,\mathrm{n.n.\,s}} \sin(\theta_{\mathbf{r}} - \theta_{\mathbf{s}}) \ . \tag{9.2}$$

This dimensionless variable u introduces a time scale $u \sim 1$ or

$$\tau_{\rm T} \sim \frac{1}{\sqrt{J}} , \qquad (9.3)$$

which is a time scale of the relaxation of the system. In particular, if there is thermalization to an equilibrium, $\tau_{\rm T}$ is a scale on which such thermalization occurs.

Thermalization in one dimension is depicted in Fig. 9.1, where the correlations stabilize on values calculated in the Appendix B. The short-range correlations also saturate for higher dimensions, as depicted in Fig. 9.2 for two dimensions and Fig. 9.3 for three dimensions.

9.2 Adiabate equation

The energy of the system in the Josephson regime is a quadratic form in the variables introduced by (8.1) and reads as

$$E[\theta_{\mathbf{s}}, f_{\mathbf{s}}] = J(t) \sum_{\mathbf{s}} \nabla \theta_{\mathbf{s}} \cdot \nabla \theta_{\mathbf{s}} + 2f_{\mathbf{s}}^2 .$$
(9.4)

This allows us to refer to the equipartition principle, which says that if the energy \mathcal{E} of the system is quadratic in its variables, then the ensemble average of the energy,

$$\langle \mathcal{E} \rangle_{\mathrm{T}} \propto \iint dq_1 dp_1 \dots dq_N dp_N \ \mathcal{E}(q_1, p_1, \dots, q_N, p_N) \times \exp\left(-\frac{\mathcal{E}(q_1, p_1, \dots, q_N, p_N)}{T}\right) ,$$

$$(9.5)$$

per degree of freedom is proportional to $\frac{1}{2}T$, [1, 2]. The integration in (9.5) runs over the entire phase space and we set the Boltzmann constant k = 1. T is the temperature of



Figure 9.1: Thermalization in one dimension after an instantaneous quench. Each panel shows the relevant correlation: C_1 , C_2 , C_3 , and C_4 , where $C_R = \langle \phi_s^* \phi_{s+R} \rangle$, after an instantaneous quench from J = 0 to three defferent final J's: J = 0.0001, J = 0.001, and J = 0.01. The data collapse onto a single curve indicating that the rescaling $u = J^{1/2}t$ introduces a common time scale. The $\tau_T \sim 1/\sqrt{J}$ is indeed a thermalization time. The plots also show the thermalized value of the correlations (the dashed line) calculated in the Appendix B.

the system. Hereafter, the thermal average is denoted as $\langle \cdot \rangle_{\rm T}$ in contrast to the average $\langle \cdot \rangle$ over the statistical realizations of the Gross-Pitaevskii equation (7.7). Therefore, thermal averages of the kinetic and potential energies, (8.5) and (8.6), yield

$$\langle E_{\rm kin} \rangle_{\rm T} = \frac{1}{2} T L^D , \qquad (9.6)$$

$$\langle E_{\rm pot} \rangle_{\rm T} = \frac{1}{2} T L^D , \qquad (9.7)$$

with the total energy

$$\langle E \rangle_{\rm T} = \langle E_{\rm kin} \rangle_{\rm T} + \langle E_{\rm pot} \rangle_{\rm T} = TL^D .$$
 (9.8)

The energy given by the Hamiltonian (8.9) is not conserved during the quench, because we drive the system by varying the parameter J with time. For quenches slow



Figure 9.2: Thermalization in two dimensions after an instantaneous quench from J = 0 to J = 0.1. The local correlations thermalize, but on larger scales it takes more time for the system to equilibrate. The four panels show C_1 , C_2 , C_3 , and C_4 respectively.

enough, however, the system is close to thermal equilibrium at each instant of time and (9.6) and (9.7) hold. From now on, this regime will be referred to as the *adiabatic regime*. Thus in this regime, the temperature also varies with time, T = T(t). Our aim is to relate it to the changing J. In order to do this, we derive the differential equation for T(t) and J(t). First, the total energy changes with time through the temperature, so we can write

$$\frac{d}{dt}\langle E\rangle_{\rm T} = \frac{dT}{dt}L^D \ . \tag{9.9}$$

Second, the total energy is also a function of time due to its dependence on J. Since only the kinetic energy depends on J, $\langle E \rangle_{\rm T}$ changes at the rate

$$\frac{d}{dt} \langle E \rangle_{\rm T} = \frac{dJ}{dt} \frac{d}{dJ} \langle E_{\rm kin} \rangle_{\rm T} = \frac{dJ}{dt} \left\langle \sum_{\rm s} \nabla \theta_{\rm s} \cdot \nabla \theta_{\rm s} \right\rangle_{\rm T} \\
= \frac{dJ}{dt} \frac{\langle E_{\rm kin} \rangle_{\rm T}}{J} = \frac{dJ}{dt} \frac{T}{2J} L^D .$$
(9.10)



Figure 9.3: Thermalization in three dimensions after an instantaneous quench from J = 0 to J = 0.1. The local correlations thermalize, but on larger scales it takes more time for the system to equilibrate. The four panels show C_1 , C_2 , C_3 , and C_4 respectively.

Equating (9.9) and (9.10) we get the said differential equation relating J and T

$$\frac{dT}{dt} = \frac{dJ}{dt} \frac{T}{2J} . \tag{9.11}$$

Simple integration of (9.11) gives a direct relation T(J):

$$T = A \sqrt{J} , \qquad (9.12)$$

which will be called the *adiabate equation*, since it relates the temperature with the external parameter in an adiabatic process.

10 Impulse-adiabatic crossover

The further we are from the critical point, the closer the system follows the equilibrium, and the better the adiabatic process describes the dynamics. On the other extreme, in the vicinity of the critical point, the relative transition rate,

transition rate
$$= \frac{1}{J} \frac{dJ}{dt}$$
, (10.1)

is much larger than the pace with which the system can react to changing parameter of the Hamiltonian. This relaxation rate is equal to the inverse of the time scale of the Josephson equations, which is also the thermalization time,

relaxation rate =
$$\tau_{\rm T} = \sqrt{J}$$
. (10.2)

The state of the system changes too slowly to catch up with the changing Hamiltonian. In the limit, in which we are very close to $J_{\rm cr}$, the evolution is impulse, i.e. the state is frozen despite the changing Hamiltonian. In the truncated Wigner approximation, the atomic density n is very large, $n \gg 1$. Since $J_{\rm cr} \approx n^{-2}$, see (7.11), the critical point is at

$$J_{\rm cr} \approx 0 \ . \tag{10.3}$$

The true dynamics of the transition is very complex, the above cases of adiabatic and impulse evolution being only the limits. Nevertheless, we can make an approximation, where we extend these idealized scenarios over the whole range of the parameter J. In this approximation, as long as the transition rate (10.1) exceeds the relaxation rate (10.2), we model the dynamics to be impulse, i.e. the state to be frozen. When the transition pace drops below the relaxation rate, we assume the dynamics to be an adiabatic process, see Fig 10.1. This picture of the dynamics goes under the name of the *impulse-adiabatic approximation*, see Section 6.

The crossover between the impulse and adiabatic regimes takes place at $\hat{J} = J(\hat{t})$, when the two rates are equal:

$$\frac{1}{\hat{J}} \left. \frac{dJ}{dt} \right|_{\hat{J}} \simeq \sqrt{\hat{J}} \ . \tag{10.4}$$

If we assume the quench to be linear with time, where J(t) has the form (5.1), then

$$\frac{1}{\hat{t}} \simeq \sqrt{\frac{\hat{t}}{\tau_Q}} , \qquad (10.5)$$

which gives us the instant of time, when the crossover happens, as a function of τ_Q :

$$\hat{t} \sim \tau_Q^{1/3} \tag{10.6}$$

and hence the scaling of \hat{J} with τ_Q

$$\hat{J} \sim \tau_Q^{-2/3}$$
 (10.7)



Figure 10.1: The impulse-adiabatic scenario for the Mott insulator to superfluid transition in the truncated Wigner approximation. Notice, that this is only 'half' of the Fig. 6.1, as the Mott insulator phase is at $J \approx 0$ (J_{cr} scales with density n as $J_{cr} \sim n^{-2}$, Eq. (7.11)). Therefore we immediately enter the superfluid phase.

11 Excitation energy

Throughout the whole impulse stage of the evolution, the state of the system is frozen, as discussed in Section 6. Therefore, at the beginning of the adiabatic process, that is at \hat{J} , the system is in the "frozen" configuration, which corresponds to the initial state. In the initial state the phases are randomly distributed over $(-\pi, \pi]$ which allows us to calculate the energy at \hat{J} ,

$$\langle E_{\rm kin} \rangle \Big|_{\hat{J}} = \hat{J} \sum_{\mathbf{s}} \langle \nabla \theta_{\mathbf{s}} \cdot \nabla \theta_{\mathbf{s}} \rangle , \qquad (11.1)$$

exactly. Since the θ 's are random and independent, the average in (11.1) can be written as

$$\langle \nabla \theta_{\mathbf{s}} \cdot \nabla \theta_{\mathbf{s}} \rangle = \left\langle \sum_{\alpha} (\theta_{\mathbf{s}+\mathbf{e}_{\alpha}} - \theta_{\mathbf{s}})^2 \right\rangle$$

= $D \left\langle (\theta_{\mathbf{s}+\mathbf{e}_{\alpha}} - \theta_{\mathbf{s}})^2 \right\rangle = 2D \left(\left\langle \theta_{\mathbf{s}}^2 \right\rangle - \left\langle \theta_{\mathbf{s}+\mathbf{e}_{\alpha}} \theta_{\mathbf{s}} \right\rangle \right) .$ (11.2)
The uniform distribution for the phases renders the calculation of $\langle \theta_{\mathbf{s}}^2 \rangle$ and $\langle \theta_{\mathbf{s}+\mathbf{e}_{\alpha}} \theta_{\mathbf{s}} \rangle$ very easy:

$$\langle \theta_{\mathbf{s}}^2 \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \, \theta^2 = \frac{\pi^2}{3} \tag{11.3}$$

$$\langle \theta_{\mathbf{s}+\mathbf{e}_{\alpha}}\theta_{\mathbf{s}}\rangle = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} d\theta \int_{-\pi}^{\pi} d\theta' \,\theta\theta' = 0 \;.$$
 (11.4)

Substitution of (11.4) to (11.2) yields the value of the kinetic energy at \hat{J} ,

$$\left\langle E_{\rm kin} \right\rangle \Big|_{\hat{J}} = \frac{2\pi^2}{3} D \hat{J} L^D \ . \tag{11.5}$$

The state of the system at \hat{J} is the initial condition for the adiabatic process. Knowledge of this state allows for fixing the unknown constant A in the adiabate equation (9.12). If we recall the equipartition and use (9.6) at \hat{J} , where we know $\langle E_{\rm kin} \rangle$ due to (11.5),

$$\frac{1}{2}T\Big|_{\hat{J}}L^{D} = \frac{2\pi^{2}}{3}D\hat{J}L^{D} , \qquad (11.6)$$

then we can determine the initial temperature as

$$T\Big|_{\hat{J}} = \frac{4\pi^2}{3}D\hat{J} \ . \tag{11.7}$$

Therefore, the adiabate equation at \hat{J} reads as

$$\frac{4\pi^2}{3}D\hat{J} = A\sqrt{\hat{J}} , \qquad (11.8)$$

and the constant of proportionality is

$$A = \frac{4\pi^2}{3} D \sqrt{\hat{J}} . (11.9)$$

Now, the full adiabate equation gives the scaling of the temperature in the adiabatic process with J and τ_Q

$$T = \frac{4\pi^2}{3} D \sqrt{\hat{J}} \sqrt{J} \sim J^{1/2} \tau_Q^{-1/3} . \qquad (11.10)$$

Heretofore, we derived all the expressions using the approximation (8.1), so the obtained scalings remain true as long as $\hat{J} < J \ll 1$. The first inequality is satisfied by quenches that are slow enough, the second is ensured by remaining in the Josephson regime.

The adiabate equation (11.10) and the temperature dependence of the energy (9.6) and (9.7) give the scalings of the kinetic and potential energies with the quench rate, in the Josephson regime,

$$\langle E_{\rm kin} \rangle = \frac{1}{2} T L^D \sim J^{1/2} \tau_Q^{-1/3} L^D , \qquad (11.11)$$

$$\langle E_{\rm pot} \rangle = \frac{1}{2} T L^D \sim J^{1/2} \tau_Q^{-1/3} L^D .$$
 (11.12)

The above result means that the energy scales with τ_Q algebraically and that the power is $-\frac{1}{3}$.

The equations (11.12) were obtained by means of the Josephson approximation and the impulse-adiabatic picture of the dynamics. To see, if this feature also pertains to the original Gross-Pitaevskii equation (7.7), we turn to the numerical evolution of the original equation (7.7). The details of the *split-step* method, which we employed, can be found in the Appendix A. The resulting kinetic and potential energies are depicted in Fig. 11.1. Therein, we can see the scalings of the kinetic and potential energy with τ_Q in one, two and three dimensions, where the respective lattice sizes were L = 4096, L = 256, L = 128. In each case the simulation was performed for three final J's: J = 0.1(the Josephson regime), J = 1 and J = 10 (the Rabi regime, $J \gg 1$). In all cases there is an algebraic scaling of energy $\langle E_{\rm kin/pot} \rangle \sim \tau_Q^{-\alpha}$ with the best fit for α consistent with the predicted $\alpha = \frac{1}{3}$. The numerical values of the fitted α 's are given in the table (Tab. 11.1). This data suggests that the employed impulse-adiabatic approximation is a good model

J	$\langle E_{\rm kin}^{\rm 1D} \rangle$	$\langle E_{\rm kin}^{\rm 2D} \rangle$	$\langle E_{\rm kin}^{\rm 3D} \rangle$	$\langle E_{\rm pot}^{\rm 1D} \rangle$	$\langle E_{\rm pot}^{\rm 2D} \rangle$	$\langle E_{\rm pot}^{\rm 3D} \rangle$
0.1	0.33	0.33	0.33	0.33	0.30	0.30
1.0	0.33	0.33	0.33	0.33	0.31	0.31
10.0	0.33	0.33	0.33	0.32	0.31	0.31

Table 11.1: The best fits to α in $\langle E_{\rm kin/pot} \rangle \sim \tau_Q^{-\alpha}$ are consistent with $\alpha = 1/3$. The fits to the data displayed in Fig 11.1; in each case, the error is not larger than ± 0.003 .

of the physics beyond the observed scalings.

12 Dynamics in the Rabi regime

The formulae we derived so far are valid in the Josephson regime, $J \ll 1$. However, the data of Fig. 11.1 and Tab. 11.1 suggests, that the obtained results extend over to $J \sim 1$ and $J \gg 1$. This section is devoted to the analysis of this regime $(J \gg 1)$, which is called the *Rabi regime*. The kinetic term in (7.7) now dominates but the nonlinear



Figure 11.1: The figure shows dependence of the kinetic energy density (left column) and potential energy density (right column) for 1D (the upper row), 2D (the middle row) and 3D lattice (the bottom row). The lattice size L = 4096, 256, 128 in 1D, 2D, 3D respectively. For large $\tau_Q \gg 1$ we observe a power-law behaviour consistent with the predicted $\langle E \rangle \sim \tau_Q^{-1/3}$. The best fits to the tails of the energy plots (the solid lines) give the exponents listed in Table 11.1.

term cannot be neglected, because it is necessary for thermalization. Thus, in the Rabi regime $\langle E_{\rm kin} \rangle \gg \langle E_{\rm pot} \rangle$ and

$$\langle E \rangle \approx \langle E_{\rm kin} \rangle \ .$$
 (12.1)

A derivation similar to the one in Subsection 9.2 leads to the equation for $\langle E_{\rm kin} \rangle$,

$$\frac{d}{dt}\langle E\rangle = \frac{d}{dt}\langle E_{\rm kin}\rangle = \frac{dJ}{dt}\frac{\langle E_{\rm kin}\rangle}{J} \ . \tag{12.2}$$

It yields a simple solution, which reads as

$$\langle E_{\rm kin} \rangle = B J , \qquad (12.3)$$

where B is a proportionality constant to be determined.

The crossover from the Josephson to the Rabi regime is roughly at $J \approx 1$. Therefore, the final state at that instant of time is the initial state for the evolution in the Rabi regime and hence the initial condition for (12.3). The equality between the energy at $J \approx 1$ calculated in the Rabi regime (E) and in the Josephson regime ($E^{(\text{Josephson})}$) allows for determination of the unknown constant B. Therefore we have

$$\langle E \rangle \Big|_{J\approx 1} = \langle E^{(\text{Josephson})} \rangle \Big|_{J\approx 1} \simeq J^{1/2} \tau_Q^{-1/3} L^D \Big|_{J\approx 1} = \tau_Q^{-1/3} L^D , \qquad (12.4)$$

and since $\langle E_{\rm kin} \rangle \Big|_{J \approx 1} = B$, we get

$$B = \tau_Q^{-1/3} L^D . (12.5)$$

Substitution of (12.5) back to (12.3) gives the full dependence of the energy on J and τ_Q in the Rabi regime:

$$\langle E \rangle \approx \langle E_{\rm kin} \rangle \simeq J \tau_Q^{-1/3} L^D .$$
 (12.6)

This shows how the scaling with the power $-\frac{1}{3}$ holds also for $J \gg 1$.

Equation (12.6) is valid as long as the impulse-adiabatic crossover takes place in the Josephson regime, which, in accordance with (10.7) $(\hat{J} \sim \tau_Q^{-2/3})$, is true for quenches that are slow enough ($\tau_Q \gg 1$). For fast quenches, however, the impulse-adiabatic crossover is located in the Rabi regime, and the significant part of the impulse stage extends into this regime. In this case, the thermalization (relaxation) time is set by the strength of the nonlinearity in the Gross-Pitaevskii equation (7.7): $\tau_T \simeq 1$. Therefore the impulse-adiabatic crossover now satisfies

$$\frac{1}{J} \left. \frac{dJ}{dt} \right|_{\hat{J}} = \frac{1}{\hat{t}} \approx \tau_{\mathrm{T}}^{-1} \simeq 1 \ . \tag{12.7}$$

This determines the time instant of the crossover, $\hat{t} \approx 1$, and \hat{J} :

$$\hat{J} = \frac{\hat{t}}{\tau_Q} \gg 1 \qquad \text{for } \tau_Q \ll 1 .$$
(12.8)

The state of the system remains frozen through the evolution until the crossover at \hat{J} . For the initial configuration of the Mott state with unit density and random phase we have

$$\langle E_{\rm kin} \rangle = J \sum_{\mathbf{s}} \langle \nabla \phi_{\mathbf{s}}^{\star} \cdot \nabla \phi_{\mathbf{s}} \rangle = J \sum_{\mathbf{s}} \langle \nabla e^{-i\theta_{\mathbf{s}}} \cdot \nabla e^{i\theta_{\mathbf{s}}} \rangle = \langle \nabla \theta_{\mathbf{s}} \cdot \nabla \theta_{\mathbf{s}} \rangle , \qquad (12.9)$$

and therefore at \hat{J} energy reads as

$$\langle E_{\rm kin} \rangle \Big|_{\hat{J}} = \hat{J}D \frac{2\pi^2}{3} L^D \simeq \hat{J}L^D$$
 (12.10)

Since in the Rabi $\langle E_{\rm kin} \rangle \sim J$, Eq. (12.3), the proportionality constant can be fixed as

$$\langle E_{\rm kin} \rangle = \frac{J}{\hat{J}} \langle E_{\rm kin} \rangle \Big|_{\hat{J}} = D \frac{2\pi^2}{3} J L^D , \qquad (12.11)$$

which gives the energy behaviour for $\tau_Q \ll 1$. The immediate observation is, that it does not depend on τ_Q . This is consistent with the numerical data (Fig. 11.1), where for fast quenches in the Rabi regime the kinetic energy is constant.

13 Quench in a 3D harmonic trap

In the experimental conditions, the gas of ultracold atoms has to be kept within a limited area. Therefore, the whole system, atoms and a lattice potential, is additionally trapped by an external field. In order to see, whether our results reproduce also in this case, we set $V_{\rm s} \neq 0$ in our model (3.1) and, consequently, in (7.7). We choose a generic trapping potential

$$V_{\mathbf{s}} = \frac{\omega^2}{2} \,\mathbf{s}^2 \,, \tag{13.1}$$

i.e. the harmonic potential; any minimum of a smooth potential can be approximated by a quadratic form.

The Gross-Pitaevskii equation (7.7) becomes

$$i\partial_t \phi_{\mathbf{s}} = -J\nabla^2 \phi_{\mathbf{s}} + |\phi_{\mathbf{s}}|^2 \phi_{\mathbf{s}} + \frac{\omega^2}{2} \,\mathbf{s}^2 \,\phi_{\mathbf{s}} - \mu \phi_{\mathbf{s}} \,\,, \tag{13.2}$$

where the initial state is again the Mott state, now modified by the presence of a trap. Thus, at J = 0, the phases θ 's are random, uniformly distributed as in (7.10), but the density is centred around the centre of the trap. Thus, $|\phi_s|$ is a solution to the stationary equation (13.2) at J = 0:

$$|\phi_{\mathbf{s}}|^2 \phi_{\mathbf{s}} + \frac{\omega^2}{2} \, \mathbf{s}^2 \, \phi_{\mathbf{s}} - \mu \phi_{\mathbf{s}} = 0 \ . \tag{13.3}$$

So, if $\phi_{\mathbf{s}} \neq 0$, the solution has the form

$$|\phi_{\mathbf{s}}|^2 = -\frac{\omega^2}{2}\mathbf{s}^2 + \mu = \frac{\omega^2}{2}\left(R_{\mathrm{TF}}^2 - \mathbf{s}^2\right) ,$$
 (13.4)

where we set $\mathbf{s}_{\text{cent}} = 0$ to be the centre of the trap. The last equality introduces a radius R_{TF} in place of the chemical potential μ . For the sites, where $\mathbf{s}^2 < R_{\text{TF}}^2$ the distribution

is given by (13.4) and for $\mathbf{s}^2 \geq R_{\text{TF}}^2$ the field vanishes, $|\phi_{\mathbf{s}}| = 0$. This distribution is called the *Thomas-Fermi distribution* and the radius R_{TF} the *Thomas-Fermi radius*.

In case of no trap present, the field has a constant density chosen to be $|\phi_s| = 1$. This sets the normalization (7.4). In case of a trap present, we still have to determine $R_{\rm TF}$, given the trap width ω . Hence, in order to make the comparison with the uniform case easier, we choose the normalization where

$$|\phi_{\mathbf{s}_{cent}}(0)|^2 = 1 \tag{13.5}$$

at the centre. Thus,

$$\omega^2 = \frac{2}{R_{\rm TF}^2} , \qquad (13.6)$$

which sets the chemical potential to $\mu = 1$.

13.1 Ground state

In contrast to the case of a uniform system, where the ground state energy was zero, in the presence of the trapping potential, the ground state energy is non-zero. Therefore, if we want to calculate the excitation energy, as we did in Section 11, we have to subtract the ground state energy from the one calculated with the formulae (7.12) and (7.13).

According to the procedure presented in Section 7, we calculate the ground state as the asymptotic stationary state of the equation (7.16):

$$-\frac{\delta}{\delta\phi_{\mathbf{s}}^{\star}}E[\phi_{\mathbf{s}},\phi_{\mathbf{s}}^{\star}] = \partial_t\phi_{\mathbf{s}} , \qquad (13.7)$$

subject to the constraint

$$\sum_{\mathbf{s}} |\phi_{\mathbf{s}}|^2 = \text{const.} , \qquad (13.8)$$

i.e. the norm should be kept constant throughout the evolution. After the evolution time long enough, the solution attains its stationary state, and the time derivative $\partial_t \phi_s$ in (13.7) vanishes. The evolution of (13.7) is presented in the Fig. 13.1, where three panels show the cross sections of the field configurations in different instants of time and for various values of J, and the last panel shows the corresponding energies. We can see that with time, the configurations converge to the limiting configuration and that the corresponding energies also stabilize. For $J \ll 1$ the solution to (13.7) is approximately the Thomas-Fermi distribution. For $J \gg 1$ (J = 10 in Fig. 13.1), the ground state is a near-Gaussian, as is discussed below. For $J \sim 1$ the ground state is some intermediate state between the two limiting cases.



Figure 13.1: The figure shows the calculation of the ground state in presence of the external trapping potential. Three panels present the evolution of (13.7) for J = 0.1 (upper left), J = 1 (upper right) and J = 10 (bottom left). The initial configuration, which has been chosen to be a Gaussian with width $(\sqrt{2J}/\omega)^{1/2}$, evolves and converges to the ground state. For $J \ll 1$, the ground state is close to the Thomas-Fermi profile (13.4) and for $J \gg 1$ it is close to the Gaussian. The corresponding energies (bottom right) also converge to the ground state energy.

13.2 Cloud expansion

When the cloud expands, the initial Thomas-Fermi profile broadens. For $J \gg 1$, when the nonlinear therm can be neglected, the equation

$$i\partial_t \phi_{\mathbf{s}} = -J\nabla^2 \phi_{\mathbf{s}} + \frac{\omega^2}{2} \,\mathbf{s}^2 \phi_{\mathbf{s}} \tag{13.9}$$

can be solved exactly. This is a discrete version of the Schrödinger equation for the three-dimensional harmonic oscillator [74], which in standard form reads as

$$i\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{m\omega^2}{2} \psi . \qquad (13.10)$$

Therefore, the ground state is known to be the Gaussian and (13.9) has the following solution

$$\phi_{\mathbf{s}}^{\mathrm{GS}} = \left(\frac{\omega}{2\sqrt{2J}}\right)^{3/2} \exp\left(-\frac{\omega}{2\sqrt{2J}} \mathbf{s}^2\right) , \qquad (13.11)$$

for $J \gg 1$, [74]. An example of the evolution of the cloud is shown in Fig 13.2, where the cross section of ϕ_s is depicted for three different instants of time. Again, the initial configuration is the Thomas-Fermi distribution, which goes through an expansion and finally reaches the profile, which is well approximated by the Gaussian.



Figure 13.2: The cross section through the centre of a 3D lattice for the system in the trapping potential. The numerical data shows $|\phi_s|^2$ in three subsequent instants of time for a single realisation from the ensemble. The black line shows the initial configuration, which is the Thomas-Fermi profile, at J = 0. The red line is an intermediate stage for J = 1. The green line is the field at J = 10, where the configuration is close to the Gaussian (13.11). The quench was performed with $\tau_Q = 102.4$.

13.3 Excitation energy

Having computed the ground state energy, we are now ready to calculate the energy of excitations above the ground state. The numerical data, presented in the Fig. 13.3 suggests, that the excitation energy

$$\langle E_{\text{excit}} \rangle = \langle E \rangle - \langle E_{\text{GS}} \rangle$$
 (13.12)

scales with $-\frac{1}{3}$ as in the uniform case. This reinforces the results of Section 11 and remains in an agreement with the experimental data obtained in [18], where the algebraic

scaling of the excitation energy was obtained, and the exponent was numerically close to $\frac{1}{3}$.



Figure 13.3: Excitation energy above the Gross-Pitaevskii ground state at a given J, $\langle E \rangle - E_{\rm GS}(J)$, as a function of τ_Q for a three dimensional lattice in a harmonic trap. The tails $\langle E \rangle - E_{\rm GS} \sim \tau_Q^{-\alpha}$ for large $\tau_Q \gg 1$ are best fitted with the exponents: $\alpha = 0.31$ for J = 0.1, $\alpha = 0.32$ for J = 1.0, and $\alpha = 0.31$ for J = 10.0. Here, the lattice size is $64 \times 64 \times 64$ and the initial Thomas-Fermi radius $R_{\rm TF} = 10$.

13.4 Breathing mode

The excitation energy discussed in the Section above comes from both the kinetic energy of the phases and the energy associated with the cloud expansion. In order to isolate the effect of expansion from the Kibble-Zurek mechanism, we repeat the simulation with a constant initial phase across the lattice. Since the choice of the constant phase is arbitrary, we choose

$$\theta_{\mathbf{s}}(0) = 0 \ . \tag{13.13}$$

The results of the simulation are presented in Fig. 13.4. The excitation energy is lower by a factor of the order of $\sim 10^2$ compared to the data in Fig. 13.3. Moreover, the decay of the energy with τ_Q is far steeper and the exponent of this decay is closer rather to 1/2. This is not too surprising, as the kinetic energy density of the random phases, $\simeq J$, far outweighs average density of kinetic energy in the Thomas-Fermi profile with a constant phase, $\simeq JR_{\rm TF}^{-2}$, for any reasonable $R_{\rm TF} \gg 1$.



Figure 13.4: The same excitation energy as in Fig. 13.3 but with constant initial phases $\theta_s = 0$. For large τ_Q the energy decays approximately like $\tau_Q^{-0.5}$ at J = 0.1 and $\tau_Q^{-0.4}$ at J = 10 i.e. faster than for the random initial phases in Fig 13.3. The size of the lattice is $64 \times 64 \times 64$.

The exponent -1/2 for the constant initial phase can be explained by an impulseadiabatic argument again. When $J \ll 1$, the Thomas-Fermi profile (13.4) is a good approximation to the ground state of the discrete Gross-Pitaevskii equation. When

$$R_{\rm TF} \gg 1$$
, (13.14)

we can decompose the field $\phi_{\mathbf{s}}$ into the Thomas-Fermi part and the Bogolyubov excitation above it,

$$\phi_{\mathbf{s}} = \phi_{\mathbf{s}}^{(0)} + \delta\phi_{\mathbf{s}} . \tag{13.15}$$

Since

Im
$$\phi_{\mathbf{s}}^{(0)} = 0$$
, Re $\delta \phi_{\mathbf{s}} = 0$, (13.16)

we can write

$$i\partial_t \,\delta\phi_{\mathbf{s}} = -J\nabla^2 \delta\phi_{\mathbf{s}} + \delta\phi_{\mathbf{s}} \,. \tag{13.17}$$

The Gross-Pitaevskii equation (7.7), simplifies to the equation for $\delta \phi_s$:

$$i\partial_t \delta\phi_{\mathbf{s}} = -J\nabla^2 \delta\phi_{\mathbf{s}} + |\phi_{\mathbf{s}}^{(0)}|^2 \delta\phi_{\mathbf{s}} + \frac{\omega^2}{2} \mathbf{s}^2 \delta\phi_{\mathbf{s}} - \mu\delta\phi_{\mathbf{s}} .$$
(13.18)

The solution for $\delta \phi_{\mathbf{s}}$ (the lowest Bogolyubov excitation) reads as

$$\delta\phi_{\mathbf{s}} = -i \text{ const. } \sin\left(\frac{\pi^2 J}{R_{\mathrm{TF}}^2}t + \varphi\right) \frac{\sin\left(\frac{\pi}{R_{\mathrm{TF}}}|\mathbf{s}|\right)}{\frac{\pi}{R_{\mathrm{TF}}}|\mathbf{s}|}$$
(13.19)

in bulk of the Thomas-Fermi distribution and $\delta \phi_{s} = 0$ otherwise. The details of the calculation can be found in Appendix C. It is a breathing mode describing radial flow of particles. In a linear quench of the tunnelling rate (5.1), the evolution is impulse as long as the transition rate,

$$\frac{1}{J}\frac{dJ}{dt} , \qquad (13.20)$$

is much less than the frequency $\frac{\pi}{R_{\rm TF}}|{f s}|,$ i.e. up to

$$\hat{J} \simeq R_{\rm TF} \tau_Q^{-1/2} , \qquad (13.21)$$

by the impulse-adiabatic argument again. At \hat{J} the wavefunction is still the initial Thomas-Fermi profile (13.4) with a constant phase, but the profile is no longer the ground state of the discrete Gross-Pitaevskii equation and its excitation energy with respect to the ground state is

$$E - E_{\rm GS} \simeq \hat{J} R_{\rm TF} \simeq R_{\rm TF}^2 \tau_Q^{-1/2}$$
 (13.22)

It decays with τ_Q with the exponent $-\frac{1}{2}$.

The kinetic energy associated with the random phases at the beginning of the evolution indeed far exceeds the energy of the harmonic confinement and the contribution of the former dominates and determines the scaling exponent. By an argument of a dimensional analysis, the kinetic energy of the random phases should scale as $1/a^2$, where *a* is the lattice constant. The energy associated with the confinement, on the other hand, scales as $1/R_{TF}^2$. Therefore, the domination of the random phases energy yields

$$\frac{1}{R_{\rm TF}^2} \ll \frac{1}{a^2}$$
 (13.23)

In our units, the lattice constant a = 1, which thereby translates the above condition into the assumed $R_{\text{TF}}^2 \gg 1$.

CHAPTER 3

Correlations and vortices

14 Correlations

While in the Mott insulator state there are no correlations between the sites of a lattice, the superfluid phase exhibits correlations. In one dimension, the correlation function,

$$C_R = \langle \phi_s^{\star} \phi_{s+R} \rangle \simeq \langle e^{-i\theta_s} e^{i\theta_{s+R}} \rangle , \qquad (14.1)$$

is exponential with the characteristic length

$$\xi \approx \frac{4J}{T} \approx \frac{J^{1/2}}{\hat{J}^{1/2}} \simeq J^{1/2} \tau_Q^{1/3} ,$$
 (14.2)

see Appendix B for a detailed derivation. Therefore, at the impulse-adiabatic crossover, \hat{J} , phases are still uncorrelated, but with growing J correlations build up with their length growing like $J^{1/2}$. Also, the slower the quench, the longer the correlations, as they have more time to spread across the system in the adiabatic process. According to (14.2), ξ grows as $\tau_Q^{1/3}$ with the quench time. These expectations remain in agreement with the numerical data shown in Fig. 14.1, where the correlations form straight lines in the *semi-log* plot with their range growing according to (14.2).

The situation is different in dimensions higher than one. Whereas in one dimension there is a finite correlation length for all temperatures, in three dimensions there is longrange order in the low-temperature phase. In two dimensions, there cannot be a longrange order, according to the Mermin-Wagner-Hohenberg theorem, [36, 5, 11]. However, there can be a Berezinskii-Kosterlitz-Thouless transition to the low-temperature phase,



Figure 14.1: Correlation functions C_R in one dimension for various quench times τ_Q for J = 0.1 (Josephson regime). The correlations decay exponentially. The slower the quench, the larger the correlation length ξ , which grows algebraically with τ_Q : $\xi \sim \tau_Q^{\alpha}$, where α can be fitted as $\alpha = 0.329$, in agreement with the predicted 1/3, see (14.2).

where there is a *quasi*-long-range order, i.e. the correlations decay in an algebraic way and the correlation length is not finite either.

However, since the rate of the adiabatic process is finite, $\tau_Q < \infty$, the (quasi-)longrange order cannot be reached, and the correlations have finite range, see Fig. 14.2 for the relevant numerical data. Although the long-range order is not achieved, and the long-range correlations thermalize slowly, the equilibration of the short-scale correlations is quick (see also Figs. 9.2 and 9.3), and the equipartition principle (9.6) and (9.7) used in Subjection 9.2 is justified. If we prepare the initial state to be correlated, and then allow it to evolve freely with a fixed value of J, then the correlation function increases its range with the time of the evolution, as depicted in Fig. 14.3.

15 Vortex excitations

In two and three dimensions, the finite rate of the transition and the resulting finite range of correlations lead to the formation of domains, whose size is of the order of ξ . In each such domain, the phase is ordered, but the whole system is a mosaic of domains, each with a different value of the phase. Since the phase is defined in $[-\pi, \pi)$, modulo 2π , the formation of domains leads to topological vortex excitations. The net phase winding along a closed path around a vortex is an integer multiplicity of 2π . For fast quenches, there is little time for the correlations to spread and, as a result, there



Figure 14.2: Correlation functions in two and three dimensions (left and right panel respectively) in the Josephson regime, J = 0.1. The local observables (short-scale correlations) equilibrate quickly, but at large scales the system does not have enough time to develop a (quasi-)long-range order. Instead, the correlations have finite range, which grows faster than $\tau_Q^{1/2}$ with the quench time.

is a big number of small domains and plethora of vortices. When the quench is slow, the resulting domains become larger with fewer, more prominent vortices. Fig. 15.2(a) presents such vortices for a slow and a fast quench in the Josephson regime. In this regime, when $J \ll 1$, the fluctuations of density $|\phi_s|$ are small, and the healing length is less than the lattice spacing. Therefore, the dips corresponding to the vortex cores are not clearly visible, see the right panel of Fig. 15.2(a). For larger J's, however, the dips associated with the vortex cores are more pronounced, see Fig. 15.1, where the vortices in phase and the corresponding dips in density are marked with arrows.

In the presence of a trapping potential, considered in Section 13, the density is centred in the middle of the trap. In quenches slow enough vortices might also be seen as in the case of the uniform system. See Fig. 15.2(b) for a cross section throughout a three dimensional lattice. The phase has a smooth, topological vortex close to the center of the trap, and the corresponding density displays a dip associated with this vortex.



Figure 14.3: Thermalization in 3D. In this figure we show the correlation function $C_R(u) = \frac{1}{n} \langle a_s^{\dagger} a_{s+R} \rangle = \langle \phi_s^{\star} \phi_{s+R} \rangle$ for several values of the rescaled time $u = J^{1/2}t$ at a fixed J = 0.01. The initial state at u = 0 has phase correlations of finite range. It is prepared by a linear quench from the initial Mott state (3.4), (7.10) at J = 0 to J = 0.01 with $\tau_Q = 512$. After this ramp, this low-energy initial state thermalizes at the fixed J = 0.01 towards a low-temperature thermal state with long-range order. While the short range correlations C_R with small R are quick to thermalize, see Fig. 9.3, the long-range correlations are slow to develop the long-range order expected at low temperature. As we can see in this figure, the range of C_R roughly doubles when the time u increases by a factor of 4, i.e. the correlation range grows like the square root of time.



Figure 15.1: A quench with $\tau_Q = 3276.8$ at J = 1 on a part of a 2D periodic 256×256 lattice. In the left panel the phase θ_s and in the right panel the density distribution $|\phi_s|^2$. The three arrows mark an isolated vortex and a vortex-antivortex pair. Unlike in the Josephson regime at J = 0.1, where density fluctuations are small and vortex cores are less than the lattice spacing, see Fig. 15.2(a), here, at J = 1, the topological vortices in the left panel are associated with clear dips in atomic density marked in the right panel.



of random vorticity. In the slower quench (middle panel), it is possible to identify smooth topological vortices (marked by the arrows). of domains of constant phase is consistent with the range of 2D correlations in Fig. 14.2. In the faster quench (left panel), there is plenty middle panel. The left and middle panel demonstrate that the range of phase correlations increases with increasing τ_Q . Average size between different sites. The associated density fluctuations in the **right panel** are small, within 10% of the average density $|\phi_s|^2 = 1$, and very weakly correlated (Middle panel): phase θ_s for a quench time $\tau_Q = 52428.8$. (Right panel): atomic density $|\phi_s|^2$ associated with the phase in the (a) Quench on a 2D periodic 256×256 lattice in the Josephson regime at J = 0.1. (Left panel): phase θ_s for a quench time $\tau_Q = 1638.4$.



plane. The arrows in the **left** and the **middle panel** point to a vortex. x - y cross section across the centre of the trap. (**Right panel**): cumulative column density in the direction perpendicular to the x - y $128 \times 128 \times 128$ lattice. (Left panel): phase in the x - y cross section across the centre of the trap. (Middle panel): density in the (b) Linear quench in the 3D trap with $\tau_Q = 204.8$ and the initial Thomas-Fermi radius $R_{\rm TF} = 25$ at the tunnelling rate J = 1 for

of harmonic trap. The finite rate of the quench causes a spontaneous vortex formation. Figure 15.2: Phase and corresponding density for the 2D lattice in Josephson regime and the 3D lattice in the presence

CHAPTER 4

Trapped winding number

16 Winding number

Until this point, we considered lattices in one, two and three dimensions. One-dimensional systems, however, turn out to have interesting properties, which are absent in higher dimensions. Now, we restrict our attention to one dimension, where the linear quench (5.1) leads to extra phenomena.

When the system is one-dimensional, which in case of periodic boundary conditions is a ring, we can define a topological quantity called *winding number*. The phase θ_s of the field ϕ_s has values in $(-\pi, \pi]$ modulo 2π , so if the field ϕ were a continuous, singlevalued function defined on the ring, $\phi = \phi(\varphi)$, then the integral of the phase along the ring,

$$\int_0^{2\pi} \theta'(\varphi) \ d\varphi = 2\pi n \ , \tag{16.1}$$

would have to be an integer multiple of 2π . Here φ parametrizes the position on the ring. In our case, the field is discrete, but we can also introduce an analogue of (16.1) with the integer winding number W given by

$$W = \frac{1}{2\pi} \sum_{s=0}^{L-1} (\theta_{s+1} - \theta_s) \Big|_{\in (-\pi,\pi]} .$$
 (16.2)

In order to account for the phase crossing the cut (exceeding the allowed range $(-\pi, \pi]$), we bring the value of each phase step between the nearest-neighbours, $\theta_{s+1} - \theta_s$, to the interval $(-\pi, \pi]$. Thus, each time we have to add or subtract 2π from the phase difference, we add a non-zero contribution to W.



Figure 16.1: An intuitive picture presenting the one-dimensional optical lattice with periodic boundary conditions, i.e. a ring. By gradually lowering the barrier separating the wells, atoms are allowed for more tunnelling and, thus, the initially isolated Bose-Einstein condensates (BEC's, depicted here as green spheres) begin to interact. We are interested in the net winding of the phase θ_s that builds up when the BEC's begin to interconnect.

The averaged variance of the winding number, $\langle W^2 \rangle$, is depicted in the Fig. 16.2 as a function of the quench time τ_Q (see Eq. (5.1)). The initial phases are independent, so with (11.3) and (11.4) the initial $\langle W^2 \rangle$ equals:

$$\langle W^2 \rangle = \frac{L}{12} , \qquad (16.3)$$

where L is the length of the ring. For small values of τ_Q , when the transition is fast, there is not enough time for the phases to correlate, so they remain close to their initial value. With τ_Q increasing, the phases enter the scaling regime and decay according to Kibble - Zurek mechanism [41]. Contrary to expectations, however, this scaling ceases to hold at a certain point and the decay does not continue. At τ_Q^c there is a crossover to a regime, where $\langle W^2 \rangle$ freezes at a finite value regardless of the final J or τ_Q , [44].

17 Josephson regime

We begin the study of the mechanism responsible for the freezing of the winding number with the investigation of the Josephson regime, akin to the procedure used in Section 8.



Figure 16.2: the averaged squared winding number, $\langle W^2 \rangle$, as a function of τ_Q . Simulation of (17.1) on a L = 512 ring, averaged over 210^4 realizations. For each J the variance of the winding number, $\langle W^2 \rangle$, saturates above a certain value of $\tau_Q = \tau_Q^c$. The saturated value does not depend on J.

The Josephson equations (8.2) in one dimension read as

$$\partial_t^2 \theta_s = 2J(t) \left\{ \sin(\theta_{s+1} - \theta_s) + \sin(\theta_{s-1} - \theta_s) \right\} . \tag{17.1}$$

Hereafter, s is a single integer numbering sites of the ring.

We can rescale time t in order to eliminate J and introduce a single parameter measuring time: u. In contrast to the change of variables in (9.1), where J was constant, here J is a function of time, J = J(t), and the following rescaling is more convenient

$$u = t \tau_Q^{-1/3} = J(t) \tau_Q^{2/3} . (17.2)$$

As a result we obtain dimensionless equations

$$\partial_u^2 \theta_s = 2u \left\{ \sin(\theta_{s+1} - \theta_s) + \sin(\theta_{s-1} - \theta_s) \right\}$$
(17.3)

with the initial conditions being random $\theta_s(0)$ and $\partial_u \theta_s(0) = 0$. The equations for L > 2 are chaotic, which means that the evolution is ergodic.



Figure 17.1: Simulation of (17.1) with the truncated Wigner method, averaged over 210^4 configurations. (a) The saturated variance $\langle W^2 \rangle$ at J = 0.01 and $\tau_Q = 52428.8$ as a function of lattice size L. The solid line is a linear fit $\langle W^2 \rangle = 0.0079 L$ for $L \ge 16$. At L = 8 the variance is below the linear fit and at L = 4 (not shown) it is zero. (b) Histograms of the modulus $|\phi_s|$ at J = 0.01 for $\tau_Q = 52428.8$ and L = 512. In the Josephson regime $J \ll 1$ fluctuations of the modulus around $|\phi_s| = 1$ are small. (c) Generic histogram of phase steps $\theta_s - \theta_{s+1}$, here at J = 0.01, $\tau_Q = 52428.8$ and L = 512. The solid line is a Gaussian fit.

18 Thermalization

The system (17.3) thermalizes approximately at $\hat{u} \approx 1$, which corresponds to a crossover to the adiabatic regime. The state of the system follows the instantaneous equilibrium with time-dependent temperature. The averages of local observables can be computed as thermal averages obtained from Boltzmann distribution.

The average of the phase step $\Delta \theta_s = \theta_{s+1} - \theta_s$ vanishes

$$\langle \theta_{s+1} - \theta_s \rangle = 0 , \qquad (18.1)$$

but its variance

$$\sigma^2 = \left\langle (\theta_{s+1} - \theta_s)^2 \right\rangle \tag{18.2}$$

remains non-zero and is shrinking after \hat{u} , see Fig. 18.1. Hence, the energy expression for the Josephson equations (17.3) (compare with the Hamiltonian (8.9) in Section 8) becomes approximately quadratic:

$$E = \frac{1}{2} \sum_{s} \left(\frac{d\theta_s}{dt} \right)^2 + 2J(t) \sum_{s} \left(1 - \cos(\theta_{s+1} - \theta_s) \right)$$
$$\approx \sum_{s} \left\{ \frac{1}{2} \left(\frac{d\theta_s}{dt} \right)^2 + J(t)(\theta_{s+1} - \theta_s)^2 \right\} .$$
(18.3)

Therefore, the Boltzmann distribution of phase steps $\Delta \theta_s$ becomes a Gaussian of zero mean,

$$f \sim e^{-\frac{1}{T}J(t)\Delta\theta^2} = e^{-\frac{\Delta\theta^2}{2\sigma^2}} , \qquad (18.4)$$

with the variance obeying

$$2 J(t) \sigma^2 = T . (18.5)$$

The equation (18.5) gives the relation between the shrinking σ and temperature as the system cools down during the evolution.

Because the energy is quadratic, the equipartition principle applies. For the Josephson system it was already discussed in Section 9. There, we derived the adiabate equation (9.12),

$$T \sim \hat{J}^{1/2} J^{1/2} \sim \frac{J^{1/2}}{\tau_O^{1/3}}$$
 (18.6)

With (18.5) we finally obtain a relation between the variance σ^2 and the dimensionless time u

$$\sigma^2 = \frac{T}{2J} \sim \frac{J^{1/2}}{J \tau_Q^{1/3}} = \frac{1}{J^{1/2} \tau_Q^{1/3}} = \left(\frac{1}{J \tau_Q^{2/3}}\right)^{1/2} = u^{-1/2} , \qquad (18.7)$$

which translates to $\sigma \sim u^{-1/4}$, a numerical evidence of which is provided in Fig. 18.1(a).

19 Breaking of ergodicity

With shrinking σ^2 the quadratic approximation for the energy (18.3) becomes more and more accurate and the system passes from a regime where its behaviour is chaotic to a regular regime. This change from the ergodic to an integrable system can be observed in the behaviour of the winding number (16.2). As Fig. 18.1(b) suggests, at the beginning of the evolution the system ergodically scans the space of the available winding numbers.



Figure 18.1: In panel (a), the dispersion σ of the phase step $\Delta \theta_s = \theta_{s+1} - \theta_s$ as a function of the rescaled time u for various quench times τ_Q (lattice of L = 2048 sites). The plot shows that the data collapse onto a single curve, i.e. the variable u eliminates the quench time τ_Q . The linear fit to the data in the *log-log* plot confirms the prediction with the fitted exponent: $\sigma \sim u^{-0.28}$. The panel (b) presents the corresponding single realizations of the winding numbers W's evolving with time measured with u. After the dispersion shrinks below σ_c , the jumps of the winding number become suppressed and eventually W gets trapped. The dispersion σ shrinks to σ_c at $u_c \simeq 20$.

As u grows larger the jumps between the winding numbers are less and less frequent and at u_c the system freezes at a fixed value of W and cannot overcome the barrier separating W from $W \pm 1$. In the Josephson regime, $J \ll 1$, the change of W is a result of a *phase slip* located on a particular link

$$\theta_{s+1} - \theta_s = \pm \pi \ . \tag{19.1}$$

An example of such a *slip* is given in Fig. 19.1 and Fig. 19.2.



Figure 19.1: The mechanism of the winding number trapping. The (left panel) shows the configuration of the phase before (black line) and after (red line) the last jump of Wfrom Fig. 18.1. The jump of the winding number results from an instability at a single link (that is between two adjoining sites). The phase step $\Delta \theta_s$ grows to just below π and in the nest step of the evolution crosses the cut acquiring the value just above $-\pi$ and therefore accounting for a -1 contribution to the overall winding number. The instability grows with time, as shown for the same realization in the (right panel) until it crosses the $\pi/-\pi$ boundary.

According to the LAMH theory [75, 76, 77], when

$$\left|\frac{W}{L}\right| \ll 1 \tag{19.2}$$

the frequency of the winding number jumps is $\propto e^{-\beta 4J}$, where the 4J is energy (18.3) of the localized phase slip. Since the temperature is $\beta^{-1} = T = 2J\sigma^2$ in (18.5), this activation coefficient is $\propto e^{-2/\sigma^2}$ and the integer winding number freezes out when σ falls below

$$\sigma_c \simeq 1 \tag{19.3}$$

From the data in Fig. 18.1(b) this happens at time $u_c \simeq 20-50$. This is when ergodicity



Figure 19.2: The picture shows the data from the Fig. 19.1 from a different perspective. It shows the segment of the chain as it evolves with time u. The intensity corresponds to the value of the phase integrated along the ring (a "partial" winding number), $\Theta_s = \sum_{j=1}^{s} (\theta_{j+1} - \theta_j) |_{\in(-\pi,\pi]}$. The time instant of the jump as well as its location in the chain are clearly visible: at $u \approx 33.07$ the winding number jumps by -1 at the link between the 355th and 356th site. In other words, the phase step $\Delta \theta_{355} = \theta_{356} - \theta_{355}$ jumps from π to $-\pi$ accounting for the net change in the winding number W.

between different W's breaks down and the winding number (distribution) gets stuck.

20 Trapped Winding Number

The phase θ_s performs a random walk and, below σ_c , the phase step dispersion is shrinking. Therefore, the random walk of $\theta_s(u)$ keeps smoothing out while u increases. Hence, when the temperature is low enough, so that it cannot induce jumps of the net winding number, the resulting frozen value of $\langle W^2 \rangle$ is determined by the state of the random walk at $\sigma = \sigma_{\rm c}$. Therefore,

$$\langle W^2 \rangle = \frac{1}{(2\pi)^2} L \,\sigma_{\rm c}^2 \,, \qquad (20.1)$$

which agrees with a linear fit to the data depicted in Fig. 17.1(a), where the fitted relation yields

$$\langle W^2 \rangle \approx 0.0079 \ L \ . \tag{20.2}$$

This corresponds to the value of $\sigma_{\rm c}$:

$$\sigma_{\rm c} \approx 0.56 \ . \tag{20.3}$$

The linear dependence of $\langle W^2 \rangle$ on L (lattice length) in (20.1) reflects the random walk performed by the phase, for which $(2\pi)^2 \langle W^2 \rangle$ is an averaged variance. For large Lthe linear scaling (20.1) gives stronger winding than typical winding originating from quantum fluctuations in the ground state that is only logarithmic in L.

The winding number assumes a fixed value at a rescaled time u_c when σ falls below σ_c . For a given final J, as in Fig. 16.2, u_c translates to a quench time

$$\tau_Q^c \simeq u_c^{3/2} J^{-3/2} , \qquad (20.4)$$

which is independent of the lattice size L and whose dependence on J is consistent with Fig. 16.2. When $\tau_Q \gg \tau_Q^c$ the variance $\langle W^2 \rangle$ saturates at the finite value in (20.1). W settles down at $J_c \simeq u_c \tau_Q^{-2/3}$ which is in the Josephson regime, $J_c \ll 1$, for slow enough quenches with $\tau_Q \gg u_c^{3/2}$.

On the other hand, for $\tau_Q \ll u_c^{3/2} \approx 10^3$, the familiar Kibble-Zurek mechanism scaling $\langle W^2 \rangle \sim \tau_Q^{-1/3}$ was observed (see [41]) in quenches that take the system beyond the Josephson regime into $J \gg 1$ territory.

21 Phonons

After the winding number freezes, there is a lot of energy deposited in the fluctuations around a smooth solution

$$\phi_s = \exp\left(i2\pi \frac{Ws}{L}\right) \ . \tag{21.1}$$

However, as σ decreases further, the configuration approaches (21.1) and the fluctuations around this solution can be conveniently viewed as a phononic field ψ_s on top of the stable solution (21.1):

$$\theta_s = 2\pi \frac{Ws}{L} + \psi_s \ . \tag{21.2}$$

The phononic filed ψ_s obeys the linearised Josephson equations (8.2). Using (21.2) and the Josephson equations, we can expand the terms therein as

$$\sin(\theta_{s+1} - \theta_s) = \sin\left(\psi_{s+1} - \psi_s + \frac{2\pi W}{L}\right)$$
$$= \sin\frac{2\pi W}{L} + (\psi_{s+1} - \psi_s)\cos\frac{2\pi W}{L}, \qquad (21.3)$$
$$\sin(\theta_{s-1} - \theta_s) = \sin\left(\psi_{s-1} - \psi_s - \frac{2\pi W}{L}\right)$$

$$= -\sin\frac{2\pi W}{L} + (\psi_{s-1} - \psi_s)\cos\frac{2\pi W}{L} . \qquad (21.4)$$

The Josephson equations become

$$\frac{d^2}{dt^2}\psi_s = 2u\cos\frac{2\pi W}{L}\left(\psi_{s+1} + \psi_{s-1} - 2\psi\right) \ . \tag{21.5}$$

With the Fourier transform of ψ_s ,

$$\psi_s = \frac{1}{\sqrt{L}} \sum_{k=0}^{L-1} \alpha_k e^{i\frac{2\pi ks}{L}} , \qquad (21.6)$$

we get the Airy equations,

$$\frac{d^2}{dt^2}\alpha_k = 4u\cos\frac{2\pi W}{L}\alpha_k\left(\cos\frac{2\pi k}{L} - 1\right) , \qquad (21.7)$$

which have solutions, whose envelopes decay like

$$\alpha_k \sim u^{-1/4} \ . \tag{21.8}$$

Therefore, the average square of the phase step reads as

$$\sigma^{2} = \left\langle (\theta_{s+1} - \theta_{s})^{2} \right\rangle = \left\langle \left(\frac{2\pi W}{L} + \psi_{s+1} - \psi_{s}\right)^{2} \right\rangle$$
$$= \left\langle \left(\frac{2\pi W}{L}\right)^{2} \right\rangle + \left\langle (\psi_{s+1} - \psi_{s})^{2} \right\rangle = \left(\frac{2\pi}{L}\right)^{2} \left\langle W^{2} \right\rangle + \left\langle (\psi_{s+1} - \psi_{s})^{2} \right\rangle$$
$$= \frac{\sigma_{c}^{2}}{L} + \frac{C}{u^{1/2}} . \tag{21.9}$$

The initial condition at u_c , $\sigma^2(u_c) = \sigma_c^2$ allows to fix the constant $C \simeq \sigma_c^2 u_c^{1/2}$. Thus, $\sigma^2(u \ll L^2 u_c) \sim u^{-1/2}$. (21.10)

For late times, however, the variance σ^2 comes from the smooth but random winding number:

$$\sigma^{2}(u \gg L^{2}u_{c}) = \langle (\theta_{s+1} - \theta_{s})^{2} \rangle = \frac{(2\pi)^{2}}{L^{2}} \langle W^{2} \rangle , \qquad (21.11)$$

see Fig 21.1.



Figure 21.1: $\langle W^2 \rangle$ and two rescaled σ^2 on L = 8 sites at J = 0.1. For small τ_Q the winding number W originates from a random walk of phase around the lattice and, consequently, $\langle W^2 \rangle \approx L \sigma^2 / (2\pi)^2$. In contrast, for large τ_Q , there is an ensemble of smooth fields $\phi_s = \exp(2\pi i W s/L)$ with a random W and, consequently, $\sigma^2 \approx \langle (2\pi W/L)^2 \rangle$ equivalent to $\langle W^2 \rangle \approx L^2 \sigma^2 / (2\pi)^2$.

The flow in the Josephson regime is not stable for $L \leq 4$, in agreement with [78], when $2\cos(2\pi W/L) \leq 0$. This is why $\langle W^2 \rangle = 0$ for L = 4 and in Fig 17.1(a) the corresponding data point is below the fit line.

CHAPTER 5

Excitation energies after a quench in a Luttinger liquid

22 Luttinger liquid

In the preceding Sections we considered the quench that leads from one phase of the Bose-Hubbard model (Mott insulator) to the other (superfluid). Such a quench crosses the phase boundary, and the system undergoes a quantum phase transition. In the remaining Sections, we turn our attention to a quench that drives the system across a gapless phase. In this case, the system also gets excited, and the excitation energy depends on how the quench is performed, i.e. if it is a smooth or a piecewise linear ramp. We compare these two cases, and we restrict ourselves to one dimension, where the gapless phase can be effectively described by the Luttinger liquid (LL), see Section 2.

Luttinger liquid Hamiltonian reads as

$$\mathcal{H}_{\rm LL} = \frac{c}{2} \int_0^L dx \; \left[K \; \Pi^2 + K^{-1} \; \left(\partial_x \Phi \right)^2 \right] \;, \tag{22.1}$$

where Π and Φ obey bosonic commutation relations and yield

$$\Pi(x) = \sum_{k \neq 0} \left(\frac{|k|}{2L}\right)^{1/2} \frac{k}{|k|} e^{-ikx} \left(a_k^{\dagger} - a_{-k}\right) , \qquad (22.2)$$

$$\Phi(x) = -i \sum_{k \neq 0} \left(\frac{|k|}{2L} \right)^{1/2} \frac{1}{k} e^{-ikx} \left(a_k^{\dagger} + a_{-k} \right) , \qquad (22.3)$$

and a_k and a_k^{\dagger} are bosonic annihilation and creation operators, and c and K are parameters of the model. A quench of one of the parameters in the Bose-Hubbard model (3.1)

along a path in its superfluid phase, see Fig. 3.1(b), maps to a quench in the LL model (22.1) along a path in the c - K plane of its two parameters. This map is accurate provided the quench does not excite high energy states beyond the low-energy LL model. In terms of a_k and a_k^{\dagger} the LL Hamiltonian (22.1) reads as

$$\mathcal{H}_{\rm LL} = \sum_{k \neq 0} c|k| \left[\left(\frac{K + K^{-1}}{2} \right) a_k^{\dagger} a_k - \frac{1}{2} \left(\frac{K - K^{-1}}{2} \right) \left(a_k a_{-k} + a_{-k}^{\dagger} a_k^{\dagger} \right) \right] .$$
(22.4)

23 Bogolyubov transformation

For time-dependent K(t) and c(t) we make a Bogolyubov transformation

$$a_{k} = u_{k}(t) \gamma_{k} + v_{-k}(t)^{\star} \gamma_{-k}^{\dagger} ,$$

$$a_{k}^{\dagger} = v_{-k}(t) \gamma_{-k} + u_{k}(t)^{\star} \gamma_{k}^{\dagger} ,$$
(23.1)

and assume that the state of the system is a Bogolyubov vacuum for γ_k 's. In the Heisenberg picture we have

$$i\frac{da_k}{dt} = [a_k, H_{\text{eff}}] \quad . \tag{23.2}$$

With the transformation (23.1) and with

$$\frac{d}{dt}\gamma_k = 0 , \qquad (23.3)$$

we obtain the Bogolyubov-de Gennes equations:

$$i\frac{d}{dt}\left(\begin{array}{c}u_k\\v_k\end{array}\right) = c|k|\mathcal{L}(K)\left(\begin{array}{c}u_k\\v_k\end{array}\right) , \qquad (23.4)$$

where $\mathcal{L}(K)$ denotes:

$$\mathcal{L}(K) = \frac{1}{2} \begin{pmatrix} K + K^{-1} & K^{-1} - K \\ K - K^{-1} & -K - K^{-1} \end{pmatrix} .$$
(23.5)

Instantaneous eigenmodes of $\mathcal{L}(K)$ with positive norm, $|u_k|^2 - |v_k|^2 = 1$,

$$(u_k, v_k) = \left(\frac{K+1}{2\sqrt{K}}, \frac{K-1}{2\sqrt{K}}\right) \equiv (U, V) , \qquad (23.6)$$

have a positive instantaneous frequency c|k|. At the same time (V, U) is an eigenmode of $\mathcal{L}(K)$ with negative norm, $|u_k|^2 - |v_k|^2 = -1$, and negative frequency -c|k|.

24 Quench at zero temperature

We drive the Hamiltonian (22.4) by time-dependent $K(t/\tau_Q)$ and $c(t/\tau_Q)$. In the adiabatic basis (23.6) we have

$$\begin{pmatrix} u_k \\ v_k \end{pmatrix} = a_k \begin{pmatrix} U \\ V \end{pmatrix} e^{-i|k|l(t)} + b_k \begin{pmatrix} V \\ U \end{pmatrix} e^{i|k|l(t)} , \qquad (24.1)$$

where

$$l(t) = \int^{t} dt' c(t') , \qquad (24.2)$$

and (23.4) becomes

$$\frac{d}{ds}a_{k} = -b_{k} e^{+2ic_{f}\tau_{Q}|k|s} \frac{d}{ds} \ln K^{1/2} ,$$

$$\frac{d}{ds}b_{k} = -a_{k} e^{-2ic_{f}\tau_{Q}|k|s} \frac{d}{ds} \ln K^{1/2} .$$
(24.3)

Here,

$$s = \int^t \frac{dt'}{c_f \tau_Q} c\left(t'/\tau_Q\right) \tag{24.4}$$

is a dimensionless time-like variable. The amplitudes $a_k(s)$, $b_k(s)$ satisfy

$$|a_k|^2 - |b_k|^2 = 1 , (24.5)$$

and initial conditions are

$$a_k(-\infty) = 1$$
, $b_k(-\infty) = 0$. (24.6)

Average number of quasiparticles of momentum k excited in the final state is

$$n_k = |b_k(\infty)|^2$$
 . (24.7)

It depends on k only through the product $c_f \tau_Q |k|$ defining a length scale

$$\xi = c_f \tau_Q \tag{24.8}$$

which is the shortest wavelength of the excited phonons. When n_k decays with |k| sufficiently fast, then average linear density of excited quasiparticles scales with τ_Q like

$$n_{\rm ex} = \int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi} n_k \sim \tau_Q^{-1} , \qquad (24.9)$$

while the more directly measurable excitation energy density scales like

$$\varepsilon = \int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi} c_f |k| \ n_k \ \sim \ \tau_Q^{-2} \tag{24.10}$$

provided that $\xi^{-1} \ll \Lambda$. These are universal scalings for quenches that do not excite beyond the range of validity of the Luttinger liquid model limited by the UV cut-off Λ .

25 Adiabatic approximation

In the most rapid limit of a sudden quench, considered in [24, 25], we have

$$\lim_{c_f \tau_Q |k| \to 0} n_k = \sinh^2 \left(\ln \sqrt{K_f / K_i} \right) , \qquad (25.1)$$

which is small when the relative change of K is small. Thus, we can try an adiabatic approximation, where $|b_k|^2 \ll 1$ and $a_k \approx 1$. Solving (24.3) perturbatively to the leading order in b_k yields a Fourier transform

$$n_k = \left| \int_{-\infty}^{\infty} ds \ e^{-2i\xi |k|s} \ \frac{d}{ds} \ln K^{1/2} \right|^2 .$$
 (25.2)

This n_k is small and the adiabatic approximation is self-consistent when relative changes of K during a quench are small. Moreover, even when they are large (25.2) is still accurate for large enough $\xi |k|$ where n_k is small, see the following examples and Fig. 25.1.

Here we consider three examples of quenches around K_0 : a smooth tanh quench

$$\ln \frac{K^{(1)}(s)}{K_0} = A \tanh(s) , \qquad (25.3)$$

a linear ramp similar as in Ref. [79, 80, 81, 82]

$$\ln \frac{K^{(2)}(s)}{K_0} = A \begin{cases} -1 & \text{, for } s < -1, \\ s & \text{, for } -1 \le s \le 1, \\ 1 & \text{, for } s > 1, \end{cases}$$
(25.4)

and a smooth shake beginning and ending at K_0

$$\ln \frac{K^{(3)}(s)}{K_0} = \frac{A}{\cosh(s)} .$$
 (25.5)

The corresponding power spectra (25.2) follow as:

$$n_{k}^{(1)} = \frac{A^{2}}{4} \left| \int_{-\infty}^{\infty} ds' e^{-2\xi|k|s'} \frac{1}{\cosh^{2}s'} \right|^{2} = A^{2} \left[\frac{\pi\xi|k|}{\sinh(\pi\xi|k|)} \right]^{2} ,$$

$$n_{k}^{(2)} = \frac{A^{2}}{4} \left| \int_{-1}^{1} ds' e^{-2\xi|k|s'} \right|^{2} = A^{2} \left[\frac{\sin(2\xi|k|)}{2\xi|k|} \right]^{2} ,$$

$$n_{k}^{(3)} = \frac{A^{2}}{4} \left| \int_{-\infty}^{\infty} ds' e^{-2\xi|k|s'} \frac{\tanh s'}{\cosh s'} \right|^{2} = A^{2} \left[\frac{\pi\xi|k|}{\cosh(\pi\xi|k|)} \right]^{2} .$$
 (25.6)



Figure 25.1: The figure displays momentum dependence of excitation density n_k as a function of $2\xi|k|$ for the tanh quench (left panels) in (25.3) and the linear ramp (right panels) in (25.4). The upper row shows results for small quenches with A = 0.1 when the adiabatic approximation (25.2) agrees with numerical evaluation of equations (24.3). For a greater A = 0.8 (lower row) it remains valid for $2\xi|k|$ large enough, but not for small $2\xi|k|$ where it underestimates n_k that tends to (25.1) for $2\xi|k| \rightarrow 0$ instead of $\ln^2 \sqrt{K_f/K_i}$ from a perturbative equation (25.2). The insets show corresponding plots in a linear scale.

They are exponentially localized on a scale $k \propto \xi^{-1}$ except the linear ramp (2), whose discontinuous time derivative results in a fat high energy tail $n_k^{(2)} \propto |k|^{-2}$. The linear density of excitations (24.9) reads as

$$n_{\rm ex}^{(1)} = \frac{A^2}{2\pi} \int_{-\Lambda}^{\Lambda} dk \, \left(\frac{\pi\xi|k|}{\sinh(\pi\xi|k|)}\right)^2 \simeq \frac{A^2}{6\xi},$$

$$n_{\rm ex}^{(2)} = \frac{A^2}{2\pi} \int_{-\Lambda}^{\Lambda} dk \, \left(\frac{\sin(2\xi|k|)}{2\xi|k|}\right)^2 \simeq \frac{A^2}{4\xi},$$

$$n_{\rm ex}^{(3)} = \frac{A^2}{2\pi} \int_{-\Lambda}^{\Lambda} dk \, \left(\frac{\pi\xi|k|}{\cosh(\pi\xi|k|)}\right)^2 \simeq \frac{A^2}{12\xi},$$
(25.7)



Figure 25.2: The upper panels of the figure represent number of excitations $|b_k(s)|^2$ in the course of time evolution of the system (24.3) for the tanh quench (left) and a ramp (right). The lower panels show the accuracy of our approximation $|\epsilon| \ll 1$ for the number of excitations $n = |b_k(\infty)|^2$ (25.2) for varying A for smooth tanh and a ramp respectively, see equations (25.6). For all four pictures the momentum k was chosen such that $2c\tau |k| = 1$.

when $\xi \Lambda \gg 1$. All three densities scale like τ_Q^{-1} in agreement with the nonperturbative Eq. (24.9).

The excitation energy densities (24.10) read as

$$\varepsilon^{(1)} = \frac{A^2}{\pi} \int_0^\Lambda dk \, k \left(\frac{\pi\xi k}{\sinh(\pi\xi k)}\right)^2 \simeq \frac{3\zeta(3)}{2\pi^3} \, \frac{A^2}{\xi^2} \,,$$
(25.8)

$$\varepsilon^{(2)} = \frac{A^2}{\pi} \int_0^{\Lambda} dk \, k \left(\frac{\sin(2\xi k)}{2\xi k}\right)^2 \simeq \frac{1}{8\pi} \, \frac{A^2}{\xi^2} \ln(2\xi\Lambda) \, ,$$
(25.9)

$$\varepsilon^{(3)} = \frac{A^2}{\pi} \int_0^\Lambda dk \, k \left(\frac{\pi\xi k}{\cosh(\pi\xi k)}\right)^2 \simeq \frac{9\zeta(3)}{8\pi^3} \, \frac{A^2}{\xi^2} \,,$$
 (25.10)

when $\xi \Lambda \gg 1$. Here, ζ is the Riemann zeta function. The energy scales like τ_Q^{-2} , in agreement with the nonperturbative equation (24.10), except for the case (2), where it logarithmically diverges with the cut-off. The discontinuous time derivative of the
linear ramp (25.4) is probing non-universal high energy excitations beyond the range of validity of the effective low-energy Luttinger liquid (22.1), see [45]. For the linear ramp, the LL is not a self-consistent approximation and the scaling of the excitation energy with the ramp time τ_Q , if any, can be different from the universal τ_Q^{-2} . A non-universal exponent was observed in numerical simulations of linear ramps in the Bose-Hubbard model [79, 80, 81, 82].



Figure 25.3: The figure shows numerical computation of a total energy (24.10) for a tanhtype quench (left) and for a ramp (right) against a dimensionless cut-off $\lambda = 2c\tau_Q\Lambda$. The plotted energy is dimensionless $\Sigma = \int_0^{\lambda} d\xi \,\xi \, n_{\xi}$ where the energy ϵ from equation (24.10) equals $\epsilon = \Sigma/4\pi c\tau_Q^2$. Results of this simulations are in accordance with equations (25.8) and (25.9), and clearly show that the energy is finite for a smooth tanh transition and divergent with a cut-off for a ramp.

The evolution of the number of excitations in the system is shown in the Fig. 25.2 for the tanh quench and for the linear ramp. The corresponding energies are depicted in Fig. 25.3, which shows, that the energy for the smooth quench is finite in contrast to the case of the ramp, where the energy diverges with a cut-off. Plots for the case of a smooth shake (3) are presented as Figs. 25.4 and 25.5.



Figure 25.4: The panels of the figure represent number of excitations $|b_k(s)|^2$ in the course of time evolution of the system (24.3) for the smooth shake (left) and the accuracy of our approximation, $|\epsilon| \ll 1$, for the number of excitations $n = |b_k(\infty)|^2$ (25.2) for varying ϵ_0 (right). The momentum k was chosen such that $2c\tau |k| = 1$.



Figure 25.5: The upper two plots compare the numerical exact evaluation of (24.3) and the perturbative approximation of n_k for small (left) and large (**right**) ϵ_0 for a smooth shake (25.5). The lower panel shows numerical computation of a total energy (24.10) against a dimensionless cut-off $\lambda = 2c\tau_Q\Lambda$. The plotted energy is dimensionless $\Sigma = \int_0^{\lambda} d\xi \, \xi \, n_{\xi}$, where the energy ϵ from (24.10) equals $\epsilon = \Sigma/4\pi c\tau_Q^2$. The exact energy remains finite with the cut-off, which supports our perturbative expression (25.10).

CHAPTER 6

Conclusions

In this thesis we considered several aspects of a quench in the Bose-Hubbard model, which describes ultracold bosons in an optical lattice. When the system is quenched from the Mott insulator state into the superfluid regime, it gets excited. In this thesis we showed, that the decay of the said excitations can be described by the impulseadiabatic scenario, a variant of the Kibble-Zurek mechanism. The excitation energy decays algebraically with the quench time τ_Q (an inverse of the quench rate), and we derived the power to be $\frac{1}{3}$ in one, two and three dimensions, in accordance with the previous calculations for one dimension [41]. Although the calculations were done in the large density limit, the value for the exponent in the power-law decay coincides numerically with the one obtained in the experiment [18], where there were only a few atoms per site.

A uniform lattice was analysed first, but we also showed, that the aforementioned result is preserved when the system is confined in a harmonic trap, i.e. quadratic potential. This is explained with the fact that the kinetic energy accumulated in the (initially random) phases of the field is much larger than the kinetic energy of the cloud expansion due to the confinement (the field distribution centred in the middle of the trap).

One dimensional system thermalizes and the correlation functions decay exponentially with the distance between the sites. In two dimensions, there is a quasi-long-range order and in three dimensions – long-range order. These cannot be attained in finite time. The system thermalizes only locally; in particular, local observables such as the energy density stabilize with time. Due to the finite rate of the transition, the domains of a broken symmetry phase appear, and size of these domains grows with τ_Q . As a result, there are topological vortices present. Also, we considered the winding of the phase in a one-dimensional system (a ring). When the tunnelling between sites grows, the phases become more and more correlated, and the random walk of phase around the ring smooths. The jumps of the net winding number become less and less frequent and, at some point, the winding number freezes and becomes topologically protected.

The variance of the winding number does not depend on the pace of the quench, as it is related to the critical value of the variance of phase.

Finally, we investigated the quench in an entirely gapless phase in one dimension. Such phase has a low-energy description of a Luttinger liquid. We showed, that if the quench is a piecewise linear ramp, then it excites the system beyond the validity of the Luttinger liquid approximation and the excitation energy is divergent with the cut-off in momentum. In contrast, if the quench is a smooth tanh-type transition, then the excitation energy is finite, and we derived its power-law decay with the quench rate.

To summarize, the thesis presented research which aims at contributing to the theoretical physics of ultracold atomic gases in optical lattices and the dynamics of quantum phase transitions therein.

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APPENDIX A

Split-step method

This Appendix describes the numerical method used for evolving the Gross-Pitaevskii equation, (7.7). The equation has the form:

$$i\partial_t \phi_{\mathbf{s}} = -J\nabla^2 \phi_{\mathbf{s}} + \left(|\phi_{\mathbf{s}}|^2 - 1\right)\phi_{\mathbf{s}} . \qquad (A.0.11)$$

The idea of the *split-step* method of a numerical evolution of ϕ_s according to the equation (A.0.11) is to evolve the linear and nonlinear parts separately in an alternating manner. This means, that we discretize time into small intervals of length ε and consecutively evolve the linear part trough time ε followed by the evolution of the nonlinear part trough time ε . The following two Sections give the details of each of the two steps.

A.1 Evolution of the linear part

Taking only the linear part of (A.0.11), we get

$$i\partial_t \phi_{\mathbf{s}} = -J\nabla^2 \phi_{\mathbf{s}} , \qquad (A.1.1)$$

which can be diagonalized by switching to the Fourier space. Therefore, we represent $\phi_{\mathbf{s}}$ as

$$\phi_{\mathbf{s}} = \frac{1}{\sqrt{L^D}} \sum_{\mathbf{k}} \tilde{\phi}_{\mathbf{k}} \exp i \frac{2\pi \,\mathbf{k} \,\mathbf{s}}{L} \,. \tag{A.1.2}$$

The ∇^2 operator is then diagonalized and $\nabla^2 \phi_{\mathbf{s}}$ read as

$$\nabla^2 \phi_{\mathbf{s}} = \sum_{\mathbf{e}_{\alpha}} \left(\phi_{\mathbf{s}+\mathbf{e}_{\alpha}} + \phi_{\mathbf{s}-\mathbf{e}_{\alpha}} - 2\phi_{\mathbf{s}} \right)$$
$$= \frac{1}{\sqrt{L^D}} \sum_{\mathbf{e}_{\alpha}} \sum_{\mathbf{k}} \tilde{\phi}_{\mathbf{k}} \left[e^{i\frac{2\pi \mathbf{k} \cdot \mathbf{e}_{\alpha}}{L}} + e^{-i\frac{2\pi \mathbf{k} \cdot \mathbf{e}_{\alpha}}{L}} - 2 \right] e^{i\frac{2\pi \mathbf{k} \cdot \mathbf{s}}{L}} .$$
(A.1.3)

The time derivative gives, on the other hand,

$$i\partial_t \phi_{\mathbf{s}} = \frac{i}{\sqrt{L^D}} \sum_{\mathbf{k}} \partial_t \tilde{\phi}_{\mathbf{k}} \exp \frac{2\pi \, \mathbf{k} \, \mathbf{s}}{L}$$
 (A.1.4)

Equating (A.1.3) and (A.1.4) and using the linear independence of the Fourier modes, $\exp\left(i\frac{2\pi \mathbf{ks}}{L}\right)$, leads to the following equation:

$$i\partial_t \tilde{\phi}_{\mathbf{k}} = -J\tilde{\phi}_{\mathbf{k}} \sum_{\mathbf{e}_{\alpha}} \left[e^{i\frac{2\pi\,\mathbf{k}\,\mathbf{e}_{\alpha}}{L}} + e^{-i\frac{2\pi\,\mathbf{k}\,\mathbf{e}_{\alpha}}{L}} - 2 \right] = -2J\tilde{\phi}_{\mathbf{k}} \sum_{\mathbf{e}_{\alpha}} \left(\cos\frac{2\pi\,\mathbf{k}\,\mathbf{e}_{\alpha}}{L} - 1 \right) \quad (A.1.5)$$

The last sum runs over the basis in **k**-space. For instance, in three dimensions, where $\mathbf{k} = (k_x, k_y, k_z)$, it yields

$$\sum_{\mathbf{e}_{\alpha}} \left(\cos \frac{2\pi \,\mathbf{k} \,\mathbf{e}_{\alpha}}{L} - 1 \right) = \cos \frac{2\pi k_x}{L} + \cos \frac{2\pi k_y}{L} + \cos \frac{2\pi k_z}{L} - 3 \,. \tag{A.1.6}$$

The immediate solution to (A.1.5) is the exponential function,

$$\tilde{\phi}_{\mathbf{k}}(t) = \text{const.} \times \exp\left(2iJ(t)\sum_{\mathbf{e}_{\alpha}} \left(\cos\frac{2\pi\,\mathbf{k}\,\mathbf{e}_{\alpha}}{L} - 1\right)t\right) \,. \tag{A.1.7}$$

Since in each step of the numerical simulation, the system evolves through a short time ε , we can write down an expression for $\tilde{\phi}_{\mathbf{k}}(t + \varepsilon)$ provided $\tilde{\phi}_{\mathbf{k}}(t)$ is given,

$$\widetilde{\phi}_{\mathbf{k}}(t+\varepsilon) = \operatorname{const.} \times \exp\left(2iJ(t)\sum_{\mathbf{e}_{\alpha}}\left(\cos\frac{2\pi\,\mathbf{k}\,\mathbf{e}_{\alpha}}{L}-1\right)t\right) \\
\times \exp\left(2iJ(t)\sum_{\mathbf{e}_{\alpha}}\left(\cos\frac{2\pi\,\mathbf{k}\,\mathbf{e}_{\alpha}}{L}-1\right)\varepsilon\right) \\
\simeq \widetilde{\phi}_{\mathbf{k}}(t) \exp\left(2iJ(t+\frac{\varepsilon}{2})\sum_{\mathbf{e}_{\alpha}}\left(\cos\frac{2\pi\,\mathbf{k}\,\mathbf{e}_{\alpha}}{L}-1\right)\varepsilon\right) . \quad (A.1.8)$$

Thus, each step of evolution of the linear part corresponds merely to a unitary phase rotation of the field $\tilde{\phi}_{\mathbf{k}}$.

A.2 Evolution of the nonlinear part

Retaining solely the nonlinear part in (A.0.11) gives a simple, but nonlinear equation:

$$i\partial_t \phi_{\mathbf{s}} = \left(|\phi_{\mathbf{s}}|^2 - 1 \right) \phi_{\mathbf{s}} . \tag{A.2.1}$$

In contrast to (A.1.1), (A.2.1) does not have an explicit solution, but the equation can be rewritten in as an integral equation, where on both sides there is the unknown field ϕ_{s} ,

$$\phi_{\mathbf{s}}(t) = \text{const.} \times \exp\left(-i \int^{t} \left(|\phi_{\mathbf{s}}|^{2} - 1\right) dt'\right) . \tag{A.2.2}$$

Nevertheless, since we are interested in a small step ε only, similarly to the procedure in the linear case, we can simplify (A.2.2) as

$$\phi_{\mathbf{s}}(t+\varepsilon) = \operatorname{const.} \times \exp\left(-i\int^{t+\varepsilon} \left(|\phi_{\mathbf{s}}|^{2}-1\right)dt'\right)$$

$$= \operatorname{const.} \times \exp\left(-i\int^{t} \left(|\phi_{\mathbf{s}}|^{2}-1\right)dt'-i\int^{t+\varepsilon}_{t} \left(|\phi_{\mathbf{s}}|^{2}-1\right)dt'\right)$$

$$= \phi_{\mathbf{s}}(t) \exp\left(-i\int^{t+\varepsilon}_{t} \left(|\phi_{\mathbf{s}}|^{2}-1\right)dt'\right)$$

$$\simeq \phi_{\mathbf{s}}(t) \exp\left(-i\varepsilon\left(|\phi_{\mathbf{s}}|^{2}-1\right)\right).$$
(A.2.3)

In the second equation we split the integral into two separate integrals, in the third equation, we used the known expression for $\phi_{\mathbf{s}}(t)$, (A.2.2). In the last equation, we approximated the integral over a short interval by multiplying the length of the integrand, ε , by the value of the integrand. The choice of the exact point t_0 at which the integrand is evaluated is irrelevant up to higher order terms in ε , as long as t_0 is in that interval, $t_0 \in (t, t+\varepsilon)$. We choose t_0 to be $t_0 = t$, which allows for calculation of $\phi_{\mathbf{s}}(t+\varepsilon)$ with the previous knowledge of $\phi_{\mathbf{s}}(t)$ only. Again, like in the linear case, the evolution through a small step ε amounts to a phase rotation, where now the phase depends on the value of $\phi_{\mathbf{s}}(t)$, which reflects the nonlinearity in the equation.

A.3 Evolution of the system

The subsequent evolution of the linear and nonlinear parts has the advantage of being unitary, i.e. the norm (7.4) is conserved during the evolution. This is, because at each step we perform a phase rotation, which leaves the amplitude $|\phi_s|^2$ unaltered.

In order to improve the method, instead of using the alternating evolution of the linear and nonlinear parts, each trough time ε , we split each step of evolution into three parts: the nonlinear evolution through time $\frac{\varepsilon}{2}$, the linear evolution through ε

with $J = J(t + \frac{\varepsilon}{2})$ (evaluated at the middle of the interval $(t, t + \varepsilon)$) and the nonlinear evolution through time $\frac{\varepsilon}{2}$ again. Such procedure should give a correct solution with higher accuracy.

${}_{\text{APPENDIX}} B$

Correlation function in one dimension

This Appendix presents the calculation of the correlation function in one dimension for the system in the Josephson regime. The correlation function has the standard definition:

$$C_{R} = \langle \phi_{s}^{\star} \phi_{s+R} \rangle \simeq \langle e^{-i\theta_{s}} e^{i\theta_{s+R}} \rangle$$

$$= \langle \exp i(\theta_{s+R} - \theta_{s+R-1} + \theta_{s+R-1} - \dots + \theta_{s+1} - \theta_{s}) \rangle$$

$$= \langle \exp \left\{ i \sum_{i=s}^{s+R-1} (\theta_{i+1} - \theta_{i}) \right\} \rangle = \langle \prod_{i=s}^{s+R-1} e^{i(\theta_{i+1} - \theta_{i})} \rangle , \qquad (B.0.1)$$

where in the first equation we neglected the density fluctuations, which are small in the Josephson regime, $|\phi_s| \approx 1$. The phase steps are approximately independent. With the arbitrary choice of s = 0:

$$C_R = \prod_{i=0}^{R-1} \langle e^{i(\theta_{i+1}-\theta_i)} \rangle .$$
 (B.0.2)

The Hamiltonian of the system reads as (see (8.9))

$$\mathcal{H}_{\rm J} = \sum_{s} \frac{p_s^2}{2} + 2J \sum_{s} (1 - \cos(\theta_{s+1} - \theta_s)) , \qquad (B.0.3)$$

and the thermal state is distributed with the Boltzmann distribution

$$f(\mathbf{p},\theta) \sim e^{-\frac{1}{T}\mathcal{H}_{\mathbf{J}}} = \exp\left(\frac{1}{2T}\sum_{s} p_{s}^{2}\right) \exp\left[\frac{2J}{T}\sum_{s}\cos\left(\theta_{s+1} - \theta_{s}\right)\right] . \tag{B.0.4}$$

Therefore, the factor $\langle e^{i\Delta\theta_s} \rangle$ in (B.0.2) can be calculated as

$$\langle e^{i\Delta\theta_s} \rangle = \iint dp_0 \dots dp_{L-1} e^{\frac{1}{2T}\sum_{s'} p_{s'}^2} \iint_{-\pi}^{\pi} d\theta_0 \dots d\theta_{L-1} e^{-\frac{2J}{T}\sum_{s'} \{1 - \cos\Delta\theta_{s'}\}} e^{i\Delta\theta_s}$$

$$\propto \iint_{-\pi}^{\pi} d\Delta\theta_0 \dots d\Delta\theta_{s-1} d\Delta\theta_{s+1} \dots d\Delta\theta_{L-1} \prod_{i\neq s} \exp(-\frac{2J}{T} (1 - \cos\Delta\theta_i)) \times$$

$$\times \int_{-\pi}^{\pi} d\Delta\theta_s \exp(-\frac{2J}{T} (1 - \cos\Delta\theta_i) + i\Delta\theta_s) = \frac{I_1(\frac{2J}{T})}{I_0(\frac{2J}{T})} ,$$
(B.0.5)

where I_n is the modified Bessel function, defined as

$$I_n(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\tau \, e^{-i(n\tau - x\sin\tau)} \,. \tag{B.0.6}$$

In (B.0.5) we used the fact, that the correlation length ξ is much smaller than the lattice length $L, \xi \ll L$, so we can get rid of the constraint for θ_0 imposed by the periodic boundary conditions. Since the relation between the new variables of integration $\Delta \theta_s$ and the old θ_s is linear, the Jacobian is a constant and the two integrals in (B.0.5) are thereby equal up to a proportionality constant.

Therefore, the correlation function yields

$$C_R = \left(\frac{I_1(\frac{2J}{T})}{I_0(\frac{2J}{T})}\right)^R , \qquad (B.0.7)$$

which results in the following correlation length

$$\xi = 1/\ln\left[\frac{I_0(2J/T)}{I_1(2J/T)}\right] \approx \frac{4J}{T}$$
, (B.0.8)

for

$$\frac{4J}{T} \gg 1 . \tag{B.0.9}$$

In the initial state, i.e. the Mott state, the momenta vanish, $p_s(0) = 0$ and the phases $\theta_s(0)$ are random. Thus,

$$E_{\text{Mott}} = 2JL . \tag{B.0.10}$$

In the Josephson regime, the system thermalizes to the temperature T and the average energy reads as

$$E_{\text{thermal}} = \frac{1}{2}TL + 2J(1 - C_1)$$
 (B.0.11)

Due to the energy conservation $E_{\text{Mott}} = E_{\text{thermal}}$ which gives the equation for $\frac{4J}{T}$:

$$2J = \frac{T}{2} + 2J \left(1 - \frac{I_1(\frac{2J}{T})}{I_0(\frac{2J}{T})} \right) .$$
 (B.0.12)

The numerical solution of (B.0.12) is

$$\frac{4J}{T} = 2.1312$$
, (B.0.13)

which implies the correlation length

$$\xi = 1.321$$
. (B.0.14)

Thus, the numerical values for the short-range correlations yield

$$C_1 = 0.469, \quad C_2 = 0.220, \quad C_3 = 0.103, \quad C_4 = 0.049, \quad (B.0.15)$$

in perfect agreement with the data in Fig 9.1.

APPENDIX C

Breathing mode

In the Subsection 13.4, we want to isolate the effect of the confinement and expansion of the atomic gas due to an external potential in the excitation energy from the contribution of the random phases. In the following, we present the details of the calculations.

The Gross-Pitaevskii equation reads as

$$i\partial_t \phi_{\mathbf{s}} = -J\nabla^2 \phi_{\mathbf{s}} + |\phi_{\mathbf{s}}|^2 \phi_{\mathbf{s}} + \frac{\omega^2}{2} \mathbf{s}^2 \phi_{\mathbf{s}} - \mu \phi_{\mathbf{s}} . \qquad (C.0.16)$$

In order to examine the lowest excitations of $\phi_{\mathbf{s}}$ above the Thomas-Fermi solution (13.4), we make an expansion

$$\phi_{\mathbf{s}} = \phi_{\mathbf{s}}^{(0)} + \delta\phi_{\mathbf{s}} , \qquad (C.0.17)$$

where $\delta \phi_{\mathbf{s}}$ is a small correction to $\phi_{\mathbf{s}}$. Since $\phi_{\mathbf{s}}^{(0)}$ is a real function and $\delta \phi_{\mathbf{s}}^{\star} = -\delta \phi_{\mathbf{s}}, |\phi_{\mathbf{s}}|^2$ simplifies significantly,

$$\begin{aligned} |\phi_{\mathbf{s}}|^{2} &= |\phi_{\mathbf{s}}^{(0)} + \delta\phi_{\mathbf{s}}|^{2} \simeq |\phi_{\mathbf{s}}^{(0)}|^{2} + \phi_{\mathbf{s}}^{(0)^{\star}}\delta\phi_{\mathbf{s}} + \phi_{\mathbf{s}}^{(0)}\delta\phi_{\mathbf{s}}^{\star} \\ &= |\phi_{\mathbf{s}}^{(0)}|^{2} + \phi_{\mathbf{s}}^{(0)}\delta\phi_{\mathbf{s}} - \phi_{\mathbf{s}}^{(0)}\delta\phi_{\mathbf{s}} = |\phi_{\mathbf{s}}^{(0)}|^{2} . \end{aligned}$$
(C.0.18)

With the expansion (C.0.17), the (C.0.16) takes the form

$$i\partial_t \delta\phi_{\mathbf{s}} = -J\nabla^2 \phi_{\mathbf{s}}^{(0)} - J\nabla^2 \delta\phi_{\mathbf{s}} + |\phi_{\mathbf{s}}^{(0)}|^2 \phi_{\mathbf{s}}^{(0)} + |\phi_{\mathbf{s}}^{(0)}|^2 \delta\phi_{\mathbf{s}} + \frac{\omega^2}{2} \mathbf{s}^2 \phi_{\mathbf{s}}^{(0)} + \frac{\omega^2}{2} \mathbf{s}^2 \delta\phi_{\mathbf{s}} - \mu \phi_{\mathbf{s}}^{(0)} - \mu \delta\phi_{\mathbf{s}} .$$
(C.0.19)

For $J \ll 1, \phi_{\mathbf{s}}^{(0)}$ satisfies

$$-J\nabla^2 \phi_{\mathbf{s}}^{(0)} + |\phi_{\mathbf{s}}^{(0)}|^2 \phi_{\mathbf{s}}^{(0)} + \frac{\omega^2}{2} \mathbf{s}^2 \phi_{\mathbf{s}}^{(0)} - \mu \phi_{\mathbf{s}}^{(0)} = 0 , \qquad (C.0.20)$$

which simplifies the (C.0.19) to

$$i\partial_t \delta\phi_{\mathbf{s}} = -J\nabla^2 \delta\phi_{\mathbf{s}} + |\phi_{\mathbf{s}}^{(0)}|^2 \delta\phi_{\mathbf{s}} + \frac{\omega^2}{2} \mathbf{s}^2 \delta\phi_{\mathbf{s}} - \mu \delta\phi_{\mathbf{s}} . \qquad (C.0.21)$$

First, let us consider the case where $r < R_{\rm TF}$, in the bulk of the Thomas-Fermi distribution. Therein, the (C.0.21) assumes the form

$$i\partial_t \delta\phi_{\mathbf{s}} = -J\nabla^2 \delta\phi_{\mathbf{s}} + \frac{\omega^2}{2}(R_{\mathrm{TF}}^2 - \mathbf{s}^2 + \mathbf{s}^2)\delta\phi_{\mathbf{s}} - \mu\delta\phi_{\mathbf{s}} , \qquad (C.0.22)$$

which, with $\mu = 1$, yields

$$i\partial_t \delta\phi_{\mathbf{s}} = -J\nabla^2 \delta\phi_{\mathbf{s}} + \frac{\omega^2}{2}R_{\mathrm{TF}}^2\delta\phi_{\mathbf{s}} - \delta\phi_{\mathbf{s}} . \qquad (C.0.23)$$

Because of our normalization choice, $\frac{\omega^2}{2}R_{TF}^2 = 1$, and the two last terms cancel. Therefore, in the bulk of the Thomas-Fermi distribution, the correction $\delta\phi_s$ satisfies a free evolution equation,

$$i\partial_t \delta \phi_{\mathbf{s}} = -J\nabla^2 \delta \phi_{\mathbf{s}} . \tag{C.0.24}$$

In order to solve (C.0.24), we refer to the well known method of separation of variables. The field $\delta \phi_{\mathbf{s}}$ factorizes into its time dependent part $\theta(t)$ and space dependent part $\chi(r)$

$$\delta\phi_{\mathbf{s}}(t,r) = \theta(t)\,\chi(r) \;. \tag{C.0.25}$$

In term of new functions, the equation (C.0.24) becomes

$$i\theta(t) \chi(r) = -J \ \theta(t) \nabla^2 \chi(r) ,$$
 (C.0.26)

or, after division by $\delta \phi_{\mathbf{s}}$,

$$i\frac{\dot{\theta}(t)}{\theta(t)} = -J\frac{\nabla^2\chi(r)}{\chi(r)} = \text{const.} = \Omega . \qquad (C.0.27)$$

Since Both sides of this equation depend solely on their own variables, each of the expressions has to be constant, should they be equal. The equation for θ ,

$$\dot{\theta}(t) = -i\Omega \,\theta(t) , \qquad (C.0.28)$$

has an immediate solution of the form

$$\theta(t) = \text{const. } e^{-i\Omega t}$$
 (C.0.29)

The radial equation,

$$-J\nabla^2 \chi(r) = \Omega \,\chi(r) , \qquad (C.0.30)$$

is slightly more complex. Since χ depends only on the radius r and not on the angular variables, the ∇^2 operator, in spherical variables, preserves only its radial part

$$\nabla^2 \chi = \frac{1}{r^2} (r^2 \partial_r^2 + 2r \partial_r) \chi . \qquad (C.0.31)$$

Eq. (C.0.30) therefore becomes

$$r^2 \partial_r^2 \chi(r) + 2r \partial_r \chi(r) + r^2 \frac{\Omega}{J} \chi(r) = 0 . \qquad (C.0.32)$$

With the change of variables $r = \sqrt{\frac{J}{\Omega}}x$, where we introduce the notation $\chi(r) = \bar{\chi}(x)$, (C.0.32) further becomes the Bessel equation of the zeroth order,

$$x^2 \partial_x^2 \bar{\chi}(x) + 2x \partial_x \bar{\chi}(x) + x^2 \bar{\chi}(x) = 0 , \qquad (C.0.33)$$

with the solution

$$\bar{\chi}(x) = j_0(x) = \frac{\sin x}{x}$$
, (C.0.34)

where $j_0(x)$ is a spherical Bessel function. Hence, eventually, the solution for χ reads as

$$\chi(r) = j_0(\sqrt{\frac{\Omega}{J}}r) . \qquad (C.0.35)$$

Finally, since $\delta \phi_{\mathbf{s}}$ is purely imaginary,

$$\delta\phi_{\mathbf{s}} = i \text{ const. Im} \left[\exp(-i\Omega t + \varphi) j_0(\sqrt{\frac{\Omega}{J}}r) \right]$$
$$= -i \text{ const. } \sin(\Omega t + \varphi) \frac{\sin(\sqrt{\frac{\Omega}{J}}r)}{\sqrt{\frac{\Omega}{J}}r} . \tag{C.0.36}$$

In case where $r > R_{\rm TF}$, (C.0.21) assumes the form

$$i\partial_t \delta\phi_{\mathbf{s}} = -J\nabla^2 \delta\phi_{\mathbf{s}} + \frac{\omega^2}{2} \mathbf{s}^2 \delta\phi_{\mathbf{s}} - \mu \delta\phi_{\mathbf{s}} , \qquad (C.0.37)$$

which can be rewritten as

$$i\partial_t \delta\phi_{\mathbf{s}} = -J\nabla^2 \delta\phi_{\mathbf{s}} + \frac{\omega^2}{2} (\mathbf{s}^2 - R_{\mathrm{TF}}^2) \delta\phi_{\mathbf{s}} . \qquad (C.0.38)$$

Therefore, for $r > R_{\rm TF}$, the field $\delta \phi_{\rm s}$ is in the area of the positive potential $\tilde{V} = \frac{\omega^2}{2}({\bf s}^2 - R_{\rm TF}^2)$, in contrast to the case of $r < R_{\rm TF}$, where the potential was $\tilde{V} = 0$, see (C.0.24). This situation is schematically depicted in Fig. C.1.



Figure C.1: The picture that represents the potential which determines the boundary conditions for the calculation of $\delta \phi_{s}$. For $R_{TF} \gg 1$ we can assume that the potential is very steep and can be effectively replaced by the infinite well potential.

When $R_{\text{TF}} \gg 1$, we can assume, that the potential in the vicinity of $r \approx R_{\text{TF}}$ is very steep and essentially can be approximated by a potential of an infinite well. Therefore, we assume that

$$\delta\phi_{\mathbf{s}} \approx 0 \tag{C.0.39}$$

outside the bulk. Thus, we can require that the boundary conditions at $|\mathbf{s}| = R_{\text{TF}}$ for $\delta \phi_{\mathbf{s}}$ should be

$$\delta\phi_{\mathbf{s}} = 0 \ . \tag{C.0.40}$$

The zeroes of the Bessel function $j_0(x)$ are

$$\sqrt{\frac{\Omega}{J}}R_{\rm TF} = \pi n , \quad n = 1, 2, 3, \dots$$
 (C.0.41)

We are interested in the lowest excitation, where there are on additional zeroes inside the well, so the lowest excitation corresponds to n = 1:

$$\sqrt{\frac{\Omega}{J}}R_{\rm TF} = \pi \ . \tag{C.0.42}$$

This condition determines the value of Ω ,

$$\Omega = \frac{\pi^2 J}{R_{\rm TF}^2} . \tag{C.0.43}$$

Finally, we get a solution for $\delta\phi_{\mathbf{s}},$ which is

$$\delta\phi_{\mathbf{s}} = -i \text{ const. } \sin\left(\frac{\pi^2 J}{R_{\rm TF}^2}t + \varphi\right) \frac{\sin\left(\frac{\pi}{R_{\rm TF}}|\mathbf{s}|\right)}{\frac{\pi}{R_{\rm TF}}|\mathbf{s}|} \tag{C.0.44}$$

in bulk of the Thomas-Fermi distribution and $\delta\phi_{\mathbf{s}}=0$ otherwise.