Comparisons between classical and quantum mechanical nonlinear lattice models

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Abstract

In the mid-1920s, the great Albert Einstein proposed that at extremely low temperatures, a gas of bosonic particles will enter a new phase where a large fraction of them occupy the same quantum state. This state would bring many of the peculiar features of quantum mechanics, previously reserved for small samples consisting only of a few atoms or molecules, up to a macroscopic scale. This is what we today call a Bose-Einstein condensate. It would take physicists almost 70 years to realize Einstein's idea, but in 1995 this was finally achieved.

The research on Bose-Einstein condensates has since taken many directions, one of the most exciting being to study their behavior when they are placed in optical lattices generated by laser beams. This has already produced a number of fascinating results, but it has also proven to be an ideal test-ground for predictions from certain nonlinear lattice models.

Because on the other hand, nonlinear science, the study of generic nonlinear phenomena, has in the last half century grown out to a research field in its own right, influencing almost all areas of science and physics. Nonlinear localization is one of these phenomena, where localized structures, such as solitons and discrete breathers, can appear even in translationally invariant systems. Another one is the (in)famous chaos, where deterministic systems can be so sensitive to perturbations that they in practice become completely unpredictable. Related to this is the study of different types of instabilities; what their behavior are and how they arise.

In this thesis we compare classical and quantum mechanical nonlinear lattice models which can be applied to BECs in optical lattices, and also examine how classical nonlinear concepts, such as localization, chaos and instabilities, can be transferred to the quantum world.

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Slutligen, tack Rebecka för det stödet du gett mig och det tålamodet du har visat under arbetet med licen. Det har varit, och du är, ovärderlig för mig.

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CHAPTER 1

Introduction

In this thesis we compare quantum mechanical lattice models, of Bose-Hubbard model types, with classical lattice models, of discrete nonlinear Schrödinger equation types, with emphasis on how classical nonlinear phenomena can be transferred to the quantum mechanical world. These models have in recent years received considerable attention in the context of Bose-Einstein condensates in optical lattices.

The outline of the thesis is as follows. In this introduction the necessary background on Bose-Einstein condensates in optical lattices and nonlinear science is presented. In chapter 2 the quantum mechanical Bose-Hubbard model is introduced, as well as extensions to the ordinary model, and relevant results are discussed. In chapter 3 the same is done for the classical discrete nonlinear Schrödinger equation. In chapter 4 it is discussed how classical nonlinear concepts can be transferred to the quantum world. In chapter 5 a summary of the appended papers is presented.

1.1 Bose-Einstein Condensation

1.1.1 Background

It is a remarkable property of nature that all particles can be classified as either fermions or bosons. Fermions are particles which have half integer spin and obey the Pauli exclusion principle, meaning that each quantum state can be occupied with at most one fermion, while bosons on the other hand have integer spin, and any number of bosons can populate a given quantum state. In this thesis, we will deal primarily with the latter type.

The statistical properties of bosons were worked out by the Indian physicist

Satyendra Nath Bose (whom they are named after) and Albert Einstein in 1924-1925 [20, 37, 38]. It was Einstein who realized that a macroscopic fraction of non-interacting massive bosons will accumulate in the lowest single particle quantum state for sufficiently low temperatures. This new phase of matter is what we today call a ‘Bose-Einstein condensate’ (BEC). The condensed atoms can be described by a single wave function, thus making the intriguing, and normally microscopic, wave-like behavior of matter in quantum mechanics a macroscopic phenomenon.

BECs were for a long time considered to be merely a curiosity with no practical importance, until in 1938 when Fritz London [76] suggested that the recently discovered superfluidity of liquid ^4He could be explained by using this concept. Also the theory of superconductivity builds on the notion of a BEC, this time of electron pairs (Cooper pairs). These are however two strongly interacting systems, and the concept of a BEC becomes quite more complicated than the simple scenario of noninteracting particles originally considered by Einstein¹. Also, only about 10% of the atoms in liquid ^4He are in the condensed phase. But to realize a purer BEC closer to the original idea would prove to be a formidable task, due to the extremely low temperatures it would require.

In the 1970’s, new powerful techniques, using magnetic fields and lasers, were developed to cool neutral atoms. This led to the idea that it would be possible to realize BECs with atomic vapors. But, as everyone knows, if a normal gas is cooled sufficiently, it will eventually form a liquid or solid, two states where interactions are of great importance. This can however be overcome by working with very dilute gases, so that the atoms stay in the gaseous form when they are cooled down, but which will also imply the need for temperatures in the micro or nano Kelvin scale for condensation².

Spin-polarized hydrogen was proposed as an early candidate³ [118], but with the development of laser cooling, which cannot be used on hydrogen, alkali atoms also entered the race. Finally in 1995, some seventy years after Einstein’s original proposal, a BEC was observed in a gas of rubidium atoms, cooled to a temperature of 170 nano Kelvin [7]. This was only a month prior to another group observing it in lithium [21], and later the same year it was also produced with sodium [29]. This would eventually render Carl Wieman, Eric Cornell (Rb-group) and Wolfgang Ketterle (Na-group) the 2001 Nobel Prize in physics. BECs have since been produced with a number of different atom species, notably with hydrogen in 1998 [47], and are nowadays produced routinely in labs around the world.

1.1.2 Theoretical Treatment

But even for a dilute gas of neutral atoms there are some interactions. The theoretical treatment of these can however be significantly simplified at low temperatures, since they then can be taken to be entirely due to low-energy binary collisions,

¹For a more formal definition of a BEC, see [95].

²The critical temperature of condensation can be estimated by when the thermal de Broglie wavelength ($\sim T^{-1/2}$) becomes equal to inter-particle spacing [92].

³Hydrogen was proposed as a candidate already in 1959 by Hecht [53], but this work was well before its time and went largely unnoticed by the scientific community.

completely characterized by only a single parameter - the s -wave scattering length a_s . This scattering length is first of all positive for certain elements (e.g. ^{23}Na and ^{87}Rb) and negative for others (e.g. ^7Li), meaning repulsive and attractive interactions respectively, but it can also, by means of Feshbach resonances, be controlled externally with magnetic field [19].

The macroscopic wave-function Ψ of the condensate is, at zero temperature and with a_s much smaller than the average inter-particle spacing, well described by the *Gross-Pitaevskii* equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\vec{r}) + \frac{4\pi\hbar^2 a_s}{m} |\Psi|^2 \right) \Psi, \quad (1.1)$$

where V_{ext} contains all the externally applied potentials, which often includes a contribution from a harmonic trapping potential with frequency $\omega_T \sim 10 - 1000$ Hz (cf. $V(x) = m\omega^2 x^2/2$). Other types of external potentials will be treated in the next section. This equation has the form of the Schrödinger equation, but with an additional nonlinear term, proportional to the local density, which accounts for the particle interactions.

The individual behavior of the condensed atoms is ‘smeared out’ in Ψ , and the validity of the Gross-Pitaevskii equation therefore relies on the number of particles in the condensate being so large that quantum fluctuations can be neglected. It will therefore be referred to as a semi-classical equation. The Gross-Pitaevskii equation has been very successful in describing many macroscopic properties [92], especially for BECs in traps, which was the focus of much of the early research after the first experimental realization [26].

But just like with electromagnetism, where certain phenomena can be explained with classical electromagnetic fields and others need a more detailed, quantum mechanical, description with photons, it is sometimes necessary to use a more microscopic (i.e. quantum mechanical) treatment also for BECs. One example, as mentioned earlier, is when there are few particles in the condensate.

1.1.3 Bose-Einstein Condensates in Optical Lattices

Utilizing *optical lattices* - periodic structures generated by the interference of laser beams - has made it possible to study effects of *periodic potentials* on BECs. The physical mechanism behind this can be illustrated by considering the simple case of two counter-propagating beams with the same amplitude, linear polarization and frequency ω . The beams will together form a standing wave with electric field⁴ $E(x, t) \propto \cos(\omega t) \cos(kx)$, which will induce electric dipole moments in atoms placed in the field. This dipole moment will in its turn couple back to the electric field, leading to a spatially varying (AC-Stark) shift of the atomic energy level, equal to

$$\Delta E(x) = -\frac{1}{2} \alpha(\omega) \langle E^2(x, t) \rangle, \quad (1.2)$$

where α denotes the atomic polarizability and $\langle . \rangle$ the average over one period of the laser [85]. All in all, this leads to a one-dimensional periodic potential for

⁴Effects of the magnetic field can generally be neglected.

the atoms, with minima at either the nodes or antinodes of the standing wave, depending on the polarizability of the atoms. Adding more lasers makes it possible to create lattices, not only simple types with higher dimensionality, but also of a more complex character, e.g. moving lattices, kagome lattices and quasi-periodic lattices [85, 125]. It is also possible to strongly suppress the movement of the atoms in a given direction, by increasing either the trapping or periodic potential that is pointing in that way. By doing this one can construct (quasi-)one or two dimensional systems, where the atoms are confined to move along either one dimensional tubes or two dimensional disks.

One of the most appealing features of experiments with BECs in optical lattices is the great external controllability of many of the system's parameters, making it possible to access fundamentally different physical regimes. One example of this was mentioned above with the different lattice geometries that are possible to create. Another is the potential depth, which is tuned by adjusting the laser intensity and can be varied over a wide range - from completely vanished lattices to very deep ones with sites practically isolated from each other. The potential depth can on top of it all also be changed in real time, making it possible to study phase transitions in detail [52].

Deeper potentials will also lead to a larger confinement (and therefore higher density) within the lattice wells, resulting in stronger on-site interactions, and it is actually possible to reach the strongly interacting regime by increasing the depth. The interaction strength, and sign, can also be changed with Feshbach resonances, which was discussed in the previous section.

Finally, the number of particles per lattice site in experiments can vary from so few that quantum fluctuations are important [19] to sufficiently many for mean-field theories to be applicable [85]. In the former case, it is necessary to use fully quantum mechanical models, for instance the Bose-Hubbard which chapter 2 will deal with in detail, while one generally uses models based on the Gross-Pitaevskii equation (1.1) in the latter case.

The diversity, and high accuracy, of experiments with BECs in optical lattices, makes it an ideal test-bed for many theoretical predictions, for instance from condensed matter physics. It has also been put forward as a candidate to realize quantum simulators [18].

1.2 Nonlinear Science

Nonlinear science can be said to be the study of generic phenomena that arise particularly in nonlinear models. The field is highly interdisciplinary, with applications in a wide variety of scientific areas, ranging from physics, chemistry and biology to meteorology, economics and social sciences. The two phenomena of nonlinear science that are of primary interest for this thesis are localization and low-dimensional chaos, both of which will be discussed in the following sections.

1.2.1 Nonlinear Localization

Continuous Models

Localized waves can appear as solutions to certain continuous nonlinear models due to a balance between the effects of dispersion and nonlinearity. The occurrence of dispersion can be illustrated by looking at the following linear equation,

$$\frac{\partial u}{\partial t} + \frac{\partial^3 u}{\partial x^3} = 0. \quad (1.3)$$

This is solved, due to the linearity, by any superposition of the exponential functions $e^{i(kx - \omega(k)t)}$, with $\omega(k) = -k^3$. The time-evolution for an arbitrary initial wave profile, $u(x, t = 0) = f(x)$, is therefore determined by

$$u(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(k) e^{i(kx - \omega(k)t)} dk \quad (1.4)$$

where

$$F(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \quad (1.5)$$

is the Fourier transform of $f(x)$. Should $f(x)$ now be spatially localized, then it must contain significant contributions from a wide range of Fourier modes,⁵ each of which traveling with a different phase velocity $v_p = \omega/k = -k^2$. This will consequently cause the wave to disperse, which is the reason we call the dependence of ω on k the *dispersion relation*.

Consider now instead the effect of a nonlinear term in the following equation⁶

$$\frac{\partial u}{\partial t} - 6u \frac{\partial u}{\partial x} = 0. \quad (1.6)$$

Plugging in a traveling wave ansatz, $u(x, t) = f(x - ct)$, into equation (1.6) leads to

$$-[c + 6f(\chi)]f'(\chi) = 0, \quad (1.7)$$

with $\chi = x - ct$, which suggests that waves with larger amplitude will move faster. For an initially localized wave, this means that parts with large amplitude will ‘catch up’ with lower amplitude parts, resulting in a steepening of the wave.

The claim in the beginning of this section was that these two effects can be balanced to create a stable, localized wave. Let us therefore consider a combination of equations (1.3) and (1.6),

$$\frac{\partial u}{\partial t} + \frac{\partial^3 u}{\partial x^3} - 6u \frac{\partial u}{\partial x} = 0. \quad (1.8)$$

⁵This is related to Heisenberg’s uncertainty principle from quantum mechanics, which states that a narrow wave-packet in real space implies a broad wave-packet in momentum (Fourier) space.

⁶The factor 6 is chosen for future convenience.

It is readily tested that this equation is satisfied by

$$u(x, t) = -\frac{v}{2} \operatorname{sech}^2 \left(\frac{\sqrt{v}}{2} (x - vt) \right), \quad (1.9)$$

a localized wave traveling with velocity $0 \leq v < \infty$. This is actually an example of a *soliton*! This term was coined in 1965 by Zabusky and Kruskal [128], to emphasize that it is not only a solitary wave, but also possesses certain particle properties (cf. electron, proton) under collisions, namely that when two solitons collide with each other, they will emerge with the same shape and velocity as before, but slightly shifted compared to the position they would have had without colliding. This is surprising, since equation (1.8) is nonlinear, and waves therefore interact with each other. One would rather expect that a collision would have a big effect on (at least) the shape and velocity. The shift also indicates that the mechanism here is something fundamentally different from the linear superposition. This property is thought to be connected to the *integrability* of the equations that support solitons, which means that they have an infinite number of conserved quantities [107]. We should however note that there is not a single, universally agreed on definition of a soliton, and that this can vary from very strict mathematical definitions to being essentially a synonym to a solitary wave⁷, which often is the case in the BEC community.

Equation (1.8) is actually the famous Korteweg-de Vries (KdV) equation, one of the classic soliton equations [31], and the particular equation that Kruskal and Zabusky considered in 1965 [128]. It is named after two dutch physicists who used it in 1895 [72] to explain the occurrence of solitary waves in shallow water. This had been observed in 1834 by Scottish engineer John Scott Russell in the Union Canal near Edinburgh [103], an observation that at the time was met with big skepticism from many leading scientists, since the current (linear) models for shallow water did not permit such solutions. The work of Korteweg and de Vries did however not initiate much further work on nonlinear localization within the scientific community. The research on nonlinear localization took off instead much later, in the 1970's. That the importance of early results was overlooked is a quite common theme within the history of nonlinear science⁸.

Another famous, and well studied, soliton equation is the nonlinear Schrödinger (NLS) equation, given in normalized units by⁹

$$i \frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} \pm |u|^2 u = 0. \quad (1.10)$$

One usually refers to the NLS equation with a plus (minus) sign as the focusing (de-focusing) NLS equation, for reasons that will be explained later. It is a generic equation which describes the evolution of a wave packet with the lowest

⁷One may also argue that a single soliton, like equation (1.9), should not be referred to as a soliton at all, but rather a solitary wave, since it does not have another soliton to collide with.

⁸The history of nonlinear science is described in an easily accessible manner in [108].

⁹This is sometimes called the *cubic* NLS equation to distinguish it from NLS equations with other types of nonlinearity. It can of course also be generalized to higher dimensions, but it is only the one-dimensional cubic NLS equation that is integrable.

order effects of nonlinearity and dispersion taken into account, and therefore appears in a wide variety of contexts, such as nonlinear optics, nonlinear acoustics, deep water waves and plasma waves [107]. The observant reader will notice that the homogeneous ($V_{ext} = 0$) one-dimensional Gross-Pitaevskii equation (1.1) can be rewritten in the form of (1.10), and the research on solitons in (quasi-)one-dimensional BECs has indeed been an active area. The de-focusing NLS equation (i.e. repulsive BEC with $a_s > 0$) supports dark solitons, i.e. localized density dips, while the focusing NLS equation (attractive BEC) instead supports bright solitons, i.e. localized density elevations. Both dark [24, 30] and bright solitons [67, 117] have been experimentally observed in BECs.

Discrete Models

Localized structures can also exist in discrete nonlinear models. An example of this is *discrete breathers* (DBs), also called *intrinsic localized modes* (ILMs), which are not only localized but also time-periodic (breathing). An intuitive example of discrete breathers can be found for a chain of masses connected with anharmonic springs. Under suitable conditions, it is possible to excite the lattice so that only one (or a few) of the masses oscillates significantly (the amplitude of oscillations may for instance decay exponentially from this point) [42].

A central paper in this field is due to MacKay and Aubry in 1994 [78], where the existence of DBs in anharmonic Hamiltonian systems with time-reversibility was rigorously proven under rather general conditions, thus showing that DBs are generic entities. This work has also been extended to more general systems [112]. The crucial point is that a non-resonance condition is fulfilled, i.e. that all multiples of the frequency of the DB fall outside the bands of the linear modes. The discreteness is essential for this, since it bounds the frequency of the linear modes (cf. the optical and acoustic branches of phonons). Compare this to a continuous, spatially homogeneous model, where the linear spectrum is unbounded, and there surely are at least some multiple of the frequency, now for the continuous breather, which falls in a linear band¹⁰.

One interesting aspect of the proof in [78] is that it also provides an explicit method for constructing discrete breathers. It starts from the so called anti-continuous limit where all sites are decoupled from each other, and one trivially can create a localized solution, let us say on one site, simply by setting this site into motion and letting all others be still.

The key idea of the method, and thus also the proof, is that when the coupling between the sites is turned up slightly, the 'old' localized solution of the uncoupled model can be mapped on a 'new' localized solution of the coupled model, if the above mentioned condition is fulfilled. This new solution can in practice be found by using the old solution as the initial guess in a Newton-Raphson algorithm that is searching for zero-points of the map, $F[\psi_{\mathbf{R}}] = \psi_{\mathbf{R}}(T) - \psi_{\mathbf{R}}(0)$ where $\psi_{\mathbf{R}}(t)$ is the

¹⁰There are some notable exceptions of integrable equations which have breather solutions, e.g. the NLS equation where a two-soliton bound state creates the breather [99]. Also the Sine-Gordon equation, $u_{xx}^2 - u_{tt}^2 = \sin(u)$ possesses an exact breather solution, which has the form $u(x, t) = 4 \arctan[\beta \sin(\omega t) / \omega \cosh(\beta x)]$ [107].

generally complex value of site $\mathbf{R}$ and T is the time period of the discrete breather one is looking for [42]. Note that the map $F[\psi_{\mathbf{R}}]$ is multidimensional, i.e. that we are looking for a solution where all sites $\mathbf{R}$ have the same periodicity. By iterating this procedure, i.e. turning up the coupling and finding a new localized solution, one can follow a family of discrete breathers as a function of the coupling [42]. Depending on which solution one starts with in the anti-continuous limit, different discrete breather families may be followed.

DBs have been studied in many different physical systems (see [42] and references therein), and experimentally observed in for example Josephson junctions [120] and coupled optical waveguides [39, 43]. But it is also an applicable concept for BECs in deep optical lattices [45, 75, 121], since one then can utilize a tight-binding approximation on the Gross-Pitaevskii equation to derive a set of discrete nonlinear equations (this will be discussed further in chapter 3). An important point is that it is generally not the amplitude, i.e. the number of atoms, that is oscillating for a DB in a BEC, but rather the phase, and it is therefore often common to instead talk about discrete solitons. This is also the case for DBs in optical waveguides.

Nonlinear localization has been observed both for BEC in weak [33] and deep periodic potentials [8], but these structures cannot really be identified with DBs, at least not few-site DBs.

1.2.2 Instabilities

The classical models that are of primary interest in this thesis are Hamiltonian systems with a discrete set of time-dependent variables, which are described by ordinary differential equations of the form

$$\begin{aligned}\dot{x}_1 &= f_1(x_1, x_2, \dots, x_n) \\ \dot{x}_2 &= f_2(x_1, x_2, \dots, x_n) \\ &\vdots \\ \dot{x}_n &= f_n(x_1, x_2, \dots, x_n),\end{aligned}\tag{1.11}$$

or, with a more compact notation,

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}),\tag{1.12}$$

where the dot denotes a time-derivative. The variables x_i are real, so if the system has complex degrees of freedom, then they have to be split up into their real and imaginary part.

By integrating the ODEs in (1.12) one can determine how some initial conditions, $\mathbf{x}(0)$, will evolve in the n -dimensional phase space. This will track out a trajectory, $\mathbf{x}(t)$, and it is common to call these systems ‘flows’, since one can think of the phase space as a flow of different initial conditions.

Consider now a fixed point $\tilde{\mathbf{x}}$ of the system, for which $\dot{\tilde{\mathbf{x}}} = \mathbf{f}(\tilde{\mathbf{x}}) = 0$. To determine whether this is an unstable or stable fixed point, we look at the time-evolution of a perturbation, $\delta\mathbf{x}$, added to $\tilde{\mathbf{x}}$. This can be determined from $\dot{\tilde{\mathbf{x}}} + \delta\dot{\mathbf{x}} =$

$\mathbf{f}(\tilde{\mathbf{x}} + \delta\mathbf{x})$, which, since the perturbation is assumed to be small, can be Taylor expanded, leading to (since $\dot{\tilde{\mathbf{x}}} = \mathbf{f}(\tilde{\mathbf{x}}) = 0$)

$$\dot{\delta\mathbf{x}} = \mathbf{Df}(\tilde{\mathbf{x}})\delta\mathbf{x} \quad (1.13)$$

where $\mathbf{Df}(\tilde{\mathbf{x}})$ is the Jacobian or functional matrix

$$\mathbf{Df}(\tilde{\mathbf{x}}) = \begin{pmatrix} \partial f_1/\partial x_1 & \partial f_1/\partial x_2 & \cdots & \partial f_1/\partial x_n \\ \partial f_2/\partial x_1 & \partial f_2/\partial x_2 & \cdots & \partial f_2/\partial x_n \\ \vdots & \vdots & \ddots & \vdots \\ \partial f_n/\partial x_1 & \partial f_n/\partial x_2 & \cdots & \partial f_n/\partial x_n \end{pmatrix} \quad (1.14)$$

evaluated at the fixed point $\tilde{\mathbf{x}}$. Let us denote the eigenvectors and eigenvalues of the functional matrix with $\mathbf{v}_i$ and h_i , respectively, so that

$$\mathbf{Df}(\tilde{\mathbf{x}})\mathbf{v}_i = h_i\mathbf{v}_i. \quad (1.15)$$

Consider now a perturbation which is parallel to an eigenvector, $\mathbf{v}_i$. Its time evolution is determined by $\dot{\delta\mathbf{x}} = h_i\delta\mathbf{x}$, which has the solution

$$\delta\mathbf{x}(t) = \delta\mathbf{x}(0)e^{h_it}. \quad (1.16)$$

It will thus stay parallel to the eigenvector, but grow if h_i is a positive real number or shrink if it is a negative real number. The eigenvalues can also be complex, but these will always appear in complex conjugated pairs, since the functional matrix is real. A perturbation in the plane spanned by the corresponding eigenvectors will then spiral, either towards $\tilde{\mathbf{x}}$ if the real part of the eigenvalues are negative, or away from $\tilde{\mathbf{x}}$ if they are positive. Should the eigenvalues be purely imaginary then the perturbation will circle the fixed point in a periodic orbit. This is called an *elliptic* fixed point.

Assuming that the eigenvectors span the whole phase space, a general perturbation can be written as $\delta\mathbf{x}(0) = \sum_i c_i\mathbf{v}_i$, which will evolve as

$$\delta\mathbf{x}(t) = \sum_i c_i e^{h_it} \mathbf{v}_i. \quad (1.17)$$

And since a random perturbation almost certainly will have at least a small component in each eigen-direction, it is enough that only one eigenvalue has a positive real part for the fixed point to be unstable.

The reasoning above is actually also valid for dissipative systems, so what is special with Hamiltonian systems? Hamiltonian systems obey Liouville's theorem, which states that all volumes in phase space are preserved [49]. This means that if one follows not the time evolution of a single point, but instead of a 'blob' of points in phase space, then the volume of this blob will not change. This will limit the possible fixed points that are allowed for a Hamiltonian system. There can for instance not be a fixed point attractor with only negative eigenvalues, since this would correspond to a volume shrinkage towards the fixed point.

Expressed in a more mathematical language, Hamiltonian systems have a symplectic structure which guarantees that all eigenvalues appear in pairs which sum

to zero [119]. In order then for the system to be stable all eigenvalues of the functional matrix must reside on the imaginary axis, since if there is an eigenvalue that has a negative real part, then there must also be one with a positive real part.

The classical pendulum can serve as an illustrative example. It has an unstable fixed point when it points straight up, since it is possible in principle to balance the pendulum like this, but even the slightest perturbation will cause the pendulum to swing around and thus deviate strongly from the fixed point. It is however possible, at least in theory, to displace the pendulum slightly and give it a little push so that it ends pointing straight up (it will take an infinite amount of time to reach this position), but this is of course extremely unlikely. This would correspond to a perturbation entirely in the direction of an eigenvector with a negative eigenvalue. The pendulum pointing straight down corresponds instead to a stable fixed point, where it still will remain in the vicinity of the fixed point if it is being perturbed, i.e. given a small push.

Consider now a system with a stable fixed point. If the system's parameters are being changed, then this fixed point can become unstable in essentially two ways. Either a pair of eigenvalues collides in the origin and goes out along the real axis. The other option is that two pairs of eigenvalues collide, one pair colliding at a positive imaginary value and the other at the corresponding negative imaginary value, and go out in the complex plane. The latter type is called a Hamiltonian Hopf bifurcation¹¹ (see e.g. [59] and references therein) and leads to an oscillatory instability, meaning that a perturbation from the fixed point will oscillate around it with an exponentially increasing amplitude.

1.2.3 Chaos

The most famous nonlinear phenomenon, at least for the public audience, is chaos. This can even be considered as part of our popular culture today, where there even are popular fictional movies and books dealing with it. We will only give a very brief description of this large area, so the interested reader is directed to any of the numerous text books on the subject, e.g. [88, 119].

Chaotic systems are characterized by their sensitive dependence of initial conditions (SIC), meaning that even minute changes of the initial conditions may cause a drastic change in the behavior of the system. This implies that, since one only can determine the configuration of a system up to a certain accuracy, the system in practice is unpredictable, even though its time evolution is governed by equations which are completely deterministic.

If one follows the time evolution of a perturbation, $\delta\mathbf{x}(0)$, from some general initial conditions $\mathbf{x}(0)$, i.e. not necessarily a fixed point as in section 1.2.2, then a chaotic trajectory, $\mathbf{x}(t)$, is characterized by an initially exponential increase of

¹¹When a system has a bifurcation, it means that its behavior changes, which in the case of the Hamiltonian Hopf bifurcation is that a stable fixed point turns unstable. Ordinary Hopf bifurcations (or supercritical Hopf bifurcations) occur in dissipative systems where the real part of a complex eigenvalue pair goes from negative to positive, turning a stable oscillatory fixed point into a stable periodic orbit surrounding the fixed point [119].

this perturbation, i.e.

$$\left| \frac{\delta \mathbf{x}(t_2)}{\delta \mathbf{x}(t_1)} \right| \approx \exp(\lambda(t_2 - t_1)), \quad (1.18)$$

for $t_2 > t_1$ and a positive value of λ . The constant λ is called the Lyapunov exponent, and it being positive is thus one of the defining properties of a chaotic trajectory. Note that we wrote ‘initial’ exponential divergence, which was to indicate that we cannot say what happens to the perturbation when it gets big, only that it will increase rapidly when it is small. Another condition for a chaotic trajectory is that it should be bounded [88], which most of physical relevance are. To understand this condition, one can easily imagine two trajectories which diverge exponentially from each other as they move towards infinity, but still behave in a regular and predictable way. The third and last condition is that the trajectory cannot be periodic, quasi-periodic or a fixed point, nor approach any of these asymptotically. Fixed points were encountered in the previous section 1.2.2, but to understand the first two (a periodic trajectory is of course nothing new for the reader) we need briefly to discuss *integrability*.

An integrable Hamiltonian system is a system with as many conserved quantities as degrees of freedom¹². It is then possible to make a canonical transformation to *action-angle variables*, P_i and Q_i , which have the property that

$$Q_i = \omega_i t + A_i \quad (1.19a)$$

$$P_i = B_i, \quad (1.19b)$$

where ω_i , A_i and B_i are constants [49]. B_i are associated with the conserved quantities, and Q_i will, as the name implies, behave like an angle, so that one can add a multiple of 2π without changing the system. This describes either a periodic trajectory, if all ω_i/ω_j are rational numbers, or a quasi-periodic trajectory if any ω_i/ω_j is irrational, which actually is the case most often since the irrational numbers are much more ‘common’ than the rational. Periodic and quasi-periodic trajectories will lie on tori in phase space, and are therefore not classified as chaotic, as they are predictable in the sense that they always will be found on their torus. Since an integrable system only can have periodic or quasi-periodic trajectories, it cannot be chaotic.

¹²There are some conditions on these conserved quantities that should be fulfilled, they are e.g. not allowed to be linear combinations of each other and their mutual Poisson brackets must be zero [119].

CHAPTER 2

Bose-Hubbard Model

In this chapter we will discuss the Bose-Hubbard model. Since the advent of BECs in optical lattices, this has received a lot of attention as a model for this kind of systems. It is however noteworthy that it was actually studied prior to this, not at least as a quantum version of the discrete nonlinear Schrödinger equation [15, 16, 110] (cf. chapter 3), when for instance studying local modes in benzene molecules [109] and vibrations in crystals [2]. Many of these papers actually refer to the model as the ‘Quantum discrete nonlinear Schrödinger equation’. We will however conduct our discussion entirely within the context of BECs in optical lattices.

2.1 Derivation of the Bose-Hubbard Model

The derivation of the Bose-Hubbard Hamiltonian can be conducted in a quite straightforward manner starting from a general bosonic many-body Hamiltonian of the form,

$$\hat{H} = \int \hat{\Psi}^\dagger(\mathbf{r}) \hat{H}^{(1)}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) d^3\mathbf{r} + \frac{1}{2} \iint \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}') \hat{H}^{(2)}(\mathbf{r}, \mathbf{r}') \hat{\Psi}(\mathbf{r}') \hat{\Psi}(\mathbf{r}) d^3\mathbf{r} d^3\mathbf{r}' \quad (2.1)$$

where $\hat{H}^{(1)}$ is the part of the Hamiltonian that acts on one particle, i.e. kinetic energy and applied potentials, and $\hat{H}^{(2)}$ the part that acts on particle pairs, i.e. interaction energies. $\hat{\Psi}(\mathbf{r})$ ($\hat{\Psi}^\dagger(\mathbf{r})$) is the bosonic field operator that destroys (creates) a particle at position $\mathbf{r}$. It can be expanded in an arbitrary complete basis

$\{f_i(\mathbf{r})\}$, so that

$$\hat{\Psi}(\mathbf{r}) = \sum_i f_i(\mathbf{r}) \hat{a}_i \quad (2.2a)$$

$$\hat{\Psi}^\dagger(\mathbf{r}) = \sum_i f_i^*(\mathbf{r}) \hat{a}_i^\dagger \quad (2.2b)$$

where $\hat{a}_i$ ($\hat{a}_i^\dagger$) is a bosonic annihilation (creation) operator from the Second Quantization formalism, that destroys (creates) a particle in a state described by the wave function $f_i(\mathbf{r})$, obeying the commutation relations¹

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{i,j} \quad (2.3a)$$

$$[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0, \quad (2.3b)$$

$\delta_{i,j}$ being the Kronecker delta function. It is also useful to introduce the *number operator* $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$, which counts the number of bosons in the i -th state.

We briefly remind ourselves that a state in the Second Quantization formalism is expressed in terms of Fock states, written as $|n_1, n_2, \dots\rangle$ where n_i specifies the number of bosons that are occupying the i -th single particle quantum state. The actions of the annihilation, creation and number operator on an associated Fock state are then given by

$$\hat{a}_i |n_1, \dots, n_i, \dots\rangle = \sqrt{n_i} |n_1, \dots, (n_i - 1), \dots\rangle \quad (2.4a)$$

$$\hat{a}_i^\dagger |n_1, \dots, n_i, \dots\rangle = \sqrt{n_i + 1} |n_1, \dots, n_i + 1, \dots\rangle \quad (2.4b)$$

$$\hat{n}_i |n_1, \dots, n_i, \dots\rangle = n_i |n_1, \dots, n_i, \dots\rangle. \quad (2.4c)$$

Notice that Fock states are eigenstates to the number operators, which actually is the defining property.

Hamiltonian (2.1) is generally too complicated to work with directly, and it is thus necessary to make suitable approximations which capture the system's main physical features. In the case of the Bose-Hubbard model, these approximations originate from that we are considering a cold, weakly interacting, dilute boson gas in a deep optical lattice². This derivation will be conducted for a three dimensional lattice, but it can equally well be done for both one and two dimensions. Remember from section 1.1.3 that it was possible to reduce the dimensionality by increasing the trapping or lattice potential in certain directions. We will return to this topic at the end of this section.

For a deep optical lattice, it seems reasonable that the field operators should be expanded in states which are localized around the lattice sites. These are readily available in the form of Wannier functions $w_{n,\mathbf{R}}(\mathbf{r})$, defined as Fourier components to the Bloch functions $\psi_{n,\mathbf{k}}(\mathbf{r})$, which should be familiar from solid state physics

¹The field operator $\hat{\Psi}(\hat{\mathbf{r}}_i)$ can be viewed as an annihilation operator connected to the eigenstate of the position operator with eigenvalue $\mathbf{r}_i$, i.e. $\delta(\mathbf{r} - \mathbf{r}_i)$. The Kronecker delta in (2.3) will then be exchanged for a Dirac delta, since $\mathbf{r}$ is a continuous set of eigenvalues.

²It is actually the validity of the approximations which defines which regimes we call cold, dilute, etc.

as the eigenstates of a single electron moving in a perfect crystal [9]. Note though that this situation is equivalent to the noninteracting Hamiltonian (2.1) with a periodic potential, which then also will have Bloch functions as eigenstates. These will have the general form

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r}) \quad (2.5)$$

where $\mathbf{k}$ is the quasimomentum, n the band index and $u_{n,\mathbf{k}}(\mathbf{r})$ a function with the same periodicity as the lattice. The relationship between Wannier and Bloch functions is thus given by

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} w_{n,\mathbf{R}}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{R}} \quad (2.6a)$$

$$w_{n,\mathbf{R}}(\mathbf{r}) = \frac{1}{V_{BZ}} \int \psi_{n,\mathbf{k}}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{R}} d\mathbf{k} \quad (2.6b)$$

where $\mathbf{R}$ denotes the lattice vectors and the integration runs over the first Brillouin zone, which has volume V_{BZ} . The Wannier functions will, just as the Bloch functions, form a complete orthonormal basis, when properly normalized. It can be readily verified, for instance by utilizing that $\psi_{n,\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}} \psi_{n,\mathbf{k}}(\mathbf{r})$, that they must have the form $w_{n,\mathbf{R}}(\mathbf{r}) = w_n(\mathbf{r} - \mathbf{R})$, i.e. that all Wannier functions in a band are copies of each other, only translated by a lattice vector.

The Wannier functions are exponentially decaying for lattices with simple bands, but with a decay rate that depends on the depth of the lattice potential [87]. They can therefore be rather wide for a shallow lattice, but should become more localized around a single lattice site for increasing depth.

For a separable periodic potential $\hat{V}_{per}(\mathbf{r}) = \sum_{i=1}^3 \hat{V}_i(x_i)$, which is e.g. the common case of an optical lattice generated by a set of perpendicular laser beams, the problem can effectively be reduced to one dimension, for which Wannier functions have been studied in detail by Kohn [71]. The form of the Wannier functions depends on the global phase of the Bloch functions³, and there is one and only one choice of the phases which will make $w_n(x)$ *i)* real, *ii)* even or odd, *iii)* exponentially decaying. This will also be the Wannier function that is optimally localized.

Because of the low temperature, one can assume that only the lowest Wannier band is occupied⁴. This also requires that the interaction energies, which are discussed later, should be smaller than the band gap, thus invoking the requirement of weak interactions. Band index will therefore be omitted hereafter.

For a deep sinusoidal lattice, the lattice wells can (locally) be approximated with harmonic oscillators, and the Wannier functions can thus be replaced with the corresponding eigenstates [19]. One should however note that no matter how deep the lattice gets, the Wannier function will never converge completely to the harmonic oscillator state, which is decaying Gaussian rather than exponential, but there will be a large overlap between the two states. This is useful for obtaining analytical expressions [19].

³This is not only the case in one dimension, but is a general property, as can be seen from equation (2.6b).

⁴It is actually possible to also create BECs in higher bands [86, 89, 126].

Assume now that the $\hat{H}^{(1)}$ -term of Hamiltonian (2.1), apart from the kinetic energy, contains contributions from a periodic potential $\hat{V}_{per}(\mathbf{r})$, due to the optical lattice, and possibly also from a slowly varying trapping potential $\hat{V}_{trap}(\mathbf{r})$. The trapping potential is taken to be essentially constant over a couple of lattice sites, so that $\int w(\mathbf{r} - \mathbf{R}') \hat{V}_{trap}(\mathbf{r}) w(\mathbf{r} - \mathbf{R}) d^3\mathbf{r} = V_{trap}(\mathbf{R}) \delta_{\mathbf{R}, \mathbf{R}'}$. Replacing the field operators in this term with the corresponding Wannier functions, will then lead to

$$\hat{H} = \sum_{\mathbf{R} \neq \mathbf{R}'} \Upsilon(\mathbf{R}' - \mathbf{R}) \hat{a}_{\mathbf{R}'}^\dagger \hat{a}_{\mathbf{R}} + \sum_{\mathbf{R}} \epsilon_{\mathbf{R}} \hat{n}_{\mathbf{R}} \quad (2.7)$$

where

$$\Upsilon(\mathbf{R}' - \mathbf{R}) = \int w(\mathbf{r} - \mathbf{R}') \left(\frac{\hat{p}^2}{2m} + \hat{V}_{per}(\mathbf{r}) \right) w(\mathbf{r} - \mathbf{R}) d^3\mathbf{r}, \quad (2.8a)$$

$$\epsilon_{\mathbf{R}} = \Upsilon(\mathbf{0}) + V_{trap}(\mathbf{R}). \quad (2.8b)$$

$\Upsilon(\mathbf{R}' - \mathbf{R})$ is the matrix element for the hopping of a boson between sites $\mathbf{R}$ and $\mathbf{R}'$. These are, just as the Wannier functions, decreasing with distance, so that only the nearest neighbor hopping is non-negligible for sufficiently deep lattices. It is thus only the nearest neighbor hopping that will be of interest and the corresponding matrix element will actually always be negative [19], and we will from now on therefore denote this Υ with $-J$. Estimations on how the ratio between matrix elements for different hopping lengths depend on the lattice depth can be obtained by replacing the Wannier functions in (2.8a) with harmonic oscillator states [19]. $\epsilon_{\mathbf{R}}$ on the other hand gives the single particle on-site energy at site $\mathbf{R}$.

The first integral in Hamiltonian (2.1) can thus be approximated with

$$-J \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} \hat{a}_{\mathbf{R}}^\dagger \hat{a}_{\mathbf{R}'} + \sum_{\mathbf{R}} \epsilon_{\mathbf{R}} \hat{n}_{\mathbf{R}} \quad (2.9)$$

where $\langle \mathbf{R}, \mathbf{R}' \rangle$ indicates summation over neighboring sites.

Let us now shift focus to the second integral in (2.1) and interactions. For a weakly interacting, dilute gas, collisions are rare events and can therefore be taken to always be between only two particles at a time. Because of the low temperatures, the collisions are also assumed to be entirely of the s -wave scattering type, since higher angular momentum scattering will be frozen out by the centrifugal barrier. The interaction potential can then be approximated with a contact pseudopotential of the form [92]

$$V_{int}(\mathbf{r}) = \frac{4\pi\hbar^2 a_s}{M_r} \delta(\mathbf{r}) \quad (2.10)$$

where M_r is the reduced mass, and a_s is the s -wave scattering length. This will be the relevant parameter that characterizes the interaction strength, larger a_s meaning stronger interactions, with positive (negative) value indicating repulsion (attraction).

Inserting $\hat{H}^{(2)}$ with (2.10) in the second integral in (2.1) leads to

$$\hat{H}_{int} = \frac{1}{2} \frac{4\pi\hbar^2 a_s}{M_r} \int \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) d^3\mathbf{r}. \quad (2.11)$$

Expanding the field operators, once again, in deep potential Wannier functions, one realizes that (2.11) is dominated by the terms $\sim \hat{a}_{\mathbf{R}}^\dagger \hat{a}_{\mathbf{R}}^\dagger \hat{a}_{\mathbf{R}} \hat{a}_{\mathbf{R}} = \hat{n}_{\mathbf{R}}(\hat{n}_{\mathbf{R}} - 1)$, and that the interaction part of (2.1) therefore can be approximated with

$$\frac{U}{2} \sum_{\mathbf{R}} \hat{n}_{\mathbf{R}}(\hat{n}_{\mathbf{R}} - 1) \quad (2.12)$$

where

$$U = \frac{4\pi\hbar^2 a_s}{M_r} \int |w(\mathbf{r})|^4 d^3\mathbf{r}. \quad (2.13)$$

Putting together (2.9) and (2.12) finally gives us the Bose-Hubbard model

$$\hat{H} = -J \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} \hat{a}_{\mathbf{R}}^\dagger \hat{a}_{\mathbf{R}'} + \frac{U}{2} \sum_{\mathbf{R}} \hat{n}_{\mathbf{R}}(\hat{n}_{\mathbf{R}} - 1) + \sum_{\mathbf{R}} \epsilon_{\mathbf{R}} \hat{n}_{\mathbf{R}}. \quad (2.14)$$

To conclude, this model describes bosons which are allowed to hop between nearest neighboring sites, corresponding essentially to the kinetic energy of the model, and that only will interact with each other when they are occupying the same site. Each particle will on top of this feel a site dependent potential.

The derivation of the Bose-Hubbard model in lower dimensions can be done in an almost identical manner. The difference is that one has to handle the confinement in the directions perpendicular to the lattice. The potential in these directions is usually taken to be approximately harmonic, and it is assumed that the frequency $\omega_\perp$, and thereby the energy separation $\hbar\omega_\perp$ between eigenstates, is sufficient large (compared to interaction and thermal energies) that only the lowest eigenstate has to be included [23]. This is analogous to why only the lowest Wannier band was considered.

Taking the one-dimensional lattice (pointing in x -direction) as an example, this means that the state localized on site $\mathbf{R} = (x_0, y_0, z_0)$ will be given by $w(x - x_0)h_0(y - y_0)h_0(z - z_0)$ instead of $w(\mathbf{r} - \mathbf{R})$, where $h_0(y)$ is the harmonic oscillator ground state. Using this state, or the corresponding one for two dimensions, will lead to essentially the same model as (2.14). The only difference lies in the lattice topology, which actually makes it possible to write the one-dimensional Bose-Hubbard model in a slightly simpler form

$$\hat{H} = -J \sum_i (\hat{a}_{i+1}^\dagger \hat{a}_i + \hat{a}_{i-1}^\dagger \hat{a}_i) + \frac{U}{2} \hat{n}_i(\hat{n}_i - 1) + \epsilon_i \hat{n}_i. \quad (2.15)$$

2.2 Eigenstates

The Hilbert space for the f -site Bose-Hubbard model is spanned by the Fock states $|n_1, \dots, n_f\rangle$, with n_i denoting the number of bosons on site i , which is infinite dimensional since n_i can take any positive integer value. It is however not necessary to work in the full Hilbert space; instead the dimensionality can be reduced to a finite size by considering only a fixed number of total particles. This seems physically reasonable since material bosons cannot be created or destroyed (unlike

photons), and is also mathematically viable since the Hamiltonian commutes with the total number operator

$$\hat{N} = \sum_{i=1}^f \hat{n}_i. \quad (2.16)$$

This implies that energy eigenstates also are eigenstates to $\hat{N}$, i.e. have specific numbers of particles.

The Hilbert space dimension $\mathcal{D}$ for fixed number of particles is indeed not infinite, but generally quite big - for f sites and N particles $\mathcal{D} = (N + f - 1)!/N!(f - 1)!$. This grows quite rapidly and one is restricted to rather modest system sizes if one wishes to use exact diagonalization when calculating eigenstates and eigenvalues.

For a translational invariant one-dimensional model, i.e. homogeneous with periodic boundary conditions ($\hat{a}_{f+1} = \hat{a}_1$), the dimensions can be reduced one step further. Defining the translation operator $\hat{T}$ as

$$\hat{T}|n_1, n_2, \dots, n_f\rangle = |n_2, \dots, n_f, n_1\rangle, \quad (2.17)$$

it is readily tested that both $\hat{H}$ and $\hat{N}$ commute with $\hat{T}$, and the Hamiltonian can therefore be further block diagonalized in a basis of mutual eigenstates to $\hat{T}$ and $\hat{N}$. It is hereafter assumed that we are in a subspace with a fixed total number of particles N . We are thus looking for states which look the same, apart from a numerical factor, when translated one site. Translating this state f sites, i.e. through the whole lattice, should give back the same state, i.e. $\hat{T}^f = \hat{I}$, where $\hat{I}$ is the identity operator. This implies that the eigenvalues of $\hat{T}$, denoted τ_k , obey $\tau_k^f = 1 \Rightarrow \tau_k = e^{ik}$, where $k = 2\pi\nu/f$ and $\nu = 0, \pm 1, \dots, \pm(f/2 - 1), +f/2$ (f even) or $\nu = 0, \pm 1, \dots, \pm(f - 1)/2$ (f odd). The eigenstates should thus have the property that $\hat{T}|\tau_k\rangle = e^{ik}|\tau_k\rangle$, and probably the simplest type of states for which this is fulfilled are

$$|\tau_k^{(\alpha)}\rangle = \sum_{j=0}^{f-1} (e^{-ik}\hat{T})^j |\phi^{(\alpha)}\rangle \quad (2.18)$$

where $|\phi^{(\alpha)}\rangle = |n_1^{(\alpha)}, n_2^{(\alpha)}, \dots, n_f^{(\alpha)}\rangle$ is a given Fock state with $\sum_i n_i^{(\alpha)} = N$. The states of type (2.18) will thus give us the basis that we are looking for. Note however that when generating this basis, one should not include two states such that $\langle \phi^{(\alpha)} | \hat{T}^s | \phi^{(\beta)} \rangle \neq 0$ for any s , since these will result in the same state when plugged into (2.18), differing only by a numerical factor. One should also note that Fock states which possess an additional translational symmetry, i.e. $\hat{T}^s |\phi^{(\alpha)}\rangle = |\phi^{(\alpha)}\rangle$ for $s < f$, will generate a null-vector when plugged into (2.18) for certain k -values. Consider the simple case of one particle in each lattice well of a two-site lattice, $|1, 1\rangle$, which for $k = 1$ gives $|1, 1\rangle - |1, 1\rangle = 0$.

These results are actually just the Bloch theorem in action. The states defined by (2.18), and also linear combinations (with the same k) of them, have the structure of Bloch states, and k (actually $\hbar k$) is the crystal momentum.

2.3 Superfluid to Mott Insulator Transition

For repulsive interactions ($U > 0$), the Bose-Hubbard model undergoes a quantum phase transition from a superfluid to Mott insulating state [130]. This transition was first discussed, for the Bose-Hubbard model, in a paper by Fisher et al [41], but with systems such as ^4He absorbed in porous media and granular superconductors in mind. It was in another seminal paper by Jaksch et al [57] where it was proposed, first of all that the Bose-Hubbard model should be applicable for ultracold atoms in optical lattices, but also that the transition could be realizable with such a system. This was experimentally observed in 2002 by Greiner et al [52] in a three-dimensional lattice, and has since also been observed in both one- and two-dimensional lattices [70, 116].

The transition illustrates the competition between the repulsive on-site interaction and kinetic energy, so that when the interaction energy 'wins', the ground state is a Mott insulator, while it becomes a superfluid when the kinetic energy prevails. To get some insight into the nature of these two states, it is instructive to look at the form the ground states take for a homogeneous Bose-Hubbard model with N particles in a f -site lattice, in the two limits $U \gg J$ and $U \ll J$.

The ground state is in the noninteracting limit ($U = 0$) given by

$$|\Psi_{SF}(N) \rangle_{(U=0)} = \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{f}} \sum_{\mathbf{R}} \hat{a}_{\mathbf{R}}^\dagger \right)^N |0 \rangle \quad (2.19)$$

with $|0 \rangle$ denoting the vacuum state where no quantum state is occupied. Noting that $f^{(-1/2)} \sum_{\mathbf{R}} \hat{a}_{\mathbf{R}}^\dagger |0 \rangle$ creates one particle in the quasimomentum state $\mathbf{k} = 0$ (c.f. (2.18)), one realizes that (2.19) is a pure BEC with all N particles in this quasimomentum state. The atoms are now in a superfluid phase [41], where each atom is completely delocalized, and allowed to move freely over the whole lattice.

In the thermodynamic limit, $N, f \rightarrow \infty$ with fixed density N/f , state (2.19) can be approximated with a coherent state [130], which in its turn, since creation operators for different sites commute, can be written as a product of local coherent states for each lattice site $\mathbf{R}$, with an average particle occupation $\langle \hat{n}_i \rangle = N/f$,

$$|\Psi_{SF}(N \rightarrow \infty) \rangle_{(U=0)} \approx \exp \left(\sqrt{\frac{N}{f}} \sum_{\mathbf{R}} \hat{a}_{\mathbf{R}}^\dagger \right) |0 \rangle = \prod_{\mathbf{R}} \exp \left(\sqrt{\frac{N}{f}} \hat{a}_{\mathbf{R}}^\dagger \right) |0 \rangle. \quad (2.20)$$

The probability of finding a specific number of particles on a site thus follows a Poisson distribution, with standard deviation $\sqrt{N/f}$.

The states (2.19) and (2.20) are examples of two types of coherent states which will be discussed in section 3.1.

In the opposite limit, $J = 0$, tunneling is completely suppressed. The repulsive interaction energy will also try to reduce the number of particles of each site as much as possible. Considering at first a system with commensurate particle filling, i.e. $\tilde{n} = N/f$ is an integer, this means that the ground state will have the particles evenly spread out, i.e. exactly $\tilde{n}$ particles on each site,

$$|\Psi_{MI}(\tilde{n}) \rangle_{(J=0)} = \left(\prod_{\mathbf{R}} \frac{(\hat{a}_{\mathbf{R}}^\dagger)^{\tilde{n}}}{\sqrt{\tilde{n}!}} \right) |0 \rangle. \quad (2.21)$$

This is a Mott insulator [41]. By tunneling a particle, so that one site has $\tilde{n} + 1$ bosons and another $\tilde{n} - 1$, the energy is increased with U . There can therefore not be a flow of particles over the lattice in this state, and the bosons thus are localized to specific sites. The site with $\tilde{n} + 1$ bosons can be referred to as a ‘particle’ and the one with $\tilde{n} - 1$ as a ‘hole’, in analogy with Dirac’s electron sea. Note also that the Mott-insulator is not a BEC, and it is therefore expected that mean-field descriptions will fail to describe this regime.

Even though the ground state only takes the simple product forms of (2.19) and (2.21) in these specific limits, classifications as Mott insulator or superfluid is valid also in the intermediate regime [19].

To illustrate the mechanism behind the phase transition, consider what will happen to state (2.21) when J is being turned up. Should an atom now hop from one site to the next, then there would on one hand be a gain of kinetic energy of order J , but also a cost in interaction energy for creating a ‘hole’ and a ‘particle’, which is of order U . Thus, if J is much smaller than U , hopping is energetically unfavorable, and the atoms will stay localized on the sites, thus still in the Mott insulating phase. But when J becomes of the same order as U the cost in interaction energy can be outweighed by the gain in kinetic energy and it will thus be beneficial to create an electron-hole pair. Also, as soon as the particle and hole have been created, they will move freely over the lattice, since they are moving over a constant background (neglecting the effect that the particle and hole have on each other) and there is no cost in interaction energy for the particle or hole to move between sites with the same number of particles, therefore making the state superfluid. The phase transition is however only sharp in the thermodynamic limit in two and three dimensions, for smaller systems it is instead more gradual [19].

What will happen if there is not a commensurate filling? Imagine that a single atom is added to the Mott insulting phase discussed above. This atom would, just as the particle and hole, be able to move freely over the constant background, and it will thereby be in the superfluid state all the way down to $J = 0$. This reasoning might suggest that the Mott insulating phase would be extremely hard to realize, but remember that the discussion so far has been for a homogeneous system. By performing the experiments in a slowly varying harmonic trap, leading to a spatially varying on-site energy, one would observe that different regions of the lattice are in the Mott insulating phase, each with different number of particles per site, and that these regions are separated by superfluid regions [57].

The two states obviously differ in many aspects. They for instance exhibit very different phase coherences, which can be understood on the basis of the Heisenberg uncertainty relation for phase and number of atoms at a site, i.e. if the number of atoms on a site is well specified the phase is uncertain, preventing phase coherence between sites, and vice versa. It is therefore low phase coherence (actually none for state (2.21)) between different sites in the Mott insulator phase, but long range phase coherence in the superfluid phase. This difference can actually be utilized to experimentally test the transition. When atoms in the superfluid phase are released from the optical lattice (this is done by simply turning the lasers off) they will lump together in clear interference peaks because of the long range phase coherence. The crossover to the Mott insulating phase can thus be identified,

essentially by looking at when these interference peaks disappear [52].

Another important difference is in the excitation spectrum, where the Mott insulator has a finite energy gap corresponding to the creation of a particle-hole pair. There is on the other hand no energy gap for the superfluid phase, which instead has sound-like excitations, with a linear relation between frequency and wave number. The energy gap in the Mott insulating phase has been experimentally verified [52, 116].

2.4 Extended Bose-Hubbard Models

It should be evident from section 2.1 that the derivation of the Bose-Hubbard model relies on a number of assumptions and approximations. There might therefore exist regimes where the validity of these approximations may come into question, and it is necessary to expand the model.

One of these assumptions was regarding the decay rate of the Wannier functions, and was used to motivate which terms of the Hamiltonian, when expanded in these functions, that should be included. Approximating the Wannier functions with harmonic oscillator ground states, Mazzarella et al [80]⁵ showed that the lowest order corrections to this assumption come from the interaction part of the Hamiltonian. Including also these terms, for a one-dimensional homogeneous ($\epsilon_i = \epsilon$) lattice, leads to the following Hamiltonian

$$\begin{aligned} \hat{H} = \sum_{m=1}^f Q_1 \hat{n}_m + Q_2 (\hat{a}_m^\dagger \hat{a}_{m+1} + \hat{a}_{m+1}^\dagger \hat{a}_m) + Q_3 \hat{n}_m^2 \\ + Q_4 [4 \hat{n}_m \hat{n}_{m+1} + (\hat{a}_{m+1}^\dagger)^2 (\hat{a}_m)^2 + (\hat{a}_m^\dagger)^2 (\hat{a}_{m+1})^2] \\ + 2Q_5 [\hat{a}_m^\dagger (\hat{n}_m + \hat{n}_{m+1}) \hat{a}_{m+1} + \hat{a}_{m+1}^\dagger (\hat{n}_{m+1} + \hat{n}_m) \hat{a}_m], \end{aligned} \quad (2.22)$$

where the parameter notation has been changed from (2.15) to agree with paper I and III. The first three terms are essentially the ordinary Bose-Hubbard model, with $Q_1 = -U/2 + \epsilon$, $Q_2 = -J$ and $Q_3 = U/2$, while the last two terms are the extension. Just as $\hat{a}_{m+1}^\dagger \hat{a}_m$ indicates nearest neighbor tunneling and $(\hat{n}_m - 1)\hat{n}_m$ is related to the on-site energy, these new terms can be associated with simple interaction or tunneling processes, which are listed below.

- $\hat{n}_m \hat{n}_{m+1}$ is related to the interaction energy between atoms at neighboring sites.
- $(\hat{a}_{m+1}^\dagger)^2 (\hat{a}_m)^2$ is coherent tunneling of two particles.
- $\hat{a}_{m+1}^\dagger \hat{n}_{m+1} \hat{a}_m$ and $\hat{a}_{m+1}^\dagger \hat{n}_m \hat{a}_m$ are density dependent tunneling, since they depend on the number of particles at the site the particle tunnels to and from, respectively. This can also be called conditioned tunneling, since $\hat{a}_{i+1}^\dagger \hat{n}_{i+1} \hat{a}_i$ vanishes when the site the particle tunnels to is empty, and $\hat{a}_{i+1}^\dagger \hat{n}_i \hat{a}_i$ vanishes when the site the particle tunnels from would become empty.

⁵This paper contains a misprint so that it appears that they are not studying the same model as we are in paper I and paper III, which they however do.

This model has been used in several theoretical [32, 74, 80, 105, 124, 129] as well as some experimental work [122].

An analogous extended model can also be produced when effects of higher bands are taken into account, in a “dressed” lowest band model [17, 77].

A similar model, with the same terms as (2.22) but with separate parameters for the neighbor interaction term and two-particle tunneling, was used for a BEC with dipolar interactions [115], i.e. with longer range interactions which are not well described by the contact potential. It is also common in this context to use a Bose-Hubbard model extended only with the nearest neighbor interaction term [14, 102, 104, 111].

These models have some new types of phases, compared to the ordinary Bose-Hubbard model, for instance a checker-board phase where every other site is populated, and the supersolid phase which has both superfluid and solid properties.

Bose-Hubbard models can also be used for BECs in higher bands [55]. This introduces new degrees of freedom for the bosons, e.g. that the orbitals can point in different directions, which leads to anisotropic tunneling and interactions [93].

CHAPTER 3

Discrete Nonlinear Schrödinger Equation

The discrete nonlinear Schrödinger (DNLS) equation is just like many of the other equations that we have encountered in this thesis quite generic, this because it arises in contexts when lowest order effects of nonlinearity and lattice dispersion are accounted for [60]. Early applications of the DNLS model include polarons in molecular crystals [54], energy transport in proteins [106] and vibrational modes in small molecules such as benzene [109], while more recent include photonic crystals [83], optical waveguide arrays [39] and, of course, BECs in optical lattices [121].

For a lattice, which may both be of any dimensionality as well as have either a finite or infinite number of lattice points $\mathbf{R}$, the DNLS equation is given by¹

$$i \frac{d\Psi_{\mathbf{R}}}{dt} + \gamma |\Psi_{\mathbf{R}}|^2 \Psi_{\mathbf{R}} + \delta \sum_{\langle \mathbf{R}' \rangle} \Psi_{\mathbf{R}'} - \epsilon_{\mathbf{R}} \Psi_{\mathbf{R}} = 0, \quad (3.1)$$

where $\langle \mathbf{R}' \rangle$ indicates the nearest neighbor sites of $\mathbf{R}$, and γ , δ , $\epsilon_{\mathbf{R}}$ the strength of the nonlinearity, the coupling between neighboring sites and the site dependent potential, respectively. Note that it is possible to rescale these parameters, by rescaling $\Psi_{\mathbf{R}}$ and t . We will take δ to be positive, but by making a staggering transformation on the model, i.e. adding a minus sign to every other site, one can change sign on this parameter. Note though that this cannot be done in all lattices in higher dimensions, e.g. triangular.

There is a connection between the DNLS and continuous NLS equation, which is most easily seen by considering the one-dimensional homogeneous DNLS equa-

¹In analogy with the NLS equation discussed in section 1.2.1, one can use the term ‘DNLS’ for a more general class of equations, but it is not uncommon, and we will also adopt this nomenclature, to with ‘DNLS equation’ mean equation (3.1) with cubic nonlinearity. It is however common to omit the site dependent potential $\epsilon_{\mathbf{R}}$.

tion

$$i \frac{d\Psi_m}{dt} + \gamma |\Psi_m|^2 \Psi_m + \delta (\Psi_{m+1} + \Psi_{m-1}) = 0, \quad (3.2)$$

in a slightly different form, produced by making the substitution $\Psi_m \mapsto e^{2it\delta} \Psi_m$,

$$i \frac{d\Psi_m}{dt} + \gamma |\Psi_m|^2 \Psi_m + \delta (\Psi_{m+1} - 2\Psi_m + \Psi_{m-1}) = 0. \quad (3.3)$$

In the continuous limit, where there are many sites and Ψ_m varies slowly between them, one can replace the discrete index of Ψ_m with a continuous variable, $\Psi_m \mapsto \Psi(m\Delta x)$. By rescaling $\delta = 1/(\Delta x)^2$, one can see that the last term of equation (3.3) will become a second order spatial derivative (Laplacian operator) when taking the limit $\Delta x \rightarrow 0$, and that the DNLS equation (3.3) turns into a NLS equation, identical to (1.10) if one also rescales γ to ± 1 (sign depending on the relative sign between γ and δ).

Equation (3.1) can be derived from the following Hamiltonian,

$$H = - \sum_{\mathbf{R}} \left(\frac{\gamma}{2} |\Psi_{\mathbf{R}}|^4 - \epsilon_{\mathbf{R}} |\Psi_{\mathbf{R}}|^2 \right) - \delta \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} \Psi_{\mathbf{R}'} \Psi_{\mathbf{R}}^* \quad (3.4)$$

with $\Psi_{\mathbf{R}}$ and $i\Psi_{\mathbf{R}}^*$ as generalized coordinates and momenta, respectively. Equation (3.1), and the complex conjugate of it, are thus given by

$$\frac{d\Psi_{\mathbf{R}}}{dt} = \frac{\partial H}{\partial (i\Psi_{\mathbf{R}}^*)}, \quad (3.5a)$$

$$i \frac{d\Psi_{\mathbf{R}}^*}{dt} = - \frac{\partial H}{\partial \Psi_{\mathbf{R}}}. \quad (3.5b)$$

The Hamiltonian is a conserved quantity, which is related, through Noether's theorem [49], to the model being time invariant. There is actually also another conserved quantity of the DNLS model, namely the norm

$$\mathcal{N} = \sum_{\mathbf{R}} |\Psi_{\mathbf{R}}|^2. \quad (3.6)$$

This is readily confirmed by plugging (3.1), and its complex conjugate, into

$$\frac{d\mathcal{N}}{dt} = \sum_{\mathbf{R}} \frac{d|\Psi_{\mathbf{R}}|^2}{dt} = \sum_{\mathbf{R}} \Psi_{\mathbf{R}} \frac{d\Psi_{\mathbf{R}}^*}{dt} + \Psi_{\mathbf{R}}^* \frac{d\Psi_{\mathbf{R}}}{dt} = 0. \quad (3.7)$$

The conservation of $\mathcal{N}$ is instead connected to the global *gauge invariance*, $\Psi_{\mathbf{R}} \rightarrow e^{i\alpha} \Psi_{\mathbf{R}}$, of the system. The conservation of norm will for BECs correspond to a conservation of particles.

These two conserved quantities make the DNLS equation with two lattice points, the *dimer*, integrable, and it can be completely solved in terms of elliptic functions. It turns out that all systems with more degrees of freedom actually are non-integrable [60].

3.1 DNLS and BECs in Optical Lattices

The DNLS equation can be applied to BECs in deep optical lattices, when there is a large number of particles on each site. Note though that the lattice should not be too deep since there needs to be phase coherence between bosons on different sites (cf. discussion on the Mott insulator in section 2.3). In this type of system, there will essentially be a separate condensate located on each site, in coherence with each other, where the $\psi_{\mathbf{R}}$ in the DNLS equation, analogous to Ψ in the Gross-Pitaevskii equation, will describe the (average) number of particles and the phase of the condensate on site $\mathbf{R}$.

When deriving the DNLS model for a BEC in an optical lattice, two different paths can be taken: either one discretizes the Gross-Pitaevskii equation (1.1), or one employs mean-field techniques on the Bose-Hubbard model (2.14). The essential difference is thus what is done first on the fundamental quantum mechanical description - the discretization or the mean-field approximation. Even though the second scheme is the most relevant for this thesis, it may be instructive to first briefly review the ideas behind the first one.

From the Gross-Pitaevskii equation

The derivation of the DNLS model by a discretization of the Gross-Pitaevskii equation was originally done in a paper by Trombettoni and Smerzi [121] to model an earlier experiment [6]. It is in many aspects similar to the derivation of the Bose-Hubbard model in section 2.1, since it also employs a tight-binding approximation, where now the macroscopic wave function in (1.1) is expanded in functions, $\phi(\mathbf{r} - \mathbf{r}_m)$, which are localized around the lattice sites $\mathbf{r}_m$

$$\Psi(\mathbf{r}, t) = \sqrt{N} \sum_m \psi_m(t) \phi(\mathbf{r} - \mathbf{r}_m), \quad (3.8a)$$

$$\sum_m |\psi_m|^2 = 1. \quad (3.8b)$$

N is the total number of particles in the condensate, and $\psi_m(t) = \sqrt{\rho_m(t)} e^{i\theta_m(t)}$ is a complex quantity which describes the (relative) number of condensed particles $\rho_m = N_m/N$ (N_m being the absolute number of particles) and phase θ_m . The conservation of norm is thus related to the conservation of particles in the BEC. Assuming that the wave functions $\phi(\mathbf{r} - \mathbf{r}_m)$ are well localized within each lattice well, and using analogous arguments about which terms that are of importance as for the Bose-Hubbard model, one can produce a DNLS equation for ψ_m [121].

Also an extended DNLS equation can be derived from the Gross-Pitaevskii equation [81, 113, 114]. This model will be discussed more in detail below, together with its connection to the extended Bose-Hubbard model (2.22).

From the Bose-Hubbard model

The other way to derive the DNLS model is to go from the Bose-Hubbard model, for instance using the so called time-dependent variational principle (TDVP),

which is an extension of the familiar time-independent Rayleigh-Ritz variational method and a quite general method for producing approximate macroscopic wave functions for many-body systems [5]. The basic idea is to describe the system with a ‘good’ state, $|\tilde{\Phi}\rangle$, which contains some variational parameters that are determined by demanding that it should fulfill the time-dependent Schrödinger equation *on average*, $\langle \tilde{\Phi} | i\hbar \partial/\partial t - \hat{H} | \tilde{\Phi} \rangle = 0$. Putting $|\tilde{\Phi}\rangle = e^{iS/\hbar} |\Phi\rangle$ leads to

$$\dot{S} = i\hbar \langle \Phi | \partial/\partial t | \Phi \rangle - \langle \Phi | \hat{H} | \Phi \rangle \quad (3.9)$$

where $|\Phi\rangle$ is the *trial macroscopic state*. It should be chosen to contain as much information as possible on the microscopic dynamics, and one should also be able to associate it with a set of parameters which describe the most important physical processes of the system. These parameters will then become the dynamical variables in the semi-classical model. One can then associate $\dot{S}$ and $\langle \Phi | \hat{H} | \Phi \rangle$ with an effective Lagrangian and Hamiltonian, respectively, and with the help of Hamilton’s equations of motion determine the time-evolution of the semi-classical system [5].

Amico and Penna [5] used this procedure with a tensor product of Glauber coherent states as the macroscopic trial state. The Glauber coherent states were originally introduced in quantum optics [48], and are defined as eigenstates to the annihilation operator, $\hat{a}_{\mathbf{R}} |\psi_{\mathbf{R}}\rangle_{(GCS)} = \psi_{\mathbf{R}} |\psi_{\mathbf{R}}\rangle_{(GCS)}$, implying that it is a state with an *average* number of particles $|\psi_{\mathbf{R}}|^2$. These are local states, i.e. they are describing only a single site, which is why it is necessary to take a tensor product to describe the full lattice. It is readily confirmed that they have the explicit form

$$|\psi_{\mathbf{R}}\rangle_{(GCS)} = \sum_{j=0}^{\infty} \frac{(\psi_{\mathbf{R}} \hat{a}_{\mathbf{R}}^{\dagger})^j}{j!} |0\rangle = \exp(\psi_{\mathbf{R}} \hat{a}_{\mathbf{R}}^{\dagger}) |0\rangle. \quad (3.10)$$

Note that (2.20), which was used to approximate the superfluid phase in the thermodynamic limit, is a special type of Glauber coherent state tensor product, with $\psi_{\mathbf{R}} = \sqrt{N/f}$. Plugging in $|\Phi\rangle = \bigotimes_{\mathbf{R}} |\psi_{\mathbf{R}}\rangle$ to $H = \langle \Phi | \hat{H} | \Phi \rangle$, $\hat{H}$ being the Bose-Hubbard Hamiltonian (2.14), gives the following semi-classical Hamiltonian,

$$H = -J \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} \psi_{\mathbf{R}}^* \psi_{\mathbf{R}'} + \frac{U}{2} \sum_{\mathbf{R}} |\psi_{\mathbf{R}}|^2 (|\psi_{\mathbf{R}}|^2 - 1) + \sum_{\mathbf{R}} \epsilon_{\mathbf{R}} |\psi_{\mathbf{R}}|^2, \quad (3.11)$$

where $\psi_{\mathbf{R}}$ and $i\hbar \dot{\psi}_{\mathbf{R}}^*$ are the canonical variables, generating the following equations of motion,

$$i\hbar \frac{d\psi_{\mathbf{R}}}{dt} = -J \sum_{\langle \mathbf{R}' \rangle} \psi_{\mathbf{R}'} + U(\psi_{\mathbf{R}} |\psi_{\mathbf{R}}|^2 - \frac{\psi_{\mathbf{R}}}{2}) + \epsilon_{\mathbf{R}} \psi_{\mathbf{R}}, \quad (3.12)$$

where the summation over $\mathbf{R}'$ runs over all the nearest neighbors of $\mathbf{R}$. These two expressions have the form of the DNLS equation (3.1) and Hamiltonian (3.4). Note that, in analogy with how (3.2) was transformed to (3.3), the term $\sim \psi_{\mathbf{R}}$ in (3.12) can be removed by $\psi_{\mathbf{R}} \mapsto \exp(iU/2\hbar) \psi_{\mathbf{R}}$, which corresponds to making a replacement of the Hamiltonian according to $H \mapsto H - UN/2$, which is just a shift of the energy scale since $\mathcal{N}$ is conserved and thereby just a number.

A different approach to derive the DNLS model is to consider the time-evolution of the annihilation operator, given by Heisenberg's equation of motion,

$$i\hbar \frac{d\hat{a}_{\mathbf{R}}}{dt} = [\hat{a}_{\mathbf{R}}, \hat{H}] = -J \sum_{\langle \mathbf{R}' \rangle} \hat{a}_{\mathbf{R}'} + U \hat{a}_{\mathbf{R}}^\dagger \hat{a}_{\mathbf{R}} \hat{a}_{\mathbf{R}} + \epsilon_{\mathbf{R}} \hat{a}_{\mathbf{R}}, \quad (3.13)$$

where $\hat{H}$ is the Bose-Hubbard Hamiltonian (2.14). Taking the expectation value of this equation with a tensor product of Glauber coherent states leads to essentially the same equation as (3.12), differing only by the insignificant term $\sim \psi_{\mathbf{R}}$ [40]. It is actually quite common in the literature to just make the substitution $\psi_{\mathbf{R}} \leftrightarrow \hat{a}_{\mathbf{R}}$ when '*studying the quantum mechanical version of...*' or vice versa.

The drawback of the Glauber coherent states is that they do not have a specified number of particles; in contrast to a Bose-Hubbard eigenstate these are only conserved on average. One can instead use $SU(f)$ -coherent states [23] (called a Hartree ansatz in [127]), f being the number of sites of the lattice, which do conserve the number of particles N , and have the form

$$|\Phi\rangle = \frac{1}{\sqrt{N!N^N}} \left(\sum_{\mathbf{R}} \psi_{\mathbf{R}} \hat{a}_{\mathbf{R}}^\dagger \right)^N |0\rangle, \quad (3.14)$$

$$\sum_{\mathbf{R}} |\psi_{\mathbf{R}}|^2 = N.$$

Note that with $\psi_{\mathbf{R}} = \sqrt{N/f}$ this becomes identical to (2.19), the superfluid state for the Bose-Hubbard model with $U = 0$. The $SU(f)$ -coherent states will produce an almost identical DNLS model as when using Glauber coherent states, the difference is a numerical factor $(N-1)/N$ attached to the nonlinear term. The two models are thus equivalent for large N .

With the same techniques as above it is also possible to derive an extended DNLS model from the extended Bose-Hubbard model (2.22). Using Glauber coherent states will lead to [58]

$$\begin{aligned} H = & \sum_m (Q_1 + Q_3) |\psi_m|^2 + Q_2 (\psi_m \psi_{m+1}^* + \psi_{m+1} \psi_m^*) \\ & + Q_3 |\psi_m|^4 + Q_4 (4 |\psi_m|^2 |\psi_{m+1}|^2 + \psi_m^2 \psi_{m+1}^{*2} + \psi_{m+1}^2 \psi_m^{*2}) \\ & + 2Q_5 [\psi_m \psi_{m+1} (\psi_m^{*2} + \psi_{m+1}^{*2}) + (\psi_m^2 + \psi_{m+1}^2) (\psi_m^* \psi_{m+1}^*)]. \end{aligned} \quad (3.15)$$

with $\sum_m |\psi_m|^2 = N$. Using $SU(f)$ -coherent states will lead to the same Hamiltonian apart from that the last two rows will contain an additional factor $(N-1)/N$. Using (3.15) in Hamilton's equations of motion leads to

$$\begin{aligned} i\hbar \frac{d\psi_m}{dt} = & \sum_m (Q_1 + Q_3) \psi_m + Q_2 (\psi_{m-1} + \psi_{m+1}) + 2Q_3 \psi_m |\psi_m|^2 \\ & + Q_4 [4\psi_m (|\psi_{m+1}|^2 + |\psi_{m-1}|^2) + 2\psi_m^* (\psi_{m+1}^2 + \psi_{m-1}^2)] \\ & + 2Q_5 [2|\psi_m|^2 (\psi_{m+1}^* + \psi_{m-1}^*) + (\psi_m^2 + \psi_{m+1}^2) \psi_{m+1}^* + (\psi_m^2 + \psi_{m-1}^2) \psi_{m-1}^*]. \end{aligned} \quad (3.16)$$

Looking at the Hamiltonians of both the ordinary and the extended DNLS model, one can see how the parameters should scale to have a well-defined classical limit $N \rightarrow \infty$, i.e. so that the Hamiltonian has a finite value. Since $|\psi_{\mathbf{R}}|$ at most can be of order $\sqrt{N}$, we can conclude that Q_1, Q_2 and J should scale as N^{-1} while Q_3, Q_4, Q_5 and U scale as N^{-2} . This also indicates how Bose-Hubbard models with different numbers of particles can be compared, i.e. in which parameter regimes one should look for similar behavior [58].

3.2 Discrete Breathers

The DNLS model possesses families of *stationary* discrete breathers (DBs), which have the general form $\Psi_{\mathbf{R}} = A_{\mathbf{R}} \exp(i\omega t)$, with time-independent amplitudes $A_{\mathbf{R}}$. Plugging in $\Psi_{\mathbf{R}} = A_{\mathbf{R}} \exp(i\omega t)$, with $\omega > 0$, to the DNLS equation (3.1) with $\epsilon_{\mathbf{R}} = 0$, leads to

$$-\omega A_{\mathbf{R}} + \gamma |A_{\mathbf{R}}|^2 A_{\mathbf{R}} + \delta \sum_{\langle \mathbf{R}' \rangle} A_{\mathbf{R}'} = 0, \quad (3.17)$$

so that finding these stationary DBs corresponds to solving this algebraic equation. Thus, when following a family of stationary DBs with the method mentioned in section 1.2.1, one is looking for zeros of (3.17).

We will mention just a few types of simple stationary DBs for the one-dimensional DNLS equation (3.1). It is assumed that the model has a focusing nonlinearity, $\gamma/\delta > 0$, but note that any solution for this convention can easily be mapped on a corresponding solution of the defocusing model with $\gamma \mapsto -\gamma$, simply by making a staggering transformation $\psi_m \mapsto (-1)^m \psi_m$. The first example is the on-site, or site-centered, DBs (Fig. 3.1a)), which can be followed to a solution in the anti-continuous limit which has only a single excited site. The second example is the inter-site, or bond-centered, DBs which in the anti-continuous limit will correspond to two neighboring sites being excited with the same amplitude². These can be either symmetric (Figure 3.1b)) or anti-symmetric (Figure 3.1c)), and the solutions in the anti-continuous limit will then have the excited sites in phase and anti-phase, respectively. Note that a staggering transformation of an inter-site DB changes its symmetry, which has to be remembered when this discussion is transferred to a defocusing model.

When following the on-site and symmetric inter-site DBs to the continuous limit, they will both become the NLS soliton [35] (not the NLS breather). The two solutions will thus become more and more similar to each other as one approaches this limit, but they will always preserve the symmetry, i.e. being either on-site or inter-site symmetric (this is of course not important in the continuous limit). The on-site DB is generally stable, while the symmetric inter-site DB is unstable (this is always true for an infinite lattice, but there can be finite-size effects on the stability) [35]. The anti-symmetric DB is, for a large system, stable in the interval $0 \leq |\delta/\omega| \leq 0.146$ [63]. This DB is sometimes called a ‘two-site localized

²Also more general breathers can have these symmetries and thus be classified as either on-site or inter-site.

Figure 3.1: Illustrations of some stationary breathers of the one-dimensional DNLS equation with a focusing nonlinearity. a) illustrates an on-site symmetric breather which in the anti-continuous limit corresponds to a single excited site. b) and c) illustrate inter-site symmetric breathers, symmetric and anti-symmetric, respectively. These will correspond to two excited neighbor sites in the anti-continuous limit, for b) in phase and c) in anti-phase.

twisted mode', and the instability it experiences for $|\delta/\omega| > 0.146$ is an oscillatory instability which will be further discussed in section 3.3

The above mentioned DBs are stationary on the lattice, but it is also interesting to learn about the mobility of DBs. One way to set a stationary breather in motion, is to give it a 'kick' in a direction by introducing a phase gradient [13]. If the site-centered breather is set into motion by a small phase gradient, assuming that it is mobile, then it will move across the lattice by transforming continuously between the on-site and inter-site profiles. A measure of how 'good' the mobility of a breather is, is the energy (Hamiltonian) difference between the on-site and inter-site DBs with the same norm - smaller energy difference meaning better mobility [34, 68]. This is called the Peierls-Nabarro barrier, and is essentially the energy it takes to translate the DB one site, if energy losses to the rest of the lattice can be neglected.

For the DNLS model, the Peierls-Nabarro barrier is generally finite. A DB that is moving through the lattice will then lose energy by emitting radiation in the form of low amplitude plane waves [50].

What was found in the work by Öster *et al* [91] was that the mobility of DBs can be greatly enhanced in the extended DNLS equation (3.16). This relies on an exchange of stability between the on-site and inter-site DB [10, 11]. In the extended DNLS equation the on-site DB can become unstable and the symmetric inter-site DB stable, and in the region where the stabilities change, the Peierls-Nabarro barrier becomes very small and the DB can then travel essentially without emitting any radiation [91]. The on-site and inter-site DB will however generally not change the stability in the same point, so there will typically be a small region where both of them are unstable and a third intermediate solution is stable, or vice versa. One can however tune the parameters so that they do exchange their

stability in the same point, which optimizes the mobility [90].

What was also found in [91] was that the extended DNLS equation supports *lattice compactons*. These are very localized solutions where only certain sites are excited and the rest of the lattice has *exact* zero amplitude. It is actually possible to have compactons with any number of excited sites. The key is that the parameters of the model can be tuned so that the coupling between an empty and an occupied site vanishes. Note though that this parameter relation actually depends on the amplitude of the occupied site. It has been suggested that compactons analogous to the ones in [91] can be realized in a BEC in an optical lattice, by using a rapidly varying magnetic field [1]. Lattice compactons have also been studied in other models [64–66].

Compactons exist also in continuous models, where they analogously are localized solutions which are exactly zero outside a given region, i.e. have compact support. The concept of a compacton was introduced in a paper by Rosenau and Hyman, for a continuous model with nonlinear dispersion [100]. But note that discretizing the continuous compacton generally do not lead to a lattice compacton, but to a solution which decays with a superexponential tail [101].

3.3 Instabilities of the DNLS Model

There are a number of different types of instabilities that the DNLS model can experience but we will only name a few of the most important ones for one-dimensional lattices.

The first one is the modulational instability of a current-carrying constant amplitude solution in an infinite lattice. This is a solution of the type $\Psi_m = |A|e^{i(\omega t - \kappa m)}$, which plugged into (3.3) gives the dispersion relation

$$\omega = \gamma|A|^2 - 4\delta \sin^2\left(\frac{\kappa}{2}\right). \quad (3.18)$$

These waves are linearly stable if and only if $(\gamma/\delta) \cos(\kappa) < 0$ [25, 69]. For $\gamma/\delta > 0$, this implies that waves with wave vectors $0 \leq |\kappa| \leq \pi/2$ are unstable through a modulational instability which typically results in that the constant amplitude is turned into a number of small-amplitude mobile excitations [28, 97, 98]. These can in their turn collapse into a small number of standing large amplitude breathers.

Another example is the self-trapping transition in a finite lattice where a bifurcation occurs for which the delocalized ground state becomes unstable and a stable localized ground state appears [25, 36]. This can be observed already in the DNLS dimer. Below a critical value of the norm (for given values of δ and γ) there exist two stable stationary solutions, corresponding to the same amplitude on both sites but either in phase or anti-phase. When the norm reaches the critical value, a bifurcation occurs for the in-phase solution which becomes unstable, and a new stable solution which breaks the permutational symmetry, i.e. has unequal amplitude on the sites, appears [36].

The third example we are going to mention is oscillatory instabilities, discussed in section 1.2.2. These appear through Hamiltonian Hopf bifurcations, where some eigenvalues of the functional matrix get both a non-zero real and imaginary part,

and a perturbation will oscillate around the fixed point with an exponentially increasing amplitude [59]. Oscillatory instabilities will typically appear when the lattice has an inhomogeneous amplitude distribution, so that it is divided into sublattices of sites with small and large amplitudes, respectively. The instability will then appear as a result of resonances between the internal oscillations of the different sublattices. Examples of this kind of configuration which experience oscillatory instabilities are discrete dark solitons ('dark breathers') [4,61], two-site localized twisted modes (mentioned in section 3.2) [27,63,79], spatially periodic or quasiperiodic nonlinear standing waves [62,84] and gap modes in diatomic chains [51,73]. The DNLS trimer, i.e. three-site periodic lattice, is arguably the simplest system which can have oscillatory instabilities. This can occur for the 'single depleted well' [46] state where one site is empty and the other two have the same amplitude but are in anti-phase with each other [59].

CHAPTER 4

Classical versus Quantum

Quantum mechanics is typically said to be the physics of microscopic objects such as atoms and molecules, while classical mechanics instead describes the macroscopic items that we encounter in our everyday life. But even macroscopic objects, such as a ball or a cat¹, is built up by atoms and molecules, and there must thus be some connection between quantum mechanics and classical mechanics. To address this issue, the great Niels Bohr formulated his correspondence principle which states, a bit vaguely expressed, that in appropriate limits of quantum mechanics, classical physics must arise. It can also be expressed that for a quantum system with a classical analog, expectation values of operators will behave like the corresponding classical quantity in the limit $\hbar \rightarrow 0$ [82].

We showed in chapter 3 that there is a connection between the quantum mechanical Bose-Hubbard model and the classical discrete nonlinear Schrödinger model. An underlying question of this thesis is how classical concepts such as nonlinear localization, chaos and instabilities can be expressed in the quantum mechanical world. More specifically, how can results from the DNLS model be transferred to the Bose-Hubbard model? We will see that there are differences between classical and quantum mechanics which make these questions far from trivial.

4.1 Quantum Discrete Breathers

When one tries to transfer the concept of discrete breathers to the quantum world, one realizes that in a translationally invariant system, all eigenstates must obey the Bloch theorem, meaning that they necessarily are delocalized. So how can localization possibly arise in quantum mechanics? We need to be a bit more

¹Ask Schrödinger about this...

specific with what we mean by delocalization here. Consider the general form of an eigenstate, with energy E_k and crystal momentum k ,

$$|E_k\rangle = \sum_{\alpha} c_{\alpha} |\tau_k^{(\alpha)}\rangle, \quad (4.1)$$

where $|\tau_k^{(\alpha)}\rangle$ is a basis state of type (2.18). Now, state (4.1) is not delocalized in the sense that upon measurement there will necessarily be an equal amount of particles on each site, but rather that the probability of finding a particular number of particles is the same for every site. The eigenstate may therefore actually have a high probability of having many particles located on a few sites, but there cannot be any sites that are more likely than others to be occupied.

But a classical breather is of course localized on specific sites, and to create a quantum state which is *truly* localized, one needs to take a superposition of eigenstates. The decoherence of such a state is then determined by the energy differences between the eigenstates in this superposition - small energy differences meaning longer decoherence times. Our expectation is therefore that a classical discrete breather corresponds in the quantum world to a superposition of eigenstates, where all the energy differences become small in the classical limit when the number of particles becomes large [94].

The eigenstates in this superposition need of course then to be localized themselves in the 'eigenstate-sense' mentioned above, and there are different quantities that can be used to characterize how well localized an eigenstate is. One example is certain correlation functions [123], e.g. $\langle \hat{n}_{\mathbf{R}} \hat{n}_{\mathbf{R}+\mathbf{d}} \rangle$ which should decrease with increasing $|\mathbf{d}|$. Another one is $\langle (\hat{a}_{\mathbf{R}}^{\dagger})^M (\hat{a}_{\mathbf{R}})^M \rangle$, M being a positive integer, which for a delocalized eigenstate should drop as M becomes large while it will remain finite for a state with a significant probability of finding many of the system's particles on one site [23, 56].

The dimensionality of the quantum lattice problem, given by $\mathcal{D} = (N + f - 1)!/N!(f-1)!$, is quite rapidly growing with the number of sites and particles, which has restricted the systems that are computationally accessible to quite modest sizes, at least if one wishes to use exact diagonalization of the Hamiltonian. This is probably also a reason why there has been much less work done on quantum discrete breathers as compared to the classical ones [44].

The work done has typically therefore been with either many particles on few lattice sites or vice versa. It is generally not sensible to talk about localization in a small lattice, but one can however study related concepts. Aubry et al [12] studied quantum signatures in the Bose-Hubbard model of a bifurcation in the DNLS dimer. This bifurcation is related to the appearance of a stationary solution which breaks the permutational symmetry of the dimer over a critical value of the norm [36], which can be compared to the breaking of translational symmetry of a localized solution. A signature of this bifurcation is a clear increase in the density of states [12].

Note that we wrote that it *generally* is not sensible to talk about localization in a small lattice. In paper I and III we actually studied quantum versions of classical lattice compactons in four-site lattices. And since the compactons are decaying so rapidly, the four-site lattice can be assumed to be a good approximation also for

a larger lattice. This made it possible to use quite many particles (up to 30) and thus better connect with the classical limit.

Regarding instead few particles in a large lattice, Scott et al [110] considered the case of two particles in a large one-dimensional lattice, for the Bose-Hubbard model (2.15) with attractive interactions ($U < 0$). The energy spectrum for this system will have a quasi-continuum, and below that a single band. This band they called the *soliton band* and the eigenstates in this band has the highest probability for the two bosons to be located close to each other. The energy of the soliton band is in the limit $f \rightarrow \infty$ given by [110]

$$E = \sqrt{1 + 16 \left(\frac{J}{U} \right)^2 \cos \left(\frac{k}{2} \right)} \quad (4.2)$$

This confirms many of our expectations for quantum breathers. To get a state for which, at least initially, there is a high probability of finding the two bosons close together, one would take a superposition of the eigenstates in the soliton band. This state would eventually spread due to the energy differences between the eigenstates. It is also noteworthy that the width of the soliton band will decrease with increasing magnitude of U , and that the decoherence time thus also will increase.

Jack and Yamashita [56] studied the one-dimensional attractive Bose-Hubbard model with $N = 10$ particles in a $f = 6$ site periodic lattice and argued that by increasing the value of $|U/J|$ it will make a transition from the superfluid regime (see section 2.3) to a soliton regime. They identified the soliton state e.g. with high values of $\langle (\hat{a}_{\mathbf{R}}^\dagger)^N (\hat{a}_{\mathbf{R}})^N \rangle$. Buonsante et al [23] used the same model but with up to $N = 10$ particles in a $f = 20$ site periodic lattice (at most 10 particles on 12 sites or 5 particles on 20 sites). They argued that the soliton regime in [56] actually could be divided into two regimes: a soliton regime for intermediate $|U/J|$ and a *Schrödinger-cat state* regime for large $|U/J|$, where a Schrödinger-cat state essentially is localized on one site². The name *Schrödinger-cat state* illustrates that this is the kind of localization that occurs for eigenstates, which was discussed above. They also argued that the observables that [56] studied actually indicated a transition, not from the superfluid to soliton regime, but from the soliton to the Schrödinger-cat state regime, but since the system considered in [56] is so small these transitions occur very close to each other [23]. The transition into the Schrödinger-cat regime is independent of the lattice size f and can be estimated with $|J/U(N-1)| \approx 1/4$ while the transition into the soliton regime is size dependent, since the size of the lattice limits how broad a soliton can be, and is approximated with $|J/U(N-1)| \approx [2f \sin^2(\pi/f)]^{-1}$.

²This is comparable to a one-site compacton, but created by a fundamentally different mechanism than in paper I and III. This can be compared to the difference between a compacton in the anti-continuous limit of the DNLS equation and the compacton created by canceling the coupling with carefully chosen parameters in the extended DNLS equation.

4.2 Quantum Signatures of Instabilities

When the instability of a fixed point is to be translated to quantum mechanics, another difficulty arises, which indeed is at the very heart of the ‘strangeness’ of quantum mechanics. Due to the Heisenberg uncertainty principle, we cannot even talk about a trajectory in phase space, since position and momentum cannot simultaneously be well defined quantities.

But the question that we can ask is: what kind of signatures of the classical instability can one see in the corresponding quantum mechanical model? This question is very much related to the field of quantum chaos which studies quantum systems which correspond to classical systems which experience chaotic dynamics. When transferring chaos to quantum mechanics similar difficulties arise as for the instability, since two initial conditions which are too close to each other in phase space cannot be distinguished from each other, due to the Heisenberg uncertainty principle.

For all the instabilities of the DNLS model that were discussed in section 3.3, there has been, at least some, studies of the quantum counterpart with the Bose-Hubbard model. The modulational instability of current-carrying constant amplitude waves was studied in [3, 96], while the self-trapping has been studied in a number of papers [12, 16, 22, 127]. The oscillatory instability was, to our knowledge, first studied in paper II for the single depleted well state in the trimer. A common result in these papers is broadening of the bifurcation point, so that the transition instead happens gradually over a critical regime.

CHAPTER 5

Summary of Appended Papers

Paper I and III are both related to quantum discrete breathers. More specifically, they are treating the quantum analogs, in the extended Bose-Hubbard model, of the classical lattice compactons, found for the extended DNLS equation [91]. An attractive model was used in paper III, unlike paper I where a repulsive one was used, but these two models can however be mapped on each other, since a staggering transformation together with the parameter substitution $Q_i \mapsto -Q_i$, $i = 1, 3, 4$, results in $\hat{H} \mapsto -\hat{H}$ in (2.22).

In paper I the concept of a m -site quantum lattice compacton (QLC) eigenstate was introduced, which was defined as an eigenstate with absolute certainty of finding all particles located on m consecutive sites. It was found that one-site QLC eigenstates actually exist and correspond to the classical one-site lattice compacton. They exist under certain parameter conditions, which when fulfilled completely cancels the tunneling from a site with all N particles to its empty neighbors. For these eigenstates the particles can actually be localized on specific sites.

Classical several-site compactons on the other hand do not correspond to exact QLC eigenstates. They correspond instead to superpositions of eigenstates, and it was shown that these eigenstates will become more and more QLC-like as the number of particles increases, i.e. the probability of finding all particles on m consecutive sites goes towards unity.

In paper III we studied how well the dynamical properties of the classical lattice compactons could be reproduced in the extended Bose-Hubbard model, with special emphasis on the mobility. In [91] it was shown that the mobility of classical discrete breathers, and actually also of classical lattice compactons, can be greatly enhanced in the extended DNLS model, by tuning the parameters close to the inversion of stability between on-site and inter-site breathers. We used two different types of states in the calculations and simulations in paper III: both what

we called ‘localized ground states’ which are superpositions of the lowest energy eigenstates from each quasi-momentum space, and also $SU(f)$ coherent states given by (3.14). It was, with the help of these states, possible for us to clearly distinguish the classical stability regimes of the extended DNLS model [91], by looking at quantities such as the average values of number operators $\langle \hat{n}_i \rangle$ and density correlation functions $\langle \hat{n}_i \hat{n}_{i+1} \rangle$. We then proceeded by studying the dynamics and mobility of $SU(f)$ coherent states with an applied phase gradient. The main conclusion was that it is possible to see clear signatures of a mobile localized structure, but that this is dependent on the magnitude of the applied phase gradient. For a small phase gradient, which classically corresponds to a slow coherent movement of the compacton, the time to travel one site is of the same order as the decoherence time and one can therefore not distinguish any clear signs of the mobility. For a larger phase gradient on the other hand, corresponding to a harder kick and a faster movement, the time-scales separate and it is possible to see a localized profile traveling several sites of the lattice before quantum fluctuations destroy it.

In paper II quantum signatures of the oscillatory instability in the Bose-Hubbard trimer were studied. The classical oscillatory instability regime could be related to avoided crossings in the energy spectrum and a strong mixing between a pure single depleted well (SDW) quantum state and other eigenstates. Several measures were also constructed which gave clear signatures on the classically unstable regime. There was for instance a clear decrease in the maximum probability, for any eigenstate, of having the particles equally distributed on two sites. Another measure was the total overlap between compact SDW basis states, having the form of $|N/2, N/2, 0\rangle$ plugged into (2.18), and basis states which are not two-site localized, summed over all eigenstates. This measure showed a pronounced plateau in the classically unstable regime. It was also possible to identify a simple superposition of quantum eigenstates with the classical SDW stationary states in the classically stable regime, while a similar identification in the unstable regime failed to capture essential features of the unstable dynamics. For example, we showed that the dynamics resulting from a small perturbation of these states cannot reproduce the development of an oscillatory instability. The classical unstable dynamics is thus a result of global properties of the eigenstates, rather than of individual eigenstates.

By instead using $SU(3)$ coherent states as initial conditions in the dynamical simulations, it was possible to reproduce several features of the transition from stable internal oscillations to oscillatory instabilities. But while the classical transition occurs in a single bifurcation point, the quantum transition happens gradually over an interval.

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