

Thermodynamics of strongly interacting bosons on a lattice: new insights and numerical approaches

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Thermodynamics of strongly interacting bosons on a lattice: new insights and numerical approaches

Thermodynamique des bosons fortement interagissants : nouveaux résultats et approches numériques

Devant le jury composé de :

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Marco Polo descrive un ponte, pietra per pietra.
Ma qual è la pietra che sostiene il ponte? - chiede Kublai Kan.
Il ponte non è sostenuto da questa o quella pietra, - risponde Marco, ma dalla linea dell'arco che esse formano.
Kublai Kan rimane silenzioso, riflettendo. Poi soggiunge:
Perchè mi parli delle pietre? È solo dell'arco che m'importa.
Polo risponde: - Senza pietre non c'è arco.

Italo Calvino, Le città invisibili

Abstract in French

Les atomes froids dans les réseaux optiques permettent d'avoir un contrôle sans précédent des états a N-corps fortement corrélés. Pour cette raison, ils représentent un excellent outil pour l'implémentation d'un « simulateur quantique », utile pour réaliser de manière expérimentale de nombreux hamiltoniens de systèmes d'intérêt physique. En particulier, ils rendent possible la création de champs de jauge artificiels; ces derniers permettant d'accéder à la physique du magnétisme frustré. Dans ce travail, il s'agit de s'intéresser à la thermodynamique des atomes froids, en abordant ce sujet de manière théorique et numérique. A ce jour, le Monte Carlo quantique est la méthode la plus efficace dans ce domaine. Néanmoins, en raison de ce qu'on appelle le « problème du signe », elle ne peut s'appliquer qu'à une classe restreinte de systèmes, et dont par exemple les systèmes frustrés ne font pas partie. L'intérêt de cette thèse est de développer une nouvelle méthode approximée fondée sur une approche Monte Carlo. La première partie de cette thèse est consacrée à des considérations de nature théorique sur la structure spatiale des corrélations classiques et quantiques. Ces résultats nous permettent de développer, dans une deuxième partie, une approximation nommée « champ moyen quantique ». Celle-ci permet de proposer, dans une troisième partie, une méthode numérique qu'on appelle « Monte Carlo du champ auxiliaire » et qu'on applique à des cas d'intérêt physique, notamment au réseau triangulaire frustré.

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Chapter 1

Introduction

When cooling down diluted atomic gases to temperatures of the order of nK, quantum statistics becomes prominent, and quantum degeneracy leads to phenomena like condensation, apparition of Fermi surfaces, etc... This physical regime remained for long inaccessible to experiments, but in the last twenty years amazing technological advances in cooling, trapping and imaging have made it possible to achieve some spectacular results. Cold atoms have become a very active and productive field of physics at the frontier between atomic physics and condensed matter physics. This field has also seen the award of two Nobel prizes, that went to Chu, Cohen-Tannoudji and Phillips in 1997 for the development of cooling and trapping techniques based on the use of laser light and to Cornell, Wiemann and Ketterle in 2001 for the realization of Bose-Einstein condensation in alkali atomic gases. The latter achievement [1], because of the ground-breaking impact it had in the nineties, is probably the best known result in the field and paved the way to many other beautiful results: the study of the BCS-BEC crossover [2], the realization of the superfluid-Mott insulator quantum phase transition [3], the realization of artificial gauge fields [4] and topological band structures [5], just to name some. The progress has been constant since then and state-ofthe-art experiments can attain an unprecedented control, even at the scale of the single atom [6].

What makes physics of quantum gases particularly interesting is the possibility of realizing the famous "quantum emulator" proposed by Feynman in the eighties [7]. When dealing with quantum systems the computational cost for exact calculations grows exponentially with the size of the system, rendering the calculations not scalable and limited to microscopic sizes. For this reason Feynman proposed not to calculate, but to simulate quantum systems experimentally. The idea is to study some "simple" experimental systems which possess quantum degrees of freedom, and which can be mapped onto more complex systems. For example, cold atoms in optical lattices (which we will cover more in detail in the next section), can be used to simulate electrons in crystals.

The main subject of this thesis is the development of a new approximation scheme for the numerical study of lattice boson models, inspired by the physics of cold atoms in optical lattices. Therefore the main themes in this thesis are of numerical and theoretical interest, with a potential relevance for state-of-the-art experiments. In the following we give a broad introduction to each of these aspects. In the first part we cover some experiments and techniques which are of interest for the models that we will deal with. In the second part we give give a broad panoramic introduction to computational methods in condensed matter theory, to contextualize the method that we will develop in the following chapters. In the last part we introduce some of the theoretical aspects which are of fundamental importance to justify our method. This tripartite introduction will set the ground for the following chapters, where the core of this thesis will be developed.

1.1 Experimental aspects: optical lattices

An optical lattice is a standing pattern of interfering laser beams. Atoms can couple to such a structure, which is periodic in space, via an induced dipole moment and therefore experience a lattice-shaped potential [8]. This scheme allows to realize many different geometric structures: a cubic lattice, for example, is created using laser beams oriented in three orthogonal directions, a bi-dimensional array of one-dimensional tubes using laser beams oriented in two orthogonal directions - see Fig. 1.1(a-b). In general, any periodic lattice structure can be realized by superimposing a finite number of laser beams. The periodic structure of optical lattices permits to use a number of theoretical tools proper to condensed matter such as, for example, the tightbinding approach. For this reason optical lattices can be used to realize experimentally models such as the (Bose)-Hubbard model. In this thesis we will focus on two-dimensional bosonic lattices and in particular on square, triangular and kagome lattices, which are shown in Fig. 1.1(c-e), and which have been realized in several experiments [9, 10, 11].

What makes optical lattices extremely interesting is their wide tunability. The lattice constant can be controlled via the wavelength of the laser beams, the depth of the lattice via the intensity of the beams and the interactions among atoms via Feshbach resonances [2]. This is in strong contrast to hard condensed matter, where the properties of solids are determined by their internal lattice structure, which in general cannot be modified continuously in the experiments. Having a light-made lattice implies also some other major advantages: there are no defects and there are no phonons, since the lattice sites are determined by minima in the interference pattern and cannot be displaced by a collective excitation.

Measurements in optical lattices are performed through imaging tech-



Figure 1.1: (a) Laser orientation and potential profile in a cubic lattice. (b) Laser orientation and potential profile in a two-dimensional square lattice of one-dimensional tubes. (c-e) Two-dimensional square, triangular and Kagome lattices. Figures (a) and (b) adapted from Ref. [12].

niques, which in recent years have reached a very high level of resolution – this is the case, for example, of absorption imaging and fluorescence imaging [8]. A widespread technique – which motivates many of the results of this thesis – is time-of-flight imaging [8], which permits to measure the momentum distribution of the atomic cloud. It consists in switching off abruptly both the trapping and the lattice potentials and, after a time interval, detecting the atoms through absorption imaging. During the expansion, the spatial distribution maps out the momentum distribution $n(\mathbf{k})$ before the trap release. This relies on the assumption that, when the potentials are switched off, atoms expand freely. One may notice that time-of-flight images – see e.g. Fig. 1.2(a) – are at most two-dimensional, given that an integration of the cloud image along the line of sight is performed by the imaging system, although recent experiments [13] have demonstrated a full tomographic reconstruction of the momentum distribution.

In the two following paragraphs we present some experimental results which show the huge potential of optical lattices and which are also significant for the themes that we will cover in the following chapters.

1.1.1 Quantum phase transitions

At zero temperature the variation of a Hamiltonian parameter (e.g. magnetic field, interaction strength, ...) can produce a quantum phase transition in the ground state of a many-body system [14]. Such a transition is not driven by thermal fluctuations, as for thermal phase transitions, but by quantum fluctuations, which are a consequence of Heisenberg's uncertainty principle. In cold atomic lattices (as well as in any other experimental system), the temperature is obviously not zero, but one can observe finite-temperature consequences of the presence of zero-temperature quantum phase transition.

One important example of quantum phase transition is the superfluid -Mott insulator transition in the aforementioned Bose-Hubbard model [14]. This model is described by a Hamiltonian

$$\hat{\mathcal{H}} = -J \sum_{\langle i,j \rangle} \left(\hat{b}_i^{\dagger} \hat{b}_j + \text{h.c.} \right) - \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i , \qquad (1.1)$$

with J the tunneling parameter, which describes the rate at which atoms tunnel from one site of the lattice to an adjacent one (here with the notation $\langle \cdot, \cdot \rangle$ we assumed nearest-neighbor tunneling only); U the interaction parameter, which accounts for on-site repulsion; and μ the chemical potential. When $J \gg U$ the hopping energy dominates, and the system is in a superfluid phase, in which atoms delocalize all over the lattice and the system possesses long-range phase coherence. This phase exhibits local density fluctuations and has no gap in the excitation spectrum. When $U \gg J$ interactions dominate and for integer lattice fillings the system enters the so-called Mott-insulator phase, in which atoms are localized at lattice sites and the system exhibits short-range phase coherence, with a gap opening in the excitation spectrum. These two phases are connected by a quantum phase transition and tuning the ratio J/U gives access to its experimental realization.

In an optical lattice such a tuning can be achieved by controlling the intensity of the laser beams, which in turn controls the lattice depth. The deeper is the lattice, the more suppressed are hopping processes, since the potential barrier to overcome is higher, and the more relevant are interactions, since atoms tend to localize at the minima of the lattice and then strongly repel each other. More quantitatively, we have that $J \sim \exp(-\sqrt{2V_0/E_R})$ [15], with V_0 the lattice potential depth and E_R a reference energy called recoil energy, which means that the ratio J/U depends exponentially on the lattice depth. The first proposal of an experimental protocol to realize the superfluid - Mott insulator transition is due to Jaksch *et al.* in 1998 [16] and the first realization to Greiner *et al.* in 2003 [3]. The experiment was realized in a cubic lattice with Rb atoms and the Hamiltonian of the system was varied continuously from the superfluid regime to the Mott insulating regime. In Fig. 1.2(a) we show the time-of-flight images reported in Greiner's

article. For weak lattices (top-left image) the system shows marked peaks in the center of the Brillouin zones (and at the reciprocal lattice vectors), which denotes the phase coherence of the superfluid state. Increasing the lattice depth, the peaks gradually disappear, until long-range coherence is lost. This same experiment was later realized also in one [17] and two [18] dimensional lattices.

We can use the superfluid - Mott insulator phase transition to introduce another important technique which is proper to optical lattices: lattice shaking. It can be shown that, when a lattice undergoes a periodic modulation of its spatial phase at a frequency ω out of resonance with respect to all transition energies of the system, and much larger than the hopping and collision rates in the lowest band, it is possible to give an effective description of the lattice in which the hopping parameters are renormalized as $J' = J \mathcal{J}_0(K/\omega)$, where \mathcal{J}_0 is a Bessel function of the first kind, K is the shaking amplitude and ω is the shaking frequency. In particular, one may suppress hopping processes by choosing amplitude and frequency such that K/ω is close to a zero of the Bessel function \mathcal{J}_0 and thus realize once again a superfluid -Mott insulator phase transition. This method was first proposed by Eckardt et al. [19] and realized by Lignier et al. in 2009 [20]. In Fig. 1.2(b) we show time-of-flight images from a lattice-shaking experiment by Zenesini et al. [21]: notice that in this case Bragg peaks appear only along one dimension, since the experiment was realized with a single pair of counter-propagating beams. The figure shows from left to right time-of-flight diffraction patterns of lattices undergoing shakings characterized by an increasingly large K/ω ratio. One may notice that a regime lacking phase coherence appears twice, since two successive zeros of the Bessel function are explored with the K/ω ratio. Moreover, in between the two zeros the Bessel function is *negative*, changing the sign of the hoppings and the position of the Bragg peaks. Lattice shaking is in principle a powerful tool, but its range of application is limited by constraints on the shaking frequency ω : the latter is required to be off-resonant with respect to the other energy scales of the system, in order to keep the effective description valid, but it cannot be too large, since it would require large amplitudes K to have sizable K/ω ratios, which in turn would produce heating as a side effect.

1.1.2 Artificial gauge fields

One of the current challenges of cold-atom experiments is to access the physics induced by strong gauge fields, even in the most general case of non abelian fields. The main limitation to the simulation of magnetism with cold atoms is the neutrality of the latters. Recently many techniques have been developed to overcome this difficulty. One possible technique is to put the atoms in rotation. At frequency close to that of the trap, the Coriolis force mimics the action of a Lorentz force acting on a charged particle



Figure 1.2: (a) Superfluid - Mott insulator quantum phase transition through tuning of the lattice depth. (b) Superfluid - Mott insulator quantum phase transition through lattice shaking. Figures adapted from Refs. [3] and [21] respectively.

in a uniform magnetic field [22]. But this method suffers from the fundamental drawback that the presence of the centrifugal force, alongside with the Coriolis one, makes the system unstable for large rotation frequencies. An alternative method for optical lattice systems is the use of laser-assisted hoppings [23], namely hoppings processes in which particles also acquire a geometric phase ϕ_{ij} , thus realizing a Hamiltonian of the form

$$\hat{\mathcal{H}} = -J \sum_{\langle i,j \rangle} \left(e^{i\phi_{ij}} \hat{b}_i^{\dagger} \hat{b}_j + \text{h.c.} \right) - \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i . \quad (1.2)$$

If assisted hoppings are organized such that particles acquire a finite phase $\Phi = \sum_{i \to j} \phi_{ij}$ on a closed loop, this scheme mimics a magnetic flux [24]. Another method is the afore-mentioned lattice shaking. The shaking frequency can be chosen such that the Bessel functions renormalizing the hopping parameter take negative values, which is equivalent to having a complex hopping process where atoms acquire a geometric phase $\Phi = \pi$. This method can be used to realize a frustrated triangular lattice [10], which will be the topic of our last chapter, or a frustrated Kagome lattice [11]. In these two lattices frustration induces different forms of degeneracy at low energies in the single-particle spectrum, namely a two-fold degeneracy in the case of



Figure 1.3: (a) Phases and associated experimental time-of-flight diffraction patterns. (b) Rectangular to spiral to staggered chain phase transition. Experimental time-of-flight diffraction patterns on the left and corresponding theoretical calculations on the right. Figures adapted from Ref. [25].

the triangular lattice and an infinite flat-band degeneracy in the case of the Kagome lattice. As a consequence, condensation of free bosons may occur at inequivalent vectors of the Brillouin zone (triangular) or not occur at all (Kagome): studying the finite-temperature physics of these lattices in the presence of interactions is therefore very interesting.

One important result due to lattice shaking is the simulation of frustrated classical magnetism, realized by Struck *et al.* in 2011 [25]. In the experiment a two-dimensional triangular lattice of one-dimensional tubes is filled with bosonic atoms. At low temperatures each tube hosts a Bose-Einstein condensate, which has a well defined phase ϕ_i . This system can be mapped onto a model of classical XY spins $\mathbf{S}_i = [\cos(\phi_i), \sin(\phi_i)]$, where the phase of the condensate corresponds to the orientation of the spin. By lattice shaking one can tune independently the hoppings in different directions, and this permits to realize a broad variety of phases (ferromagnetic as well as anti-ferromagnetic). Fig. 1.3(a) gives a visual representation of these phases in terms of spins and of the associated experimental diffraction pattern in time-of-flight experiments. This experiment also permits to study a variety of phase (shown in Fig. 1.3(a)) to a spiral phase, and then to staggered one-dimensional chains.

1.2 Theoretical aspects: correlations and entanglement

In this thesis we will focus on some important theoretical aspects of quantum many-body theory. In particular, our second chapter will be dedicated to entanglement and quantum correlations. Entanglement is an essential quantum property of many-body states that manifests itself in the impossibility of describing the state of a quantum degree of freedom independently of the others. According to the seminal work of Werner [26], a most general mixed state is called entangled if it is not separable; and a state is separable (or classically correlated) if, given two subsystems A and B, its density matrix can be expressed as $\hat{\rho} = \sum_{s} p_s \hat{\rho}_A^{(s)} \otimes \hat{\rho}_B^{(s)}$, with p_s a normalized classical distribution function.

In the case of pure states (for which $\hat{\rho}^2 = \hat{\rho}$), a generic state can always be determined as separable or not by using the Schmidt rank criterion, which is based on a Schmidt decomposition of the vector state (using orthonormal bases for the Hilbert spaces of A and B) [27]. In the case of mixed states (for which $\hat{\rho}^2 \neq \hat{\rho}$) the situation complicates considerably: the Schmidt rank criterion is not applicable and, in general, determining if a state is entangled or not is an NP-hard problem [28]. A necessary, yet not sufficient, criterion for separability is the Peres-Horodecki criterion [29], which is based on positive definiteness of a partial transpose of the density matrix.

Defining quantum correlations is also, in general, a non-trivial task. In the case of pure states one can unambiguously associate quantum correlations with entanglement, but in the case of mixed states it appears more complicated to give a precise definition, since thermal correlations are always present at T > 0. A possible definition could be extracted from the non local disturbance produced by a local measurement, which is revealed by the so-called quantum discord [30]. In Chap. 3 we will give a new alternative observable-dependent definition, calculated as the difference between the usual total correlation function and a response function. This quantity, unlike quantum discord, will prove to be completely insensitive to classical thermal critical phenomena. We will also study the spatial structure of this newly-defined correlation function and show that its rapid decay justifies the introduction of a criterion for effective separability of quantum systems.

1.3 Numerical aspects: computational methods

The impressive development of experiments in cold atoms has been accompanied by a parallel development of a zest of computational methods. Calculations for quantum systems are particularly challenging because their computational cost grows generally esponentially with the size of the system. For this reason most methods rely either on approximations or on a stochastic approach. One of the core topics of this thesis is the proposal of a new numerical approach to the thermodynamics of lattice boson systems. For this reason we find it instructive to give an overview over some of the most common methods approaching the same problem. We shall review their strengths and weaknesses, and we will set the stage for our approach, that we briefly introduce in the last paragraph. A few of these methods will be analyzed more in details in Chap. 2.

1.3.1 Exact Diagonalization

The very first approach to a many-body system would be to try and solve its associated eigenvalue problem through full diagonalisation of the Hamiltonian. This method can be applied to any kind of system but, as we explained in the previous paragraphs, the exponential growth of Hilbert space with the size of the system limits its use to small sizes, where results are strongly affected by finite-size effects. Speed-ups are possible by exploiting symmetries of the system or by using, for example, the Lanczos algorithm [31]. This algorithm calculates the first m eigenvalues and eigenvectors of an nxn matrix, with $m \ll n$, and it is particularly useful if one is only interested in the ground state of the system or in very low temperatures, where a few eigenstates can successfully describe the system. State-of-the-art Lanczos-based techniques permit to diagonalize systems of S = 1/2 Heiseneberg spins on lattices of up to around 40 sites [32, 33]. Despite its limitations, this method remains very important for models to which other methods are not applicable in general (e.g. fermionic systems, frustrated quantum magnets).

1.3.2 Mean-field theory

A first approximated approach to many-body systems is mean-field (MF) theory, which consists in decoupling the fluctuations of some degrees of freedom of the system and then coupling them through their average values. This technique can be applied to a large variety of systems ranging from fermionic gases (see e.g. the famous Hartree-Fock theory [34]) to the bosonic lattice models of interest in our work. In this latter case, MF theory decouples the bosonic modes associated to each lattice site or, in its improved cluster version (cMF), to clusters of sites [35]. Despite being correct at a semi-quantitative level in many situations, MF and cMF miss systematically the long-wavelength fluctuations that dominate e.g. the physics of critical points. For example, they completely miss the peculiar nature of the superfluid phase of two-dimensional lattice bosons - see Chap. 2.

1.3.3 DMRG and variational approaches

The Density Matrix Renormalization Group (DMRG) [36] is a variational method which is best suited for one-dimensional or quasi-one-dimensional

systems at zero temperature. DMRG realizes a systematic truncation of the Hilbert space of the system and it constructs a wave-function by keeping a small number of important states (the most probable eigenstates of a reduced density matrix) in a series of increasingly large subsystems. DMRG can be applied to virtually all one-dimensional systems, and it has proven to be extremely accurate thanks to the weak entanglement content of most one-dimensional Hamiltonians of physical interest. It can be applied to equilibrium systems which reach a few thousands of sites, and it can be used as well to study non-equilibrium phenomena (on smaller lattices) [37]. Extensions of DMRG are possible to finite temperature [38] and to cylinder-shaped two-dimensional lattices [39].

Variational methods which are similar to DMRG in spirit are based on Matrix Product States (MPS), which are restricted to one-dimensional systems, and their generalization to any dimension, the so-called Tensor Network States (TNS) [40]. These methods are particularly suited for the study of ground states, but there exist some very recent extensions to finitetemperature [41].

1.3.4 Quantum Monte Carlo

The name Quantum Monte Carlo (QMC) denotes a family of stochastic methods based on a Monte Carlo approach, which includes e.g. variational MC, diffusion MC, path integral MC - [42, 43, 44] for a brief introduction to the Monte Carlo method, in its Metropolis version, we refer the reader to appendix A. The common ground of these methods is the calculation of multi-dimensional integrals through a guided stochastic sampling of the integrand (importance sampling). QMC is statistically exact in the sense that an ideal infinite-time simulation converges to the exact result. This method reveals to be very effective in describing long-range correlations and critical phenomena. The main weakness of QMC is that its use is limited to a broad, yet restricted class of models. The domain of applicability of QMC is limited by the so-called "sign problem", which prevents the application of QMC to generic fermionic systems, or to bosonic systems in gauge fields (including frustrated magnetism). The sign problem arises from negative (or imaginary) probability amplitudes appearing in the simulations [45]. In the case of fermions the origin of this problem resides in the properties of the wave-function, which is anti-symmetric for the exchange of two particles. The impossibility of applying QMC to systems which are currently of great interest for experiments, such as frustrated lattices, requires for the search of new alternative methods.

1.3.5 Auxiliary Field Monte Carlo

In the last chapter of this thesis we introduce a method called auxiliary-field Monte Carlo (AFMC), which is similar in spirit to approaches such as that used in Ref. [46] for spins and bosons, or to some others used in the context of lattice fermions [47]. In its general version AFMC suffers from a heavy sign problem, that we overcome by using a semi-classical approximation that we develop in Chap. 4 and we call quantum mean-field (QMF) approximation. The AFMC method supplemented with the QMF approximation is readily suited for the study of the thermodynamics of a large class of bosonic systems, including frustrated lattice bosons.

1.4 Outline of the thesis

The thesis is organized as follows.

In Chap. 2 we analyze more in detail some of the methods commonly in use for the study of the thermodynamics of lattice systems.

In Chap. 3 we study quantum and classical correlations and show how they live on very different length scales. We focus in particular on the Bose-Hubbard model in the limits of hard-core bosons and quantum rotors.

In Chap. 4, on the basis of this length-scale separation, we introduce the aforementioned quantum mean-field approximation and apply it to the test model of quantum rotors.

In Chap. 5 we introduce the auxiliary-field Monte Carlo approach (AFMC), and apply its QMF-approximated version to the study of frustrated bosons in a triangular lattice.

Chap. 6 is devoted to conclusions.

Chapter 2

Some numerical approaches to lattice-boson systems

In this chapter we recall and illustrate more in detail some of the numerical methods mentioned in the introduction. We use Quantum Monte Carlo results, which are statistically exact, as a reference, and compare them to cluster mean-field theory (cMF) and Gutzwiller Monte Carlo (GMC), two methods based on a Gutzwiller mean-field Ansatz. cMF is a self-consistent method which can be improved systematically by considering clusters of larger size. Being limited to small-sized cluster, this method is unable to capture long-ranged correlations. GMC, conversely, thanks to its stochastic nature, is able to describe thermal fluctuations at all scales. It captures therefore the correct nature of thermal phases and phase transitions, but it is less accurate then cMF close to zero temperature, because in that limit it reduces to single-site MF.

The focus of this chapter is on hard-core bosons on a square lattice at finite temperature, which will often serve as a test system also in the following chapters. The choice of this model is motivated by the limited computational cost required by simulations (with respect to, for example, the more general case of "softcore" bosons) due to the minimal size of the local Hilbert space. Nonetheless, in order to keep the treatment as general as possible, all the equations will refer to "softcore" bosons, while all the plots will show results for hard-core bosons. Both cMF and GMC could be used for systems with magnetic frustration, for which we shall not have a reference method to compare with.

2.1 Hard-core bosons in two dimensions

We recall the Hamiltonian of the Bose-Hubbard model, which has already been mentioned in the introduction:

$$\hat{\mathcal{H}} = -J \sum_{\langle ij \rangle} \left(\hat{b}_i^{\dagger} \hat{b}_j + \text{h.c.} \right) - \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i . \qquad (2.1)$$

The various phases of the system are best characterized by studying the first-order correlation function $g(i,j) = \langle \hat{b}_i^{\dagger} \hat{b}_j \rangle$. When considering a twodimensional system, Mermin-Wagner's theorem predicts the absence of true condensation, namely of long-range phase coherence at any temperature, imposing that g(i,j) decays to zero at large distances. Nonetheless the system still exhibits a Berezinskii-Kosterlitz-Thouless (BKT) phase transition [48, 49, 50] between a low temperature and a high temperature phase. At low temperature the correlation function exhibits an algebraic decay in the form

$$g(r) \sim r^{-\eta(T)} , \qquad (2.2)$$

where $r = |\mathbf{r}_i - \mathbf{r}_j|$ is the inter-site distance. The system is in a regime called "quasi-condensate" [51], in which the number of particles in the condensate, $n(k = 0) = (1/L^2) \sum_{ij} \langle \hat{b}_i^{\dagger} \hat{b}_j \rangle$ scales as $L^{2-\eta(T)}$, namely it diverges (as $\eta(T) < 2$), but is not extensive. This happens because thermal effects are strong enough to prevent full condensation even at very low temperatures. Conversely, at high temperature the correlation function shows an exponential decay

$$g(r) \sim e^{-r/\xi(T)}$$
, (2.3)

characterizing a normal phase, in which n(k = 0) remains finite for $L \to \infty$. Therefore there must be a transition between the two regimes at some T_{BKT} . It is not possible to associate an order parameter to such a transition (it is said to be of "infinite order" [49]), but it is nevertheless characterized by the divergence of the correlation length $\xi(T)$ while approaching T_{BKT} from above.

In the limit of large on-site interaction $U/J \gg 1$, and filling n < 1, bosons reach the "hard-core" limit, in which one may neglect the multiple occupation of each lattice site. In this limit one may incorporate the hardcore constraint into the commutation relations of the operators, by requesting that

$$\begin{aligned} [\hat{a}_i, \ \hat{a}_j^{\dagger}] &= 0 \quad \text{for } i \neq j , \\ (\hat{a}_i^{\dagger})^2 &= (\hat{a}_i)^2 = 0 , \\ \{\hat{a}_i, \hat{a}_i^{\dagger}\} &= 1 , \end{aligned}$$
(2.4)

2.2. QUANTUM MONTE CARLO

where we renamed the bosonic operators as $a^{(\dagger)}$, to highlight that they refer to bosons of hard-core type. The interaction term can then be dropped in Eq. (2.1), and the Hamiltonian becomes

$$\hat{\mathcal{H}}_{\rm hc} = -J \sum_{\langle ij \rangle} \left(\hat{a}_i^{\dagger} \hat{a}_j + \text{h.c.} \right) - \mu \sum_i \hat{n}_i . \qquad (2.5)$$

The commutation relations of hard-core-boson operators are the same as those of the Pauli matrices σ^+ and σ^- , implying the mapping from hard-core bosons to S = 1/2 spins as [52]

$$\hat{a}_i \to \hat{S}_i^- = \hat{S}_i^x - i\hat{S}_i^y ,$$
 (2.6)

$$\hat{a}_{i}^{\dagger} \to \hat{S}_{i}^{+} = \hat{S}_{i}^{x} + i\hat{S}_{i}^{y} .$$
 (2.7)

By introducing the new operators in the Hamiltonian and removing the constant terms, one gets the new Hamiltonian

$$\hat{\mathcal{H}}_{XY} = -2J \sum_{\langle i,j \rangle} \left(\hat{S}_i^{x\dagger} \hat{S}_j^x + \hat{S}_i^{y\dagger} \hat{S}_j^y \right) - \mu \sum_i \hat{S}_i^z , \qquad (2.8)$$

which is precisely that of the S = 1/2 quantum XY model in a transverse magnetic field μ . This exact mapping allows one to express results either in the language of spins or of lattice bosons.

2.2 Quantum Monte Carlo

Hard-core bosons on a square lattice can be efficiently simulated using Quantum Monte Carlo, here in the Statistic Series Expansion (SSE) formulation [42, 43, 44]. Without going into the details of this formulation, we shall limit ourselves to saying that it is based on a Taylor expansion of the density operator $e^{-\beta \hat{\mathcal{H}}}$ in powers of the inverse temperature β . In Figs. 2.1 we show some results obtained using a code developed by T. Roscilde. With these plots we do not intend to study the system in detail, but just to give a quantitative reference for the other methods that we present in the following sections. For this reason we limit ourselves to small lattices.

Figs. 2.1(a-b) show the kinetic energy and the k = 0 peak of the momentum distribution $n(\mathbf{k})$ for different lattice sizes. Both quantities are divided by the number of sites of the lattice. As one may expect the kinetic energy grows with the transition from superfluid to normal phase, whereas the momentum peak decreases, since coherence is progressively lost. Fig. 2.1(c) shows a peak for the specific heat, which normally appears just above the BKT transition [54]. The specific heat does not show any discontinuity since, as said previously, the transition is an infinite-order one. At the transition the n(k = 0) scales as $L^{7/4}$, since $\eta(T_{BKT}) = 1/4$ [55]. One may extract an estimate for the infinite-size system BKT transition temperature by finitesize scaling, as shown in Fig. 2.1(d).



Figure 2.1: (a-b) Kinetic energy and n(k = 0), both expressed per site. (c) Specific heat. (d) Finite-size scaling for $n(k = 0)L^{-7/4}$. The vertical line marks the reference BKT transition temperature as obtained in [53]. All plots refer to hard-core bosons and employ the temperature $t = k_B T/J$, with k_B the Boltzmann constant.

2.3 Cluster mean-field approach

As we mentioned in the introduction, a mean-field (MF) approximation [56] amounts to decoupling the fluctuations of selected degrees of freedom of a system, and coupling the latter only through their average values. In the

case of lattice bosons, these degrees of freedom might be the bosonic modes associated to single sites of the lattice, or to clusters of sites, in order to gain a more accurate description - see Fig. 2.2.

When considering the ground state of the system, a cluster MF approach amounts to minimizing the ground-state energy

$$E[\psi_{MF}] = \langle \psi_{MF} | \hat{\mathcal{H}} | \psi_{MF} \rangle \tag{2.9}$$

of a wave function in the form

$$|\psi_{\rm MF}\rangle = \otimes_c |\psi_c\rangle, \qquad (2.10)$$

where c is the cluster index. In the finite temperature case it amounts to minimizing the free energy

$$F[\rho;T] = \operatorname{Tr}[\hat{\rho}\hat{\mathcal{H}} + T\hat{\rho}\log\hat{\rho}]$$
(2.11)

of a factorized density matrix $\hat{\rho}$

$$\hat{\rho}_{\rm MF} = \otimes_c \hat{\rho}_c \ . \tag{2.12}$$

Both Eq. (2.10) and Eq. (2.12) show how MF theory neglects any form of correlations and entanglement among degrees of freedom belonging to different clusters. On the other hand, one may notice that such an approach becomes exact in the limit of an infinite lattice connectivity, since entanglement gets spread among all degrees of freedom and then becomes negligible.

In the following we present the self-consistent cluster MF method [35, 57, 58] based on the Gutzwiller ansatz, both for zero and finite temperatures.

2.3.1 Single-site Gutzwiller mean field

The conventional Gutzwiller Ansatz [59] amounts to factorizing the wavefunction into clusters composed of single sites. In a homogeneous lattice, each site i will have a local wave function

$$|\psi_i\rangle = \sum_{n=0}^{n_{\text{max}}} f_{n_i} |n_i\rangle , \qquad (2.13)$$

where $|n_i\rangle$ is a local Fock state with n particles and n_{\max} is a convenient cutoff. We focus on a specific site j and express the wave function of the system as $|\psi_{\chi_j}\rangle \otimes |\psi_j\rangle$, where $|\psi_{\chi_j}\rangle = \otimes_{i\neq j} |\psi_i\rangle$ is the wave function of the rest of the system but the site j (χ_j stands for the complement to j). Notice that this equation is in the form of Eq. (2.10). The Bose-Hubbard Hamiltonian Eq. (2.1) can then be written as a sum of three contributions

$$\hat{\mathcal{H}} = \hat{H}_j + \hat{H}_{\chi_j} + \hat{H}_{j\chi_j} , \qquad (2.14)$$

which describe respectively the site j, the rest of the system, and the interaction between j and the rest of the system:

$$\hat{H}_{j} = \frac{U}{2}\hat{n}_{j}(\hat{n}_{j}-1) - \mu\hat{n}_{j} ,$$

$$\hat{H}_{\chi_{j}} = -J \sum_{\langle i\neq j, l\neq j \rangle} \left(\hat{b}_{i}^{\dagger}\hat{b}_{l} + h.c.\right) + \frac{U}{2} \sum_{i\neq j} \hat{n}_{i}(\hat{n}_{i}-1) - \mu \sum_{i\neq j} \hat{n}_{i} ,$$

$$\hat{H}_{\chi_{j}j} = -J \sum_{\langle j' \rangle} \left(\hat{b}_{j}^{\dagger}\hat{b}_{j'} + h.c.\right) ,$$
(2.15)

where $\langle j' \rangle$ denotes the sum over the nearest neighbors of site j. We can define an effective on-site Hamiltonian $\hat{H}_{\text{eff}}^{j} = \langle \psi_{\chi_{j}} | \hat{\mathcal{H}} | \psi_{\chi_{j}} \rangle$ for the site j, that in the local basis $\{ |n_{j} \rangle \}$ has a matrix form

$$\begin{pmatrix} \hat{H}_{\text{eff}}^{j} \end{pmatrix}_{m_{j}n_{j}} = \langle m_{j} | \hat{H}_{j} | n_{j} \rangle + \langle \psi_{\chi_{j}} | \hat{H}_{\chi_{j}} | \psi_{\chi_{j}} \rangle \delta_{m_{j}n_{j}} - J \sum_{\langle j' \rangle} \left(\langle m_{j} | \hat{b}_{j}^{\dagger} | n_{j} \rangle \langle \psi_{\chi_{j}} | \hat{b}_{j'} | \psi_{\chi_{j}} \rangle + \text{h.c.} \right) .$$
 (2.16)

Here $\langle m_j | \hat{H}_j | n_j \rangle$ can be easily expressed in the local basis $\{ |n_j \rangle \}$, whereas $\langle \psi_{\chi_j} | \hat{H}_{\chi_j} | \psi_{\chi_j} \rangle \delta_{m_j n_j}$ represents an energy offset, which can then be neglected. One can make initially an arbitrary choice for the coefficients $\{ f_n \}$ and, since the lattice is homogeneous, express the expectation values for the sites j' in Eq. (2.15) as

$$\langle \psi | \hat{b}_{j'} | \psi \rangle = \langle \psi_j | \hat{b}_j | \psi_j \rangle = \sum_{n_j} f_{n_j}^* f_{n_j+1} \sqrt{n+1} . \qquad (2.17)$$

This permits to diagonalize the Hamiltonian and to obtain a new set of coefficients $\{f_{n'_j}\}$ from the ground state. The process can be iterated until it reaches convergence and the final ground state can be used to calculate expectation values for the observables.

This procedure is consistent with a variational approach to the groundstate energy, which can be minimized using the method of Lagrange multipliers. One has

$$E_{\lambda} = \langle \psi | \hat{\mathcal{H}} | \psi \rangle - \lambda \langle \psi | \psi \rangle , \qquad (2.18)$$

where λ is a Lagrange multiplier which accounts for the normalization of the wave function. Imposing the vanishing of the derivative with respect to the local wave-function $\langle \psi_i |$, we obtain

$$\frac{\partial E_{\lambda}}{\partial \langle \psi_j |} = \langle \psi_{\chi_j} | \hat{\mathcal{H}} | \psi_{\chi_j} \rangle | \psi_j \rangle - \lambda | \psi_j \rangle = \hat{H}^j_{\text{eff}} | \psi_j \rangle - \lambda | \psi_j \rangle = 0 , \qquad (2.19)$$

which is precisely the eigenvalue problem of \hat{H}_{eff}^{j} .

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The self-consistent method here presented for zero temperature, can be easily extended to finite temperature, by considering a system in the form of Eq. (2.12), namely $\hat{\rho} = \bigotimes_i \hat{\rho}_i$. One can obtain an effective Hamiltonian at site j as

$$\hat{H}_{\text{eff}}^{j} = \text{Tr}_{\chi_{j}}[\hat{\mathcal{H}}\hat{\rho}] = \hat{H}_{j} - Jz \left(\Phi \hat{b}_{j}^{\dagger} + \text{h.c.}\right), \qquad (2.20)$$

where $\operatorname{Tr}_{\chi_j}$ denotes a partial trace over the complement to j. Here z is the coordination number of the lattice and Φ is the MF parameter, which is the same is the same for all the z neighbors of the lattice site j, since the lattice is homogeneous. One can make a convenient initial assumption for Φ (which accounts for making an initial assumption for $\hat{\rho}$) and calculate a new MF parameter as

$$\Phi = \frac{\operatorname{Tr}[\hat{b}_j e^{-\beta \hat{H}_{\mathrm{eff}}^j}]}{\operatorname{Tr}[e^{-\beta \hat{H}_{\mathrm{eff}}^j}]} .$$
(2.21)

This procedure can be iterated as in the case of zero temperature until it reaches convergence. Thermal averages for the observables can be calculated using the final form of the effective Hamiltonian.

2.3.2 Cluster Gutzwiller mean field

The previous approach can be easily generalized to clusters of sites. One can focus on a specific cluster c of s sites, with a local wave-function in the form

$$|\psi_c\rangle = \sum_{N_c=1}^{N_{\text{max}}} f_{N_c} |N_c\rangle .$$
 (2.22)

Here $|N_c\rangle = |n_0, n_1, ..., n_s\rangle_c$, with n_i the number of particles on the *i*-th site of the cluster and $N_{max} = s(n_{max} + 1)$ a convenient cut-off. The effective local Hamiltonian of *c* results

$$(H_{\text{eff}}^{c})_{M_{c}N_{c}} = \langle \psi_{\chi_{c}} | \hat{H}_{\chi_{c}} | \psi_{\chi_{c}} \rangle \delta_{M_{c}N_{c}} + \langle M_{c} | \hat{H}_{c} | N_{c} \rangle - J \sum_{j \in \partial c} \nu_{j} \left(\Phi \langle M_{c} | \hat{b}_{j}^{\dagger} | N_{c} \rangle + \text{h.c.} \right) , \qquad (2.23)$$

where \hat{H}_c (\hat{H}_{χ_c}) indicates Bose-Hubbard Hamiltonian Eq. (2.1) restricted to sites *i* and *j* (not) belonging to the cluster *c*, Φ denotes the MF parameter, ∂c is the frontier of the cluster and ν_j is the number of connections linking the site *j* to sites outside the cluster. For example, for a square lattice and a square cluster, ν_j is 2 for a corner site and 1 for a site along an edge – see Fig. 2.2(a). This form of Eq. (2.23) relies once again on the assumption that the MF to which border sites couple is the same in all the directions, which is a consequence of considering a homogeneous lattice. Once made an initial



Figure 2.2: (a) Cartoon of a square lattice divided into 3x3 clusters. (b-c) Momentum peak and kinetic energy per site calculated with cMF for different cluster sizes, compared to QMC (data from 36x36 lattice). (d) Extrapolation of the transition temperature with the surface-to-bulk ratio of clusters. The horizontal line represents the reference value $T_{BKT} = 0.685 k_B/J$. All plots refer to hard-core bosons and employ the reduced temperature $t = k_BT/J$, with k_B the Boltzmann constant.

assumption for the coefficients $\{f_{N_c}\}$, a new MF parameter can be obtained

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as

$$\Phi = \sum_{M_c,N_c} f_{M_c}^* f_{N_c} \langle M_c | \hat{b}_t | N_c \rangle , \qquad (2.24)$$

where t denotes a target site belonging to the cluster. This site, if possible, should belong to the bulk of the cluster, or at least be minimally coupled to the MF, in order to avoid the effects of the cluster boundaries as much as possible. As in the case of single-site MF, this procedure can be iterated until convergence is reached, and expectation values for the observables can be calculated from the final ground state.

This method can be straightforwardly generalized to finite temperatures in complete analogy to what is done in the single-site case.

Results obtained with cMF for 2d hard-core bosons on the square lattice are reported in Fig. 2.2(b-c), where they are compared to QMC. Applying the cMF approach to hard-core bosons amounts to rephrase all the previous formulas involving bosonic operators \hat{b}_i , \hat{b}_i^{\dagger} in terms of hard-core boson operators \hat{a}_i , \hat{a}_i^{\dagger} (or simply to set $n_{max} = 1$). The comparison is drawn using QMC data for the largest of the lattices considered so far (the 36x36 lattice), which is the least affected by finite-size effects. One can notice how results slowly move closer to those of QMC upon increasing the size of the clusters. However, the cMF approach completely misses the nature of the low-temperature phase, which is described by cMF as possessing true longrange order in contradiction to Mermin-Wagner's theorem; as well as the nature of the transition, which is inevitably represented as belonging to the MF universality class. One may extract an estimate for the exact transition temperature by using a polynomial extrapolation in the surface-to-bulk ratio λ of the clusters, defined as

$$\lambda = \frac{N_{\text{ext}}}{N_{\text{int}} + N_{\text{ext}}} , \qquad (2.25)$$

where N_{ext} is the number of bonds linking the degrees of freedom within the cluster to those external to the cluster, while N_{int} is the number of bonds within the cluster. Hence $\lambda = 1$ for the basic (single-site) mean-field approximation, while $\lambda = 0$ corresponds to the exact result of a single cluster covering the whole system. We performed a linear fit to the cMF estimates of the transition temperature for each cluster size, corresponding to the temperature at which n(k = 0) vanishes. The result is shown in Fig. 2.2(d). The infinite-size estimate takes a value $T_{\lambda=0} = (0.86 \pm 0.05) k_B/J$, which appears to be quite far from the best estimate $T_{BKT} = 0.685 k_B/J$ [53]. One may also notice that cMF results strongly depend on the cluster size, with the infinite-size estimated transition temperature being almost half the single-site one ($\lambda = 1$). This result will be useful for the following chapters, where a similar procedure of extrapolation will be used, albeit in a different context.

2.4 Gutzwiller Monte Carlo

We present now a "hybrid" method which relies on both a MF and a Monte Carlo approach, and which has been used in a few recent works dealing with frustrated bosons and spins [60, 61].

The Gutzwiller wave-function introduced in the previous section can be cast in its most general form as

$$|\psi(\vec{f})\rangle = \bigotimes_{i=1}^{N} |\psi_i\rangle = \bigotimes_{i=1}^{N} \left(\sum_{n_i=0}^{n_{max}} f_{n_i}^{(i)} |n_i\rangle \right), \qquad (2.26)$$

where $\vec{f} = \{f_{n_i}^{(i)}\}\$ is an array of $N(n_{max}+1)$ complex coefficients, normalized as $\sum_{n_i=0}^{n_{max}} |f_{n_i}^{(i)}|^2 = 1$ on each site. Notice that now coefficients can differ from site to site. Because of the normalization constraint we have that $f_{n_i}^{(i)} = \alpha_{n_i}^{(i)} e^{i\phi_{n_i}^{(i)}}$, with $0 \le \alpha_{n_i}^{(i)} \le 1$. We can calculate the partition function of the system as

$$\mathcal{Z} = \sum_{\{n_i\}} \langle \{n_i\} | e^{-\beta \hat{\mathcal{H}}} | \{n_i\} \rangle = C \int \mathcal{D}[\vec{f}] \langle \psi(\vec{f}) | e^{-\beta \hat{\mathcal{H}}} | \psi(\vec{f}) \rangle , \qquad (2.27)$$

where C is a numerical factor and we have set

$$\mathcal{D}[\vec{f}] = \prod_{i,n_i} \frac{df_{n_i}^{(i)} df_{n_i}^{*(i)}}{2\pi i} = \prod_{i,n_i} d\phi_{n_i}^{(i)} d\alpha_{n_i}^{(i)} \ \alpha_{n_i}^{(i)} \ \delta\left(\sum_{n_i} (\alpha_{n_i}^{(i)})^2 - 1\right) \ . \tag{2.28}$$

We notice that the metric for the amplitude can be chosen arbitrarily, since it only modifies the numerical factor C. Here we have chosen the one naturally emerging from the integral of the coefficients on the complex plane.

The weights $\langle \psi(\vec{f}) | e^{-\beta \hat{\mathcal{H}}} | \psi(\vec{f}) \rangle$ are still unknown without diagonalizing the Hamiltonian. A drastic approximation consists in assuming that a Gutzwiller state $|\psi(\vec{f})\rangle$ indeed diagonalizes $\hat{\mathcal{H}}$, so that

$$\langle \psi(\vec{f}) | e^{-\beta \hat{\mathcal{H}}} | \psi(\vec{f}) \rangle \approx e^{\langle \psi(\vec{f}) | -\beta \hat{\mathcal{H}} | \psi(\vec{f}) \rangle} = e^{-\beta E(\vec{f})} , \qquad (2.29)$$

where

$$E(\vec{f}) = - 2J \sum_{\langle i,j \rangle} \sum_{n_i, n_j=1}^{n_{max}} \gamma_{ij}(n_i, n_j) \cos\left(\theta_{n_i}^{(i)} - \theta_{n_j}^{(j)}\right) + \sum_{i, n_i} \left(\alpha_{n_i}^{(i)}\right)^2 \left(\frac{U}{2} n_i(n_i - 1) - \mu n_i\right)$$
(2.30)

and

$$\gamma_{ij}(n_i, n_j) = \sqrt{n_i n_j} \alpha_{n_i}^{(i)} \alpha_{n_i-1}^{(j)} \alpha_{n_j}^{(j)} \alpha_{n_j-1}^{(j)} , \qquad (2.31)$$



Figure 2.3: (a-b) Kinetic energy and k = 0 peak in momentum distribution calculated using QMC and GMC. (c) Finite-size scaling for $n(k = 0)L^{-7/4}$. All plots refer to hard-core bosons and employ the reduced temperature $t = k_B T/J$, with k_B the Boltzmann constant.

with $\theta_{n_i}^{(i)} = \phi_{n_i}^{(i)} - \phi_{n_i-1}^{(i)}$. This model represents a generalized XY model with fluctuating couplings, with the XY spins living on a (d+1)-dimensional lattice with sites (i, n_i) , where the extra dimension is provided by the occupation number. The XY interactions involve all sites (i, n_i) and (j, n_j) with (i, j) nearest neighbors. One can approximate the partition function as

$$\mathcal{Z} \approx \mathcal{Z}_{GMF} = C \int \mathcal{D}[\vec{f}] \ e^{-\beta E(\vec{f})} ,$$
 (2.32)

which is suitable for a Monte Carlo approach. One may notice that, at sufficiently high temperatures (such that βU , $\beta J \ll 1$), Eq. (2.29) becomes exact:

$$\langle \psi(\vec{f})|e^{-\beta\hat{\mathcal{H}}}|\psi(\vec{f})\rangle \approx 1 - \beta\langle \psi(\vec{f})|\hat{\mathcal{H}}|\psi(\vec{f})\rangle = 1 - \beta E(\vec{f}) \approx e^{-\beta E(\vec{f})} , \quad (2.33)$$

whereas at T = 0 the approach reproduces the Gutzwiller mean-field ground state.

A Monte Carlo simulation of the partition function Eq. (2.32) should contain two types of moves: an update of $\alpha_{n_i}^{(i)}$ coefficients, preserving the constraint $\sum_{n_i} (\alpha_{n_i}^{(i)})^2 - 1$, and an update of the $\theta_{n_i}^{(i)}$ coefficients. Observables can be obtained as

$$\langle \hat{O} \rangle \stackrel{\text{\tiny GMC}}{=} \left\langle \langle \psi(\vec{f}) | \hat{O} | \psi(\vec{f}) \rangle \right\rangle_T = C \int \mathcal{D}[\vec{f}] \left\langle \psi(\vec{f}) | \hat{O} | \psi(\vec{f}) \right\rangle \frac{e^{-\beta E(f)}}{\mathcal{Z}} \quad (2.34)$$

For example, the two-point operator $\langle \hat{b}_i^{\dagger} \hat{b}_j \rangle$ takes the form

$$\langle \hat{b}_i^{\dagger} \hat{b}_j \rangle = \left\langle \sum_{n_i, n_j=1}^{n_{max}} \gamma_{ij}(n_i, n_j) \left[\cos \left(\theta_{n_i}^{(i)} - \theta_{n_j}^{(j)} \right) + i \sin \left(\theta_{n_i}^{(i)} - \theta_{n_j}^{(j)} \right) \right] \right\rangle.$$
(2.35)

This can be used to calculate the kinetic energy and the n(k = 0) peak, which are shown in Fig. 2.3.

This approximation gives by construction a quantitative description of the thermodynamics of the Bose-Hubbard model at a sufficiently high temperature for the expression Eq. (2.33) to be valid. Given that Eq. (2.30)has the same symmetries and range of the intersite couplings as the original Bose-Hubbard Hamiltonian, thermal transitions are expected to be reproduced with the correct universality class, even though the correct value of the transition temperature is largely missed. This can be seen in Fig. 2.3(c), where the estimate $T_{BKT} \approx 0.36 k_B/J$ is roughly one half of the exact value. This shows how a better description of quantum fluctuations, that here are approached in a MF way, is fundamental for a correct quantitative picture of finite-temperature physics. At low temperatures the essential classical nature of the field theory defined by Eq.(2.30) emerges. One may notice that the kinetic energy, in Fig. 2.3(a), is linear at low temperatures, thus implying a constant specific heat C_v . This is a classical result, which is a consequence of the equipartition of energy and is in strong contrast with the $C_v \sim T^2$ dependence, determined by Bose statistics, that one would expect for our model [62]. Moreover, this overestimation of temperature effects at low temperature is arguably at the origin of the underestimation of the transition temperature. One may also notice that at zero temperature the method provides the single-site MF ground state, as can be seen comparing the low-temperature values for kinetic energy and n(k = 0) in Fig. 2.3(a-b) to those in Fig. 2.2(b-c).

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As a final remark, we notice that one may naively think of generalizing the GMC approach to the case of cluster decoupling in the form

$$|\psi_{cMF}\rangle = \bigotimes_{c=1}^{N_c} |\psi_c\rangle , \qquad (2.36)$$

$$\langle \psi_{cMF} | e^{-\beta \hat{\mathcal{H}}} | \psi_{cMF} \rangle \simeq e^{-\beta \langle \psi_{cMF} | \hat{\mathcal{H}} | \psi_{cMF} \rangle}.$$
 (2.37)

But this approximation turns out not to be useful: the vector \vec{f} parametrizing the cluster MF state grows exponentially with the cluster size, and Eq. (2.37) does not become more accurate upon increasing the cluster size, not even in the limit in which the cluster coincides with the whole system.

Chapter 3

Quantum and classical correlations

In this chapter we investigate the spatial structure of quantum correlations by introducing a quantum correlation function, defined as the difference between the total correlation function and a response function. We show how this newly-defined quantum correlation function – in contrast with the commonly used quantum discord – only captures the truly quantum aspects of many-body quantum states. We also observe that its very rapid spatial decay naturally defines a criterion for effective separability of subsystems. These arguments, besides being of specific theoretical interest themselves, constitute a fundamental justification for the approach to lattice systems that we will develop in Chap. 4.

3.1 Quantum correlation functions

We consider a generic quantum model with Hamiltonian $\hat{\mathcal{H}}$, in thermal equilibrium at a temperature T, or at an inverse temperature $\beta = (k_B T)^{-1}$. Let \hat{O}_A and \hat{O}_B be some local observables associated with two non overlapping regions A and B of the system. We define the two-point quantum correlation function (QCF) between A and B as follows:

$$\langle \delta \hat{O}_A \delta \hat{O}_B \rangle_Q = \langle \delta \hat{O}_A \delta \hat{O}_B \rangle - \frac{\partial \langle \hat{O}_A \rangle_{\lambda_B}}{\partial \lambda_B} \Big|_{\lambda_B = 0}$$

$$= \langle \delta \hat{O}_A \delta \hat{O}_B \rangle - \frac{1}{\beta} \int_0^\beta d\tau \langle \delta \hat{O}_A(\tau) \delta \hat{O}_B(0) \rangle .$$

$$(3.1)$$

Here $\langle ... \rangle = \text{Tr}(...\hat{\rho})$ denotes the thermal average, with $\hat{\rho} = e^{-\beta\hat{\mathcal{H}}}/\mathcal{Z}$ and $\mathcal{Z} = \text{Tr}(e^{-\beta\hat{\mathcal{H}}})$; $\delta\hat{O} = \hat{O} - \langle \hat{O} \rangle$ is the fluctuation with respect to the average; λ_B is a field coupling to \hat{O}_B via a term $-\lambda_B\hat{O}_B$ added to the Hamiltonian and $\langle ... \rangle_{\lambda_B} = \text{Tr}[...\hat{\rho}(\lambda_B)]$ with $\hat{\rho}(\lambda_B) = e^{-\beta(\hat{\mathcal{H}} - \lambda_B\hat{O}_B)}/\text{Tr}[e^{-\beta(\hat{\mathcal{H}} - \lambda_B\hat{O}_B)}]$;
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 $\hat{O}(\tau) = e^{\tau \hat{\mathcal{H}}} \hat{O} e^{-\tau \hat{\mathcal{H}}}$ is the imaginary-time-evolved operator. A simple physical example of this could be a two-site system with sites A and B where $\hat{O}_A = \hat{n}_A$, $\hat{O}_B = \hat{n}_B$ and $\lambda_B = \mu_B$ is a local chemical potential.

The QCF evaluates the difference between the conventional two-point correlation function (CF) involving the regions A and B, and the response function of region A upon perturbing region B with a field λ_B . In any classical system, these two quantities are identified via a fluctuation-dissipation relation [63], and therefore the QCF is identically zero. In a quantum system, the QCF is non-zero since, in general, both commutators $[\hat{O}_A, \hat{\mathcal{H}}]$ and $[\hat{O}_B, \hat{\mathcal{H}}]$ are non-vanishing. It is immediate to verify that if one of them vanishes, then the QCF vanishes. The QCF probes how the \hat{O}_A and \hat{O}_B are jointly incompatible with $\hat{\mathcal{H}}$, namely how the Heisenberg's uncertainties of \hat{O}_A and \hat{O}_B on eigenstates of $\hat{\mathcal{H}}$ correlate with each other. One may notice that the fact that both \hat{O}_A and \hat{O}_B possess quantum uncertainty is not sufficient to have a non-zero QCF. For example, for a Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B$, where A and B are two uncorrelated subsystems (namely $[\hat{\mathcal{H}}_A, \hat{\mathcal{H}}_B] = 0$), one can easily show that the QCF vanishes even if both $[\hat{O}_A, \hat{\mathcal{H}}_A]$ and $[\hat{O}_B, \hat{\mathcal{H}}_B]$ are non-zero. Correlations between the subsystems A and B are necessary in order to have a non-zero QCF.

It is interesting to explore the low (T = 0) and high $(T = \infty)$ temperature limits of the QCF. One would expect that the QCF coincides with the total CF at T = 0, where no thermal contribution is present, and that it vanishes at $T = \infty$, where quantum effects disappear. In the following we show that these expectations are matched.

Proving the coincidence of QCF and total CF at zero temperature amounts to proving that the imaginary-time correlation function, evaluated on the ground state of the system $\langle \delta \hat{O}_A(\tau) \delta \hat{O}_B(0) \rangle_0$, decreases to zero for $\tau \to \infty$. This is true if the integral

$$\left| \int_{0}^{\beta} d\tau \langle \delta \hat{O}_{A}(\tau) \delta \hat{O}_{B}(0) \rangle_{0} \right| \leq \int_{0}^{\beta} d\tau \left| \langle \delta \hat{O}_{A}(\tau) \delta \hat{O}_{B}(0) \rangle_{0} \right|$$
(3.2)

grows slowlier than linearly with β , so that it vanishes when divided by β . One can make use of the basis $|n\rangle$ of eigenstates of $\hat{\mathcal{H}}$ with eigenenergies E_n , and assume that the system admits a non-degenerate ground state $|0\rangle$. One has that

$$\left| \langle \delta \hat{O}_A(\tau) \delta \hat{O}_B(0) \rangle_0 \right| = \left| \sum_{n>0} \langle 0 | \delta \hat{O}_A | n \rangle \langle n | \delta \hat{O}_B | 0 \rangle e^{-\Delta E_n \tau} \right|$$

$$\leq \sum_{n>0} \left| \langle 0 | \delta \hat{O}_A | n \rangle \langle n | \delta \hat{O}_B | 0 \rangle \right| e^{-\Delta E_n \tau}, \tag{3.3}$$

where $\Delta E_n = E_n - E_0 > 0$, and the ground-state term disappears because $\langle 0|\delta \hat{O}_{A(B)}|0\rangle = 0$ by construction. Hence the imaginary-time correlation

function is a sum of exponentially decreasing terms, and it decreases to zero in the limit $\tau \to \infty$, thus proving what announced previously. We deliberately assumed that the ground state is unique, since the case of a degenerate ground state is somehow pathological. Anyway, in the hypothetic case of a degenerate ground state, one could lift the degeneracy with an infinitesimal perturbation, and remark that the identity between quantum and total correlation function at T = 0 is completely independent of the perturbation.

In the opposite limit of $T = \infty$ one can expand the exponentials $e^{\pm \tau \mathcal{H}}$ and easily show that the QCF, as expected, vanishes.

3.2 Hamiltonian separability

According to the previously mentioned Werner's definition [26] a state is defined as separable (or classically correlated) if its density matrix can be written as

$$\hat{\rho} = \sum_{s} p_s \hat{\rho}_A^{(s)} \otimes \hat{\rho}_B^{(s)}, \qquad (3.4)$$

where p_s is a normalized, classical distribution function weighing different factorized forms for $\hat{\rho}$. In general, owing to the semi-positive definiteness of density operators, we can always write them as exponential of (effective) Hamiltonian operators:

$$\hat{\rho} = e^{-\beta\hat{\mathcal{H}}} = \sum_{s} p_s \ e^{-\beta\hat{\mathcal{H}}_A^{(s)}} \otimes e^{-\beta\hat{\mathcal{H}}_B^{(s)}}$$
(3.5)

where $\hat{\tilde{\mathcal{H}}} = \hat{\mathcal{H}} - \ln \mathcal{Z}$. In order to calculate the QCF, it is necessary to know explicitly how the density matrix is deformed upon applying a field term, namely upon shifting the Hamiltonian $\hat{\tilde{\mathcal{H}}}$ by $-\lambda_A \hat{O}_A - \lambda_B \hat{O}_B$. This invites us to restrict the concept of separability – see Fig. 3.1 – to that of *Hamiltonian* separability, namely to interpret $\hat{\mathcal{H}}_{A(B)}^{(s)}$ as physical Hamiltonians which are affected linearly by the corresponding field terms. Hence we shall say that a separable density matrix $\hat{\rho}$ (as in Eq. (3.5)) is Hamiltonian-separable if

$$\hat{\rho}(\lambda_A, \lambda_B) = e^{-\beta(\hat{\mathcal{H}} - \lambda_A \hat{O}_A - \lambda_B \hat{O}_B)}$$

=
$$\sum_s p_s \ e^{-\beta(\hat{\mathcal{H}}_A^{(s)} - \lambda_A \hat{O}_A)} \otimes e^{-\beta(\hat{\mathcal{H}}_B^{(s)} - \lambda_B \hat{O}_B)} .$$
(3.6)

(notice that $\hat{\rho}(\lambda_A, \lambda_B)$ has no longer a unit trace). Physically, Hamiltonianseparability amounts to imagining that – as sketched in Fig. 3.1 – A and Bare physical systems individually in thermal equilibrium states with Hamiltonians $\hat{\mathcal{H}}_{A(B)}^{(s)}$, and both coupled to a source of classical noise – namely a



Figure 3.1: (a) Hamiltonian-separable states are a subset of separable states: ruling out Hamiltonian separability does not prove entanglement. (b) A quantum Hamiltonian acting coherently on the subsystems A and B correlates quantum mechanically the uncertainties on the local observables \hat{O}_A and \hat{O}_B , generating a non-vanishing quantum correlation function; (c) The opposite scenario is the one in which the two subsystems are locally in an equilibrium state governed by two separated Hamiltonians, correlated to a common classical noise source; in this case the quantum correlation function $\langle \delta \hat{O}_A \delta \hat{O}_B \rangle_Q$ vanishes identically; (d) When two sites *i* and *j* of a lattice system are separated by a distance far exceeding the quantum coherence length ξ_Q , the sites in between mediate their correlations in a similar way as a classical statistical field coupling the two sites.

classical statistical field – whose configurations are parametrized by the parameter s, and which correlate A and B in a classical sense. We can make the following statement:

Theorem: A non-zero QCF, $\langle \delta \hat{O}_A \delta \hat{O}_B \rangle_Q \neq 0$, for some observables \hat{O}_A and \hat{O}_B implies that A and B are not Hamiltonian-separable.

Proof: Considering a Hamiltonian-separable density matrix for subsystems A and B, $\hat{\rho}(\lambda_A, \lambda_B)$ as in Eq. (3.5), and the corresponding partition function $\mathcal{Z}(\lambda_A, \lambda_B) = \text{Tr}[\hat{\rho}(\lambda_A, \lambda_B)]$, we have that

$$\frac{\partial \langle \hat{O}_A \rangle}{\partial \lambda_B} \Big|_{\lambda_B = 0} = \frac{1}{\mathcal{Z}(0,0)} \sum_s p_s \operatorname{Tr}_A \{ \hat{O}_A e^{-\beta \hat{\mathcal{H}}_A^{(s)}} \} \frac{\partial}{\partial \lambda_B} \operatorname{Tr}_B \{ e^{-\beta (\hat{\mathcal{H}}_B^{(s)} - \lambda_B \hat{O}_B)} \} \Big|_{\lambda_B = 0} - \langle \hat{O}_A \rangle \frac{1}{\mathcal{Z}(0,0)} \frac{\partial \mathcal{Z}(0,\lambda_B)}{\partial \lambda_B} \Big|_{\lambda_B = 0} = \langle \hat{O}_A \hat{O}_B \rangle - \langle \hat{O}_A \rangle \langle \hat{O}_B \rangle .$$
(3.7)

As a consequence, Hamiltonian separability implies the vanishing of all QCFs $\langle \delta \hat{O}_A \delta \hat{O}_B \rangle_Q$, and the presence of at least one non-vanishing QCF negates Hamiltonian separability. \Box

Therefore, finding a finite QCF rules out that the correlations between the fluctuations of local observables \hat{O}_A and \hat{O}_B are generated purely by correlated classical noise. Disproving Hamiltonian separability does not imply disproving the most general form of separability in Eq. (3.4) – see Fig. 3.1 – which would be equivalent to proving entanglement, and which remains a challenging task. Nonetheless the absence of Hamiltonian separability is tightly related to the existence of some form of quantum correlations. As a final remark we observe that the above result is not limited to bipartitions of the system, but it applies to A and B being any two subsystems in arbitrary multi-partitions of the total system.

3.2.1 An example of Hamiltonian inseparability

We find it instructive to show an example of a non Hamiltonian separable system and of its Hamiltonian separable version.

We consider a two-mode bosonic system, equivalent to a two site Bose-Hubbard model, with Hamiltonian

$$\hat{\mathcal{H}} = -J(\hat{b}_A^{\dagger}\hat{b}_B + \text{h.c.}) + U(\hat{b}_A^{\dagger})^2\hat{b}_A^2 + U(\hat{b}_B^{\dagger})^2\hat{b}_B^2$$
(3.8)

containing a hopping term (J) and a repulsion (U) term. In this system the field correlations $\langle \hat{b}_A^{\dagger} \hat{b}_B \rangle$ have a non-zero quantum component $\langle \hat{b}_A^{\dagger} \hat{b}_B \rangle_Q$ determined by the hopping term, and the density matrix is not Hamiltonian separable, once again because of the hopping term.

The Hamiltonian-separable version of this system would have a Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B$, where

$$\hat{\mathcal{H}}_{A}(\Psi, \Psi^{*}) = -(\Psi^{*}\hat{b}_{A} + \text{h.c.}) + U(\hat{b}_{A}^{\dagger})^{2}\hat{b}_{A}^{2}
\hat{\mathcal{H}}_{B}(\Psi, \Psi^{*}) = -(\Psi^{*}\hat{b}_{B} + \text{h.c.}) + U(\hat{b}_{B}^{\dagger})^{2}\hat{b}_{B}^{2}$$
(3.9)

are dependent on a complex classical field $\Psi,$ and a corresponding density operator

$$\hat{\rho} = \frac{1}{\mathcal{Z}} \int \frac{d\Psi d\Psi^*}{2\pi i} P(\Psi, \Psi^*) \ e^{-\beta \hat{\mathcal{H}}_A} \otimes e^{-\beta \hat{\mathcal{H}}_B} \ . \tag{3.10}$$

In this case the field correlations $\langle \hat{b}_A^{\dagger} \hat{b}_B \rangle$ are induced uniquely by the classical field term, and do not admit a quantum part, namely $\langle \hat{b}_A^{\dagger} \hat{b}_B \rangle_Q = 0$. Indeed, introducing the notation

$$\langle \hat{b}_{A(B)} \rangle_{\Psi} = \operatorname{Tr} \left[\hat{b}_{A(B)} e^{-\beta \hat{\mathcal{H}}_{A(B)}(\Psi, \Psi^*)} \right]$$
(3.11)

one has that

$$\langle \hat{b}_A^{\dagger} \hat{b}_B \rangle = \frac{1}{\mathcal{Z}} \int \frac{d\Psi d\Psi^*}{2\pi i} P(\Psi, \Psi^*) \langle \hat{b}_A^{\dagger} \rangle_{\Psi} \langle \hat{b}_B \rangle_{\Psi} \neq 0.$$
(3.12)

Even if the averages $\langle \hat{b}_A^{\dagger} \hat{b}_B \rangle_{\Psi}$ factorize, correlations do exist between the average values $\langle \hat{b}_{A(B)} \rangle_{\Psi}$ via the common coupling to the Ψ field. On the other hand, quantum correlations vanish as a consequence of the theorem discussed in the previous section.

3.3 Quantum coherence length

The QCF of any observable is readily accessible to analytical and numerical computations for all models which admit an efficient calculation of the correlation and response functions. Here we exploit this property to explicitly calculate the QCF for Bose fields in two very different regimes of the two-dimensional Bose-Hubbard model, of which we recall the Hamiltonian

$$\hat{\mathcal{H}} = -J \sum_{\langle ij \rangle} \left(\hat{b}_i^{\dagger} \hat{b}_j + \text{h.c.} \right) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i . \qquad (3.13)$$

One regime shall be that of hard-core bosons, which we have already introduced in Sec. 2.1 and which is described by a Hamiltonian

$$\hat{\mathcal{H}} = -J \sum_{\langle ij \rangle} (\hat{a}_i^{\dagger} \hat{a}_j + \text{h.c.}) - \mu \sum_i \hat{n}_i , \qquad (3.14)$$

with $\hat{a}_i^{(\dagger)}$ bosonic operators for hard-core bosons, and the other one that of quantum rotors. The latter model is best understood rewriting Eq. (3.13) (up to an additive constant) as

$$\hat{\mathcal{H}} = -J \sum_{\langle ij \rangle} (\hat{b}_i^{\dagger} \hat{b}_j + \text{h.c.}) + \frac{U}{2} \sum_i (\hat{n}_i - \nu)^2 , \qquad (3.15)$$

where $\nu = \mu/U + 1/2$ is the average density. Taking ν to be an integer $\delta \hat{n}_i = \hat{n}_i - \nu$ can be considered as being an angular momentum operator canonically conjugated to a phase operator $\hat{\theta}_i$ with commutation relations $[\hat{\theta}_i, \delta \hat{n}_i] = i$, so that $\delta \hat{n}_i = -i \frac{\partial}{\partial \theta_i}$. Moreover, in the limit of very large average filling, $\nu \gg 1$, one can adopt a phase-number decomposition of the Bose operator, $\hat{b}_i \approx e^{i\hat{\theta}_i}\sqrt{\hat{n}_i}$, and neglect number fluctuations in the hopping term of Eq. (3.15), $\hat{b}_i \approx \sqrt{\nu} e^{i\hat{\theta}_i}$. This then leads to the quantum-rotor Hamiltonian

$$\hat{\mathcal{H}}_{QR} = -2J\nu \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) - \frac{U}{2} \sum_i \frac{\partial^2}{\partial \theta_i^2} , \qquad (3.16)$$

where we have dropped the operator notation for θ_i , as we are now working in an explicit phase representation of the Hamiltonian.

In both cases, we probe the first-order total correlation function $g(i, j) = \langle \hat{c}_i^{\dagger} \hat{c}_j \rangle$ and the first-order QCF

$$g_Q(i,j) = \langle \hat{c}_i^{\dagger} \hat{c}_j \rangle_Q = \langle \hat{c}_i^{\dagger} \hat{c}_j \rangle - \frac{1}{\beta} \int d\tau \langle \hat{c}_i^{\dagger}(\tau) \hat{c}_j(0) \rangle$$
(3.17)

for the Bose field, where $\hat{c}_i = \hat{a}_i$ for hard-core bosons and $\hat{c}_i = e^{i\theta_i}$ for quantum rotors (we normalized the field operator by $\sqrt{\bar{n}}$). Since first-order

correlations are the dominant ones in the above models, one may naturally expect that the first-order QCF are also the dominant ones among all QCFs. This was explicitly verified in our numerical simulations in the case of hardcore bosons, by comparing with the second-order, or density-density QCF, $\langle \delta \hat{n}_i \delta \hat{n}_j \rangle_Q$. We calculated the first order QCF for hard-core bosons using quantum Monte Carlo (here in the Stochastic Series expansion formulation [42, 43, 44]), and for quantum rotors using path-integral Monte Carlo [64, 65], making use in both cases of a code developed by T. Roscilde.

Figs. 3.2(a-b) show the total first-order QCF in the superfluid phase of hard-core bosons and quantum rotors as a function of temperature. We notice that, in both cases, the QCF lays orders of magnitudes below the total correlation function g(i, j) down to very low temperatures. Most importantly, it decays *exponentially* at *all* finite temperatures, revealing the existence of a characteristic quantum coherence length ξ_Q which is completely insensitive to the divergent correlation length associated with the superfluid phase.

Figs. 3.2(c-d) show the temperature dependence of the quantum coherence length ξ_Q in both models. Data were extracted from the integrated Lorentzian width of the k = 0 peak of the "quantum momentum distribution" $n_Q(\mathbf{k}) = \frac{1}{L^2} \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} g_Q(i,j)$. The figures clearly show a divergence of ξ_Q upon lowering the temperature, but its asymptotic temperature dependence, while presumed to follow a power law ($\xi_Q \sim T^{-\alpha}$) is difficult to extract from the numerics: one can clearly observe crossovers between at least two temperature behaviors with $\alpha = 1/2$ and 1. The temperature behavior in the thermodynamic limit can be predicted analytically on the basis of spin-wave theory, which gives $\xi_Q \sim T^{-1}$ [66].

The quantum coherence length sets the characteristic scale beyond which two subsystems can be considered as nearly Hamiltonian-separable – in explicit physical terms, when $g_Q(i,j) \ll 1$, the correlations between the two points *i* and *j* could have been prepared by coupling two independent subsystems (containing sites *i* and *j* respectively) to the same source of classical noise. Obviously this source does not exist physically, but one can consider the degrees of freedom spatially separating the sites *i* and *j* as the effective "classical bus" for correlations among the two sites – classical because the distance between *i* and *j* exceeds the quantum coherence length (see Fig. 3.1(c)).

A few other criteria for separability have been recently introduced for lattice systems based on the quantum Fisher information [67, 68], skew information [69] and quantum variance [70] of a collective observable. In the following paragraph we verify the consistency of the QCF-based method with these other approaches.



Figure 3.2: Upper panels. Quantum correlation function g_Q of Bose fields for (a) hard-core bosons with L = 64 and different temperatures $t = k_B T/J$; (b) quantum rotors with $u = U/(2J\bar{n}) = 1$, L = 32 and different temperatures $t = k_B T/(2J\bar{n})$. The g_Q function is compared to the total correlations g(r). Here r is the short-hand notation for (r, 0). Solid lines are exponential fits $A'e^{-d(x|L)/\xi_Q}d(x|L)^{-\eta'}$ for g_Q , where $d(x|L) = (L/\pi)\sin(\pi x/L)$ is the cord length. All data refer to the superfluid phase. Lower panels. Quantum coherence length ξ_Q vs. temperature for (c) hard-core bosons; (d) quantum rotors with u = 1. The solid and dashed lines indicate t^{-1} and $t^{-1/2}$ power laws.

3.4 Quantum variance of a collective observable

In the following we briefly introduce quantum variance (QV) for a collective observable [70] and show how it defines an "inseparability length" expressing the minimal linear size of clusters into which the density matrix can be effectively separated. We calculate this length for hard-core bosons on a square lattice and compare the result to that obtained for the quantum coherence length. This comparison would also indirectly account for a comparison to the aforementioned Quantum Fisher Information and Skew Information, to which QV represents a tight lower bound.

3.4.1 Definition of quantum variance

Given a generic operator \hat{O} , its quantum variance on a generic thermal state $\hat{\rho}$ is defined as

$$\langle \delta^2 \hat{O} \rangle_Q = \langle \hat{O}^2 \rangle - \frac{1}{\beta} \int_0^\beta d\tau \ \langle \hat{O}(\tau) \hat{O}(0) \rangle \ , \tag{3.18}$$

and it is such that $\langle \delta^2 \hat{O} \rangle_Q \leq \langle \delta^2 \hat{O} \rangle = \langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2$ [70].

In the following we shall focus on a collective operator $\hat{O} = \sum_i \hat{o}_i$, which is the sum of local operators \hat{o}_i with a bounded spectrum in $[o_{\min}, o_{\max}]$. For such an operator the QV represents the integral of the QCF $\langle \delta \hat{o}_i \delta \hat{o}_j \rangle_Q$. We consider a state $\hat{\rho}$ which can be separated into clusters of size p (or p-separable), namely which admits the separable form

$$\hat{\rho} = \sum_{s} p_s \otimes_c \hat{\rho}_c^{(s)} \tag{3.19}$$

where $\hat{\rho}_c^{(s)}$ is the density matrix for a single cluster. For such a state $\langle \delta^2 \hat{O} \rangle_Q$ is upper-bounded as

$$\langle \delta^2 \hat{O} \rangle_Q \leq \sum_s p_s \sum_c \langle \delta^2 \hat{O}_c \rangle_{Q,s}$$

$$\leq \sum_s p_s \sum_c \langle \delta^2 \hat{O}_c \rangle_s ,$$
 (3.20)

where $(\langle \delta^2 \hat{O}_c \rangle_{Q,s}) \langle \delta^2 \hat{O}_c \rangle_s$ is the (quantum) variance of the cluster operator $\hat{O}_c = \sum_{i \in c} \hat{o}_i$. Considering a partition of the system of total size N into identical clusters of size p (such that N/p is an integer), one can show that the variance of the observable \hat{O}_c is easily upper-bounded using a bimodal distribution for the observable \hat{O}_c with values po_{max} and po_{min} both having probability 1/2 [70], which gives

$$\langle \delta^2 \hat{O}_c \rangle \le \frac{p^2}{4} (o_{\max} - o_{\min})^2 .$$
 (3.21)

As a consequence, for all *p*-separable states, the QV satisfies the bound:

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$$\langle \delta^2 \hat{O} \rangle_Q \le \frac{Np}{4} \left(o_{\max} - o_{\min} \right)^2 \,. \tag{3.22}$$

This bound is obviously a necessary but not sufficient condition for *p*-separability, namely states which are not *p*-separable but are p'-separable with p' > p (up to $p' = \infty$) may still comply with the bound.

As a consequence of the bound given above, one could use the quantum variance as a witness of entanglement. Given a thermal state with quantum variance $\langle \delta^2 \hat{O} \rangle_Q$, in order to approximate it with a *p*-separable state one needs to use clusters with *p* at least taking the value which saturates the bound of Eq. (3.22), namely $p \geq p_{\min} = 4 \langle \delta^2 \hat{O} \rangle_Q / [N(o_{\max} - o_{\min})^2]$. Hence the quantum variance witnesses entanglement among at least p_{\min} sites. Considering then the local observables \hat{o}_i with unit spectral width, $\Delta o = o_{\max} - o_{\min} = 1$, which maximize the quantum variance of the corresponding collective observable \hat{O} among all collective observables, for a *d*-dimensional system one can define an *inseparability length* l_I as

$$l_I = \left[\frac{4}{N} \sup_{\hat{O}:\Delta o = 1} \langle \delta^2 \hat{O} \rangle_Q \right]^{1/d} . \tag{3.23}$$

This length indicates the minimal linear size of clusters building a separable state of the kind of Eq. (3.19), which is compatible with the maximum quantum variance of collective observables. It is therefore to be considered as a lower bound to the length beyond which two subsystems can be considered as effectively separable in the state of the system. Hence it is meaningful to compare it to the quantum coherence length ξ_Q , which is the natural (Hamiltonian-)separability length, and to which l_I may be expected to act as a lower bound.

3.4.2 Quantum variance vs quantum coherence length

The length l_I can be easily calculated both in the case of hard-core bosons and of quantum rotors. One can maximize the quantum variance of a collective observable with $\Delta o = 1$ by considering: 1) for hard-core bosons, $\hat{o}_i = (\hat{a}_i + \hat{a}_i^{\dagger})/2$; 2) for quantum rotors, $\hat{o}_i = [\cos(\theta_i) + \sin(\theta_i)/(2\sqrt{2})]$. In both cases the quantum correlation function $\langle \hat{o}_i \hat{o}_j \rangle_Q = g_Q(i,j)/2$ (for hard-core bosons) and $\langle \hat{o}_i \hat{o}_j \rangle_Q = g_Q(i,j)/8$ (quantum rotors). As a consequence, the corresponding quantum variance is related to the k = 0 peak in the "quantum momentum distribution" $n_Q(\mathbf{k}) = \frac{1}{L^2} \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r_i}-\mathbf{r_j})}g_Q(i,j)$, namely $\langle \delta^2 \hat{O} \rangle_Q = Nn_Q(0)/2$ (hard-core bosons at half filling) and $\langle \delta^2 \hat{O} \rangle_Q =$ $Nn_Q(0)/8$ (quantum rotors). Given that the $g_Q(i,j)$ is the dominant quantum correlation function, and it is positive definite, the quantum momen-



Figure 3.3: Quantum coherence length ξ_Q and inseparability length l_I vs. temperature for (a) hard-core bosons; (b) quantum rotors with u = 1. The solid and dashed lines indicate t^{-1} and $t^{-1/2}$ power laws.

tum distribution, which is its integral, will give the dominant quantum variance among all observables, as requested in Eq. (3.23). This defines the inseparability lengths $l_I = \sqrt{2n_Q(k=0)}$ for hard-core bosons and $l_I = \sqrt{n_Q(k=0)/2}$ for quantum rotors, which can be extracted from Monte Carlo simulations. The results for the two models are shown in Fig. 3.3, where they are compared to the data previously shown for the quantum coherence length. As expected, l_I proves to be a lower bound to the ξ_Q . The two lengths show a similar temperature dependence, thus supporting the interpretation of ξ_Q as the characteristic length scale beyond which two subsystems can be considered as nearly (Hamiltonian)-separable.

One can also try to establish a scaling relationship between the two lengths l_I and ξ_Q . Indeed, one can expect the quantum correlation function to decay as:

$$g_Q(r) \sim \frac{e^{-r/\xi_Q}}{r^{d-2+\tilde{\eta}}} \tag{3.24}$$

(which is verified by the fits of the numerical data in Fig. 3.3). Therefore, integrating $g_Q(r)$ one obtains

$$n_Q(k=0) \sim \int_a^\infty dr \ r^{d-1} g_Q(r) \sim \xi_Q^{2-\tilde{\eta}} \int_{a/\xi_Q}^\infty dx \frac{e^{-x}}{x^{\tilde{\eta}-1}}$$
(3.25)

where a is the lattice spacing. Under the assumption that $\xi_Q/a \gg 1$, the

integral loses its dependence on ξ_Q , and hence one obtains the scaling relation

$$l_I \sim [n_Q(\mathbf{k}=0)]^{1/d} \sim \xi_Q^{\frac{2-\tilde{\eta}}{d}}.$$
 (3.26)

The temperature dependence of the two lengths is generically different unless $\phi = (2 - \tilde{\eta})/d = 1$. The data in Fig. 3.3(a-b) suggest that, for the models of interest, $1/2 \leq \phi \leq 1$ in the low-temperature regime of $\xi_Q/a \ll 1$. In general one can expect that $\phi \leq 1$, so that the inequality $l_I \leq \xi_Q$ holds for $T \to 0$, where both quantities diverge.

3.5 Quantum discord

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The QCF that we introduced in this chapter captures an essential form of quantum correlation between local observables belonging to distinct subsystems of an extended quantum system in thermal equilibrium. An alternative definition of quantum correlations has been given using quantum discord (QD) [30, 71, 72], which is an observable-independent quantity that expresses to what extent a density matrix violates an identity valid for classical, joint probability distributions of several variables. In the following we briefly introduce QD and then draw a comparison to our definition of QCF, in the case of hard-core bosons.

3.5.1 Definition of quantum discord

Let us take two sites *i* and *j* in the lattice, and define the reduced density matrices $\hat{\rho}_i$, $\hat{\rho}_j$ and $\hat{\rho}_{ij}$ for the single sites *i* and *j*, and for the two-site compound *ij*, respectively. The total amount of correlations (of classical *and* quantum origin) among the two sites is generally expressed via the mutual information

$$I(i,j) = S(\hat{\rho}_i) + S(\hat{\rho}_j) - S(\hat{\rho}_{ij})$$
(3.27)

where $S(\hat{\rho}) = -\text{Tr}(\hat{\rho} \log_2 \hat{\rho})$ is the von Neumann entropy. [27] The mutual information expresses the "missing" entropy in the compound state due to correlations in the fluctuations: namely, there exists information on *i* which can be gained by making observations on *j*, and vice-versa. Indeed $S(\hat{\rho}_{ij}|\hat{\rho}_j) = S(\hat{\rho}_{ij}) - S(\hat{\rho}_j)$ is the entropy of *ij* conditioned on the knowledge of the state of *j*, and the fact that this entropy is less than that of $\hat{\rho}_i$ (ignoring completely *j*) implies the existence of correlations between *i* and *j*, which provide information on *i* when measuring *j*.

This observation invites to analyze the density matrix conditioned on measurements on site j. Considering the local observable \hat{O}_j on site j with eigenvalues $o_k^{(j)}$ and projectors $\mathcal{P}_k^{(j)}$ on the associated eigenspaces, one can define the compound density matrix of sites ij conditioned upon the outcome

3.5. QUANTUM DISCORD

 $o_k^{(j)}$ of the measurement of the observable \hat{O}_j as

$$\hat{\rho}_{ij,k} = \frac{1}{p_k} \left(\mathbb{I}_i \otimes \mathcal{P}_k^{(j)} \right) \ \hat{\rho}_{ij} \ \left(\mathbb{I}_i \otimes \mathcal{P}_k^{(j)} \right), \tag{3.28}$$

where $p_k = \text{Tr}\left[\left(\mathbb{I}_i \otimes \mathcal{P}_k^{(j)}\right) \hat{\rho}\left(\mathbb{I}_i \otimes \mathcal{P}_k^{(j)}\right)\right]$ [27]. The compound entropy conditioned on the measurement of the observable \hat{O}_j , and averaged on all possible outcomes of the measurement, can be therefore expressed as

$$S(\hat{\rho}_{ij}|\hat{O}_j) = \sum_k p_k S(\hat{\rho}_{ij,k}) , \qquad (3.29)$$

which expresses the average entropy that the system has after a measurement of the observable \hat{O}_j – averaged over all the possible outcomes of the measurement, with their *a priori* probabilities p_k . In a classical system the p_k would be the statistical weights of the configurations of site j, and therefore Eq. (3.29) would represent the entropy of ij conditioned upon the knowledge of j, $S(\hat{\rho}_{ij}|\hat{\rho}_j)$. In a quantum-mechanical system, this is no longer the case, because measurements on j not only give information on i, but also perturb its state. The amount by which measurements on j perturb i is then quantified by the quantum discord

$$D(i,j) = I(i,j) - C(i,j)$$
(3.30)

where

$$C(i,j) = S(\hat{\rho}_i) - \min_{\hat{O}_i} S(\hat{\rho}_{ij} | \hat{O}_j)$$

$$(3.31)$$

expresses the (so-called) "classical" correlations, namely the maximum amount of information that can be gained on i by making measurements on j. The function D(i, j) captures the fundamental discrepancy (or "discord") between the entropy associated with the correlations among sites i and j, and the maximal information that one can gain on i by making projective measurements on j: the latter does not saturate the former because local measurements disturb the state and they reduce correlations between i and j.

In summary, seen as a generalized correlation function, D(i, j) probes how much a measurement on *i* can affect the state of *j*. Even for states in which two subsystems are separable, the measurement on one system can affect the state of the other (this is true when the factorized density matrices $\hat{\rho}_{A(B)}^{(s)}$ in the separable form do not commute with each other). Hence quantum discord can be non-zero even in the presence of separability.

3.5.2 Quantum discord vs quantum correlation function

Quantifying discord for generic degrees of freedom is in general a hard problem, due to the maximization operation implied in Eq. (3.31), but a quantitative comparison between QCF and QD is possible in the case of hard-core



Figure 3.4: (a) Comparison between QCF and QD. (b) Zero-momentum peak in the total and "quantum" momentum distribution for 2d hard-core bosons. Full symbols refer to $n_Q(k=0)$, while open ones to n(k=0).

bosons. According to Refs. [73, 74] in the limit $|\mathbf{r}_i - \mathbf{r}_j| \to \infty$, QD takes the form

$$D(i,j) \approx (C_1^2 + C_2^2)/(2\log 2)$$
 (3.32)

with $C_1 = g(i, j)/2$ and $C_2 = \langle \hat{n}_i \hat{n}_j \rangle - \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle$. Therefore the quantum discord, being asymptotically proportional to the square of the correlation functions, has their exact same range – as was already discussed in Ref. [75] in a variety of different models. For 2d hard-core bosons the two-point QD decays algebraically throughout the superfluid phase and exponentially only in the normal phase, in a similar way as ordinary correlations do – and it is singular at the BKT transition, even though this transition is uniquely driven by thermal fluctuations and quantum fluctuations and correlations are not supposed to exhibit singularities at thermal phase transitions. This is to be contrasted with the QCF, not bearing any signature of the BKT transition and decaying exponentially at all finite temperatures.

These observations are supported by the plots shown in Fig. 3.4. Fig. 3.4(a) shows that the "quantum" momentum distribution $n_Q(k = 0)$, namely the integral of the quantum correlation function, does not exhibit any singularity at the BKT transition of hard-core bosons (occurring for $t = k_B T/J \approx 0.685$ [76]). On the other hand, at the BKT critical temperature the integral of the total correlations, n(k = 0), exhibits a well-known divergence. Fig. 3.4(b) shows a comparison between the QD and the QCF in the superfluid phase of hard-core bosons. The QCF, as already observed in the previous plots, decays exponentially, whereas the QD decays algebraically.

The dramatic difference between QD and QCF, and the sensitivity of QD to classical critical phenomena, suggest that the notion of quantum correlations attributed to QD should be critically re-examined. The sensitivity of the two-point QD to ordinary correlations can be simply traced back to

its definition in terms of the reduced two-point density matrix $\hat{\rho}_{ij}$ which is in turn fully expressed through correlation functions. On the other hand, the QCF depends on the reduced density matrix and its deformation upon applying a field at site *i* (or *j*). As a consequence the QCF provides information beyond that contained in ordinary correlations and in the two-point QD.

Chapter 4

Quantum mean-field approximation

In this chapter we introduce an approach to lattice systems that we name quantum mean-field (QMF) approximation, or cluster QMF (cQMF), in its most general cluster version. This latter relies on the findings of our previous chapter, and in particular on the different spatial structure found for thermal and quantum correlations, which permits to develop an approximation that affects quantum correlations only, thus preserving a full description of thermal correlations. In the following we develop the formalism of cMF, using a path-integral approach, and we show numerical results for two-dimensional quantum rotors, which already served as a test model in the previous chapter.

4.1 Path-integral approach for lattice bosons

In this section we introduce the coherent-state path-integral approach to the partition function, which will be the reference formalism throughout the remaining chapters. Let us consider once again a Bose-Hubbard Hamiltonian

$$\hat{\mathcal{H}} = \sum_{i \neq j} \left[J_{ij} \hat{b}_i^{\dagger} \hat{b}_j + \frac{V_{ij}}{2} \hat{n}_i \hat{n}_j \right] + \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right] , \qquad (4.1)$$

to which we also added a term (V_{ij}) for interactions between different sites. More general models (including spin degrees of freedom, non-abelian gauge fields, etc.) can also be treated similarly, but we keep working with our usual spinless Bose-Hubbard model for the sake of simplicity in the exposition.

We can now introduce the path-integral expression of the partition function in terms of coherent bosonic states. These states represent the eigenstates $\hat{b}_i |\phi\rangle = \phi |\phi\rangle$ of the bosonic operators, form an over-complete nonorthonormal basis of the Hilbert space and satisfy a completeness relation $\int \frac{d\phi^* d\phi}{2\pi i} e^{\phi^* \phi} |\phi\rangle \langle \phi| = 1$. They consent to express the partition function of the system as [14, 77, 78]

$$\mathcal{Z} = \int \mathcal{D}[\{\phi_i(\tau)\}] \ e^{-S[\{\phi_i(\tau)\}]} , \qquad (4.2)$$

where

$$S[\{\phi_i(\tau)\}] = \int_0^\beta d\tau \left[\sum_i \phi_i^*(\tau) \frac{\partial}{\partial \tau} \phi_i(\tau) + \hat{\mathcal{H}}(\{\phi_i(\tau), \phi_i^*(\tau)\})\right] , \quad (4.3)$$

$$\hat{\mathcal{H}}(\{\phi_i(\tau), \phi_i^*(\tau)\}) = - \int_0^\beta d\tau \sum_{i \neq j} \left[\phi_i^*(\tau) J_{ij} \phi_j(\tau) + |\phi_i(\tau)|^2 \frac{V_{ij}}{2} |\phi_j(\tau)|^2\right] \\ + \sum_i \left[\frac{U}{2} |\phi_i(\tau)|^4 - \mu |\phi_i(\tau)|^2\right], \qquad (4.4)$$

where $S[\{\phi_i(\tau)\}]$ is the Euclidean action for the complex field $\phi_i(\tau)$ dependent on imaginary time $\tau \in [0,\beta]$ where $\beta = (k_B T)^{-1}$. We would like to stress the fact that the coupling terms among different sites in Eq. (4.3) are uniquely contained in $\hat{\mathcal{H}}$, and they are therefore completely *local* in imaginary time. This observation will be very important in the following.

4.2 From cluster-mean-field states to cluster-separable states

In Sec. 2.3 we presented a cluster mean-field approach to lattice systems based on a factorized Ansatz for the density matrix. In this paragraph we briefly reformulate it in the language of path-integral and then introduce a new approach, which stems from a more general Ansatz for the density matrix.

4.2.1 Cluster mean field

Cluster mean field assumes a factorized density matrix

$$\hat{\rho}_{\rm cMF} = \otimes_c \hat{\rho}_c \ , \tag{4.5}$$

which has a partition function in the form

$$\mathcal{Z}_{\rm cMF} = \prod_{c} \mathcal{Z}_{c} \tag{4.6}$$

where

$$\mathcal{Z}_c = \int \mathcal{D}[\{\phi_{i\in c}(\tau)\}] \ e^{-S_c^{(\mathrm{MF})}}$$
(4.7)

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and

$$S_{c}^{(\mathrm{MF})}[\{\phi_{i\in c}(\tau)\}] = \int d\tau \ \hat{\mathcal{H}}_{c}(\{\phi_{i\in c}(\tau), \phi_{i\in c}^{*}(\tau)\})$$
$$+ \int d\tau \sum_{i\in c, j\notin c} \left[-\left(J_{ij}\phi_{i}^{*}(\tau)\langle\hat{b}_{j}\rangle + \mathrm{c.c.}\right) + V_{ij}n_{i}(\tau)\langle\hat{n}_{j}\rangle \right]$$
$$- \frac{\beta}{2} \sum_{i\in c, j\notin c} \left[-\left(J_{ij}\langle\hat{b}_{i}^{\dagger}\rangle\langle\hat{b}_{j}\rangle + \mathrm{c.c.}\right) + V_{ij}\langle\hat{n}_{i}\rangle\langle\hat{n}_{j}\rangle \right]$$
(4.8)

where we have introduced the notation $n_i(\tau) =: |\phi_i(\tau)|^2$ and $\hat{\mathcal{H}}_c$ denotes a Hamiltonian of the form Eq. (4.4) restricted to sites belonging to the same cluster c. Here $\langle ... \rangle$ indicates the thermal average, to be calculated self-consistently using the partition function in the form of Eq. (4.6).

Both Eq. (4.5) and Eq. (4.6) show how the cMF approach retains the quantum nature of the bosonic field, as well as its correlations within each cluster, but discards correlations of all forms between clusters. This results in neglecting long-wavelengths fluctuations and prevents a correct description of critical phenomena below the upper critical dimension

4.2.2 Incorporating classical correlations into cMF

On the basis of the observations made in Sec. 3.2, classical correlations can be included in the cMF Ansatz for the density matrix, by promoting Eq. (4.5) to the most general separable form

$$\hat{\rho}_{\rm sep} = \sum_{\{\Psi\}} p(\{\Psi\}) \ [\otimes_c \hat{\rho}_c(\{\Psi\})] , \qquad (4.9)$$

where $\{\Psi\}$ is a set of (possibly continuous) variables parameterizing the form of the cluster density matrix $\hat{\rho}_c(\{\Psi\})$, and $p(\{\Psi\}) \geq 0$ is the probability of the associated factorized form [26]. It is important to notice that the temperature is contained in the functional form of both $\hat{\rho}_c$ and p. A variational optimization of Eq. (4.9) to minimize the free energy is essentially impossible, given the extreme freedom of the function $p(\{\Psi\})$. In the following section we show how an approximation that we will name quantum meanfield (QMF) provides an explicit educated Ansatz for the density matrix of a bosonic lattice model in the form of Eq. (4.9).

4.3 Quantum mean-field approximation

Let us consider the partition function as introduced in Sec. 4.1 in the pathintegral formalism. The hopping and off-site potential terms, coupling sites together in the action Eq. (4.3), as we observed previously, are fully *local* in imaginary time. The QMF approximation consists in treating them as completely non-local, namely imagining that full connectivity exists along the imaginary-time dimension, namely an all-to-all coupling – see Fig. 4.1 for a cartoon. In terms of equations, calling $S_{ij}^{(\text{hop})}$ and $S_{ij}^{(\text{pot})}$ the terms of the action coupling two sites *i* and *j* (with $i \neq j$), the QMF approximation amounts to taking

$$S_{ij}^{(\text{hop})}[\phi_{i}(\tau),\phi_{j}(\tau)] = -\int_{0}^{\beta} d\tau \ (\phi_{i}^{*}(\tau) \ J_{ij} \ \phi_{j}(\tau) + \text{c.c.})$$

$$\stackrel{\text{QMF}}{\approx} -\frac{1}{\beta} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \ (\phi_{i}^{*}(\tau) \ J_{ij} \ \phi_{j}(\tau') + \text{c.c.})$$

$$= -\beta \ \bar{\phi_{i}}^{*} \ J_{ij} \ \bar{\phi_{j}} = S_{ij}^{(\text{hop})}[\bar{\phi}_{i},\bar{\phi}_{j}] \qquad (4.10)$$

 and

$$S_{ij}^{(\text{pot})}[n_i(\tau), n_j(\tau)] = -\int_0^\beta d\tau \ n_i(\tau) \ V_{ij} \ n_j(\tau)$$
$$\stackrel{\text{QMF}}{\approx} -\frac{1}{\beta} \int_0^\beta d\tau \int_0^\beta d\tau' \ n_i(\tau) \ V_{ij} \ n_j(\tau')$$
$$= -\beta \ \bar{n}_i \ V_{ij} \ \bar{n}_j = S_{ij}^{(\text{pot})}[\bar{n}_i, \bar{n}_j] \ , \qquad (4.11)$$

where we have introduced the time-averaged field and density

$$\bar{\phi}_i = \frac{1}{\beta} \int_0^\beta d\tau \ \phi_i(\tau) \ , \qquad \bar{n}_i = \frac{1}{\beta} \int_0^\beta d\tau \ n_i(\tau) \ . \tag{4.12}$$

Equivalently, the QMF approximation amounts to substituting the coupling between the imaginary-time evolutions of the field ϕ_i , and of its squared amplitude $|\phi_i|^2$, at different sites with the coupling between the *averages* over such evolutions – whence the concept of quantum (or imaginary-time) mean field.

4.3.1 Cluster QMF approximation

This approximation can be easily cast in a cluster form, by dividing the ij bonds into intra-cluster and inter-cluster ones, and applying the mean-field approximation in imaginary time to all inter-cluster couplings. Under this approximation, the coherent state action in Eq. (4.3) takes the form

$$S[\{\phi_i(\tau)\}] \stackrel{\text{QMF}}{\approx} \sum_c S_c[\{\phi_{i\in c}(\tau)\}] + \sum_{c< c'} \sum_{i\in c, j\in c'} S_{ij}[\bar{\phi}_i, \bar{\phi}_j; \bar{n}_i, \bar{n}_j] \qquad (4.13)$$

where we have introduced the cluster action

$$S_{c}[\{\phi_{i\in c}(\tau)\}] = \sum_{i\in c} S_{i}[\{\phi_{i}(\tau)\}] + \sum_{i,j\in c} S_{ij}[\phi_{i}(\tau),\phi_{j}(\tau);n_{i}(\tau),n_{j}(\tau)] .$$
(4.14)



Figure 4.1: Cartoon of the cluster quantum mean-field (cQMF) approximation: (a) Coherent-state path integral configuration: to each site one associates a variable $\phi_i(\tau)$ in the complex plane \mathbb{C} , evolving in imaginary time τ , and coupled to the other variables *instantaneously* in imaginary time via the hopping J_{ij} and the off-site interactions V_{ij} (dashed orange lines); (b) the cQMF approximation consists in dividing the system into clusters (rounded boxes) and approximating the instantaneous J_{ij} and V_{ij} couplings between clusters with all-to-all couplings in imaginary time, namely couplings between the imaginary-time-averaged variables ϕ_i (see text) – but fully preserving the spatial structure of the couplings in real space.

Here S_i is the part of the action containing exclusively the on-site terms (on-site interaction and chemical potential), while $S_{ij} = S_{ij}^{(\text{hop})} + S_{ij}^{(\text{pot})}$ is the off-site part, which becomes

$$S_{ij}[\bar{\phi}_i, \bar{\phi}_j; \bar{n}_i, \bar{n}_j] = S_{ij}^{(\text{hop})}[\bar{\phi}_i, \bar{\phi}_j] + S_{ij}^{(\text{pot})}[\bar{n}_i, \bar{n}_j]$$
(4.15)

under the QMF approximation.

The path integral over coherent states $\int \mathcal{D}[\{\phi_i(\tau)\}]$ can then be decomposed into two integrals: an integral over average values of the fields $\bar{\phi}_i$ and of the densities \bar{n}_i , and a path-integral over paths realizing those average values [79, 80]:

$$\begin{aligned} \mathcal{Z} \approx & \int \left(\prod_{j} \frac{d\bar{\phi}_{j} \ d\bar{\phi}_{j}^{*} \ d\bar{n}_{j}}{2\pi i} \right) e^{-\sum_{c \neq c'} \sum_{i \in c, j \in c'} S_{ij}[\bar{\phi}_{i}, \bar{\phi}_{j}; \bar{n}_{i}, \bar{n}_{j}]} \\ & \prod_{c} \int_{\{\bar{\phi}_{i \in c}, \bar{n}_{i \in c}\}} \mathcal{D}[\{\phi_{i \in c}(\tau)\}] \ e^{-S_{c}[\{\phi_{i \in c}(\tau)\}]} \ . \end{aligned}$$

4.3.2 cQMF approximation and classically correlated states

Here we show that the cQMF expression for the partition function can be cast into the form of the trace of a cluster-separable density matrix, as in Eq. (4.9). We introduce two auxiliary fields, a complex-valued one (Ψ_i) and a real-valued one (ϱ_i) , and perform a Hubbard-Stratonovich transformation [78] as in the following:

$$e^{-\sum_{ij}' S_{ij}^{(\text{hop})}[\bar{\phi}_{i},\bar{\phi}_{j}]} = \frac{1}{\det J'} \int \mathcal{D}\psi \ e^{-\beta \sum_{ij}' \Psi_{i}^{*}[(J')^{-1}]_{ij}\Psi_{j} - \beta \sum_{i}' (\Psi_{i}\bar{\phi}_{i}^{*} + \Psi_{i}^{*}\bar{\phi}_{i})},$$

$$e^{-\sum_{ij}'' S_{ij}^{(\text{pot})}[\bar{n}_{i},\bar{n}_{j}]} = \frac{1}{\det V''} \int \mathcal{D}\rho \ e^{-\beta \sum_{ij}'' \varrho_{i}[(V'')^{-1}]_{ij}\varrho_{j} - \beta \sum_{i}'' \varrho_{i}\bar{n}_{i}}, \quad (4.16)$$

where $\mathcal{D}\psi = \left(\prod_j \frac{\beta^2 d\Psi_j d\Psi_j^*}{2\pi i}\right)$ and $\mathcal{D}\rho = (\prod_i \beta \ d\varrho_i)$, the primed (and doubleprimed) sums $\sum' (\sum'')$ are restricted to those sites which are indeed involved in an inter-cluster bond for the kinetic energy (the potential energy), and the matrices J' and V'' are connectivity matrices restricted to inter-cluster bonds (for the kinetic energy and potential energy respectively). We shall here assume that J' and V'' are positive definite, so that the HS transformation is well defined, otherwise they can be appropriately redefined, leaving the essence of the present argument intact – see Chap. 5 for further discussion.

The HS transformation allows therefore to cast the partition function within the cQMF approximation into the separable form, $\mathcal{Z} \approx \text{Tr}(\rho_{\text{cQMF}})$ with (up to multiplicative constants)

$$\hat{\rho}_{cQMF} \sim \int \left(\prod_{j} \frac{d\Psi_{j} d\Psi_{j}^{*} d\varrho_{j}}{2\pi i} \right) e^{-S_{aux}[\{\Psi_{i}, \Psi_{i}^{*}; \varrho_{i}\}]} (\otimes_{c} \hat{\rho}_{c}[\{\Psi_{i \in c}, \Psi_{i \in c}^{*}; \varrho_{i \in c}\}])$$

$$(4.17)$$

where we have introduced the auxiliary-field action

$$S_{\text{aux}}[\{\Psi_i, \Psi_i^*; \varrho_i\}] = \beta \sum_{ij}' \Psi_i^*[(J')^{-1}]_{ij}\Psi_j + \beta \sum_{ij}'' \varrho_i[(V'')^{-1}]_{ij}\varrho_j , \quad (4.18)$$

and the single-cluster density matrix

$$\hat{\rho}_{c}[\{\Psi_{i\in c}, \Psi_{i\in c}^{*}; \varrho_{i\in c}\}] = e^{-\beta \hat{\mathcal{H}}_{c}^{(\text{eff})}[\{\Psi_{i\in c}, \Psi_{i\in c}^{*}; \varrho_{i\in c}\}]}, \qquad (4.19)$$

with the effective single-cluster Hamiltonian

$$\hat{\mathcal{H}}_{c}^{(\text{eff})} = \hat{\mathcal{H}}_{c} - \sum_{i \in c}' \left(\Psi_{i} \hat{b}_{i}^{\dagger} + \Psi_{i}^{*} \hat{b}_{i} \right) - \sum_{i \in c}'' \varrho_{i} \hat{n}_{i} , \qquad (4.20)$$

where $\hat{\mathcal{H}}_c$ is the physical Hamiltonian, Eq. (4.1), restricted to intra-cluster bonds (for the off-site terms) and cluster sites (for the on-site terms). Therefore the effective cluster Hamiltonian has the form of the physical Hamiltonian plus "boundary" source terms (containing the auxiliary fields Ψ_i, Ψ_i^*) and a "boundary" potential term (containing the auxiliary field ϱ_i) involving the sites coupled to other sites outside the cluster.

As one may already notice from the previous equations, the cQMF approach reduces to the standard cMF approach in the limit of zero temperature, as we will further elucidate with an example in Sec. 5.3.1.

4.4 Theoretical basis for the cQMF approximation

In this section, we provide a justification for the cQMF approximation, which stems from the formal separation between classical and quantum correlations introduced in our previous chapter. We start by briefly recalling the first-order correlation functions that we introduced and by giving their path-integral expressions, in order to be coherent with the formalism used throughout this chapter. We defined the total correlation function

$$g(l,m) = \langle \hat{b}_l^{\dagger} \hat{b}_m \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\{\phi_i(\tau)\}] \ \phi_l^*(\tau') \phi_m(\tau') \ e^{-S} \ , \tag{4.21}$$

for any arbitrary time $\tau' \in [0, \beta]$, the thermal correlation function

$$g_T(l,m) = \frac{1}{\beta} \int d\tau \ \langle \hat{b}_l^{\dagger}(\tau) \hat{b}_m(0) \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\{\phi_i(\tau)\}] \ \bar{\phi}_l^* \bar{\phi}_m \ e^{-S} \ , \quad (4.22)$$

and the quantum correlation function

$$g_{Q}(l,m) = g(l,m) - g_{T}(l,m)$$

$$= \frac{1}{\mathcal{Z}} \int \mathcal{D}[\{\phi_{i}(\tau)\}] \left[\frac{1}{\beta} \int d\tau' (\phi_{l}^{*}(\tau') - \bar{\phi}_{l}^{*})(\phi_{m}(\tau') - \bar{\phi}_{m})\right] e^{-S} ,$$
(4.23)

where S stands for the action $S[\{\phi_i(\tau)\}]$ in Eq. (4.3). Applying a cQMF approximation, which relies on a density matrix in the form Eq. (4.9), amounts to considering the various cluster as Hamiltonian-separable. According to the theorem proved in Sec. 3.2 this implies that, within the cQMF approximation, all the quantum correlation functions are zero between sites belonging to different clusters, namely that $g_Q(l,m) = 0$ for $l \in c$ and $m \in c'$, with $c \neq c'$. Therefore the cQMF approximation truncates quantum correlations to distances not exceeding the linear size of the clusters and "confuses" the total correlations among different clusters with their thermal part only.

4.4.1 Two different length scales

In the previous chapter (see Fig. 3.2), we showed that, for hard-core bosons and quantum rotors, the first-order correlation function decays exponentially at *any* finite temperature. This decay is characterized by a quantum coherence length ξ_Q , which is independent of the correlation length ξ for the decay of the total correlations, and which is such that $\xi_Q < \xi$. This length-scale separation between thermal and quantum correlations constitutes the main motivation behind the cQMF approximation. The latter, introducing a spatial cutoff in the quantum correlations at a length scale $l_c/2$ (the maximum distance between the bulk of the cluster and its boundaries), would be in fact completely arbitrary if the quantum correlation function did not posses an exponential decay. One can then expect the quality of the approximation to depend on the ratio $\vartheta = 2\xi_Q/l_c$, being more accurate when $\vartheta \ll 1$.



Figure 4.2: (a) Sketch of the correlations in quantum many-body system at finite temperature. Beyond a characteristic quantum coherence length ξ_Q total correlations (g) are very closel to the thermal part (g_T) ; (b) Sketch of the cQMF account for correlations in quantum many-body systems at finite temperature. Beyond a length proportional to the cluster size (αl_c) the total correlations are described as *identical* to (approximate) thermal correlations \tilde{g}_T .

The existence of a finite quantum coherence length ξ_Q defines a distance beyond which thermal and total correlations are nearly identical, as sketched in Fig. 4.2(a). This in turn implies that, for $r \gg \xi_Q$, correlations in a quantum many-body system can be regarded – to within a very good approximation – as those generated by an effectively classical system. One can then design a classical model, which would capture the long-range $(r \gg \xi_Q)$ correlations, and whose local degrees of freedom (on the scale ξ_Q) are renormalized in their effective couplings by short-range quantum fluctuations. The cQMF approach is precisely a systematic way of building effective classical theories which describe short-range quantum correlations up to a scale proportional to the cluster linear size l_c , and which then identify the total correlations with (approximate) thermal ones (\tilde{g}_T) beyond that scale. This is sketched in Fig. 4.2(b).

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4.4.2 Effects of the cluster decomposition

We can make some general considerations about the influence of using a cQMF approximation on the description of the system. The general asymptotic form of correlation functions reads

$$A\frac{e^{-r/\xi}}{r^{d-2+\eta}}\tag{4.24}$$

where A, ξ and η depend generically on the temperature and on the size of the system when extracted from finite-size data. The cQMF adds to these dependencies a further cluster-size dependence, namely $A = A(\vartheta; T, L)$, $\xi = \xi(\vartheta; T, L)$, $\eta = \eta(\vartheta; T, L)$. Being restricted to quantum fluctuations, the cQMF is able to capture the correct divergence of the correlation length at a thermal transition, as well as the correct exponent η at the critical point. The position (T_c) of the critical point, anyway, may depend significantly on the ϑ parameter, namely $T_c = T_c(\vartheta)$. In general we expect $T_c(\vartheta > 0) > T_c(0)$ since, by systematically underestimating quantum effects, the cQMF overestimates the transition points. This can be intuitively understood from Fig. 4.1: the cQMF approximation amounts to increasing locally the connectivity of the couplings appearing in the action that weighs the path integral, and this is expected to stabilize correlations against thermal fluctuations.

Moreover, if $\xi \sim \xi_Q$, the short-range properties of the correlation function are dominated by quantum effects, and therefore ξ will depend very strongly on ϑ . Only the condition $\vartheta \ll 1$ would ensure a good description of the correlation function in this regime. Conversely, when $\xi \gg \xi_Q$, thermal and quantum correlations acquire a true separation of scales, which could permit to accurately describe the long-range aspects of thermal correlations, while only partially accounting for quantum correlations.

The next sections are dedicated to a quantitative test of the abilities and limitations of the cQMF scheme. Due to its convenient path-integral solution, we will use once again the two-dimensional quantum-rotor model as a reference, and we will study in particular the convergence of relevant physical observables upon increasing the cluster size.

4.5 Quantum rotors and the QMF approximation

We recall the Hamiltonian of quantum rotors

$$\mathcal{H}_{\text{QR}} = -2J\nu \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) - \frac{U}{2} \sum_i \frac{\partial^2}{\partial \theta_i^2} , \qquad (4.25)$$

which was already presented in the previous chapter, in Eq. (3.16). In what follows we shall first describe the path-integral representation of this model and the implementation of a cQMF approximation, and then discuss numerical results concerning the convergence of the cQMF approach.

The path-integral representation of the partition function for the quantum rotor can be realized by using coherent states with unit norm, namely $\phi_i = e^{i\theta_i}$. The partition function takes then the form

$$\mathcal{Z}_{\text{QR}} = \int \mathcal{D}[\{e^{i\theta_i(\tau)}\}] \ e^{-S_{\text{QR}}[\{e^{i\theta_i(\tau)}\}]} \ . \tag{4.26}$$

The action S_{QR} , as shown in Refs. [64, 81], can be cast in the form of an effective classical XY model in (d + 1) dimensions. One can discretize the imaginary time in M slices of length $\delta \tau = \beta/M$ using Trotter-Lie discretization [77] and take the limit $M \to \infty$. The quality of such an expansion is controlled by the ratio $\epsilon = \delta \tau U$. In particular, for $\epsilon \to 0$, one can use the Villain approximation [82], which gives an action in the form

$$S_{\text{QR}} \approx \sum_{k=1}^{M} \left[-K \sum_{\langle ij \rangle} \cos(\theta_{i,k} - \theta_{j,k}) - K_{\tau} \sum_{i} \cos(\theta_{i,k} - \theta_{i,k+1}) \right], \quad (4.27)$$

where we have introduced the coupling constants $K = \epsilon/u$ and $K_{\tau} = 2/\epsilon$ for the "space-like" and "(imaginary)-time-like" couplings respectively, the reduced repulsion parameter u = U/(2Jn) and the Trotter-discretized phase field $\theta_i(\tau) \to \theta_{i,k}$.

Applying cQMF to Eq. (4.27) amounts to simply redefining the effective XY couplings. Indeed the cQMF approximation addresses the space-like (K) couplings between sites belonging to different clusters, and it redefines them from local in imaginary time to completely non-local (which is the same as assuming that clusters interact via imaginary-time averaged bosonic fields, $\overline{e^{i\theta_i}}$). Then the cQMF effective action, as usual, breaks up into an intracluster part and an inter-cluster part:

$$S_{\text{QR}} \stackrel{\text{QMF}}{\approx} \sum_{c} S_{c} + \sum_{c \neq c'} S_{cc'} , \qquad (4.28)$$

where c, c' are pairs of interacting clusters. The intra-cluster Hamiltonian is simply the effective Hamiltonian Eq. (4.27) specified to the sites and links within a given cluster c:

$$S_c = \sum_{k=1}^{M} \left[-K \sum_{\langle ij \rangle, i, j \in c} \cos(\theta_{i,k} - \theta_{j,k}) - K_\tau \sum_{i \in c} \cos(\theta_{i,k} - \theta_{i,k+1}) \right], \quad (4.29)$$

while the inter-cluster Hamiltonian contains the mean-field couplings in imaginary time between neighboring clusters:

$$S_{cc'} = -\frac{K}{M} \sum_{k,k'=1}^{M} \sum_{\langle ij \rangle, i \in c, j \in c'} \cos(\theta_{i,k} - \theta_{j,k'}) .$$
(4.30)



Figure 4.3: (a-c) Total correlations within the cQMF approximation with variable cluster size l_c for quantum rotors on the square lattice. Here u = 3 and L = 36. (d) Temperature dependence of the η exponent extracted from power-law fits to the correlation function with $l_c = 1$ and $l_c = L = 36$ (see text), over the range $r \in [3, L/2]$; the result is contrasted to that of classical spin-wave (SW) theory, $\eta(t) = t/(2\pi)$.

A path-integral evaluation of the partition function within the cQMF approximation amounts therefore to simulating a classical XY model with spatially anisotropic couplings and all-to-all couplings in imaginary time for inter-cluster links (see again Fig. 4.1 for a cartoon).

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4.6 cQMF results for quantum rotors

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In this section we finally test numerically the ability of the cQMF of describing our test model of quantum rotors in a square lattice. This model possesses a superfluid phase with algebraically decaying correlation function g for temperatures below a critical BKT transition $t < t_{BKT}$. The critical t_{BKT} temperature is a decreasing function of the interaction u, and it vanishes at a quantum critical point $u_c \approx 5.8$, beyond which the ground state of the system becomes a gapped Mott insulator with exponentially decaying correlations [83]. The cQMF action, Eq. (4.28), lends itself naturally to a path-integral Monte Carlo (PIMC) study. For this reason simulations are realized using a PIMC code developed by T. Roscilde.

4.6.1 Description of correlations

We start by studying how clusters behave in the description of the total correlation function, focusing on a strongly interacting superfluid regime (u = 3). Figs. 4.3(a-c) show that for most values of the distance r (namely for $r \ge 2$), the correlation function g(r) obtained via cQMF converges from above to the exact result. The cQMF approximation therefore overestimates the strength of correlations by underestimating quantum effects. The logarithmic scale of the plots permits also to observe something rather remarkable: despite the clear difference in the very value of the correlation function, the long-range tails of the correlation functions for different l_c values appear as nearly parallel. This suggests that the asymptotic behavior of the correlation function is captured by the cQMF up to a multiplicative constant, which accounts for the incomplete description of short-range quantum fluctuations.

One can use the previous data to extract the exponent η , by fitting the correlation function to a power-law $A/d(r|L)^{\eta}$, where $d(r|L) = (L/\pi)\sin(\pi r/L)$ is the chord length, which is well suited for systems defined on a torus, namely with periodic boundary conditions. The so-extracted η exponent is shown as a function of temperature in Fig. 4.3(d), where it is compared to the classical limit $\eta = t/(2\pi)$, which comes the spin-wave theory, valid at low T for u = 0. It is clear that cQMF captures the substantial speed-up in the increase of the η exponent with respect to spin waves. This is due to the fact that $\eta = t/(2\pi \ \varrho_s(u,t=0))$, with $\varrho_s(u,t=0)$ the superfluid density, decreases as u increases. Moreover, we can observe that using the cQMF for the smallest cluster $(l_c = 1)$ already produces a very accurate result compared to the exact one $(l_c = 36)$. This proves the remarkable ability of cQMF to describe quantitatively long-range correlations, which is a non-trivial result, as quantum fluctuations are indeed strong in this example. This possibility of effectively describing thermal fluctuations even by discarding quantum correlations between different sites – which is the case for $l_c = 1$ – provides an interesting insight into the physics of quantum ro-



Figure 4.4: Thermal vs. quantum correlations in the superfluid phase of 2d quantum rotors (t = 0.1, u = 3, L = 36) within the cQMF approximation. (a) Thermal correlations g_T for different cluster sizes, normalized by the value at maximum distance r = L/2; (b) Quantum correlations g_Q for different cluster sizes.

tors. It shows that, sufficiently far from the quantum critical point $u = u_c$, the quantum renormalization of the η exponent for the power-law decay of superfluid correlations comes from very-short-ranged quantum fluctuations.

The form of the long-range tail of the correlation function, and the accuracy of the $(l_c = 1)$ -cQMF in describing the η exponent, suggest that the approximation could describe the thermal correlations g_T very accurately, but only up to an overall multiplicative factor. This latter would account for the fact that, in the real system, the effective classical degrees of freedom are recovered by tracing out quantum fluctuations correlated within a volume ~ ξ_Q^2 . This can be tested by plotting the normalized thermal correlation function $g_T(r)/g_T(L/2)$, where the normalization to the asymptotic value eliminates the above-mentioned multiplicative factor. Fig. 4.4(a) compares the normalized thermal correlations for different cluster sizes with the exact result $(l_c = 36)$: remarkably the *full* structure of the thermal correlation function is well captured by the cQMF approach. Moreover, we can observe that the thermal correlation function exhibits a power-law behavior (very well fitted by $A/d(r|L)^{\eta}$ across the entire range of separations r, whereas the total correlation function clearly deviates from a simple power law, as shown in Fig. 4.3(a-c), when approaching r = 0. This implies that the short-range deviation from a power-law comes entirely from the quantum



Figure 4.5: Total vs. thermal correlations of 2d quantum rotors (t = 0.1, u = 3, L = 36) for three different cluster sizes. The deviation of total correlations g from a power-law decay at short distance comes entirely from the quantum correlations.



Figure 4.6: Correlations in the superfluid phase of 2d quantum rotors with u = 5, L = 36. (a) Normalized thermal correlations at t = 0.15 for various cluster sizes. (b) η exponent extracted from power-law fits of the thermal correlation function over the range [3, L/2].



Figure 4.7: Scaling of the energy density e with the cluster parameter λ (see text) for quantum rotors on the square lattice. λ values correspond to cluster linear sizes $l_c = 1, 2, 3, 4, 6, 12$ and 24 (in decreasing order). The solid and dashed line are a linear fit (excluding the points at $\lambda = 0$ and 1) and a power-law fit $a_1 + a_2\lambda^{a_3}$ (retaining all points), respectively. Model parameters are u = 3 and L = 24.

correlations, which are progressively captured by the cQMF approach with an increasingly large cluster size (Fig. 4.4(b)).

Fig. 4.5 summarizes all these considerations by showing how thermal correlations contribute to total correlations. The total correlation function reproduces a power-law thermal correlation function at large distances, once an exponentially decaying short-range quantum component has died out over a distance $r \gg \xi_Q$ for the real system, or an imposed distance $r \ge l_c$ for its cQMF approximation. This is in agreement with the cartoon proposed in Fig. 4.2.

We can now test the behavior of cQMF when approaching the quantum critical point: we choose the value u = 5, which is close to $u_c \simeq 5.8$. Fig. 4.6 reports results for the normalized thermal correlations and for the η exponent. The plots show that the convergence with the cluster size is much slower than in the u = 3 case, and that large clusters are necessary to give a satisfactory description of the system. The reason behind this behavior is that ξ_Q is significantly larger with respect to the previous case. Therefore, the effective classical degrees of freedom, whose correlations are probed by



Figure 4.8: Scaling of the condensate peak $n_{k=0}$ with the cluster parameter λ for quantum rotors on the square lattice. Lines and parameters as in Fig. 4.7.

g(r) (or $g_T(r)$) at $r \gg \xi_Q$, emerge from integrating out short-range quantum fluctuations over larger quantum-correlated volumes. As a result, the exponent η for the decay of g(r) is affected by increasingly longer-range quantum fluctuations, and a simple cQMF approach with $l_c = 1$ is not sufficient any more.

4.6.2 Cluster-size scaling

In order to determine the precise form of the convergence of observables upon increasing the cluster size, we focus our attention on the energy density and on the momentum-distribution peak n(k = 0), which can be calculated from the correlation function

$$\langle \hat{b}_i^{\dagger} \hat{b}_j \rangle = \langle e^{i(\theta_i - \theta_j)} \rangle . \tag{4.31}$$

Figs. 4.7 and 4.8 show the cluster-size scaling of the kinetic energy and of the n(k = 0) respectively, both calculated in the superfluid phase, for u = 3. We observe that, when plotted against the surface-to-bulk ratio λ , the two quantities scale generically as a power law towards the exact $(\lambda = 0)$ result, which validates the choice of the λ parameter to extrapolate the finite-cluster results towards the exact one. In particular the exponent of the power law seemingly approaches 1 when $T \to 0$, which is consistent



Figure 4.9: Scaling of the condensate peak $n_{k=0}$ with the cluster parameter λ for quantum rotors on the square lattice. λ values correspond to cluster linear sizes $l_c = 1, 2, 3, 6, 9$, and 18 (in decreasing order). Model parameters are u = 5.8 and L = 18. Lines as in Fig. 4.8.

with the numerical observation of linear scaling in ground-state studies of lattice boson models, based on the cMF [35, 84, 85, 86]. On the other hand, the power-law exponent appears to grow gradually upon increasing the temperature, namely the convergence towards the exact result is slightly faster, the higher the temperature.

Finally, it is interesting to observe that the cluster-size scaling of the cQMF results holds not only in the superfluid phase, but also along the quantum-critical trajectory, namely for finite temperatures above the quantum critical point $u = u_c \approx 5.8$ for the superfluid Mott-insulator transition. As shown in Fig. 4.9, a power-law scaling is well consistent with the numerical results, with a nearly linear scaling which persists at higher temperatures, and a much larger prefactor. The slower scaling reveals a strong enhancement of quantum correlations in the quantum critical region, in spite of the fact that the total correlations have in fact acquired an exponentially decreasing form at finite temperature, in contrast with the superfluid phase. This reveals once again the semi-classical nature of the cQMF approximation, limited by the strength of quantum correlations and not by that of thermal ones.

Chapter 5

Auxiliary-field Monte Carlo

In this chapter we introduce a numerical approach to lattice systems called auxiliary-field Monte Carlo (AFMC), which is similar in spirit to approaches such as that used in Ref. [46] for spins and bosons, or to some others used in the context of lattice fermions [47]. In its general version AFMC suffers a heavy sign (or, more generally, "phase") problem, which can be eliminated by making approximations. We show that a possible approximation casts the density matrix of the system in a cluster quantum mean-field (cQMF) form, as that introduced in Chap. 4. Therefore the results of our previous chapters constitute a fundamental justification for such an operation, that a priori would be completely arbitrary.

In the end of the chapter we apply the AFMC method supplemented with the cQMF approximation to the study of the thermodynamics of hard-core bosons both on a square lattice – which admits a numerically exact solution via quantum Monte Carlo – as well as on a triangular frustrated (π -flux) lattice – which instead prevents the use of quantum Monte Carlo because of a severe sign problem. This latter system is particularly interesting because it could be implemented experimentally using ultra-cold atoms in an optical lattice in the presence of an artificial gauge field [87].

5.1 Partition function as a path-integral over auxiliary fields

We consider the Bose-Hubbard Hamiltonian

$$\hat{\mathcal{H}} = -\sum_{ij} \left(J_{ij} \hat{b}_i^{\dagger} \hat{b}_j + \text{h.c.} \right) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i , \qquad (5.1)$$

where $J_{ij} = J_{ji}^*$ is the most general Hermitian hopping matrix, possibly including a gauge field. With respect to Chap. 4, for the sake of simplicity in the exposition, we have restricted ourselves to the case of an on-site interaction only. Analogously to what done in the previous chapter, we express

the partition function of the system in terms of coherent-state path-integrals [14, 77, 88] as

$$\mathcal{Z} = \operatorname{Tr}[e^{-\beta\hat{\mathcal{H}}}] = \int \mathcal{D}[\{\phi_i(\tau)\}] \exp\{-S[\{\phi_i(\tau)\}\}, \qquad (5.2)$$

with

$$S[\phi_i(\tau)] = \sum_i S_i[\phi_i(\tau)] + \sum_{ij} S_{ij}[\phi_i(\tau), \phi_j(\tau)] , \qquad (5.3)$$

$$S_{i}[\phi_{i}(\tau)] = \int_{0}^{\beta} d\tau \left[\phi_{i}^{*}(\partial_{\tau} - \mu)\phi_{i} + \frac{U}{2} |\phi_{i}|^{4} \right] , \qquad (5.4)$$

$$S_{ij}[\phi_i(\tau), \phi_j(\tau)] = -\int_0^\beta d\tau \ \phi_i^* J_{ij} \phi_j \ .$$
 (5.5)

The hopping matrix is in general not positive definite, but one can always add a diagonal constant $J_{ij} \rightarrow \tilde{J}_{ij} = J_{ij} + K\delta_{ij}$ to achieve this property, and redefine accordingly the chemical potential as $\mu \rightarrow \mu - K$. For instance, in the case of the square lattice, whose energy minimum is -4J, we need a term $K = 4J + \epsilon$ (with $\epsilon > 0$) to render J_{ij} positive definite.

Once the positive definiteness of the hopping matrix is ensured, one can use the Hubbard-Stratonovich decoupling [14, 77]

$$\exp \left[\Delta \tau \sum_{ij} \phi_i^* \tilde{J}_{ij} \phi_j\right] =$$

$$\underbrace{\frac{1}{\sum ij}}_{ij} \int \prod \frac{d(\operatorname{Re}\Psi_i) d(\operatorname{Im}\Psi_i)}{ij} e^{-\Delta \tau \left[\sum_{ij} \Psi_i^* \tilde{J}_{ij}^{-1} \Psi_j - \sum_i (\Psi_i^* \phi_i + \text{c.c.})\right]}$$
(5.6)

$$\frac{1}{\det(\tilde{J}/\Delta\tau)} \int \prod_{i} \frac{1}{2\pi} e^{-\Delta\tau} \left[\sum_{ij} \Psi_{i} J_{ij} \Psi_{j} - \sum_{i} (\Psi_{i} \psi_{i} + 0.0.) \right]$$

ch imaginary-time step, using a set of complex *auxiliary fields* { $\Psi_{i}(\tau)$ }

at each imaginary-time step, using a set of complex *auxiliary fields* $\{\Psi_i(\tau)\}$. Concerning the spatial structure of the \tilde{J}_{ij}^{-1} couplings, one may say that, e.g. on the square lattice, \tilde{J}_{ij}^{-1} behaves at large distances as the Bessel function $\mathcal{K}_0(|\vec{r}_i - \vec{r}_j|/\lambda)$ decaying exponentially over the length-scale λ , where $\lambda = \sqrt{J/\epsilon}$ [89]. The partition function takes the form

$$\mathcal{Z} = \int \frac{\mathcal{D}[\{\Psi_i(\tau)\}]}{\det J} \ e^{-S_{\Psi}[\{\Psi_i(\tau)\}]} \ \prod_i \mathcal{Z}_i[\Psi_i(\tau)] , \qquad (5.7)$$

where

$$S_{\Psi}[\{\Psi_{i}(\tau)\}] = \int d\tau \sum_{ij} \Psi_{i}^{*}(\tau) (\tilde{J}^{-1})_{ij} \Psi_{j}(\tau)$$
(5.8)

 and

$$\mathcal{Z}_{i}[\Psi_{i}(\tau)] = \int \mathcal{D}[\phi_{i}(\tau)] \ e^{-\{ S_{i}[\phi_{i}(\tau)] + \int_{0}^{\beta} [\Psi_{i}^{*}(\tau)\phi_{i}(\tau) + \Psi_{i}(\tau)\phi_{i}^{*}(\tau)] \}}$$
(5.9)

is the effective partition function of a single site. This latter can be rewritten in the form

$$\mathcal{Z}_{i}[\Psi_{i}(\tau)] = \operatorname{Tr}\left\{T_{\tau} \exp\left[-\int_{0}^{\beta} d\tau \ \hat{\mathcal{H}}_{i}(\tau)\right]\right\}$$
(5.10)

where T_{τ} is the imaginary-time-ordering operator. The effective single-site partition function is most explicitly written upon discretizing the imaginarytime direction: $\tau \to \tau_k = k\Delta \tau$, with k = 1, ..., M and $\Delta \tau = \beta/M$:

$$\mathcal{Z}_{i}[\Psi_{i}(\tau)] = \lim_{M \to \infty} \operatorname{Tr} \left\{ \prod_{k=1}^{M} \exp\left[-\Delta \tau \ \hat{\mathcal{H}}_{i}(k\Delta \tau) \right] \right\}$$
(5.11)

where the "instantaneous" Hamiltonian in imaginary time is

$$\hat{\mathcal{H}}_i(k\Delta\tau) = -\left[\Psi_i^*(k\Delta\tau)\hat{b}_i + \text{h.c.}\right] + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - (\mu - K)\sum_i \hat{n}_i . \quad (5.12)$$

In recent years the coherent-state path-integral has come under scrutiny because of some essential ambiguities it exhibits, and it therefore may not seem as a solid basis for a numerical approach [90]. We would like to point out that the path-integral formalism is not strictly necessary to obtain Eq. (5.7), but we used it for the convenience of the presentation. Moreover the path-integral of Eq. (5.9) is exactly calculated to give Eq. (5.11), which is expressed in operatorial form, and which will be the basis of our subsequent analysis. In App. B we show a possible alternative derivation of Eq. (5.7) which does not make use of the coherent-state path-integral.

5.2 Auxiliary-field Monte Carlo and sign problem

We may express Eq. (5.7) in the form

$$\mathcal{Z} = \int \mathcal{D}[\{\Psi_i(\tau)\}] \ w[\{\Psi_i(\tau)\}]$$
(5.13)

with $w[\{\Psi_i(\tau)\}]$ weights given by

$$w[\{\Psi_i(\tau)\}] = e^{-S_{\Psi}[\{\Psi_i(\tau)\}]} \prod_i \mathcal{Z}_i[\Psi_i(\tau)] , \qquad (5.14)$$

which suggests the possibility of implementing a Monte Carlo approach that is usually called auxiliary-field Monte Carlo (AFMC), by performing amplitude and phase updates for the auxiliary fields $\{\Psi_i(\tau)\}$. The calculation of each local partition function $\mathcal{Z}_i[\Psi_i(\tau)]$ would require M diagonalizations of $(n_{\max} + 1) \times (n_{\max} + 1)$ matrices, namely the $\mathcal{H}_i(k\Delta\tau)$ matrices which need to be exponentiated to produce the infinitesimal propagators $\exp\left[-\Delta\tau \mathcal{H}_i(k\Delta\tau)\right]$. \mathcal{Z}_i would then be obtained as the trace of the product
of the M exponentiated matrices. Thermal averages of observables could be estimated as

$$\langle \hat{O}_i \rangle = \langle [\hat{O}_i] \rangle_{\mathrm{MC}} = \frac{\int \mathcal{D}[\{\Psi_i(\tau)\}] w[\{\Psi_i(\tau)\}] [\hat{O}_i]}{\int \mathcal{D}[\{\Psi_i(\tau)\}] w[\{\Psi_i(\tau)\}]}$$
(5.15)

where

$$[\hat{O}_i] = \frac{1}{\mathcal{Z}_i} \operatorname{Tr} \left\{ \hat{O}_i \ T_\tau \exp\left[-\int_0^\beta d\tau \ \hat{\mathcal{H}}_i(\tau) \right] \right\} , \qquad (5.16)$$

for single-site observables and

$$\langle \hat{O}_{i_1} ... \hat{O}_{i_n} \rangle = \langle [\hat{O}_{i_1}] ... [\hat{O}_{i_n}] \rangle_{\mathrm{MC}}$$
(5.17)

for n-site observables.

But in order for this numerical approach to be effective, to perform such a simulation one has to ensure that all the weights $w[\{\Psi_i(\tau)\}]$ are real positive or zero. This is the case for the component $e^{-S_{\Psi}[\{\Psi_i(\tau)\}]}$, which is a product of Gaussians, but there is no reason in principle to say that the local partition functions $\prod_i \mathcal{Z}_i[\Psi_i(\tau)]$ are also real positive, because the operator appearing in Eq. (5.11) under the trace is the product of more than two Hermitian operators. Such a product admits a non-zero trace for both its Hermitian part (which gives a real contribution) as well as its anti-Hermitian part (which gives an imaginary contribution). With complex weights, the statistical averages $\langle \hat{O}_i \rangle$ (which are real numbers) are the result of the sum of both positive and negative terms coming from the real as well as the imaginary part of $w[\{\Psi_i(\tau)\}]$ and $[\hat{O}_i]$, hence the sign problem (that one may call here "phase" problem, since it emerges from complex numbers). Therefore, in order to implement a meaningful numerical approach, it is essential to develop some form of approximations, as we discuss in the following.

5.3 Time-independent auxiliary fields: a quantum mean-field approximation

A first, simple approximation consists in ignoring the imaginary-time dependence of the auxiliary fields:

$$\Psi_i(\tau) \approx \bar{\Psi}_i \ . \tag{5.18}$$

This amounts to decouple the imaginary-time dynamics of the different sites, that remain coupled only through the mean fields in imaginary time. In this case the single-site partition function \mathcal{Z}_i becomes a *physical* partition function (namely the trace of the exponential of an Hermitian operator), and therefore the Monte Carlo simulation can be done straightforwardly, as it amounts to the sampling of the following object

$$\mathcal{Z} = \int \prod_{i} \frac{d(\operatorname{Re}\Psi_{i})d(\operatorname{Im}\Psi_{i})}{2\pi} w(\{\bar{\Psi}_{i}\})$$
(5.19)

5.3. TIME-INDEPENDENT AUXILIARY FIELDS

with positive-definite $w(\{\bar{\Psi}_i\})$ weights.

One can easily observe that the approximation of time-independent auxiliary fields (TIAF) sets the density matrix in a form which is precisely that of a cQMF density matrix (see Eq. (4.17)) for single-site clusters. Moreover, as we show in the following section, for $T \rightarrow 0$, this approach reduces to a MF approximation.

5.3.1 T = 0 limit of the time-independent-auxiliary-field approximation: Gutzwiller mean-field solution

In the limit $T \to 0$ the single-site partition functions become

$$\mathcal{Z}_i[\bar{\Psi}_i] \to e^{-\beta E_0[\bar{\Psi}_i]} , \qquad (5.20)$$

with $E_0[\bar{\Psi}_i]$ the ground-state energy of the Hamiltonian $\hat{\mathcal{H}}_i(\bar{\Psi}_i)$. This reduces the statistical sum to the form

$$\mathcal{Z} \approx \int \prod_{i} \frac{d(\operatorname{Re}\bar{\Psi}_{i})d(\operatorname{Im}\bar{\Psi}_{i})}{2\pi} \ e^{-\beta E_{\operatorname{eff}}[\{\bar{\Psi}_{i}\}]} , \qquad (5.21)$$

where the effective auxiliary field energy $E_{\rm eff}$ has the form

$$E_{\text{eff}}[\{\bar{\Psi}_i\}] = \sum_{ij} \bar{\Psi}_i^* [\tilde{J}^{-1}]_{ij} \bar{\Psi}_j + \sum_i \langle \psi_{0,i} | \hat{\mathcal{H}}_i(\bar{\Psi}_i) | \psi_{0,i} \rangle .$$
(5.22)

Here $|\psi_{0,i}\rangle$ is the ground state of the single-site Hamiltonian $\hat{\mathcal{H}}_i[\bar{\Psi}_i]$. The ground-state value of the auxiliary fields is then found upon minimizing the effective energy

$$\frac{\delta E_{\text{eff}}}{\delta \Psi_i^*} = \sum_j [\tilde{J}^{-1}]_{ij} \bar{\Psi}_j - \langle \hat{b}_i \rangle_0 = 0 \tag{5.23}$$

where $\langle \hat{b}_i \rangle_0 = \langle \psi_{0,i} | \hat{b}_i | \psi_{0,i} \rangle$, and we have used Hellman-Feynman's theorem to evaluate the derivative of the ground-state energy. Inverting this relation we find that the ground-state auxiliary field configuration satisfies the self-consistent condition

$$\bar{\Psi}_{i,0} = \sum_{j} \tilde{J}_{ij} \langle \hat{b}_j \rangle_0 = \sum_{j} J_{ij} \langle \hat{b}_j \rangle_0 + K \langle \hat{b}_i \rangle_0 , \qquad (5.24)$$

where the expectation value of \hat{b}_j is taken on the ground state of the singlesite Hamiltonian containing the auxiliary field itself. This condition is similar to that satisfied by the ground state in the Gutzwiller mean-field approximation – see Eqs. (2.16) and (2.17), but it shall be exactly the same only in the case of K = 0. One can show that, in a square lattice, Eq. (5.24) is the same as the Gutziller mean-field condition for a Hamiltonian with redefined parameters $J \to J + K/4$ and $\mu \to \mu - K$. This shall give a first idea of how the use of the diagonal shift K affects the correct description of the model.



Figure 5.1: The time-independent AFMC with cluster decomposition simulates an effective classical field theory for auxiliary fields living on the boundaries of clusters. The effective couplings among the classical auxiliary fields are obtained by inverting the (shifted) matrix $(\tilde{J}^{(inter)})$ of the inter-cluster couplings, indicated in blue in the picture.

5.3.2 Cluster decomposition and time-independent auxiliary fields

The use of the approximation $\Psi_i(\tau) \approx \overline{\Psi}_i$ can be systematically improved by dividing the system into clusters and applying the approximation only on the borders of clusters. We define a matrix $J_{ij}^{(\text{inter})}$ containing hoppings connecting only sites belonging to different clusters and a matrix $J_{ij}^{(\text{intra})}$ containing hoppings connecting only sites belonging to the same cluster. This amounts to writing the kinetic-energy term in the action Eq. (5.5) as

$$\sum_{ij} \phi_i^* J_{ij} \phi_j = \sum_{ij \in \mathcal{B}} \phi_i^* J_{ij}^{(\text{inter})} \phi_j + \sum_{ij} \phi_i^* J_{ij}^{(\text{intra})} \phi_j , \qquad (5.25)$$

where \mathcal{B} denotes the set containing the boundary sites of all clusters. One can then apply a Hubbard-Stratonovich transformation to the inter-cluster couplings only, which indeed may require the redefinition of the hopping matrix as $\tilde{J}_{ij}^{(\text{inter})} = J_{ij}^{(\text{inter})} + K\delta_{ij}$, in order to render the matrix positive definite, as well as a redefinition of the chemical potential for the boundary sites of the cluster, $\mu_{i\in\mathcal{B}} \to \mu_{i\in\mathcal{B}} - K$. The partition function becomes

$$\mathcal{Z} = \int \frac{\mathcal{D}[\{\Psi_{i\in\mathcal{B}}(\tau)\}]}{\det(\tilde{J}^{(\text{inter})})} \ e^{-S_{\Psi}[\{\Psi_{i\in\mathcal{B}}(\tau)\}]} \ \prod_{c} \mathcal{Z}_{c}[\{\Psi_{i}(\tau)\}_{c}]$$
(5.26)

where

$$S_{\Psi}[\{\Psi_{i\in\mathcal{B}}(\tau)\}] = \int d\tau \sum_{ij\in\mathcal{B}} \Psi_i^*(\tau) \ [(\tilde{J}^{(\text{inter})})^{-1}]_{ij} \ \Psi_j(\tau)$$
(5.27)

and

$$\mathcal{Z}_{c}[\{\Psi_{i\in c}(\tau)\}] = \int \mathcal{D}[\{\phi_{i\in c}(\tau)\}] \ e^{-\{S_{c}[\{\phi_{i\in c}(\tau)\}] + \int_{0}^{\beta} \sum_{i\in\mathcal{B}_{c}} [\Psi_{i}^{*}(\tau)\phi_{i}(\tau) + \text{c.c.}]\}}.$$
(5.28)

Here c is the cluster index, \mathcal{B}_c is the boundary of the cluster c, and S_c is the action describing the bulk of the cluster:

$$S_{c}[\{\phi_{i\in c}(\tau)\}] = \sum_{i\in c} S_{i}[\phi_{i}(\tau)] - \sum_{ij\in c} \int_{0}^{\beta} d\tau \ \phi_{i}^{*} J_{ij}^{(\text{intra})} \phi_{j} \ . \tag{5.29}$$

The cluster effective partition function is easily rewritten in operatorial form as

$$\mathcal{Z}_{c}[\{\Psi_{i\in c}(\tau)\}] = \operatorname{Tr}\left\{T_{\tau}\exp\left[-\int_{0}^{\beta}d\tau \ \hat{\mathcal{H}}_{c}(\tau)\right]\right\}$$
(5.30)

where the cluster Hamiltonian is given by

$$\hat{\mathcal{H}}_{c}(\tau) = - \sum_{i \in \mathcal{B}_{c}} \left[\Psi_{i}^{*}(\tau) \hat{b}_{i} + \text{h.c.} \right] - \sum_{ij \in c} \left[J_{ij}^{(\text{intra})} \hat{b}_{i}^{\dagger} \hat{b}_{j} + \text{h.c.} \right]$$
$$+ \frac{U}{2} \sum_{i \in c} \hat{n}_{i} (\hat{n}_{i} - 1) - \mu \sum_{i \in c, i \notin \mathcal{B}_{c}} \hat{n}_{i} - (\mu - K) \sum_{i \in \mathcal{B}_{c}} \hat{n}_{i} . (5.31)$$

We would like to stress that so far the approach is exact: no approximation has been employed. At this point one can employ the approximation $\Psi_i(\tau) \approx \bar{\Psi}_i$ in the previous equation. This allows us to achieve positive weights and to simulate the model through a Monte Carlo approach, using amplitude and phase updates for the auxiliary fields $\{\bar{\Psi}_i\}$.

One may also observe that the approximation on the boundary of the cluster casts the density matrix in the form of a cQMF density matrix, as in Eq. (4.17). In the previous chapter, we proved cQMF approximation to be effective in the description of lattice bosons at finite temperature. This was in turn a consequence of a length scale separation of classical and thermal correlations already shown in Chap. 3. Therefore, the AFMC with cluster decomposition and time-independent auxiliary fields can be regarded as a physically motivated approach applicable to a wide class of lattice systems, since it permits the study of models involving complex hopping processes. This approach constitutes a systematic construction of effective classical field theories for classical auxiliary fields living on the boundary of the clusters, characterized by an action

$$S_{\text{eff}}[\{\bar{\Psi}_{i\in\mathcal{B}}\}] = S_{\Psi}[\{\bar{\Psi}_{i\in\mathcal{B}}\}] - \sum_{c} \log \mathcal{Z}_{c}[\bar{\Psi}_{i\in\mathcal{B}_{c}}] .$$
(5.32)



Figure 5.2: Kinetic energy density (a) and n(k = 0) (b) for different cluster sizes with AMFC, compared to QMC. Plots show a L = 12 lattice and employ the temperature $t = k_B T/J$, with k_B the Boltzmann constant.

The division into clusters realizes a spatial renormalization of the lattice (see Fig. 5.1), with both quantum and thermal fluctuations being integrated on the scale of the clusters.

In the following we apply the method to the test model of hard-core bosons on a square lattice, and we then approach the problem of hard-core bosons on a frustrated triangular lattice.

5.4 Application of AFMC to hard-core bosons on a square lattice

Let us recall the $(\mu = 0)$ Hamiltonian of hard-bosons in a square lattice:

$$\hat{\mathcal{H}} = -\sum_{ij} \left(J_{ij} \hat{a}_i^{\dagger} \hat{a}_j + \text{h.c.} \right) .$$
(5.33)

As discussed in the previous sections, the Hubbard-Stratonovich transformation requires the introduction of a diagonal shift K to the hopping matrix in order to make it positive definite. In the following we choose $K = |\alpha_{min}|(1 + \varepsilon)$, where α_{min} is the minimum eigenvalue of the matrix $J_{ij}^{(\text{inter})}$ and $\varepsilon > 0$. The chosen ε shall be big enough to ensure positive definiteness of the hopping matrix, but also small, in order to minimally affect the results. In the following we always take $\varepsilon = 0.05$; moreover, we noticed that for small ε results depend weakly on its specific choice.



Figure 5.3: Finite-size scaling for n(k = 0) for different cluster sizes.

As already pointed out in Sec. 5.1, the shift in the hopping matrix is compensated by the one of the chemical potential. Under the TIAF approximation this seemingly harmless shift remains imprinted on the boundary of the cluster, affecting the cluster physics in a way that only disappears upon growing the cluster size. To accelerate the cluster-size convergence, we make the choice of removing the chemical-potential shift altogether, and thereby assuring particle-hole symmetry when $\mu = 0$ on each cluster, whatever the cluster size.

In Fig. 5.2 we report plots showing the kinetic energy and the n(k=0)



Figure 5.4: Linear fit to extrapolate the $\lambda = 0$ estimate of the BKT transition. Results are compared to those previously shown in Fig. 2.2 for cMF.

peak in momentum distribution (for different cluster sizes), and compare them to QMC results. First of all one can observe that AFMC results get closer to the exact results upon increasing the cluster size. Analogously to what done in Secs. 2.2 and 2.4, we extract estimates for the BKT transition temperature using finite-size scaling for n(k=0). This is done for all the available cluster sizes – see Fig. 5.3. The so-obtained estimates can be extrapolated linearly in the surface-to-bulk ratio λ and then give an infinitesize $(\lambda = 0)$ estimate, as previously done in Sec. 4.6.2. In Fig. 5.4, we realize a linear fit in λ , which gives a value $T_{\lambda=0} = (0.69 \pm 0.02) k_B/J$, compatible with the reference value $T_{BKT} = 0.685 k_B/J$ [53]. The choice of a linear interpolation (with respect to a polynomial one, as done in Sec. 4.6.2) is motivated by the limited number of points available, which is in turn imposed by the excessive computational cost of larger-size clusters. In Fig. 5.4 we also show the results previously obtained using cluster mean field (Sec. 2.3). One can appreciate how AFMC – which, at variance with cMF, can capture long-wavelength thermal fluctuations that govern the transition - can capture the correct universality class of the transition for each cluster size, and is significantly more accurate in the estimate than cMF. Moreover, AFMC results appear to be much less scattered than cMF ones, thus showing a much less steep linear interpolation function.

As a final remark, we notice that AFMC points (contrarily to cMF points)



Figure 5.5: (a) Chiral ground states for the anti-ferromagnetic classical XY model on a triangular lattice. + and - denote the chirality of a single plaquette $\kappa_{\Delta} = \sum_{(i \to j) \in \Delta} \sin(\theta_i - \theta_j)$, which is positive for spins turning clock-wise and negative for spins turning anti-clockwise. (b) Single-site, triangular and rhombic clusters on a triangular lattice.

converge to the $\lambda = 0$ estimate from below, and not from above, as one may expect from a method that underestimates quantum effects. This is due to the K term that we artificially introduced in the Hamiltonian. This additional shift modifies the estimates of the T_{BKT} transition temperature for $\lambda > 0$, thus deforming the shape of the convergence, but it shall not modify the infinite-size estimate, as already observed.

5.5 Application of AFMC to hard-core bosons in a frustrated triangular lattice

We can now apply the cluster AFMC approach with time-independent approximation to a more challenging model: hard-core bosons in a triangular frustrated lattice (or anti-ferromagnetic quantum XY model, using the mapping in Sec. 2.1), which cannot be studied using QMC because of sign problem. Our results constitute the first numerical study to our knowledge of the phase transitions in this model. This model is particularly interesting because it can be experimentally realized using artificial gauge fields for cold atoms in an optical lattice [87]. We start by briefly introducing the classical version of the model (in the language of XY spins), and then present our results for its quantum counterpart. In general, we expect the quantum model to show the same transitions as the classical one, with transition temperature strongly renormalized by the presence of quantum effects.

5.5.1 Classical anti-ferromagnetic XY model on a triangular lattice

The classical S = 1/2 anti-ferromagnetic XY model on a triangular lattice is described by a Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) , \qquad (5.34)$$

with $\mathbf{S}_i = (\cos \theta_i, \sin \theta_i)$ and J < 0. This model shows frustration, since spins cannot orient anti-ferromagnetically with respect to all bonds in which they are involved. The ground state exhibits a 3-sublattice structure with spins forming 120 degrees angles with one another. This ground state possesses a \mathcal{Z}_2 chiral degeneracy, with the two chiral ground states characterized by the configurations shown in Fig. 5.5 (up to a U(1) symmetry). At finite temperatures this model shows two phase transitions: a spin transition, and a chiral transition, associated with the spontaneous symmetry breaking of the inversion symmetry. The spin transition is assessed to happen at a lower temperature than the chiral one, thus showing a "spin-chirality decoupling". The nature of both transitions is somehow debated: some works claimed the chiral transition to belong to standard Ising universality class [91, 92, 93], whereas some others reported possible deviations of the critical exponents from the standard Ising ones [94, 95]; some works claimed the spin transition to belong to standard BKT universality class [94, 95, 96], whereas some others reported possible deviations of the critical exponents from the standard BKT ones [91, 92, 93]. In the following we will not enter this debate, but we will assume the transitions to belong to Ising and BKT classes respectively and use the corresponding critical exponents for the finite-size scaling analysis. As reference values for the transitions we give those presented in a recent work by Obuchi and Kawamura [93], which estimates $T_{BKT} \simeq 0.505 \ k_B/J$ and $T_{Is} \simeq 0.513 \ k_B/J$, therefore with the spin transition occurring at a temperature around 1.5% lower than chiral one.

5.5.2 Hard-core bosons on a frustrated triangular lattice

We study the quantum XY model in the language of hard-core bosons, relying on the exact mapping presented in Sec. 2.1. The Hamiltonian, for the case of $\mu = 0$, will be

$$\hat{\mathcal{H}} = -\sum_{ij} \left(J_{ij} \hat{a}_i^{\dagger} \hat{a}_j + \text{h.c.} \right) , \qquad (5.35)$$

which has the same form as in Eq. (5.33), but with the non-zero elements of the hopping matrix such that $J_{ij} = -J < 0$ (there is a π -flux). This model as well requires the introduction of a K shift (that we choose as in Sec. 5.4) in order to make the hopping matrix positive definite, therefore the same



Figure 5.6: Kinetic energy, density peak and current structure factor for the triangular lattice.

observations as in Sec. 5.4 apply. We focus in particular on two observables, which will serve to characterize the BKT and Ising transitions. One shall be captured by the peak in the momentum distribution, which for the two chiral ground states shown before occurs respectively at $\mathbf{k} = (-4\pi/3; 0)$ and $\mathbf{k} = (4\pi/3; 0)$, and equivalent points in the Brillouin zone. We define an observable

$$n_{4/3} = \left[n(-4\pi/3;0) + n(4\pi/3;0) \right] / 2 , \qquad (5.36)$$



Figure 5.7: Finite-size scaling for $n_{4/3}$ on a triangular lattice.

which is the average of the peaks of the two chiral configurations. The other observable shall be a structure factor for currents, defined as

$$S(q=0) = \frac{1}{N_{\Delta}^2} \sum_{\Delta\Delta'} \langle \hat{\kappa}_{\Delta} \hat{\kappa}_{\Delta'} \rangle , \qquad (5.37)$$

where Δ denotes a triangular plaquette oriented in a chosen direction (upwards or downwards) and

$$\hat{\kappa}_{\Delta} = \sum_{(i \to j) \in \Delta} i(\hat{a}_i^{\dagger} \hat{a}_j - \hat{a}_j^{\dagger} \hat{a}_i)$$
(5.38)



Figure 5.8: Finite-size scaling for S(q=0) on a triangular lattice.

is the bosonic current over a closed loop on such plaquette, whose sign depends on the chirality of the plaquette. The structure factor is designed such that it is maximal for configurations in which all triangular plaquettes oriented in the same direction have the same chirality – which is the case for the two ground states. In Fig. 5.6 we show time-independent AFMC results for the kinetic energy, the momentum peak and the current structure factor for single-site, triangular and rhombic clusters (see Fig. 5.5 for the clusters shape).

We can make some more comments on the simulation. As done in the previous section for the square lattice, we introduce a diagonal shift on the



Figure 5.9: Linear fits for T_{BKT} and T_{Is} in the surface-to-bulk ratio for single-site, triangular and rhombic clusters.

hopping matrix that we do not counterbalance with a new shift for the chemical potential. This is done again with the aim of preserving half filling for all cluster matrices. Moreover, in the case of triangular and rhombic clusters the sum (5.37) is restricted to triangles entirely contained in a cluster, in order to have all bonds described in the same way. All data in Fig. 5.6 (as well as those in the following section) are the result of an average over 20 independent simulations. This was done in order to have smooth curves. Moreover, all simulations (and in particular those for triangular and rhombic clusters) showed a very slow convergence, which required the use of annealing (see App. A).

5.5.3 Finite-size and cluster-size scaling

We follow now the same approach as in Sec. 5.5 and derive estimates for the BKT and Ising transition temperatures through finite-size scaling and cluster-size scaling. In Figs. 5.7 and 5.8 we show finite-size scaling for singlesite, triangular and rhombic clusters for both momentum peak $n_{4/3}$ and current structure factor S(q = 0). We use the η exponent for the 2d BKT universality class and the 2d Ising class, which is in both cases $\eta = 1/4$, and for each cluster size we extract an estimate for the transition temperatures. Then we perform linear fits for the so-extracted finite-size estimates in order to have infinite-size estimates for the two transition temperatures, as shown in Fig. 5.9.

The plot suggests that the decoupling of the two transitions is preserved in the quantum model. In particular, for all the three cluster sizes investigated (and for the infinite-size estimates as well) $T_{BKT} < T_{Is}$, as found in the classical model. The plot also seems to suggest that quantum effects enhance the separation between the two transitions. Our linearly extrapolated estimates for the transitions are $T_{BKT} = (0.272 \pm 0.007) k_B/J$ and $T_{Is} = (0.290 \pm 0.004) k_B/J$, with T_{BKT} approximately 6% lower than T_{Is} . Conversely, in the classical model T_{BKT} is found to be around 1.5% lower than T_{Is} [93].

Chapter 6

Conclusions

In this thesis we approached lattice quantum systems both from a theoretical and a numerical point of view. In the first part we made some considerations of general interest for equilibrium many-body states, mainly concerning the nature and structure of correlations. In the second part, on the basis of these results, we developed an approximated framework which is particularly suited for the numerical study of bosonic models (including frustrated lattices) currently at interest in experimental physics.

We introduced a new quantum correlation function (QCF), that we defined as the difference between the conventional two-point correlation function involving the regions A and B, and the response function of region Aupon perturbing region B with a field λ_B . In the classical case these two quantities are identified by a fluctuation-dissipation relation, which breaks down quantum-mechanically. We studied the spatial structure of the QCF and of its classical counterpart, and showed a length-scale separation, with quantum correlations decaying exponentially (with a characteristic quantum coherence length) at all temperature and classical correlations decaying either algebraically or exponentially, depending on the temperature. We showed that finite QCFs rule out a specific form of separability that we named Hamiltonian separability, thus suggesting that the quantum coherence length can be regarded as an effective separability length of the system, which is also compatible with a similar separability length defined by quantum variance [70]. Moreover, we compared the quantum correlation function with an important reference quantity in the physics of quantum information, the quantum discord [30], which measures the non-local disturbance that a local measure produces in a quantum system. Quantum discord is regarded as an observable measuring truly quantum correlations, but we showed that (at variance with the QCF) it is sensitive to purely classical phenomena, thus suggesting the necessity of critically revise its use.

On the basis of the observed length-scale separation in the spatial structure of classical and quantum correlations, we introduced an approximation to lattice systems that we named quantum mean-field (QMF). The latter realizes a decomposition of the system into clusters: quantum correlations are cut at the cluster edges, whereas thermal correlations are properly described by a form of classical correlation introduced in the density matrix. As long as the ratio between the quantum coherence length and the cluster linear size is much bigger than one, the approximation is extremely accurate. We tested the approximation for a model of quantum rotors in a square lattice, for which we studied several cluster sizes and extracted estimates for the infinite-size cluster performing a fit in the surface-to-bulk ratio of the clusters.

Finally, we made use of the QMF approximation in the general framework of the so-called auxiliary-field Monte Carlo (AFMC) [46]. This allowed us to circumvent the severe sign problem which characterizes AFMC and develop a widely applicable approximate method. In particular, we applied such a method to the study of the thermodynamics of hard-core bosons in a frustrated (or π -flux) triangular lattice (equivalent to the anti-ferromagnetic quantum XY model). This constitutes to our knowledge the first numerical study of the transitions of this model. Simulations showed the same transitions (a BKT and an Ising one) as in the classical model, but with temperatures strongly renormalized by quantum effects. The renormalization of the BKT transition temperature is more severe than that of the Ising one, increasing the width of the in-between chiral phase.

These results suggest the possibility of applying the new method we developed to many other models of current interest both in ultra-cold atoms and in condensed matter. One may study e.g. frustrated lattices such as the kagome lattice [11] or the anisotropic triangular lattice [97]. But one may also move away from the π -flux case and investigate the Hofstadter model for bosons [98], which represents one of the "holy grails" of current experimental efforts in ultra-cold atoms. Introducing a second, real-valued auxiliary field allows one to describe as well arbitrary density-density interactions (as discussed in Sec. 4.3): this opens the path to studying e.g. XXZ models or dipolar atoms in a gauge field, to cite a few examples. Finally, using a spinor auxiliary field { $\vec{\Psi}_i$ } allows one to treat spinful bosons, potentially extending the purpose of our method to non-abelian gauge fields.

Chapter 7

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Appendix A

Monte Carlo method

Since the Monte Carlo method [99, 100, 101] is a central concept throughout this thesis, we find it instructive to give a short pedagogical introduction, which might interest a reader with no previous knowledge in this field. We focus in particular on the application of Monte Carlo to a (classical) physical system and on the implementation of the Metropolis algorithm.

A.1 Basics

Let us consider a physical system at thermal equilibrium. The expectation value for some extensive quantity Q (internal energy, entropy, magnetization...) will be of the form:

$$\langle Q \rangle = \frac{\sum_{\boldsymbol{x}} Q(\boldsymbol{x}) e^{-\beta E_{\boldsymbol{x}}}}{\sum_{\boldsymbol{x}} e^{-\beta E_{\boldsymbol{x}}}} \equiv \sum_{\boldsymbol{x}} p(\boldsymbol{x}) Q(\boldsymbol{x}) , \qquad (A.1)$$

where the sums are carried out on the \mathcal{N} microstates of the system, $Q(\boldsymbol{x})$ is the value of Q measured on a microstate \boldsymbol{x} and $e^{-\beta E_{\boldsymbol{x}}}$ is the Boltzmann weight of such a microstate. Unfortunately, this expression can only be evaluated exactly for very small systems, since \mathcal{N} is typically a very large number. This can be easily understood by thinking to a system of n particles with z possible internal states: the number of microstates is $\mathcal{N} = z^n$, which grows exponentially with the number of particles.

One could then think of selecting $N < \mathcal{N}$ microstates through a uniform sampling of the phase space and approximating the thermal average with an estimator

$$Q_U \equiv \frac{\sum_{i=1}^{N} Q(\boldsymbol{x}_i) e^{-\beta E_{\boldsymbol{x}_i}}}{\sum_{i=1}^{N} e^{-\beta E_{\boldsymbol{x}_i}}} .$$
(A.2)

But this operation, in general, does not give a satisfactory result. Often, and in particular at low temperatures, the thermal average is dominated by very few states with respect to the total number of states. A finite-time uniform sampling of phase space would most likely select almost only states with a negligible Boltzmann weight and then give a biased estimator.

One could then use another approach. The expectation value in Eq. (A.1) is a weighed average of the elements $\{Q(\boldsymbol{x})\}$, where the weight of any $Q(\boldsymbol{x})$ is its Boltzmann weight. One could generate a set of N states $\{\boldsymbol{x}_1, ..., \boldsymbol{x}_N\}$, where a state \boldsymbol{x} occurs with a frequency proportional to its Boltzmann weight (or equivalently to its normalized probability $p(\boldsymbol{x})$ introduced in Eq. (A.1)). This allows to build an estimator of the form

$$Q_{MC} \equiv \frac{1}{N} \sum_{i=1}^{N} Q(\boldsymbol{x}_i) . \qquad (A.3)$$

In the following we show how to use a stochastic process to generate a set of states distributed as a probability distribution p.

A.2 Markov chain: ergodicity and detailed balance

Let us consider an initial microstate x_1 . One can introduce an arbitrary probability distribution $t(\boldsymbol{x} \to \boldsymbol{y}) \geq 0 \quad \forall \boldsymbol{x}, \boldsymbol{y}$, which gives the probability of transitioning from a state \boldsymbol{x} to a state \boldsymbol{y} . A new state \boldsymbol{x}_2 can be generated using the transition probability $t(\boldsymbol{x}_1, \boldsymbol{y})$. This process can be iterated until one has produced a chain of states $\{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$. Such a chain is called a Markov chain and its most remarkable feature is that the state at step idepends only on the state at step i - 1 and not on the previous history. It is costumary to say that the chain has no memory. This is a consequence of the fact that the probabilities $t(\boldsymbol{x} \to \boldsymbol{y})$ do not depend on time.

One can require the chain to converge asymptotically to a probability distribution p, by imposing some conditions on the choice of $t(\boldsymbol{x} \to \boldsymbol{y})$. A first condition could be to ask that at equilibrium the system transitions to and from any state \boldsymbol{x} at the same rate:

$$\sum_{\boldsymbol{y}} p(\boldsymbol{x}) t(\boldsymbol{x} \to \boldsymbol{y}) = \sum_{\boldsymbol{x}} p(\boldsymbol{y}) t(\boldsymbol{y} \to \boldsymbol{x}) .$$
 (A.4)

But one can show that this condition alone is not sufficient to determine such a convergence, because of a mechanism called "loop cycle" [100]. It is necessary to make further assumptions.

The previous condition could be made more strict by imposing that at equilibrium any transition occurs with a probability which is equal to the one of the inverse transition:

$$p(\boldsymbol{x})t(\boldsymbol{x} \to \boldsymbol{y}) = p(\boldsymbol{y})t(\boldsymbol{y} \to \boldsymbol{x})$$
. (A.5)

This equation is customarily called the detailed balance equation.

We would like to make a remark about the transition probabilities. One is free to set to zero some of the probabilities $t(\boldsymbol{x}, \boldsymbol{y})$ (as tipically done in Monte Carlo algorithms), but there must always exist a non-zero probability path connecting two states \boldsymbol{x} and \boldsymbol{y} (ergodicity condition [100]). This is necessary to ensure the convergence to the probability distribution regardless to the initial state. Otherwise the chain could be stuck in a region of the phase space which not connected to the regions where the most relevant states are situated.

It is possible to show [100] that under these conditions the Markov chain converges to a set distributed as the probability distribution p. In the following paragraph we see how to practically choose the transition probabilities to realize such a process.

A.3 Metropolis algorithm

The transition probability is often written as

$$t(\boldsymbol{x} \to \boldsymbol{y}) = q(\boldsymbol{x}, \boldsymbol{y}) \alpha(\boldsymbol{x}, \boldsymbol{y}) , \qquad (A.6)$$

where $q(\boldsymbol{x}, \boldsymbol{y})$ selects the pair of states to be connected by the transition, and $\alpha(\boldsymbol{x}, \boldsymbol{y})$ provides the transition state.

Let us choose at random an initial configuration x_1 for the system. The algorithm is constituted of N-1 steps and the protocol to move from step i to step i+1 is the following, where x_i is the configuration at the *i*-th step:

- Generate a configuration \boldsymbol{y} from the probability $q(\boldsymbol{x}_i, \cdot)$.
- Generate a random value ξ from the uniform distribution on (0, 1).
- Calculate the acceptance probability

$$\alpha(\boldsymbol{x}_i, \boldsymbol{y}) = \min\left\{1, \frac{e^{-\beta E_{\boldsymbol{y}}}q(\boldsymbol{y}, \boldsymbol{x}_i)}{e^{-\beta E_{\boldsymbol{x}_i}}q(\boldsymbol{x}_i, \boldsymbol{y})}\right\} , \qquad (A.7)$$

where the ratio inside the brackets is the so-called acceptance ratio.

• If $\xi \leq \alpha(\boldsymbol{x}_i, \boldsymbol{y})$, then set $\boldsymbol{x}_{i+1} = \boldsymbol{y}$, otherwise set $\boldsymbol{x}_{i+1} = \boldsymbol{x}_i$.

It can easily be checked that equation Eqs. (A.7) and (A.6) satisfy the detailed balance condition. One should notice that a set of states distributed as the probability distribution p has been generated without the explicit knowledge of the probabilities p, of which we do not know explicitly the normalization factor (represented by the partition function).

At the end of the process one has generated a sample $(x_1, ..., x_N)$ and can calculate the estimator

$$Q_{MC} \equiv \frac{\sum_{i=1}^{N} Q(\boldsymbol{x}_i)}{N} . \tag{A.8}$$

It is important to notice that the variance of this estimator cannot be estimated as $\operatorname{Var}[Q_{MC}] = \sum_{i=1}^{N} (Q(\boldsymbol{x}_i) - Q_{MC})^2 / N$, since the variables considered are not independent. Typically, for practical reasons, most of the probabilities $t(\boldsymbol{x} \to \boldsymbol{y})$ are chosen to be zero, which determines a correlation between the configurations at each step, since two subsequent configurations have similar physical properties. This calls for the necessity of considering some methods to properly account for correlations.

A.4 Autocorrelation time

One could say that in a stochastic process, correlations decay over a characteristic time scale (a certain number of steps), that is called autocorrelation time. An autocorrelation function can be defined as:

$$C_Q(j) = \frac{1}{(N-j)\sigma^2} \sum_{i=1}^{N-j} \left(Q(\boldsymbol{x}_i) - Q_{\rm MC} \right) \left(Q(\boldsymbol{x}_{i+j}) - Q_{\rm MC} \right) , \qquad (A.9)$$

where $\sigma^2 = \sum_{i=1}^{N} (Q(\boldsymbol{x}_i) - Q_{MC})^2 / N$ in the denominator is used to normalize the ratio, such that $C_Q(0) = 1$. If one assumes that the correlations decay exponentially as $C_Q(j) \sim e^{-\frac{j}{\tau_Q}}$, then it is possible to estimate the autocorrelation time by integration as

$$\tau_Q \sim \sum_{j=0}^{N-1} C_Q(j) ,$$
(A.10)

where one may notice that we kept an index Q, since this quantity is in principle observable-dependent. This implies that the effective number of uncorrelated measurements is not N, but $N/(2\tau_Q)$, which means that if we consider a point in the Markov chain, it will have τ_Q correlated elements on his left and τ_Q correlated elements on his right. As a consequence over a block of $2\tau_Q$ steps width, measures are correlated. The statistical error for the estimate of Q will then result

$$\Delta_Q = \sqrt{(2\tau_Q)\frac{\sigma^2}{N}} . \tag{A.11}$$

A.5 Reducing correlations with blocks

One way to circumvent the presence of a finite auto-correlation time is to divide the series into a set of blocks whose width is much bigger than the auto-correlation time itself. Namely, one divides the set $\{x_1, ..., x_N\}$ into k blocks of $b > \tau_Q$ elements each, such that N = kb:

$$\{x_1, ..., x_b, x_{b+1}, ..., x_{2b}, ..., x_{(k-1)b+1}, ..., x_{kb}\}$$
 (A.12)

and calculate the average of each block:

$$\{\langle Q(\boldsymbol{x})\rangle_1, ..., \langle Q(\boldsymbol{x})\rangle_b\}$$
. (A.13)

By increasing the size b of the blocks, non-consecutive blocks are less and less correlated. Once b is sufficiently big, we can assume that averages in Eq. (A.13) are independent and then calculate the variance as

$$\operatorname{Var}[Q_{MC}] = \frac{1}{k(k-1)} \sum_{i=1}^{k} \operatorname{Var}[(\langle Q \rangle_i - Q_{MC})^2] .$$
 (A.14)

Throughout this thesis error bars were estimated by making use of this formula.

A.6 Dependence on the initial configuration

As shown in Eq. (A.11), in the limit of an infinite simulation $N \to \infty$, the results of Monte Carlo tend to the exact result and do not depend on the initial configuration. But real simulations always have a finite number of steps, and the dependence on the initial configuration might result in a bias on the results, in particular if the chosen configuration is very far away (in terms of Monte Carlo steps) from the region where the most relevant states (from the point of view of Boltzmann weights) are located, or in case the system exhibits metastable states for the stochastic dynamics generated by the Monte Carlo simulation.

To eliminate any dependence on the initial configuration, and let the configuration move to the region of phase space contributing the most to the statistical sums, the first part of the MC simulation is devoted to thermalization, during which measurements of observables are not recorded. For thermalization to be effective, the length of the thermalization process should exceed the autocorrelation time of all observables of interest.

For some kind of systems thermalization might not be sufficient or might require a very large number of steps. For this reason one can use an alternative process called annealing [102]. A random configuration is chosen at a temperature much higher than the one at which the system will be studied. At high temperatures a completely random configuration is often a proper configuration of the system. A short thermalization is performed at that temperature. Then the temperature is lowered of a certain ΔT and the process is repeated. The process is iterated until the desired temperature is reached. In this way the system is guided towards the low temperature gradually with a reduced probability of getting trapped in metastable states, and it can establish the correct equilibrium regime at low temperatures. All the simulations presented in Chap. 5, for example, make use of annealing. 96

Appendix B

Formulation of AFMC without the coherent states

In the following we derive Eq. (5.7) without using the coherent-state pathintegral formalism. We make use anyway of the Hubbard-Stratonovich transformation, which is the only truly essential ingredient to obtain such a result. One can express the infinitesimal propagator exp $\left(-\Delta \tau \ \hat{\mathcal{H}}\right)$ as

$$\exp\left(-\Delta\tau \ \hat{\mathcal{H}}\right) = \exp\left[-\Delta\tau \left(\sum_{\alpha} (\epsilon_{\alpha} - K)\hat{b}_{\alpha}^{\dagger}\hat{b}_{\alpha} + \hat{\mathcal{H}}_{U,\mu-K}\right)\right]$$
(B.1)
$$= 1 - \Delta\tau \left[\sum_{\alpha} (\epsilon_{\alpha} - K)\hat{b}_{\alpha}^{\dagger}\hat{b}_{\alpha} + \hat{\mathcal{H}}_{U,\mu-K}\right] + \mathcal{O}(\Delta\tau^{2}) ,$$

where we expanded the hopping part of the Hamiltonian in terms of the eigenvalues $\{\epsilon_{\alpha}\}$ of the hopping matrix J_{ij} and corresponding density operators $\{\hat{b}_{\alpha}^{\dagger}\hat{b}_{\alpha}\}$ and we defined $\hat{\mathcal{H}}_{U,\mu-K} = \frac{U}{2}\sum_{i}\hat{n}_{i}(\hat{n}_{i}-1) - (\mu-K)\sum_{i}\hat{n}_{i}$. The density operators can be decoupled using a Hubbard-Stratonovich transformation as

$$\exp\left(-\Delta\tau \ \hat{\mathcal{H}}\right) = \int \mathcal{D}\Psi \ \mathcal{G} \left\{ 1 - \Delta\tau \left[\sum_{\alpha} \left(\Psi_{\alpha} \hat{b}^{\dagger}_{\alpha} + \Psi^{*}_{\alpha} \hat{b}_{\alpha} + \Delta\tau |\Psi_{\alpha}|^{2} \hat{b}^{\dagger}_{\alpha} \hat{b}_{\alpha} \right) + \hat{\mathcal{H}}_{U,\mu-K} \right] + \mathcal{O}(\Delta\tau^{2}) \right\}$$
$$= \int \mathcal{D}\Psi \ \mathcal{G} : e^{-\Delta\tau \left[\sum_{\alpha} (\Psi_{\alpha} \hat{b}^{\dagger}_{\alpha} + \text{h.c.}) + \hat{\mathcal{H}}_{U,\mu-K} \right]} : + \mathcal{O}(\Delta\tau^{2})$$
(B.2)

where : ... : denotes normal ordering, $\mathcal{G} = e^{-\Delta \tau \sum_{\alpha} \frac{|\Psi_{\alpha}|^2}{K - \epsilon_{\alpha}}} / \mathcal{N}$, \mathcal{N} is the normalization of the Gaussian distribution for the auxiliary field Ψ_{α} and $\mathcal{D}\Psi = \prod_{\alpha} \frac{d\Psi_{\alpha} d\Psi_{\alpha}^*}{2\pi i}$. Changing variables in the auxiliary-field integral from

 Ψ_{α} to Ψ_i , one obtains for the density operator $\hat{\rho}$ the following form:

$$\hat{\rho} = \lim_{M \to \infty} \left[\exp\left(-\Delta \tau \ \hat{\mathcal{H}}\right) \right]^{M}$$
(B.3)
$$= \lim_{M \to \infty} \left[\int \prod_{i} \prod_{k=1}^{M} \frac{d\Psi_{i,k} d\Psi_{i,k}^{*}}{2\pi i} \ \frac{e^{-\Delta \tau \sum_{k} \sum_{ij} \Psi_{i,k}^{*} \tilde{J}_{ij}^{-1} \Psi_{j,k}}}{\mathcal{N}} \ \otimes_{i} \hat{\rho}_{i} + \mathcal{O}(M\Delta \tau^{2}) \right]$$

where the local density operators read

$$\hat{\rho}_{i} = \prod_{k} : e^{-\Delta \tau \left(\Psi_{i,k}^{*} \hat{b}_{i} + \Psi_{i,k} \hat{b}_{i}^{\dagger} + \hat{\mathcal{H}}_{i}^{(d)}(U, \mu - K)\right)} : .$$
(B.4)

Taking the trace of this density operator gives precisely Eq. (5.7), thus proving the equivalence of this approach with the path-integral one.

We may observe that in the case of ordinary bosons normal ordering is not essential, and neglecting it leads to an overall multiplicative constant which appears in front of the density operator. On the other hand, for hardcore bosons the normal ordering is essential to obtain the correct density operator.

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