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Il Modello di Bose-Hubbard Disordinato

Disordered Bose-Hubbard Model

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Abstract

The interplay of disorder and interactions in condensed matter physics remains a compelling challenge, particularly in the context of the Bose-Hubbard model. This thesis explores the phase transitions that occur within the disordered Bose-Hubbard model, specifically the emergence of the Bose Glass phase.

We begin by presenting an overview of second quantization, laying the groundwork for the theoretical framework necessary to describe many-body quantum systems. From there, we delve into the functional integral formalism, providing the mathematical tools to address many-body quantum systems with statistical methods.

We then transition to the Bose-Hubbard model, where optical lattices provide the experimental realization for studying quantum phase transitions. By introducing Landau theory, we describe how phase transitions occur in pure systems and highlight the significance of the superfluid-to-Mott insulator transition in the non-disordered Bose-Hubbard model. However, introducing disorder into the system complicates this picture significantly. Using the theorem of inclusion we show that, with bounded disorder, a direct phase transition from the superfluid phase to the Mott insulating phase is not possible. Instead, a Bose Glass phase emerges: a state characterized by localized, non-superfluid regions coexisting with superfluid puddles. This phase is compressible, lacks a gap, and fundamentally alters the phase diagram of the disordered system. Given the difficulty of deriving an exact analytical solution for the disordered system's phase transition, we propose a variational approach using the overlap matrix criterion. This method allows us to capture the qualitative features of the phase transition and to predict the emergence of the Bose Glass phase with reasonable accuracy.

Through these investigations, this thesis provides new insights into the rich physics of the disordered Bose-Hubbard model and presents a method that could be extended to other disordered quantum systems. The results contribute to a deeper understanding of how disorder and interactions interplay to create new phases of matter in condensed systems.

Abstract

La comprensione del rapporto tra disordine e interazioni nei sistemi di materia condensata rappresenta una delle sfide più affascinanti, e ciò particolarmente nel contesto del modello di Bose-Hubbard. La presente tesi esplora le transizioni di fase che si verificano all'interno del modello di Bose-Hubbard disordinato, concentrandosi sull'emergenza della fase di Bose Glass.

Iniziamo presentando una panoramica della seconda quantizzazione, che costituisce la base teorica necessaria per descrivere i sistemi quantistici a molti corpi. Da qui, passiamo al formalismo dell'integrale funzionale, che fornisce gli strumenti matematici per affrontare sistemi quantistici complessi tramite metodi statistici.

Successivamente, analizziamo il modello di Bose-Hubbard, dove i reticoli ottici offrono una realizzazione sperimentale per lo studio delle transizioni di fase quantistiche. Introducendo la teoria di Landau, descriviamo come avvengono le transizioni di fase nei sistemi puri, con particolare attenzione alla transizione da superfluido a isolante di Mott nel modello di Bose-Hubbard non disordinato. Tuttavia, l'introduzione del disordine complica notevolmente questo quadro. Utilizzando il teorema delle inclusioni, mostriamo che in presenza di un disordine limitato, una transizione diretta dalla fase superfluida alla fase isolante di Mott non è possibile. Invece, emerge una fase di Bose Glass: uno stato caratterizzato dalla presenza di regioni localizzate non superfluide che coesistono con pozze superfluide. Questa fase è comprimibile, priva di gap e altera profondamente il diagramma di fase. Derivare una soluzione analitica esatta per la transizione di fase del sistema disordinato è estremamente complesso, e per tale ragione proponiamo un approccio variazionale basato sul criterio della matrice di sovrapposizione. Tale metodo mette in luce le caratteristiche qualitative fondamentali della transizione di fase e permette di prevedere l'emergenza della fase di Bose Glass con una buona accuratezza.

Attraverso queste indagini, la tesi fornisce nuove prospettive sulla fisica del modello di Bose-Hubbard disordinato e presenta un metodo generale estendibile ad altri sistemi quantistici disordinati. I risultati contribuiscono a una comprensione più profonda di come il disordine e le interazioni possano combinarsi per creare nuove fasi della materia nei sistemi condensati.

Contents

1 An Overview of Second Quantization

Quantization is the transition procedure of going from a classical theory to a quantum theory. An important example, dating back to the early days of quantum mechanics, is the canonical[1] quantization procedure: it consisted in replacing the classical dynamical variables and their Poisson brackets by quantum mechanical operators and their commutators, with the purpose to preserve the formal structure, such as symmetries, of the classical theory to the greatest extent possible.[2] Within this first approach, originally introduced by P. Dirac [3] and denoted as *First Quantization*, only the motion of the particles was quantized while the applied fields were treated classically.

This method was further used by P. Dirac in the context of quantum field theory, in his construction of quantum electrodynamics. As it turned out, the canonical quantization procedure could also be extended to field theory, such that the classical fields were replaced by quantum mechanical creation and annihilation operators: this led the wavefunctions to actually become quantized themselves. Since the resulting formulation allowed for the quantization of the fields that were in the original quantum theory still treated classically, it is commonly referred to as *Second Quantization*.

The reason for introducing the language of second quantization is that it turns out to be an extremely efficient framework in which to formulate many-particle quantum systems. As we will see, one of the major problems in dealing with many-particle quantum systems is the indistinguishability of particles in quantum mechanics, which ultimately leads to the spin-statistics theorem. While the first-quantized representation of the many-body wavefunction is clumsy, the second quantization formalism provides the means to heavily simplify the notation through the occupation number representation. The power of this formalism will become even more evident in the following chapters, as it will allow us to transition from the canonical ensemble to the grand canonical ensemble with great ease. The main references for this chapter are [11], [14] and [17].

1.1 Background

Let us start by considering a many-particle quantum system made of N identical particles. Within the context of the first quantization method, the system is described by a complex and square-integrable wave function that lives in the tensor product of Hilbert spaces $\mathscr{H}_N$.[3] If $\{\langle\alpha\rangle\}$ is an orthonormal basis of $\mathscr{H}$, the canonical orthonormal basis of $\mathscr{H}_N$ is constructed from the tensor products:

$$|\alpha_1\alpha_2\alpha_3\dots\alpha_N) := |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_N\rangle \tag{1.1}$$

Through the multilinearity of the tensor product and thanks to the completeness of the basis $\{|\alpha\rangle\}$, the following relations naturally emerge:

$$\begin{gathered}(\alpha_1\alpha_2\dots\alpha_N\,|\,\alpha_1{}'\alpha_2'\dots\alpha_N') = \langle\alpha_1|\alpha_1'\rangle\,\langle\alpha_2|\alpha_2'\rangle\cdots\langle\alpha_N|\alpha_N'\rangle \\ \sum_{\alpha_1,\dots,\alpha_N} |\alpha_1\alpha_2\dots\alpha_N)(\alpha_1\alpha_2\dots\alpha_N| = \mathbb{I}_{\mathscr{H}_N}\end{gathered} \tag{1.2}$$

Thus far we have introduced a way to describe a general system of identical particles without considering the possible symmetries of the wave function. In contrast to the multitude of pure and mixed symmetry states one could define mathematically, only totally symmetric systems $\mathcal{B}$ (bosonic) and totally antisymmetric systems $\mathcal{F}$ (fermionic) are observed in nature. Bosonic systems, being totally symmetric, are invariant under permutation $\mathcal{P}$ of elements while fermionic systems, being totally antisymmetric, change sign with the parity of permutation. For convenience, we shall adopt a unified notation for bosons and fermions[4]

$$\Psi_{\alpha_1\alpha_2\dots\alpha_N}(\vec{r}_1\vec{r}_2\dots\vec{r}_N) = (\zeta)^{\tilde{P}}\Psi_{\alpha_1\alpha_2\dots\alpha_N}(\vec{r}_{P1}\vec{r}_{P2}\dots\vec{r}_{PN}) \quad \forall P\in\mathcal{P} \tag{1.3}$$

where P is the parity of the permutation, ζ is $+1$ or -1 for bosons or fermions respectively, and $\tilde{P}$ is the minimum number of transpositions necessary to restore the permutation $(P1, P2, ..., PN)$ to its original order $(1, 2, ..., N)$.

[1] The word canonical arises from the Hamiltonian approach to classical mechanics, in which a system's dynamics is generated via canonical Poisson brackets. All transformations of variables which preserve these brackets are known as *canonical transformations* in classical mechanics.

[2] As we know, this structure is only partially preserved in canonical quantization, as it leads to the Heisenberg's Uncertainty Principle.

[3] This is true in any representation of the quantum system. As an example, in the space representation we have $\Psi_N(\vec{r}_1,\vec{r}_2,\dots,\vec{r}_N) = \Psi_N \in \mathscr{H}_N = \bigotimes_{i=1}^{N}\mathscr{H}_i$

[4] From now on, for simplicity of notation, we will not indicate the states $\{\alpha_i\}$ in the wave function.

These symmetry requirements imply corresponding restrictions to the Hilbert space $\mathcal{H}_N$ in which the system is described. Indeed, if we consider a wave function $\Psi(\vec{r}_1\vec{r}_2\dots\vec{r}_N)$ in $\mathcal{H}_N$ describing N identical particles, it will belong to the Hilbert space of N bosons $\mathcal{B}_N$, or to Hilbert space of N fermions $\mathcal{F}_N$, if it is symmetric or antisymmetric under a permutation of the particles. In order to easily project the wavefunction into the right subspace, we will define the symmetrization operator $\mathcal{P}_{\mathcal{B}}$ and the antisymmetrization operator $\mathcal{P}_{\mathcal{F}}$, both acting in $\mathcal{H}_N$, by their action on a wave function $\Psi\left(\vec{r}_1\vec{r}_2\dots\vec{r}_N\right)$

$$\mathcal{P}_{\left\{\begin{smallmatrix}\mathcal{B}\\ \mathcal{F}\end{smallmatrix}\right\}}\Psi(\vec{r}_1,\vec{r}_2,\dots,\vec{r}_N) \coloneqq \frac{1}{N!}\sum_P \zeta^P \Psi(\vec{r}_{P1}\vec{r}_{P2}\dots\vec{r}_{PN}) \tag{1.4}$$

The manifestly hermitian operator $\mathcal{P}$ is a projector, as it turns out to also be idempotent $\mathcal{P}=\mathcal{P}^2$. These operators project $\mathcal{H}_N$ into the Hilbert space of Bosons $\mathcal{B}_N$ and Fermions $\mathcal{F}_N$

$$\mathcal{B}_N \coloneqq \mathcal{P}_{\mathcal{B}}\mathcal{H}_N \qquad \mathcal{F}_N \coloneqq \mathcal{P}_{\mathcal{F}}\mathcal{H}_N \tag{1.5}$$

In these spaces, a generic state with a particle in a state α_1, another in α_2 etc. is defined in a natural way as follows

$$|\alpha_1\alpha_2\dots\alpha_N\} \coloneqq \sqrt{N!}\,\mathcal{P}_{\left\{\begin{smallmatrix}\mathcal{B}\\ \mathcal{F}\end{smallmatrix}\right\}}|\alpha_1\alpha_2\dots\alpha_N) = \frac{1}{\sqrt{N!}}\sum_P \zeta^P |\alpha_{P1}\rangle\otimes\dots\otimes|\alpha_{PN}\rangle \tag{1.6}$$

Note that these symmetrized or antisymmetrized states utilize a curly bracket in the ket symbol. From equations (1.2) and thanks to the properties of the projector operators, it follows that if $|\alpha_1\dots\alpha_N)$ is a basis of the Hilbert space $\mathcal{H}_N$ then $\mathcal{P}_{\left\{\begin{smallmatrix}\mathcal{B}\\ \mathcal{F}\end{smallmatrix}\right\}}|\alpha_1\dots\alpha_N)$ is a basis of $\mathcal{B}_N$ or $\mathcal{F}_N$. Therefore, the closure relation (1.2) in $\mathcal{H}_N$ becomes a closure relation in $\mathcal{B}_N$ or $\mathcal{F}_N$.

$$\sum_{\alpha_1,\dots,\alpha_N}\mathcal{P}_{\left\{\begin{smallmatrix}\mathcal{B}\\ \mathcal{F}\end{smallmatrix}\right\}}|\alpha_1\alpha_2\dots\alpha_N)(\alpha_1\alpha_2\dots\alpha_N|\,\mathcal{P}_{\left\{\begin{smallmatrix}\mathcal{B}\\ \mathcal{F}\end{smallmatrix}\right\}} = \frac{1}{N!}\sum_{\alpha_1,\dots,\alpha_N}|\alpha_1\alpha_2\dots\alpha_N\}\{\alpha_1\alpha_2\dots\alpha_N| = \mathbb{I}_{\left\{\begin{smallmatrix}\mathcal{B}\\ \mathcal{F}\end{smallmatrix}\right\}} \tag{1.7}$$

With the same reasoning, if the basis $|\alpha)$ is orthogonal in $\mathcal{H}$, then the basis $|\alpha_1\dots\alpha_N)$ is orthogonal in $\mathcal{B}_N$ or $\mathcal{F}_N$. The scalar product of two such vectors constructed from the same basis $|\alpha\rangle$ is:

$$\begin{aligned}
\{\alpha_1\alpha_2\dots\alpha_N\,|\,\alpha'_1\alpha'_2\dots\alpha'_N\} &= N!\left(\alpha_1\alpha_2\dots\alpha_N\left|\mathcal{P}^2_{\left\{\begin{smallmatrix}\mathcal{B}\\ \mathcal{F}\end{smallmatrix}\right\}}\right|\alpha'_1\alpha'_2\dots\alpha'_N\right)\\
&= N!\left(\alpha_1\alpha_2\dots\alpha_N\left|\mathcal{P}_{\left\{\begin{smallmatrix}\mathcal{B}\\ \mathcal{F}\end{smallmatrix}\right\}}\right|\alpha'_1\alpha'_2\dots\alpha'_N\right)\\
&= N!\,\frac{1}{N!}\sum_P \zeta^P\left(\alpha_{P1}\dots\alpha_{PN}\,|\,\alpha'_1\dots\alpha'_N\right)\\
&= \sum_P \zeta^P\,\langle\alpha_{P1}|\alpha'_1\rangle\,\langle\alpha_{P2}|\alpha'_2\rangle\cdots\langle\alpha_{PN}|\alpha'_N\rangle
\end{aligned} \tag{1.8}$$

Because of the orthogonality of the basis $|\alpha\rangle$, the only non-vanishing terms in the right hand side of (1.8) are the permutations P such that

$$\alpha'_1=\alpha_{P1}\,,\ \alpha'_2=\alpha_{P2}\,,\dots,\alpha'_N=\alpha_{PN}$$

For fermions, since there is at most one particle per state $|\alpha\rangle$, no two identical states can be present in the set $\alpha_1,\dots,\alpha_N$ and therefore there exists only one permutation P which transforms $\alpha_1,\dots,\alpha_N$ into $\alpha'_1,\dots,\alpha'_N$. The sum in (1.4) then reduces to one term, and if the states $|\alpha_i\rangle$ are normalized, we obtain

$$\text{Fermions}\ \longrightarrow\ \{\alpha_1\alpha_2\dots\alpha_N\,|\,\alpha'_1\alpha'_2\dots\alpha'_N\} = (-1)^P \tag{1.9}$$

For bosons there are not limitation for the number of particles in the same state, so any permutation which does interchange particles in the same state contributes to the sum (1.8). By defining the occupation number n_{α_i} as the number of particles in the state α_i, we have that the bra-ket between two different states is given by the sum of all the permutation in each state:

$$\text{Bosons}\ \longrightarrow\ \{\alpha_1\alpha_2\dots\alpha_N\,|\,\alpha'_1\alpha'_2\dots\alpha'_N\} = n_{\alpha_1}!n_{\alpha_2}!\dots n_{\alpha_N}! \tag{1.10}$$

Finally, an orthonormal basis for the Hilbert space $\mathcal{B}_N$ or $\mathcal{F}_N$ is obtained by utilizing (1.9)-(1.10) to normalize the states $|\alpha_1\alpha_2\dots\alpha_N\}$

$$|\alpha_1\alpha_2\dots\alpha_N\rangle = \frac{1}{\sqrt{N!}}\frac{1}{\sqrt{\prod_\alpha n_\alpha!}}\sum_P \zeta^P\,|\alpha_{P1}\dots\alpha_{PN}) \tag{1.11}$$

Note that in contrast to the states defined in (1.1) and (1.6), the normalized symmetric or antisymmetric states defined in (1.11) utilize an angular bracket in the ket symbol. Because orthonormality was used in the calculation of the normalization factor, it will be understood henceforth that whenever the symbol $|\alpha_1\dots\alpha_N\rangle$ is utilized, the basis

$|\alpha_i\rangle$ is orthonormal. Finally using (1.11) and the normalization condition, the closure relation in $\mathcal{B}_N$ or $\mathcal{F}_N$ is given by

$$\sum_{\alpha_1,\ldots,\alpha_N} \frac{\prod_\alpha n_\alpha!}{N!} |\alpha_1 \ldots \alpha_N\rangle\langle\alpha_1 \ldots \alpha_N| = \mathbb{I}_{\{\substack{\mathcal{B}\\\mathcal{F}}\}} \tag{1.12}$$

The overlap between two normalized and symmetrized or antisymmetrized states $|\beta_1 \ldots \beta_N\rangle$ and $|\alpha_1 \ldots \alpha_N\rangle$ can be written as follows, where $\mathcal{S}(M_{ij})$ denotes a permanent for bosons and a determinant for fermions.

$$\begin{aligned}\langle\beta_1 \ldots \beta_N|\alpha_1 \ldots \alpha_N\rangle &= \frac{1}{\sqrt{\prod_\beta n'_\beta! \prod_\alpha n_\alpha!}} \sum_P \zeta^P \langle\beta_1|\alpha_{P1}\rangle \langle\beta_2|\alpha_{P2}\rangle \cdots \langle\beta_N|\alpha_{PN}\rangle \\ &= \frac{\mathcal{S}(\langle\beta_i|\alpha_j\rangle)}{\sqrt{\prod_\beta n'_\beta! \prod_\alpha n_\alpha!}} = \begin{cases} \frac{1}{\sqrt{N!}} \mathrm{Det}(M_{ij}) & \text{Fermions} \\ \frac{1}{\sqrt{N! \prod_\alpha n_\alpha!}} \mathrm{Per}(M_{ij}) & \text{Bosons} \end{cases}\end{aligned} \tag{1.13}$$

1.2 Creation and Annihilation operators

As we have seen, a fundamental postulate of quantum mechanics is that identical particles are intrinsically indistinguishable. We have dealt with this fundamental property of many-body quantum systems in the previous section, however the expression (1.11) makes it clear that the first quantised representation of the many-body wavefunction is clumsy. First quantization complicates the description of many-body states for indistinguishable particles, requiring intricate symmetrization, because it redundantly associates each particle with a specific state - a meaningless approach when the particles are identical.

The second quantisation provides the means to heavily condense the formalism by shifting the focus from associating individual particles with specific states, to counting the number of particles in each state. This defines the occupation number representation, where the basis states are written as

$$|\mathbf{n}\rangle \equiv |n_1, n_2, \ldots\rangle \quad \text{where} \quad \textstyle\sum_i n_i = N \tag{1.14}$$

with n_i representing the occupation number of the i-th single particle state, and N being the total number of particles. In the case of bosons n_i can be any non-negative integer, whereas for fermions the *Pauli exlusion principle* restricts n_i to either 0 or 1. Because this description does not refer to the labeling of particles, it contains no redundant information, and hence leads to a precise and simpler description of the quantum many-body state. As a result, any bosonic (or fermonic) many-particle state in $\mathcal{B}_N$ (or $\mathcal{F}_N$) can be obtained by a linear superposition of the basis states $|n_1, n_2, \ldots\rangle$.

In order to make our argument more general, we will eventually have to emancipate ourselves from the condition of a fixed particle number N. In the occupation number representation, this can be done straightforwardly. A Hilbert space large enough to accommodate a state with an undetermined number of particles is given by

$$\mathcal{B} := \mathcal{B}_0 \oplus \mathcal{B}_1 \oplus \ldots \oplus \mathcal{B}_\infty = \bigoplus_{i=0}^{\infty} \mathcal{B}_i \qquad \mathcal{F} := \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \ldots \oplus \mathcal{F}_\infty = \bigoplus_{i=0}^{\infty} \mathcal{F}_i$$

where the spaces $\mathcal{F}$ (for identical fermions) and $\mathcal{B}$ (for identical bosons) are called *Fock spaces* and ultimately define the principal arena of quantum many-body theory.[5] To obtain a basis for $\mathcal{F}$ (or $\mathcal{B}$), known as *Fock states*, it is sufficient to take the complete set of our previous basis states $|n_1, n_2, \ldots\rangle$ and remove the condition $\sum_i n_i = N$ on the occupation numbers. A general many-body state $|\Psi\rangle$ can then be represented by a linear superposition

$$|\Psi\rangle = \sum_{n_1,n_2,\ldots} c_{n_1 n_2 \ldots} |n_1, n_2, \cdots\rangle \tag{1.15}$$

The occupation number representation is a step forward, but it does not fully resolve our main challenge, as we have not yet addressed the symmetrization or antisymmetrization of the quantum many-particle state. For each single particle state $|\alpha\rangle$ of the single particle space $\mathcal{H}$, we define a bosonic or fermionic **creation operator** $a^\dagger_\alpha$ by its action on any symmetrized or antisymmetrized Fock state in the occupation number representation $|n_1, n_2, \cdots\rangle$, living in $\mathcal{B}$ or $\mathcal{F}$. The creation operator is defined as a linear map $a^\dagger_\alpha : \mathcal{F}^N \to \mathcal{F}^{N+1}$ (or $a^\dagger_\alpha : \mathcal{B}^N \to \mathcal{B}^{N+1}$) such that

$$a^\dagger_\alpha |n_1, \ldots, n_i, \ldots\rangle \equiv (n_\alpha + 1)^{1/2} \zeta^{s_\alpha} |n_1, \ldots, n_\alpha + 1, \ldots\rangle \tag{1.16}$$

where $s_\alpha = \sum_{j=1}^{\alpha-1} n_j$, and n_α is the occupation number of the state $|\alpha\rangle$ in $|\alpha_1 \ldots \alpha_N\rangle$. In the fermionic case, the occupation numbers n_i have to be understood mod 2: since there can be at most one fermion in a given state, the

[5] Here we are implicitly denoting $\mathcal{B}_0 = \mathcal{F}_0 = |0\rangle$ and $\mathcal{B}_1 = \mathcal{F}_1 = \mathcal{H}$. As it will be clear in a moment, $|\mathbf{0}\rangle$ is the **vacuum state** or the state with zero particles.

result will be evidently zero if the state $|\alpha\rangle$ is present in $|\alpha_1 \dots \alpha_N\rangle$, thanks to the *Pauli exclusion principle*. Physically the operator $a^\dagger_\alpha$ adds a particle in state $|\alpha\rangle$ to the state on which it operates, and symmetrizes or antisymmetrizes the new state.

In addition to the many-particle states we have used thus far, it is now useful to define the **vacuum state** $|\mathbf{0}\rangle$, which represents a state with zero particles.[6] As a consequence of (1.16), we are able to generate every basis state of $\mathcal{F}$ (or $\mathcal{B}$) by repeatedly applying $a^\dagger_\alpha$ to the vacuum state.

$$a^\dagger_\alpha |\mathbf{0}\rangle = |\alpha\rangle\,, \qquad |n_1, n_2, \dots\rangle = \prod_i \frac{1}{(n_i!)^{1/2}} \left(a^\dagger_i\right)^{n_i} |\mathbf{0}\rangle \tag{1.17}$$

This result makes a significant claim: the complex permutation entanglement inherent in (1.11) can be produced through the simple application of a set of linear operators to a single reference state. As a result, the creation operators generate the entire Fock space by repeated action on the vacuum state.

Now, since quantum mechanics is a unitary theory, whenever a new operator is introduced it is important to determine the hermitian adjoint. The operators $a^\dagger_\alpha$ are not self-adjoint, and therefore we define the annihilation operators a_α as the adjoints of the creation operators $a^\dagger_\alpha$. The action of a_α on bras follows from the action of the adjoint, while their action on a ket can be deduced by observing the matrix element between two arbitrary states:

$$\overbrace{\{\alpha_1 \dots \alpha_N \mid a_\alpha}^{N+1 \text{ components}} \underbrace{\mid \beta_1 \dots \beta_M\}}_{M \text{ components}} \qquad \begin{aligned} \langle n_1, \dots, n_\alpha, \dots | a^\dagger_\alpha | n'_1, \dots, n'_\alpha, \dots\rangle &= (n'_\alpha + 1)^{1/2}\, \zeta^{s'_\alpha}\, \delta_{n_1, n'_1} \dots \delta_{n_\alpha, n'_\alpha + 1} \dots \\ \langle n'_1, \dots, n'_\alpha, \dots | a_\alpha | n_1, \dots, n_i, \dots\rangle &= n_\alpha^{1/2} \zeta^{s_\alpha} \delta_{n'_1, n_1} \dots \delta_{n'_\alpha, n_\alpha - 1} \dots \end{aligned}$$

where, on the left, the braket is non-zero only if $N + 1 = M$. As a result, the annihilation operator consists in the (adjoint) linear map $a_\alpha : \mathcal{F}^N \to \mathcal{F}^{N-1}$ (or $a_\alpha : \mathcal{B}^N \to \mathcal{B}^{N-1}$) whose effect is to decrease the number of particles in the state on which it acts by one, according to the equation

$$a_\alpha |n_1, \dots, n_\alpha, \dots\rangle = n_\alpha^{1/2} \zeta^{s_\alpha} |n_1, \dots, n_\alpha - 1, \dots\rangle \tag{1.18}$$

which identifies a_α as the **annihilation operator**. As a result, when acting on the vacuum $|0\rangle$ for any state $|\alpha\rangle$, we find $a_\alpha |0\rangle = 0$, which means that the vacuum is the kernel of the annihilation operators.

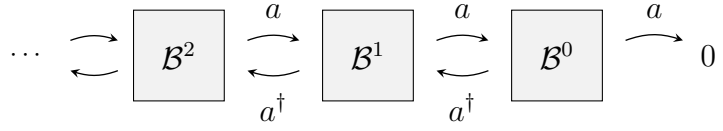

Figure 1.1: Representation of the bosonic Fock subspaces $\mathcal{F}^N$ generated by the repeated application of creation operators to the vacuum space $\mathcal{F}^0$. An identical representation can be given for the fermionic Fock subspaces.[7]

In order to preserve the integrity of the theory we have developed, it is crucial that the operators respect the symmetries of the wavefunction. This is achieved when the creation and annihilation operators satisfy the following algebraic closure relations:

$$\left[a_\lambda, a^\dagger_\mu\right]_{-\zeta} = \delta_{\lambda,\mu} \qquad \left[a^\dagger_\lambda, a^\dagger_\mu\right]_{-\zeta} = 0 \qquad \left[a_\lambda, a_\mu\right]_{-\zeta} = 0 \tag{1.19}$$

where $[\hat{A}, \hat{B}]_{-\zeta} \equiv \hat{A}\hat{B} - \zeta \hat{B}\hat{A}$ denotes the commutator ($\zeta = 1$) or the anticommutator ($\zeta = -1$), corresponding to bosons or fermions, respectively. In the fermionic case, $[a^\dagger_\lambda, a^\dagger_\lambda]_{-\zeta} = 0$ leads to $(a^\dagger_\lambda)^2 = 0$ indicating that the creation operator is nihilpotent, which reflects the *Pauli exclusion principle*.

1.3 Applications

The framework of second quantization has successfully described many-body quantum systems and the inherent indistinguishability of identical particles. However, to fully reformulate many-body quantum mechanics, we need to connect these definitions with standard quantum mechanical operations. Specifically, we must understand how changes in single-particle bases affect the operator algebra, and how generic operators in many-particle Hilbert spaces can be expressed using creation and annihilation operators.

[6] It is important to point out that $|\mathbf{0}\rangle$ is a physical state with no particles, and must be distinguished from the zero of the Hilbert space.
[7] Creation and annihilation operators do not operate within a single Fock subspace $\mathcal{B}_N$ or $\mathcal{F}_N$; rather, they act between adjacent Fock subspaces. Collectively, they allow us to navigate between subspaces of the entire Fock space.

Basis change. Let us consider the linear transformation $|\tilde{\alpha}\rangle = \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle\,|\alpha\rangle$ which maps the orthonormal basis $\{|\alpha\rangle\}$ into another basis $\{|\tilde{\alpha}\rangle\}$. By using the Dirac completeness $\mathbb{I} = \sum_{\alpha=0}^{\infty} |\alpha\rangle\langle\alpha|$ and the definitions above, for any set of a basis state $|\alpha_1 \dots \alpha_N\rangle$ we obtain

$$a^\dagger_{\tilde{\alpha}} = \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle\, a^\dagger_\alpha \qquad a_{\tilde{\alpha}} = \sum_\alpha \langle\tilde{\alpha}|\alpha\rangle\, a_\alpha \tag{1.20}$$

from which analogous algebraic closure relations can be deduced. Explicitly, commutation and anticommutation relations for $a^\dagger_{\tilde{\alpha}}$ and $a_{\tilde{\alpha}}$ result to be[8]

$$\left[a_{\tilde{\beta}}, a^\dagger_{\tilde{\alpha}}\right]_{-\zeta} = \langle\tilde{\beta}|\tilde{\alpha}\rangle \qquad \left[a^\dagger_{\tilde{\alpha}}, a^\dagger_{\tilde{\beta}}\right]_{-\zeta} = 0 \qquad \left[a_{\tilde{\alpha}}, a_{\tilde{\beta}}\right]_{-\zeta} = 0 \tag{1.21}$$

As we will see in the proceedings, within the context of the functional integral formulation of quantum statistical mechanics, the spatial coordinate basis $\{|x\rangle\}$ is of utmost importance. In this basis the creation and annihilation operators, now called **field operators**, are traditionally denoted by $\hat{\psi}^\dagger(x)$ and $\hat{\psi}(x)$. Their expansion on a basis $\{|\alpha\rangle\}$ and their commutation and anticommutation relations can be found straightforwardly

$$\hat{\psi}^\dagger(x) = \sum_\alpha \langle\alpha|x\rangle\, a^\dagger_\alpha = \sum_\alpha \Phi^*_\alpha(x)\, a^\dagger_\alpha \qquad \hat{\psi}(x) = \sum_\alpha \langle x|\alpha\rangle\, a_\alpha = \sum_\alpha \Phi_\alpha(x)\, a_\alpha \tag{1.22}$$

$$\left[\hat{\psi}(x), \hat{\psi}^\dagger(y)\right]_{-\zeta} = \delta(x-y) \qquad \left[\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(y)\right]_{-\zeta} = 0 \qquad \left[\hat{\psi}_(x), \hat{\psi}(y)\right]_{-\zeta} = 0 \tag{1.23}$$

Representation of operators. In addition to generating all the many-particle states in the Fock space by repeated action on the vacuum state, a fundamental property of creation and annihilation operators is that they provide a basis for all operators in the Fock space. That is, any operator can be expressed as a linear combination of the set of all products of the operators $a^\dagger_\alpha$ and a_α.[9] As compared to the conventional description, the formulation of interaction processes within the language of second quantisation is considerably more effective.

In order to show this, we must start by considering matrix elements of many-body operators in the canonical basis (1.1) of $\mathcal{H}_N$. Their corresponding representation in the spaces $\mathcal{B}_N$ and $\mathcal{F}_N$ can be obtained using the symmetrization and antisymmetrization operators. That being said, a convenient method to move to the second quantization representation is to diagonalize the above operators in a suitable basis, and then transform them to a general basis. In order to represent the operator in the diagonal basis, we define the **occupation number operator** $\hat{n}_\alpha$

$$\hat{n}_\alpha := a^\dagger_\alpha a_\alpha = a_\alpha a^\dagger_\alpha - 1 \qquad \hat{n}_{\alpha_j}\,|n_{\alpha_1}, n_{\alpha_2}, \dots\rangle = n_{\alpha_j}\,|n_{\alpha_1}, n_{\alpha_2}, \dots\rangle \tag{1.24}$$

This operator counts the number of particles in the state $|\alpha_j\rangle$ within the many-particle state $|\Phi\rangle$.[10] If the orthonormal basis $\{|\alpha\rangle\}$ is transformed into another basis $\{|\tilde{\alpha}\rangle\}$, the number operator will change accordingly to equations (1.20). Additionally, we define the **total occupation number operator** as $\hat{N} = \sum_\alpha \hat{n}_\alpha = \sum_\alpha a^\dagger_\alpha a_\alpha$ which counts the total number of particles in the system.

We begin by considering an hermitian **single-particle operator** $\hat{\mathcal{U}}$ acting in a N-particle Fock subaspace, assumed to be diagonal in the basis $\{|\alpha\rangle\}$. Since one-body operators affect one particle at a time, its action on a state $|\alpha_1 \dots \alpha_N\rangle$ of N particles is the sum of the action of $\hat{\mathcal{U}}$ on each particle

$$\begin{aligned} \hat{\mathcal{U}}\,|\alpha_1 \dots \alpha_N) &= \textstyle\sum_{i=1}^N \hat{\mathcal{U}}^i\,|\alpha_1 \dots \alpha_N) \\ \hat{\mathcal{U}}\,|\alpha\rangle &= \mathcal{U}_\alpha\,|\alpha\rangle \quad \text{with} \quad \mathcal{U}_\alpha = \langle\alpha|\hat{\mathcal{U}}|\alpha\rangle \end{aligned} \tag{1.25}$$

where the operator $\hat{\mathcal{U}}^i$ acts only on the i-th particle. As we will show in the next page, a single-particle operator in the diagonal representation can be found by simply counting the number of particles in a state $|\alpha\rangle$ and multiplying by the correspondent eigenvalue $\mathcal{U}_\alpha$. Finally, by transforming from the diagonal representation to a general basis, we obtain the following general result

$$\hat{\mathcal{U}} = \sum_\alpha \mathcal{U}_\alpha \hat{n}_\alpha = \sum_\alpha \langle\alpha|\hat{\mathcal{U}}|\alpha\rangle\; a^\dagger_\alpha a_\alpha \quad \xrightarrow{\text{basis change}} \quad \hat{\mathcal{U}} = \sum_{\mu\nu} \langle\mu|\hat{\mathcal{U}}|\nu\rangle\, a^\dagger_\mu a_\nu \tag{1.26}$$

[8] In the event that the basis $\{|\tilde{\alpha}\rangle\}$ is orthonormal, the commutation relations for $a^\dagger_{\tilde{\alpha}}$ and $a_{\tilde{\alpha}}$ reduce to those of $a^\dagger_\alpha$ and a_α.

[9] This argument can be made quantitative by group theoretical reasoning. Equations (1.21) and (1.11) define the **irreducible representation** of an operator algebra: an algebra because commutation relations define products in the space of generators a_λ and $a^\dagger_\lambda$; a representation because the operators act in a vector space, namely the Fock space, which is irreducible since all states $|\lambda_1, \dots, \lambda_N\rangle$ can be reached by iterative application of operators onto a unique reference state, namely the vacuum state.

[10] This works because $\hat{n}_\alpha$ commutes with all $a^\dagger_{\alpha' \neq \alpha}$. Indeed, momentarily shifting to the first quantization formalism:

$$\hat{n}_\alpha\,|\alpha_1 \dots \alpha_N\} = a^\dagger_\alpha a_\alpha\,|\alpha_1 \dots \alpha_N\} = \textstyle\sum_{i=1}^N \zeta^{i-1}\delta_{\alpha\alpha_i}\, a^\dagger_\alpha\,|\alpha_1 \dots \alpha_i \dots \alpha_N\} = \left[\sum_{i=1}^N \delta_{\alpha\alpha_i}\right]|\alpha_1 \dots \alpha_i \dots \alpha_N\}$$

Proof.
$$\begin{aligned}
\{\beta_1\dots\beta_N|\hat{\mathcal{U}}|\alpha_1\dots\alpha_N\} &= N!\,(\beta_1\dots\beta_N|\mathcal{P}\,\hat{\mathcal{U}}\,\mathcal{P}|\alpha_1\dots\alpha_N)\\
&= \frac{1}{N!}\sum_{\mathbf{P}'',\mathbf{P}'}\zeta^{\mathbf{P}''+\mathbf{P}'}\sum_i\prod_{k\neq i}\langle\beta_{\mathbf{P}'k}|\alpha_{\mathbf{P}''k}\rangle\,\langle\beta_{\mathbf{P}'i}|\mathcal{U}_\alpha^{\mathbf{P}''i}|\alpha_{\mathbf{P}''i}\rangle\,\langle\beta_{\mathbf{P}'i}|\alpha_{\mathbf{P}''i}\rangle\\
\mathbf{P}'=\mathbf{P}\circ\mathbf{P}'' \qquad &= \frac{1}{N!}\sum_{\mathbf{P},\mathbf{P}''}\zeta^{\mathbf{P}}\sum_i\prod_{k\neq i}\langle\beta_{\mathbf{P}\mathbf{P}''k}|\alpha_{\mathbf{P}''k}\rangle\,\langle\beta_{\mathbf{P}\mathbf{P}''i}|\alpha_{\mathbf{P}''i}\rangle\,\mathcal{U}_\alpha^{\mathbf{P}''i}\\
&= \frac{N!}{N!}\sum_{\mathbf{P}}\zeta^{\mathbf{P}}\sum_i\prod_{k\neq i}\langle\beta_{\mathbf{P}k}|\alpha_k\rangle\,\langle\beta_{\mathbf{P}i}|\mathcal{U}_\alpha^i|\alpha_i\rangle = \left[\textstyle\sum_i\mathcal{U}_\alpha^i\right]\sum_{\mathbf{P}}\zeta^{\mathbf{P}}\prod_k\langle\beta_{\mathbf{P}k}|\alpha_k\rangle\\
&= \textstyle\sum_i\mathcal{U}_\alpha^i\{\beta_1\dots\beta_N|\alpha_1\dots\alpha_N\} = \{\beta_1\dots\beta_N|\sum_\alpha\mathcal{U}_\alpha\hat{n}_\alpha|\alpha_1\dots\alpha_N\}
\end{aligned}$$

In the last line, we have substituted the sum over the states of each particle with the sum over every possible state by means of the particle number operator. Since this equality holds for any set of states, the result is indeed proven.

Similarly, a **two-particle operator** $\hat{\mathcal{V}}$ may be expressed in terms of creation and annihilation operators. Two-body operators are needed to describe pairwise interactions between particles, and essentially consist into the quantum mechanical analogue of the classical two-body interaction potential. Following the same reasoning, we will start by considering the basis $\mathcal{V}_{\alpha\beta}$ in which $\hat{\mathcal{V}}$ is diagonal. Since two-body operators affect pairs of two particles at a time, its action is obtained by summing over pairs of single-particle states $|\alpha\rangle$ and $|\beta\rangle$ and multiplying the matrix element $(\alpha\beta|V|\alpha\beta)$ by the number of pairs of such particles present in the physical state.

$$\begin{aligned}
\hat{\mathcal{V}}\,|\alpha_1\dots\alpha_N) &= \tfrac{1}{2}\textstyle\sum_{i\neq j}\hat{\mathcal{V}}_{\alpha_i\alpha_j}\,|\alpha_1\dots\alpha_N)\\
\hat{\mathcal{V}}|\alpha\beta) = \mathcal{V}_{\alpha\beta}|\alpha\beta) \quad &\text{with} \quad \mathcal{V}_{\alpha\beta} = (\alpha\beta|\hat{\mathcal{V}}|\alpha\beta)
\end{aligned} \tag{1.27}$$

As a result, we need to construct an operator $\hat{\mathcal{P}}_{\alpha\beta}$ which counts the number of pairs of particles in the states $|\alpha\rangle$ and β. If $|\alpha\rangle$ and β are different, the number of pairs is $n_\alpha n_\beta$; whereas if $|\alpha\rangle = |\beta\rangle$, the number of pairs is $n_\alpha(n_\alpha-1)$. Hence, the operator which counts pairs may be written:

$$\begin{aligned}
\hat{\mathcal{P}}_{\alpha\beta} &= \hat{n}_\alpha\hat{n}_\beta - \delta_{\alpha,\beta}\hat{n}_\alpha = a_\alpha^\dagger a_\alpha a_\beta^\dagger a_\beta - \delta_{\alpha,\beta}a_\alpha^\dagger a_\alpha\\
&= a_\alpha^\dagger\zeta a_\beta^\dagger a_\alpha a_\beta + a_\alpha^\dagger\delta_{\alpha\beta}a_\beta - \delta_{\alpha\beta}a_\alpha^\dagger a_\alpha = \zeta a_\alpha^\dagger a_\beta^\dagger a_\alpha a_\beta\\
&= \zeta^2 a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha = a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha
\end{aligned} \tag{1.28}$$

and the two-particle operator $\hat{\mathcal{V}}$ in its diagonal representation immediately follows.[11] Finally, transforming from the diagonal representation to an arbitrary basis, the general expression far a two-body operator is

$$\hat{\mathcal{V}} = \frac{1}{2}\sum_{\alpha\beta}\mathcal{V}_{\alpha\beta}\hat{\mathcal{P}}_{\alpha\beta} = \frac{1}{2}\sum_{\alpha\beta}\mathcal{V}_{\alpha\beta}\,a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha \quad\xrightarrow{\text{basis change}}\quad \hat{\mathcal{V}} = \tfrac{1}{2}\sum_{\lambda\mu\nu\rho}(\lambda\mu|\mathcal{V}|\nu\rho)a_\lambda^\dagger a_\mu^\dagger a_\rho a_\nu \tag{1.29}$$

Proof.
$$\begin{aligned}
\left\{\beta_1\dots\beta_N|\hat{\mathcal{V}}|\alpha_1\dots\alpha_N\right\} &= \frac{1}{2}\sum_{\mathbf{P}}\zeta^{\mathbf{P}}\sum_{i\neq j}\prod_{k\neq i,j}\langle\beta_{\mathbf{P}k}|\alpha_k\rangle\,(\beta_{\mathbf{P}i}\beta_{\mathbf{P}j}|\hat{\mathcal{V}}|\alpha_i\alpha_j)\\
&= \left[\tfrac{1}{2}\textstyle\sum_{i\neq j}\mathcal{V}_{\alpha_i\alpha_j}\right]\{\beta_1\dots\beta_N|\alpha_1\dots\alpha_N\}\\
&= \left\{\beta_1\dots\beta_N|\tfrac{1}{2}\textstyle\sum_{\alpha\beta}\mathcal{V}_{\alpha\beta}\hat{\mathcal{P}}_{\alpha\beta}|\alpha_1\dots\alpha_N\right\}
\end{aligned}$$

By generalizing the preceding arguments, we can use a and $a^\dagger$ to build up every N particle operator, with the result

$$\hat{\mathcal{R}} = \frac{1}{N!}\sum_{\lambda_1\dots\lambda_N}\sum_{\mu_1\dots\mu_N}(\lambda_1\dots\lambda_N|\hat{\mathcal{R}}|\mu_1\dots\mu_N)\,a_{\lambda_1}^\dagger\cdots a_{\lambda_N}^\dagger a_{\mu_N}\cdots a_{\alpha_1} \tag{1.30}$$

Normal Ordering. As we have shown previously, within the framework of second quantization, any operator can be expressed as a linear combination of the set of all products of the operators $a_\alpha^\dagger$ and a_α. For the proceeding, as we will introduce the path integral in quantum field theory, it is important to introduce the concept of **normal ordering** (or **Wick ordering**). An operator is said to be normal ordered (or **Wick ordered**) when all creation operators are to the left of all annihilation operators in the product

$$A = A\left(a^\dagger, a\right) \quad\xrightarrow{\text{Normal Order}}\quad A = a^\dagger a^\dagger a^\dagger\cdots a^\dagger a\cdots aaa$$

The process of normal ordering is particularly important for a quantum mechanical Hamiltonian. When quantizing a classical Hamiltonian there is some freedom when choosing the operator order, and these choices lead to differences

[11] Note the order of annihilation operators in this expression which is required to remove the factor ζ.

in the ground state energy.[12] The second-quantized form of the first-quantized N-body Hamiltonian can be most generically expressed as follows

$$\hat{H}(a^\dagger, a) = \sum_i \varepsilon_i a_i^\dagger a_i + \sum_{ijkl} V_{ii'jj'} a_i^\dagger a_{i'}^\dagger a_j a_{j'} \tag{1.31}$$

The non-interacting part, on the left, is expressed in its diagonal basis and can be easily understood: $a_i^\dagger a_i$ counts the number of particles in each single particle state $|n_i\rangle$, which is then multiplied by the single-particle eigenenergy ε_i to give the total energy of the noninteracting system. On the right, the two-body interaction term[13] has been expressed in a non-diagonal basis, where the matrix elements of the two-body interaction are given by:

$$V_{i,i',j,j'} = \int d\mathbf{x} \int d\mathbf{x}' \chi_i^*(\mathbf{x}) \chi_{i'}^*(\mathbf{x}') V(\mathbf{x} - \mathbf{x}') \chi_j^*(\mathbf{x}) \chi_{j'}^* \tag{1.32}$$

The second-quantized expression for the interacting part of the Hamiltonian is also intuitively clear: two particles that are initially in a state $|i\rangle$ and $|i'\rangle$ can scatter into the states $|j\rangle$ and $|j'\rangle$ under the influence of the interaction potential $V(\mathbf{x} - \mathbf{x}')$. Moreover, the probability amplitude for this process to happen is given by $V_{i,i',j,j'}$.

Coherent States. In single-particle quantum mechanics, the Hamiltonian is naturally expressed using coordinate and momentum eigenstates. Transitioning to many-body quantum mechanics, however, requires a new formalism - the framework of second quantization - where operators, including the Hamiltonian, are efficiently represented with creation and annihilation operators. Our next goal, similar to what we did in first quantization, is to determine the eigenstates of such operators a_α and $a_\alpha^\dagger$, known as **coherent states**.

A coherent state is defined to be the (unique) eigenstate of the annihilation operator a corresponding to the eigenvalue α. These coherent states form an extremely useful basis of Fock space, known as the **coherent state basis**. While this basis is not orthonormal, it does span the whole Fock space, leading to what is known as the **coherent state representation**.

The reason for focusing on the annihilation operator, rather than the creation operator, is that *creation operators cannot have eigenstates*. To see this, consider an arbitrary vector $|\phi\rangle$ in the Fock space, which can expanded as

$$|\phi\rangle = \sum_{n_1,n_2,\ldots} \Phi_{n_1,n_2,\ldots} |n_1, n_2, \cdots\rangle = \sum_{n_1,n_2,\ldots} \Phi_{n_1,n_2,\ldots} \left[\frac{a_1^\dagger}{\sqrt{n_1!}} \frac{a_2^\dagger}{\sqrt{n_2!}} \cdots \right] |\mathbf{0}\rangle \tag{1.33}$$

Occupation numbers have a minimum value but no maximum. When $a^\dagger |\phi\rangle$ is applied, it increases by one the minimum occupation number for every ket, making it impossible for $|\phi\rangle$ to be an eigenvector. On the other hand, applying $a |\phi\rangle$ reduces the maximum occupation number by one. Since the occupation number cannot be infinite, it is possible for the annihilation operator to have an eigenvector.

Let us assume we have successfully constructed an eigenstate $|\phi\rangle$ of the annihilation operator. This means that the state $|\phi\rangle$ simultaneously diagonalizes all annihilation operators

$$\begin{array}{c} a_i |\phi\rangle = \phi_i |\phi\rangle \ \text{ for all } i \\ [\phi_i, \phi_j]_\zeta = 0 \end{array} \quad \xrightarrow[\text{eigenstate}]{\text{bosonic}} \quad |\phi\rangle \equiv \exp\left(\sum_i \phi_i a_i^\dagger \right) |\mathbf{0}\rangle \tag{1.34}$$

where the correspondent eigenvalues ϕ_i are, in general complex numbers.[14] Although the general form of these states is similar for both bosons and fermions, the key difference lies in their *algebraic structure*, particularly when multiple annihilation operators act on a coherent state. The commutation or anticommutation relations of the operators lead to corresponding relations for the eigenvalues. For fermions, these eigenvalues anticommute, which requires the introduction of anticommuting variables called **Grassmann numbers** to handle this feature. For bosons, however, the eigenvalues commute, allowing us to proceed using ordinary numbers without additional complications. Since our focus is on developing a formalism for bosons, we will focus on the bosonic case (where such issues do not arise) for which the **boson coherent state** was already presented in (1.34).

To prove it, let us apply the eigenvalue conditions (1.34) to an arbitrary coherent state $|\phi\rangle$ in the Fock space, which can be expaned as in (1.33). As a result, we find:[15]

[12] That's why the process can also be used to eliminate the infinite vacuum energy of a quantum field.

[13] As in the case of first quantization, we are implicitly supposing that the interaction occurs only between pairs of particles

[14] Since $\hat{a}$ is not hermitian, ϕ is in general a complex number. Writing $\phi = |\phi| \exp^{i\theta}$, $|\phi|$ and θ are called amplitude and phase of the coherent state $|\phi\rangle$.

[15] The eigenvalue condition for an annihilation operator a_i acting on $|\phi\rangle$ implies the following condition on the coefficients:

$$\begin{aligned} \langle n_1 \cdots (n_i - 1) \cdots | a_\alpha | \phi \rangle &= \sqrt{n_i} \langle n_1 \cdots (n_i - 1) \cdots | \sum_{n_1,n_2\ldots} \Phi_{n_1 \ldots n_i \ldots} | n_1, n_2 \cdots \rangle = \sqrt{n_i}\, \Phi_{n_1 \ldots n_i \ldots} \\ &= \phi_i \langle n_1 \cdots (n_i - 1) \cdots | \phi \rangle = \phi_i\, \Phi_{n_1 \ldots (n_i - 1) \ldots} \end{aligned}$$

$$\Phi_{n_1\dots n_i\dots} = \frac{\phi_i}{\sqrt{n_i}}\Phi_{n_1\dots(n_i-1)\dots} = \frac{\phi_i}{\sqrt{n_i}}\frac{\phi_1^{n_1}}{\sqrt{n_1!}}\frac{\phi_2^{n_2}}{\sqrt{n_2!}}\cdots\frac{\phi_{i-1}^{n_i-1}}{\sqrt{(n_i-1)!}}\cdots = \prod_i \frac{\phi_i^{n_i}}{\sqrt{n_i!}} \tag{1.35}$$

from which, by substituting (1.35) in the expansion (1.33), we finally obtain the explicit expression for the boson coherent state

$$|\phi\rangle = \sum_{\{n_i\}}\left(\prod_i \frac{\phi_i^{n_i}}{\sqrt{n_i!}}\right)\left(\prod_i \frac{\left(a_i^\dagger\right)^{n_i}}{\sqrt{n_i!}}\right)|\mathbf{0}\rangle = \exp\left[\sum_i \phi_i a_i^\dagger\right]|\mathbf{0}\rangle \quad \xrightarrow{adjoint} \quad \langle\phi| = \langle\mathbf{0}|\exp\left[\sum_i \phi_i^* a_i\right] \tag{1.36}$$

While field integration does not strictly require an in-depth understanding of coherent states, gaining further insights into their properties can be helpful when constructing the path integral. First, the action of the creation operator on a bosonic coherent state satisfies the following identity:

$$a_i^\dagger|\phi\rangle = a_i^\dagger \exp\left[\sum_j \phi_j a_j^\dagger\right]|\mathbf{0}\rangle = \frac{\partial}{\partial\phi_i}|\phi\rangle \quad \xrightarrow{\text{adjoint}} \quad \langle\phi| a_i = \langle\mathbf{0}|\exp\left[\sum_j \phi_j a_j\right] a_i = \frac{\partial}{\partial\phi_i^*}\langle\phi| \tag{1.37}$$

Second, and most importantly, the coherent states form a complete – specifically, an **overcomplete** – set of states in Fock space. This means that any vector in the Fock space can be expressed as a linear combination of coherent states, though this representation is not unique.[16] This overcompleteness is reflected in the closure relation:

$$\int\prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i}\exp\left[-\sum_\alpha \phi_\alpha^*\phi_\alpha\right]|\phi\rangle\langle\phi| = \mathbb{I}_{\mathbb{F}} \quad \text{where} \quad \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} = \frac{d\left(\operatorname{Re}\phi_\alpha\right)d\left(\operatorname{Im}\phi_\alpha\right)}{\pi} \tag{1.38}$$

where $\mathbb{I}_{\mathbb{F}}$ is the identity operator in Fock space, and the integration extends over all possible values of $\operatorname{Re}\phi_\alpha$ and $\operatorname{Im}\phi_\alpha$. To prove equation (1.38), an elegant method involves applying *Shur's lemma* [2].

Lemma [Schur] *An operator $\hat{A}$ commutes with all representation matrices of an irreducible group representation if and only if $\hat{A}$ is proportional to the identity operator.*

Thus, a way to prove equation (1.38) is to show that the *l.h.s* commutes with every creation and annihilation operators, since they provide the **irreducible representation** of an operator algebra. From the eigenstate condition (1.34) it follows that:

$$\begin{aligned}
a_\alpha\int\prod_{\alpha'}\frac{d\phi_{\alpha'}^* d\phi_{\alpha'}}{2\pi i}\; e^{-\sum_{\alpha'}\phi_{\alpha'}^*\phi_{\alpha'}}|\phi\rangle\langle\phi| &= \int\prod_{\alpha'}\frac{d\phi_{\alpha'}^* d\phi_{\alpha'}}{2\pi i}e^{-\sum_{\alpha'}\phi_{\alpha'}^*\phi_{\alpha'}}\phi_\alpha|\phi\rangle\langle\phi| \\
&= -\int\prod_{\alpha'}\frac{d\phi_{\alpha'}^* d\phi_{\alpha'}}{2\pi i}\left(\partial_{\phi_\alpha^*}e^{-\sum_{\alpha'}\phi_{\alpha'}^*\phi_{\alpha'}}\right)|\phi\rangle\langle\phi| \\
&\xrightarrow{\text{integrating by parts}} \quad = -\prod_{\alpha'}\frac{e^{-\sum_{\alpha'}(\operatorname{Re}\{\phi_\alpha\})^2+(\operatorname{Im}\{\phi_\alpha\})^2}}{\pi}|\phi\rangle\langle\phi|\Bigg|_{\substack{\operatorname{Re}\{\phi_\alpha\},\operatorname{Im}\{\phi_\alpha\}\to\infty \\ \\ \operatorname{Re}\{\phi_\alpha\},\operatorname{Im}\{\phi_\alpha\}\to-\infty}} \\
&\quad + \int\prod_{\alpha'}\frac{d\phi_{\alpha'}^* d\phi_{\alpha'}}{2\pi i}\; e^{-\sum_{\alpha'}\phi_{\alpha'}^*\phi_{\alpha'}}|\phi\rangle\,\partial_{\phi_\alpha^*}\langle\phi| \\
&= \int\prod_{\alpha'}\frac{d\phi_{\alpha'}^* d\phi_{\alpha'}}{2\pi i}\; e^{-\sum_{\alpha'}\phi_{\alpha'}^*\phi_{\alpha'}}|\phi\rangle\langle\phi|\, a_\alpha
\end{aligned}$$

and the correspondent relation for the creation can be found similarly. As a result, the *l.h.s* of (1.38) is proportional to the identity operator $\mathbb{I}_{\mathbb{F}}$. To determine the proportionality factor, we evaluate the expectation value of the *l.h.s* in the vacuum state:[17]

$$\int\prod_{\alpha'}\frac{d\phi_{\alpha'}^* d\phi_{\alpha'}}{2\pi i}e^{-\sum_{\alpha'}\phi_{\alpha'}^*\phi_{\alpha'}}\langle 0|\phi\rangle\langle\phi|0\rangle = \int\prod_{\alpha'}\frac{d\phi_{\alpha'}^* d\phi_{\alpha'}}{2\pi i}e^{-\sum_{\alpha'}\phi_{\alpha'}^*\phi_{\alpha'}} = 1$$

[16] Formally, a subset of the vectors $\{\phi_i\}_{i\in J}$ in a Banach space $\mathcal{X}$ (also known as a *system*) is complete if every element in $\mathcal{X}$ can be approximated arbitrarily well in norm by finite linear combinations of elements from $\{\phi_i\}_{i\in J}$. A system is **overcomplete** if it contains more vectors than necessary to be complete; that is, there exist vectors $\{\phi_j\}_{j\in J}$ that can be removed without losing completeness.

[17] To calculate this expectation value, it is useful to first compute the overlap between two coherent states $|\phi\rangle$ and $|\phi'\rangle$:

$$\langle\phi|\phi'\rangle = \langle\mathbf{0}|\exp\left[\textstyle\sum_i \phi_i^* a_i + \sum_j \phi_j' a_j^\dagger\right]|\mathbf{0}\rangle = \sum_{n_i,n_j'}\left(\prod_i\frac{(\phi_i)^{n_i}}{\sqrt{n_i!}}\right)\left(\prod_j\frac{(\phi_j')^{n_j}}{\sqrt{n_j!}}\right)\underbrace{\langle n_1 n_2\cdots|n_1' n_2'\cdots\rangle}_{\delta_{(n_1 n_1')}\delta_{(n_2 n_2')}\cdots}$$

$$= \sum_{n_i}\prod_i\frac{(\phi_i^*\phi_i')^{n_i}}{n_i!} = \exp\left[\textstyle\sum_\alpha \phi_\alpha^*\phi_\alpha'\right]$$

Thanks to the bosonic overcompleteness relation, we can straightforwardly represent any bosonic state $|\psi\rangle \in \mathcal{B}$ in the coherent state representation

$$|\psi\rangle = \int \prod_\alpha \frac{d\phi_\alpha d\phi_\alpha^*}{2\pi i} e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \underbrace{\langle\phi|\psi\rangle}_{\psi(\phi^*)} |\phi\rangle = \int \prod_\alpha \frac{d\phi_\alpha d\phi_\alpha^*}{2\pi i} e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \psi(\phi^*) |\phi\rangle$$

where $\langle\phi|\psi\rangle \equiv \psi(\phi^*)$ is the coherent state representation of $|\psi\rangle$. The coherent state representation for bosons is often referred to as the **holomorphic representation**, which arises from the fact that ψ is an analytic function of the variables ϕ_α^*. Physically, $\psi(\phi_\alpha^*)$ is simply the wavefunction of the state $|\psi\rangle$ in the coherent state representation; that is, the probability amplitude to find the system in the coherent state $|\phi\rangle$.

Having stated the coherent state overcompleteness relation, let us now focus on deriving some results that will be useful for the proceedings. As we will see, an important task is computing the trace of an operator in the coherent state representation. Let A be any operator and let $\{|n\rangle\}$ denote a complete set of states, then by inserting the bosonic overcompleteness above we find

$$\begin{aligned} \mathrm{Tr}(A) = \sum_n \langle n|A|n\rangle &= \sum_n \int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} \exp\left[-\sum_\alpha |\phi_\alpha|^2\right] \langle n|\phi\rangle \langle\phi|A|n\rangle \\ &= \int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} \exp\left[-\sum_\alpha |\phi_\alpha|^2\right] \sum_n \langle\phi|A|n\rangle \langle n|\phi\rangle \\ &= \int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} \exp\left[-\sum_\alpha |\phi_\alpha|^2\right] \langle\phi|A|\phi\rangle \end{aligned} \tag{1.39}$$

For normal ordered operators, calculating the matrix elements in the coherent state representation is straightforward. Denoting $A(\phi_\alpha^*, \phi_\alpha)$ as a generic combination of ϕ_α and ϕ_α^*, we have that

$$\langle\phi|A\big(a_\alpha^\dagger, a_\alpha\big)|\phi'\rangle = A(\phi_\alpha^*, \phi'_\alpha)\ e^{\sum_\alpha \phi_\alpha^* \phi'_\alpha}$$

Finally, just as it is useful to know how the operators $\hat{x}$ and $\hat{p}$ act in the coordinate representation, it is useful to exhibit how the operators $a_\alpha^\dagger$ and a_α act in the coherent state representation. From what we have stated, it follows that

$$\begin{aligned} \langle\phi|a_\alpha^\dagger|\psi\rangle = \phi_\alpha^* \langle\psi|\psi\rangle = \phi_\alpha^* \psi(\phi^*) \qquad &\longrightarrow \qquad a_\alpha^\dagger = \phi_\alpha^* \\ \langle\phi|a_\alpha|\psi\rangle = \frac{\partial}{\partial\phi_\alpha^*} \langle\phi|\psi\rangle = \frac{\partial}{\partial\phi_\alpha^*} \psi(\phi^*) \qquad &\longrightarrow \qquad a_\alpha = \frac{\partial}{\partial\phi_\alpha^*} \end{aligned}$$

which is consistent with the bosonic commutation relations for $a_\alpha^\dagger$ and a_α we found in the previous chapter (1.21)

$$\left[\frac{\partial}{\partial\phi_\alpha^*}, \phi_\beta^*\right] = \delta_{\alpha,\beta} \qquad \left[\phi_\alpha^*, \phi_\beta^*\right] = 0 \qquad \left[\frac{\partial}{\partial\phi_\alpha^*}, \frac{\partial}{\partial\phi_\beta^*}\right] = 0$$

2 Functional Integral Formulation

Functional integrals provide a powerful framework for studying many-particle quantum systems. In this chapter, we briefly depart from many-body physics and second quantization to revisit single-particle quantum mechanics through the Feynman path-integral formulation. This approach extends the classical Lagrangian and Hamiltonian formalisms into the quantum realm, where the system's dynamics are governed by a central object known as the action functional. By expressing quantum evolution as a sum over all possible trajectories, each weighted by the action, the path integral not only introduces us to field integral methods but, when examined closely, already embodies the essence of a field theoretical approach.

Establishing the path integral for quantum mechanics will prepare us to apply functional integrals to many-body systems. This method provides a unifying perspective that bridges quantum mechanics with classical statistical mechanics, making it especially useful for describing complex quantum phase transitions. By the end of this chapter, we will have laid the foundation necessary for exploring many-body physics by means of the functional integral techniques. The main references for this chapter are [11] and [14].

2.1 The Feynman path integral

Consider a particle in an initial position x_i at time t_i that eventually reaches a position x_f at a certain time t_f. As postulated by quantum mechanics, the time evolution of a state $|\psi(t)\rangle$ is governed by the Schrödinger equation. As a result, if we know the state at time t, in quantum mechanics we can deterministically obtain the state at $t' > t$ by means of the time evolution operator U

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(\hat{p},\hat{x})|\psi(t)\rangle \quad &\xrightarrow{\text{resulting in}} \quad |\psi(t')\rangle = U(t',t)|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}(\hat{p},\hat{x})(t'-t)}|\psi(t)\rangle \\ \psi(x',t') = \langle x'|\psi(t')\rangle = \langle x'|U|\psi(t)\rangle = \int dx\,\langle x'|U(t',t)|x\rangle\,\langle x|\psi(t)\rangle &= \int dx\,\underbrace{\langle x'|e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|x\rangle}_{U(x',t';x,t)}\psi(x,t) \end{aligned} \tag{2.1}$$

This means that, in order to find the final wavefunction $\psi(x',t')$, we must determine the matrix elements of the time evolution operator

$$\langle x_f|U(t_f,t_i)|x_i\rangle \equiv U(x_f,t_f;\,x_i,t_i) = \langle x_f|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|x_i\rangle$$

However, the computation of this object over finite time intervals Δt can be difficult, or even impossible. As we will see later, we can calculate these matrix elements with arbitrary precision over infinitesimal intervals: Feynman's idea was to break the time interval in infinite components, estimate the matrix elements of U for each step, and chain the matrix elements together to obtain the result for the finite interval. This is, essentially, **Feynman's path integral**. Before diving into the path integral formulation of quantum mechanics, let us firstly fix the notation by introducing

$$\epsilon = \frac{t_f - t_i}{M} = \frac{\Delta t}{M} \qquad \begin{aligned} t_0 \equiv t_i \quad &\text{and} \quad x_0 \equiv x_i \\ t_n = t_i + (n-1)\epsilon \\ t_M \equiv t_f \quad &\text{and} \quad x_M \equiv x_f \end{aligned}$$

where the entire time interval $\Delta t = t_f - t_i$ has been divided into M equal steps of size ϵ. With this in mind, by inserting the closure relation in the coordinate representation $M-1$ times, the matrix element of the evolution operator may be written as

$$\begin{aligned} U(x_f,t_f;x_i,t_i) = \langle x_f|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_i\rangle &= \langle x_f|\left(e^{-\frac{i}{\hbar}\hat{H}\epsilon}\right)^M|x_i\rangle \\ \int dx_k\,|x_k\rangle\langle x_k| = \mathbb{I} \quad \longrightarrow \quad &= \int\left[\prod_{k=1}^{M-1}dx_k\right]\langle x_f|e^{-\frac{i}{\hbar}\hat{H}\epsilon}|x_{M-1}\rangle\,\langle x_{M-1}|e^{-\frac{i}{\hbar}\hat{H}\epsilon}|x_{M-2}\rangle\cdots\langle x_1|e^{-\frac{i}{\hbar}\hat{H}\epsilon}|x_i\rangle \\ &= \int\left[\prod_{k=1}^{M-1}dx_k\right]\prod_{k=1}^{M}\langle x_k|e^{-\frac{i}{\hbar}\hat{H}\epsilon}|x_{k-1}\rangle \end{aligned} \tag{2.2}$$

Now, the following step would be to determine the generic matrix element of the infinitesimal evolution operator, or equivalently an appropriate approximation.[1] The most generic one-particle Hamiltonian describing the particle's

[1] Here *appropriate* means that the approximation ultimately converges to the right solution, for infinitely small steps.

dynamics is depicted in (2.1). As a result, a possible solution would be to introduce a set of completeness relations in the momentum representation, and compute the corresponding braket for every time step. However, we find ourselves irremediably stuck. Indeed, while being tempted to apply $\langle p_k|$ and $|x_k\rangle$ to their correspondent operator, it is hindered by the fact that operators $\hat{X}$ and $\hat{P}$ do not commute: this prevents us to expand the exponential matrix and use the binomial theorem.

$$\langle x_k|e^{-\frac{i\epsilon}{\hbar}H(\hat{p},\hat{x})}|x_{k-1}\rangle = \langle x_k|e^{-\frac{i\epsilon}{\hbar}\left[\frac{\hat{p}^2}{2m}+V(\hat{x})\right]}|x_{k-1}\rangle = \int dp_k\, \langle x_k|p_k\rangle\, \langle p_k|e^{-\frac{i\epsilon}{\hbar}\left[\frac{\hat{p}^2}{2m}+V(\hat{x})\right]}|x_{k-1}\rangle$$

For our purposes in obtaining a practical functional integral, we desire an approximation of the infinitesimal evolution operator which not only reproduces the exact evolution of a wave function in the limit $\epsilon \to 0$, but also yields acceptable results when acting on position and momentum eigenstates. We obtain such an approximation by considering a form of normal ordered exponential. Similarly to what we did for creation and annihilation operators, we may define normal ordering for operators expressed in terms of $\hat{p}$ and $\hat{x}$, since they provide an equivalent irreducible representation. An operator is said to be in normal form when all the momentum operators $\hat{p}$ appear to the left of all the position operators $\hat{x}$, and the result of reordering an operator $A(\hat{p},\hat{x})$ into normal form will be denoted as $:A(\hat{p},\hat{x}):$

Lemma [Ordering correction] *Let A and B be two generic operators such that $[A,B] \neq 0$, and let $e^{\epsilon(A+B)}$ be the infinitesimal exponential operator of their sum. The following relation holds:*

$$e^{\epsilon(A+B)} - :e^{\epsilon(A+B)}: = \mathcal{O}(\epsilon^2)$$

By ordering the time-evolution operator in the same manner, we can finally decompose the exponential function using the binomial theorem. The normal-order time-evolution operator is indeed a successful approximation of the not-ordered one: the error we commit in the reordering procedure is of order $\mathcal{O}(\epsilon^2)$.

$$e^{-\frac{i\epsilon}{\hbar}\hat{H}(\hat{p},\hat{x})} = :e^{-\frac{i\epsilon}{\hbar}\hat{H}(\hat{p},\hat{x})}: + \mathcal{O}(\epsilon^2) = \sum_{n=0}^{\infty}\left[\frac{-i\epsilon}{\hbar}\right]^n \frac{1}{n!}\sum_k^n \binom{n}{k}\left[\frac{\hat{p}^2}{2m}\right]^k (V(\hat{x}))^{n-k} + \mathcal{O}(\epsilon^2)$$

$$\begin{aligned}
\langle x_k|\, :e^{-\frac{i\epsilon}{\hbar}\hat{H}(\hat{p},\hat{x})}:\, |x_{k-1}\rangle &= \int dp_k\, \langle x_k|p_k\rangle\, \langle p_k|\, :e^{-\frac{i\epsilon}{\hbar}\hat{H}(\hat{p},\hat{x})}:\, |x_{k-1}\rangle + \mathcal{O}(\epsilon^2) \\
&\xrightarrow[\text{ordering approximation}]{\text{only possible with}} = \int dp_k\, \langle x_k|p_k\rangle\, \langle p_k|e^{-\frac{i\epsilon}{\hbar}\frac{\hat{p}^2}{2m}}\cdot e^{-\frac{i\epsilon}{\hbar}V(\hat{x})}|x_{k-1}\rangle + \mathcal{O}(\epsilon^2) \\
&= \int \frac{dp_k}{(2\pi\hbar)^3}\, \langle x_k|p_k\rangle\, \langle p_k|x_{k-1}\rangle\; e^{-\frac{i\epsilon}{\hbar}\frac{p_k^2}{2m}}\; e^{-\frac{i\epsilon}{\hbar}V(x_{k-1})} + \mathcal{O}(\epsilon^2) \qquad (2.3) \\
&\xrightarrow{\text{Gaussian Integral}} = \int \frac{dp_k}{(2\pi\hbar)^3}\, \underbrace{e^{\frac{i\epsilon p_k}{\hbar}(x_k-x_{k-1})}\; e^{-\frac{i\epsilon}{\hbar}\frac{p_k^2}{2m}}}\; e^{-\frac{i\epsilon}{\hbar}V(x_{k-1})} + \mathcal{O}(\epsilon^2) \\
&\xrightarrow{\text{resulting in}} = \int \frac{dq_k}{(2\pi\hbar)^3}\, e^{-\frac{i\epsilon q_k^2}{2m\hbar}}\, e^{\frac{im}{2\epsilon\hbar}(x_k-x_{k-1})^2}\, e^{-\frac{i\epsilon}{\hbar}V(x_{k-1})} + \mathcal{O}(\epsilon^2) \\
&\xrightarrow{\text{resulting in}} = \frac{1}{(2\pi\hbar)^3}\left(\frac{2\pi m\hbar}{\epsilon i}\right)^{3/2} e^{\frac{im}{2\epsilon\hbar}(x_k-x_{k-1})^2}\, e^{-\frac{i\epsilon}{\hbar}V(x_{k-1})} + \mathcal{O}(\epsilon^2)
\end{aligned}$$

where we have solved the gaussian integral through the variable change $q_k = p_k - \frac{m}{\epsilon}(x_k - x_{k-1})$. By chaining these evolution steps, we obtain an approximation of the time-evolution matrix element over a finite time interval Δt

$$U(x_f,t_f,x_i,t_i) = \int \prod_{k=1}^{M-1} dx_k \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{\frac{3M}{2}} e^{\frac{i\epsilon}{\hbar}\sum_{k=1}^{M}\left[\frac{m}{2}\left(\frac{x_k-x_{k-1}}{\epsilon}\right)^2 - V(x_{k-1})\right]} + \mathcal{O}(\epsilon^2) \qquad (2.4)$$

Here the set of points $\{x_0, x_1, \ldots, x_M\}$ defines a trajectory. In the limit $M \to \infty$, for notation convenience, we will often denote this trajectory by $x(t)$ with starting point $x(t_i) = x_i$ and endpoint $x(t_f) = x_f$, but it is crucial to note that this notation does not imply continuity or differentiability. Rather, the trajectory should always be thought as a set of M points $x(t_k)$ indexed by the discrete times t_k. With this in mind, it is convenient to introduce the following notation convention

$$\epsilon\sum_{k=1}^{M}\frac{m}{2}\left(\frac{x_k-x_{k-1}}{\epsilon}\right)^2 \to \int_{t_i}^{t_f} dt\,\frac{m}{2}\left(\frac{dx(t)}{dt}\right)^2 \qquad \text{and} \qquad \epsilon\sum_{k=1}^{M} V(x_{k-1}) \to \int_{t_i}^{t_f} dt\, V(x(t))$$

Finally, by taking the limit of (2.4) as $M \to \infty$, and hence as $\epsilon \to 0$, we obtain the time-evolution operator's matrix element over a finite time interval, notoriously denoted as Feynman path integral

$$U(x_f,t_f;x_i,t_i) = \int_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)]\; e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\left[\frac{m\dot{x}^2(t)}{2} - V(x(t))\right]} = \int_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\;\mathcal{L}[x(t)]} \qquad (2.5)$$

$$\text{where} \quad \int_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)] = \lim_{M\to\infty}\int \prod_{k=1}^{M-1} dx_k \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{\frac{3M}{2}} \qquad (2.6)$$

where (2.6) represents a sum over all possible trajectories starting at position x_i at instant t_i and ending at x_f at t_f. Also, if the condition of Legendre transformations holds, then the time-integral over bounded trajectories of the Lagrangian $\mathcal{L}[x(t)]$ consists in the action functional $\mathcal{S}[x(t)]$

$$U\left(x_f,t_f,x_i,t_i\right)=\int_{(x_i,t_i)}^{(x_f,t_f)}\mathcal{D}\left[x(t)\right]\,e^{\frac{i}{\hbar}S[x(t)]}\quad\text{where}\quad\mathcal{S}[x(t)]=\int_{(x_i,t_i)}^{(x_f,t_f)}dt\;\mathcal{L}(x(t),\dot{x}(t),t)\tag{2.7}$$

The functional integral in (2.7) is said to be in the *Lagrangian form* and requires the Hamiltonian to have quadratic momentum dependence, as in equation (2.1). On the other hand, a more general form of the functional integral is obtained by substituting (2.3) in (2.2) without performing the momentum integration, in which case the matrix element of the evolution operator becomes

$$U\left(x_f,t_f,x_i,t_i\right)=\lim_{M\to\infty}\int\prod_{k=1}^{M-1}dx_k\prod_{k=1}^{M}\frac{dp_k}{(2\pi\hbar)^3}\;e^{\frac{i\epsilon}{\hbar}\sum_{k=1}^{M}\left[\frac{p_k(x_k-x_{k-1})}{\epsilon}-H(p_k,x_k)\right]}\tag{2.8}$$

$$=\int_{(x_i,t_i)}^{(x_f,t_f)}\mathcal{D}[x(t)]\,\mathcal{D}[p(t)]\,e^{\frac{i}{\hbar}\int_{t_i}^{t_f}dt\,[p(t)\dot{x}(t)-H(p(t),x(t))]}\tag{2.9}$$

where the resulting functional integral (2.8) is said to be the *Hamiltonian form*. In this case, the trajectories $x(t)$ obey the same boundary conditions as in the Lagrangian form and the momenta $p(t)$ have no boundary conditions. The Hamiltonian from of the functional integral is a priori more general than the Lagrangian form, but requires care in the ordering of the non-commuting operators $\hat{x}$ and $\hat{p}$ when H contains mixed terms in $\hat{x}$ and $\hat{p}$.

Path integrals for statistical mechanics. As we have seen, Feynman's path integral formulation of quantum mechanics consists in a generalization of the classical least action principle. Its importance in theoretical physics cannot be overstated enough, especially because of its natural ability to describe a multitude of phenomena. One of its major applications is in quantum statistical mechanics. Let's start from the definition of the partition function

$$Z=\mathrm{Tr}\big(e^{-\beta H}\big)=\int dx\;\langle x|e^{-\beta H}|x\rangle\quad\text{where}\quad\beta=\frac{1}{k_bT}\tag{2.10}$$

which in the context of the one-particle problem, because we are working in the *canonical ensemble*, does not include the chemical potential. We can relate this expression to the previous Feynman integral setting by a dimensional comparison of the exponents:

$$\beta=\frac{i}{\hbar}\Delta t\quad\Longrightarrow\quad\tau_f-\tau_i=\hbar\beta,\quad\tau\in\mathbb{C}$$

As a result, by means of a simple variable change, Z may be thought as the sum over the diagonal matrix elements of an imaginary time evolution operator $U(x_f,\tau_f;x_i,\tau_i)$, evaluated for the interval $\tau_f-\tau_i=\beta\hbar$. By paying the price of detaching, for a moment, from the physical sense, we can construct an astounding conceptual bridge between quantum mechanics and statistical mechanics, with the bridge being the path integral formulation. Indeed, all the steps in the derivation of the real-time path integral may be repeated for the case of imaginary time. For the Hamiltonian, by dividing the imaginary-time interval in M steps of length $\epsilon\equiv\frac{\tau_f-\tau_i}{M}$, we then obtain

$$\begin{aligned}U\left(x_f,\tau_f;x_i,\tau_i\right)&=\langle x_f|e^{-\frac{(\tau_f-\tau_i)\,\hat{H}}{\hbar}}|x_i\rangle=\langle x_f|\left(e^{-\frac{\epsilon}{\hbar}\hat{H}}\right)^M|x_i\rangle=\lim_{M\to\infty}\int\prod_{k=1}^{M-1}dx_k\prod_{k=1}^{M}\langle x_k|e^{-\frac{\epsilon\hat{H}}{\hbar}}|x_{k-1}\rangle\\&=\lim_{M\to\infty}\int\prod_{k=1}^{M-1}dx_k\prod_{k=1}^{M}dp_k\,\langle x_k|p_k\rangle\,\langle p_k|\,{:}e^{-\frac{\epsilon}{\hbar}\hat{H}(\hat{p},\hat{x})}{:}\,|x_{k-1}\rangle+\mathcal{O}(\epsilon^2)\\&=\lim_{M\to\infty}\int\prod_{k=1}^{M-1}dx_k\prod_{k=1}^{M}\frac{dp_k}{(2\pi\hbar)^3}\,e^{\sum_{k=1}^{M}\left[\frac{ip_k}{\hbar}(x_k-x_{k-1})-\frac{\epsilon}{\hbar}\left(\frac{p_k^2}{2m}+V(x_{k-1})\right)\right]}+\mathcal{O}(\epsilon^2)\\&=\lim_{M\to\infty}\int\prod_{k=1}^{M-1}dx_k\left(\frac{m}{2\pi\hbar\epsilon}\right)^{\frac{3M}{2}}\,e^{-\frac{\epsilon}{\hbar}\sum_{k=1}^{M}\left[\frac{m}{2}\frac{(x_k-x_{k-1})^2}{\epsilon^2}+V(x_{k-1})\right]}+\mathcal{O}(\epsilon^2)\\&=\int_{(x_i,\tau_i)}^{(x_f,\tau_f)}\mathcal{D}[x(\tau)]\;e^{-\frac{1}{\hbar}\int_{\tau_i}^{\tau_f}d\tau\left[\frac{m}{2}\dot{x}^2(\tau)+V(x(\tau))\right]}=\int_{(x_i,\tau_i)}^{(x_f,\tau_f)}\mathcal{D}[x(\tau)]\;e^{-\frac{1}{\hbar}\int_{\tau_i}^{\tau_f}d\tau\hat{H}[x(\tau)]}\end{aligned}$$

Thus, the imaginary-time path integral is a sum over trajectories starting at (x_i,τ_i) and ending at (x_f,τ_f) weighted by the exponential of a modified action. Indeed, while in Feynman path integrals we work with the action functional $S[x(t)]$, in statistical mechanics the sign of the potential V changes: this results in a modified action, called **Euclidean action**

$$U\left(x_f,\tau_f,x_i,\tau_i\right)=\int_{(x_i,\tau_i)}^{(x_f,\tau_f)}\mathcal{D}[x(\tau)]\;e^{-\frac{1}{\hbar}\mathcal{S}[x(\tau)]}\quad\text{where}\quad\mathcal{S}[x(t)]=\int_{(x_i,\tau_i)}^{(x_f,\tau_f)}d\tau\,H[x(t)]\tag{2.11}$$

An alternative derivation, which shows explicitly how the Lagrangian in the real time case is transformed into the Hamiltonian in the imaginary time case, is to perform an analytic continuation of equation (2.5) to imaginary time. This continuation, also known as **Wick rotation**[2], is effected by the variable transformation:

$$t = -i\tau \qquad \longrightarrow \qquad \begin{aligned} dt &= -id\tau \\ \frac{dx}{d\tau} &= \frac{dx}{dt}\frac{dt}{d\tau} = -i\frac{dx}{d\tau} \end{aligned}$$

As a result, under the Wick rotation the kinetic energy changes sign because each time derivative acquires a factor i, resulting in the **Euclidean action**

$$\frac{i}{\hbar}\int_{t_u}^{t_f} dt\left[\frac{m}{2}\dot{x}^2(t) - V(x(t))\right] = -\frac{1}{\hbar}\int_{\tau_i}^{\tau_f} d\tau\left[\frac{m}{2}\dot{x}^2(\tau) + V(x(\tau))\right]$$

In conclusion, using equations (2.10)-(2.11), the partition function may be expressed as the sum over periodic trajectories of period $\beta\hbar$.

$$Z = \int dx \int_{(x,0)=x}^{(x,\hbar\beta)=x} \mathcal{D}[x(\tau)] e^{-\frac{1}{\hbar}\int_{\tau_i}^{\tau_f} d\tau\left[\frac{m}{2}\dot{x}^2(\tau)+V(x(\tau))\right]} \tag{2.12}$$

2.2 Path integral for many-particle systems

The Feynman path integral in real or imaginary time may be straightforwardly extended to many-particle systems. Describing the evolution of a many-particle system in the path integral formulation not only requires the framework of statistical mechanics, but also the second quantization formalism for many-particle quantum states. The recipe is essentially the same: the real (complex) time interval may be divided into infinitesimal steps, which can be treated separately by inserting suitable closure relations. Either choice yields the exact evolution, while the symmetry or antisymmetry of the final states in the trace sufficies to impose the proper statistics.

Let us start by considering a close system of N bosons or fermions, whose Hamiltonian describes a system of N particles that are locally interacting.

$$H = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} v\left(\hat{x}_i - \hat{x}_j\right)$$

The partition function in the *canonical ensemble*, which has to be thought as an N-particle operator, can be computed straightforwardly: the use of product states yields the simplest formal result completely analogous to (2.12)

$$\begin{aligned} Z = \mathrm{Tr}(e^{-\beta H}) &= \frac{1}{N!}\int \prod_{i=1}^{N} dx_i \left\{x_1 \dots x_N\right| e^{-\beta H} \left|x_1 \dots x_N\right\} \\ &= \frac{1}{N!}\sum_P \xi^P \int \prod_{i=1}^{N} dx_i \left(x_{P1} \dots x_{PN}\right| e^{-\beta H} \left|x_1 \dots x_N\right) \\ &= \frac{1}{N!}\sum_P \xi^P \int_{x(0)=x_P(\hbar\beta)} \mathcal{D}[x_1(t)] \cdots \mathcal{D}[x_N(t)]\, e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\left[\sum_i \frac{m\dot{x}_i^2(\tau)}{2} + \frac{1}{2}\sum_{i\neq j} v(x_i - x_j)\right]} \end{aligned} \tag{2.13}$$

Coherent-state functional integral. For a general many-particle Hamiltonian expressed in second quantized form, the functional integral representation for the many-body evolution operator may be obtained using the coherent-state representation, instead of the position and momentum eigenstates used for the Feynman path integral. As it will be clear, the coherent state over-basis manifests its true advantages in the context of the many-body path integral formulation, as it allows to elegantly describe the system in different ensembles. By working in the coherent state representation, we will evaluate the matrix element of the evolution operator between an initial coherent state $|\phi_i\rangle$ having components $\phi_{\alpha,i}$ and a final state $\langle\phi_f|$ with components $\phi^*_{\alpha,f}$.

$$U\left(\phi^*_{\alpha,f}, t_f; \phi_{\alpha,i}, t_i\right) = \langle\phi_f| e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} |\phi_i\rangle$$

As before, the integral $[t_i, t_f]$ is broken into M time steps of size $\epsilon \equiv (t_f - t_i)/M$ and the generalized closure relation for bosonic (fermionic) coherent states[3]

$$\mathbb{I} = \int \prod_{\alpha} \frac{d\phi^*_{\alpha k} d\phi_{\alpha k}}{\mathcal{A}}\, e^{-\sum_\alpha \phi^*_{\alpha k}\phi_{\alpha k}} |\phi_{\alpha k}\rangle\langle\phi_{\alpha k}| \quad \text{where} \quad \mathcal{A} = \begin{cases} 1 & \text{fermions} \\ 2\pi i & \text{bosons} \end{cases}$$

[2] The term *rotation* comes from the fact that it may be viewed as a rotation of the integration contour in the complex t-plane.

[3] As it turns out, the difference between the bosonic and the fermionic coherent-state overcompleteness relation only amounts to a different normalization parameter, which we will call $\mathcal{A}$. The reason for this ultimately relies on the Grassmann algebra for fermions.

is inserted at the k^{th} time step. Analogously to the single-particle case, in order to proceed with the computation, it is necessary to expand the exponential matrix and use the binomial theorem. Being this approach precluded by the fact that $a^\dagger$ and a do not commute, the concept of normal order operators is again needed. For second-quantized operators, the appropriate form of normal ordering is that defined in the previous chapter, with all creation operators to the left of annihilation operators. As shown in the **ordering correction lemma**, the error we commit in the reordering procedure is of order $\mathcal{O}(\epsilon^2)$, for which the matrix element of the evolution operator may be written[4]

$$\begin{aligned}
U(\phi^*_{\alpha,f}, t_f;\, \phi_{\alpha,i}, t_i) &= \lim_{M\to\infty} \langle \phi_f | e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} | \phi_i \rangle \\
&= \lim_{M\to\infty} \int \prod_{k=1}^{M-1} \left[\prod_\alpha \frac{d\phi^*_{\alpha k} d\phi_{\alpha k}}{\mathcal{A}}\, e^{-\sum_\alpha \phi^*_{\alpha k}\phi_{\alpha k}} \right] \prod_{k=1}^{M} \langle \phi_k | e^{-\frac{i}{\hbar}\hat{H}\epsilon} | \phi_{k-1} \rangle \\
&= \lim_{M\to\infty} \int \left[\prod_{k=1}^{M-1} \prod_\alpha \frac{d\phi^*_{\alpha k} d\phi_{\alpha k}}{\mathcal{A}} \right] e^{-\sum_{k=1}^{M-1}\sum_\alpha |\phi_{\alpha k}|^2} \prod_{k=1}^{M} \langle \phi_k | :e^{-\frac{i}{\hbar}\hat{H}\epsilon}: | \phi_{k-1} \rangle + \mathcal{O}(\epsilon^2) \\
&= \lim_{M\to\infty} \int \left[\prod_{k=1}^{M-1} \prod_\alpha \frac{d\phi^*_{\alpha k} d\phi_{\alpha k}}{\mathcal{A}} \right] e^{-\sum_{k=1}^{M-1}\sum_\alpha |\phi_{\alpha k}|^2}\, e^{\sum_{k=1}^{M}\left[\sum_\alpha \phi^*_{\alpha k}\phi_{\alpha(k-1)} - \frac{i\epsilon}{\hbar} H(\phi^*_k, \phi_{k-1})\right]}
\end{aligned}$$

Similarly to the path integral formulation, the set of coherent states $\{\phi_{\alpha 1}, \phi_{\alpha 2}, \ldots, \phi_{\alpha M}\}$ can be imagined as a discrete trajectory-like state path. In the limit $M \to \infty$, for notation convenience, it is useful to introduce a continuous trajectory of states $\phi_\alpha(t)$ together with the following notation

$$\phi^*_{\alpha k} \frac{(\phi_{\alpha,k} - \phi_{\alpha,k-1})}{\epsilon} \;\to\; \phi^*_\alpha(t) \frac{\partial}{\partial t} \phi_\alpha(t) \qquad \text{and} \qquad H(\phi^*_{\alpha,k}; \phi_{\alpha,k-1}) \;\to\; H(\phi^*_\alpha(t); \phi_\alpha(t))$$

Remembering that $\phi_{\alpha,M} = \phi_{\alpha,f}$ and $\phi_{\alpha,0} = \phi_{\alpha i}$, we can arrange the summations in the exponent and rewrite it symbolically

$$\begin{aligned}
(*) &= \sum_\alpha \phi^*_{\alpha,M}\phi_{\alpha,M-1} - i\frac{\epsilon}{\hbar} H(\phi^*_{\alpha,M}; \phi_{\alpha,M-1}) + \sum_{k=1}^{M-1} \left[\sum_\alpha \phi^*_{\alpha,k}\phi_{\alpha,k-1} - \phi^*_{\alpha,k}\phi_{\alpha,k} - \frac{i\epsilon}{\hbar} H(\phi^*_{\alpha,k}; \phi_{\alpha,k-1}) \right] \\
&= \sum_\alpha \phi^*_{\alpha,M}\phi_{\alpha,M-1} - i\frac{\epsilon}{\hbar} H(\phi^*_{\alpha,M}; \phi_{\alpha,M-1}) + \frac{i\epsilon}{\hbar} \sum_{k=1}^{M-1} \left[i\hbar \sum_\alpha \phi^*_{\alpha,k} \left(\frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} \right) - H(\phi^*_{\alpha,k}; \phi_{\alpha,k-1}) \right] \\
&= \sum_\alpha \phi^*_\alpha(t_f)\phi_\alpha(t_f) + \frac{i}{\hbar} \int_{t_i}^{t_f} dt \left[\sum_\alpha i\hbar \phi^*_\alpha(t) \frac{\partial \phi_\alpha(t)}{\partial t} - H(\phi^*_\alpha(t), \phi_\alpha(t)) \right] \\
&= \sum_\alpha \phi^*_\alpha(t_f)\phi_\alpha(t_f) + \frac{i}{\hbar} \int_{t_i}^{t_f} dt\, \mathcal{L}(\phi^*_\alpha(t), \phi_\alpha(t))
\end{aligned}$$

where, in the last line, we have introduced the **Schrödinger Lagrangian operator**. As in the Feynman path integral, it is important to emphasize that the trajectory and derivative notation is purely symbolic: indeed the correct physical quantity is calculated by performing the integral over the discrete action, and by taking the limit $M \to \infty$. Either way, the time-evolution operator's matrix element results to be

$$U(\phi^*_{\alpha,f}, t_f;\, \phi_{\alpha,i}, t_i) = \int_{\phi_\alpha(t_i)=\phi_{\alpha,i}}^{\phi^*_\alpha(t_f)=\phi^*_{\alpha,f}} \mathcal{D}\left[\phi^*_\alpha(t)\phi_\alpha(t)\right]\, e^{\sum_\alpha \phi^*_\alpha(t_f)\phi_\alpha(t_f) + \frac{i}{\hbar}\int_{t_i}^{t_f} dt \left[\sum_\alpha i\hbar\phi^*_\alpha(t)\frac{\partial\phi_\alpha(t)}{\partial t} - H(\phi^*_\alpha(t),\phi_\alpha(t))\right]} \tag{2.14}$$

$$\propto \int_{\phi_\alpha(t_i)=\phi_{\alpha,i}}^{\phi^*_\alpha(t_f)=\phi^*_{\alpha,f}} \mathcal{D}\left[\phi^*_\alpha(t)\phi_\alpha(t)\right]\, e^{\frac{i}{\hbar}S[\phi^*(t),\phi(t)]} \tag{2.15}$$

$$\text{where} \quad \int_{\phi_\alpha(t_i)}^{\phi^*_\alpha(t_f)} \mathcal{D}\left[\phi^*_\alpha(t)\phi_\alpha(t)\right] = \lim_{M\to\infty} \int \prod_{k=1}^{M-1} \prod_\alpha \frac{d\phi^*_{\alpha,k} d\phi_{\alpha,k}}{\mathcal{A}} \tag{2.16}$$

One significant difference between the coherent state functional integral (2.14) and the Feynman path integral is the dependence upon $\hbar$. While in the Feynman case $1/\hbar$ appears as a constant multiplying the entire exponent, here the action contains $\hbar$ within the Schrodinger Lagrangian operator.

Having determined the time evolution operator for many-particle systems, we now move on to statistical mechanics. As stated in the end previous chapter, in order to properly describe a many-particle system it is convenient (or even necessary) to work within the second quantization formalism, and specifically in the coherent state representation. Indeed, this framework allows us to efficiently describe not only the *canonical ensemble*, but also the *grancanonical ensemble*.

[4]Note that in the case of fermions, since there is no metric in the Grassman algebra, all the following integrals are finite. For bosons, the argument is analogous to that for the path integral case.

As stated in equation (2.13), the grancanonical partition function for a many-particle system may be expressed as the trace of an imaginary-time evolution operator. By using equation (1.39) for computing the trace in the bosonic or fermionic coherent state representation, and by assuming $\hbar = 1$, we find

$$Z_{gc} = \mathrm{Tr}\Big(e^{-\beta(\hat{H}-\mu\hat{N})}\Big) = \int \prod_{\alpha} \frac{d\phi^*_\alpha d\phi_\alpha}{\mathcal{A}} e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \langle \phi | e^{-\beta(\hat{H}-\mu\hat{N})} | \phi \rangle \qquad \begin{cases} \phi_{\alpha,0} = \phi_\alpha \\ \phi^*_{\alpha,M} = \phi^*_\alpha \end{cases} \tag{2.17}$$

where $\hat{N} = \sum_\alpha a^\dagger_\alpha a_\alpha$ and $\hat{H}(a^\dagger_\alpha, a_\alpha)$ is assumed to be in normal order. When the analytical continuation of (2.10) to imaginary time is substituted in (2.17), the trace imposes the periodic or antiperiodic boundary conditions summarized above. The choice of considering $\hat{H}(a^\dagger_\alpha, a_\alpha)$ in normal order, as we have shown, is not an oversimplification of the problem but rather a successful approximation of the general not-ordered one. With this in mind, by expanding the exponential operator and using the binomial theorem, we thus obtain

$$\begin{aligned} Z_{gc} &= \lim_{M\to\infty} \int \prod_{\alpha} \frac{d\phi^*_\alpha d\phi_\alpha}{\mathcal{A}} e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \left[\prod_{k=1}^{M-1} \prod_{\alpha} \frac{d\phi^*_{\alpha k} d\phi_{\alpha k}}{\mathcal{A}} e^{-\sum_{k=1}^{M-1} \sum_\alpha \phi^*_{\alpha k} \phi_{\alpha k}} \right] \prod_{k=1}^{M} \langle \phi_k | e^{-\frac{\beta}{M}(\hat{H}-\mu\hat{N})} | \phi_{k-1} \rangle \\ &= \lim_{M\to\infty} \int \prod_{k=1}^{M} \prod_{\alpha} \frac{d\phi^*_{\alpha k} d\phi_{\alpha k}}{\mathcal{A}} \; e^{\sum_{k=1}^{M} \sum_\alpha \phi^*_{\alpha k} \phi_{\alpha,k-1} - \phi^*_{\alpha k}\phi_{\alpha k}} \times e^{-\frac{\beta}{M} \sum_{k=1}^{M} \sum_\alpha [H(\phi_{\alpha k}, \phi_{\alpha,k-1}) - \mu \phi^*_{\alpha k} \phi_{\alpha,k-1}]} \end{aligned}$$

where we have merged the summations by using *periodic* and *antiperiodic* boundary conditions. By fixing $\epsilon = \beta/M$ and using the continuous trajectory notation this may be rewritten as follows, with the usual understanding that derivatives and integrals are defined in terms of discrete expressions.

$$\begin{aligned} Z_{gc} &= \lim_{M\to\infty} \int \prod_{k=1}^{M} \prod_{\alpha} \frac{d\phi^*_{\alpha k} d\phi_{\alpha k}}{\mathcal{A}} \; e^{-\epsilon \sum_{k=2}^{M} \left[\sum_\alpha \left(\phi^*_{\alpha k} \frac{\left(\phi_{\alpha k} - \phi_{\alpha(k-1)}\right)}{\epsilon} - \mu \phi^*_{\alpha k} \phi_{\alpha(k-1)} \right) + H(\phi^*_{\alpha k}, \phi_{\alpha(k-1)}) \right]} \\ &= \int_{\phi_\alpha(\beta) = \xi \phi_\alpha(0)} \mathcal{D}[\phi^*_\alpha(\tau), \phi_\alpha(\tau)] \; e^{-\int_0^\beta d\tau \sum_\alpha \left[\phi^*_\alpha(\tau) \left(\frac{\partial}{\partial \tau} - \mu \right) \phi_\alpha(\tau) + H(\phi^*_\alpha(\tau), \phi_\alpha(\tau)) \right]} \end{aligned} \tag{2.18}$$

3 Bose-Hubbard Model

The Hubbard model is a foundational concept in solid-state and condensed-matter physics, originally proposed by J. Hubbard, M. Gutzwiller, and J. Kanamori [5]. It provides a simplified yet powerful approximation for understanding electron motion in transition metals, with a particular focus on explaining their magnetic properties. Over time, the Hubbard model has been extended to study phenomena such as high-temperature superconductivity and charge density waves, and it remains a vibrant area of research.

In this chapter, we turn our attention to the bosonic counterpart of the Hubbard model, known as the Bose-Hubbard model. In this version, the spin-1/2 electrons of the original model are replaced by spinless bosons, which can represent various systems such as Cooper pairs tunneling between superconducting islands, helium atoms on a substrate, or ultracold atoms in optical lattices.

We focus specifically on bosonic gases of ultracold atoms trapped in optical lattices, which are periodic potentials formed by standing waves of laser light. Optical lattices provide a highly tunable system, as the depth of the potential can be adjusted by changing the laser intensity. This high degree of control, combined with the absence of the complex lattice dynamics present in traditional solid-state systems, makes ultracold atoms in optical lattices an ideal platform for realizing the Bose-Hubbard model experimentally. The main reference for this chapter is [17].

3.1 Optical Lattice

Let us do a brief review of how a (dilute) Bose gas can be trapped through an optical lattice. We will start by studying the interference pattern caused by a set of crossed laser beams, and then proceed to examine the coupling between atoms and light.

Laser beams. A laser with wavelength λ consists of photons with energy $2\pi\hbar c/\lambda$, and therefore has to be treated within the framework of quantum mechanics. That said, it is possible to treat the laser beam and the corresponding electromagnetic field classically, and move to the quantized version at the end. For a single plane wave travelling in the positive z direction, the electric field is given by

$$\mathbf{E}(\mathbf{x},t) = \boldsymbol{\varepsilon} E_0 \cos(kz-\omega t)\exp\left\{-\frac{x^2+y^2}{2w^2(z)}\right\} \tag{3.1}$$

where $\omega = 2\pi c/\lambda$ is the angular frequency, $k = 2\pi/\lambda$ is the wavenumber and $\boldsymbol{\varepsilon}$ is the polarization unit vector, living in the $x-y$ plane. The quantity $w(z)$ is called the *waist* of the Gaussian laser beam and defines its extension in the radial direction.[1] By superimposing two counter-propagating laser beams of the same wavelength and frequency, we can create a standing wave. Assuming they also share the same linear polarization, the electric field is then given by

$$\mathbf{E}(\mathbf{r},t) = 2\boldsymbol{\varepsilon} E_0 \cos(\omega t)\cos(kz)\exp\left\{-\frac{x^2+y^2}{2w^2}\right\} \equiv \boldsymbol{\varepsilon} E(\mathbf{x})\left(\frac{\mathrm{e}^{\mathrm{i}\omega t}+\mathrm{e}^{-\mathrm{i}\omega t}}{2}\right) \tag{3.2}$$

which can be easily quantized by simply replacing $\sqrt{\langle N_{\mathrm{ph}}\rangle}\,\mathrm{e}^{-\mathrm{i}\omega t}$ with the annihilation operator of a photon $\hat{a}$, where $\langle N_{\mathrm{ph}}\rangle = \langle \hat{a}^\dagger \hat{a}\rangle$ denotes the average number of photons present in the standing wave.[2] As a result, the electric-field operator in the Schrödinger picture is given by

$$\hat{\mathbf{E}}(\mathbf{x}) = \boldsymbol{\varepsilon} E(\mathbf{x})\left(\frac{\hat{a}+\hat{a}^\dagger}{2\sqrt{\langle N_{\mathrm{ph}}\rangle}}\right) \tag{3.3}$$

Atom-light coupling. A single laser beam, by coupling with an atom of the ultracold gas, gives rise to a potential that is constant in the axial direction and Gaussian in the radial direction. Depending on the frequency of the laser, this potential can be both repulsive and attractive. By superimposing two counter-propagating laser beams as stated above, we create standing wave which acts as a periodic potential for the atoms. This is known as an optical lattice.

[1] The waist depends in general on the z coordinate, in particular when the laser beam is focused, which is used experimentally to create an optical trap for atoms. For our purposes we can take the waist to be a constant, i.e. $w(z) = w$.

[2] Interestingly, we are here making use of the fact that a laser can be seen as a Bose-Einstein condensate of photons if the number of photons is much larger than one. In addition, the Hamiltonian for the photons is $\hat{H}_{\mathrm{ph}} = \hbar\omega \hat{a}^\dagger \hat{a}$.

For the sake of simplicity, we will consider ground-state Alkali atoms[3] which couple to the electromagnetic field mainly because of the quadratic Stark effect, i.e. via an induced electric dipole moment $\mathbf{d}(\mathbf{x}) = \alpha(\omega)\mathbf{E}(\mathbf{x})$ (the coupling to the magnetic dipole moment of the atom can be neglected). Here $\alpha(\omega)$ is the polarizability of the atom, which in general depends on the frequency of the electric field. Classically, the resulting potential is expected to be

$$V^{\mathrm{ex}}(\mathbf{x}) = -\mathbf{d}(\mathbf{x}) \cdot \mathbf{E}(\mathbf{x}) = -\alpha(\omega) E^2(\mathbf{x}) \tag{3.4}$$

which can be either attractive or repulsive depending on the sign of the polarizability.

In the context of quantum mechanics, the above potential can be deduced by taking into account laser-induced excitations of alkali atoms to an excited state. Once again, we will simplify the problem by considering a two-level atom whose ground state $|g\rangle$ has energy E_{g} and whose single excited state $|\mathrm{e}\rangle$ has energy E_{e}. The interaction between the atom and the electric field is described by the Hamiltonian

$$\hat{H} = -\hat{\mathbf{d}} \cdot \hat{\mathbf{E}}(\mathbf{x}) \tag{3.5}$$

where $\hat{\mathbf{d}}$ is now the dipole operator.[4] Because only the electrons in the outer shell are important, in the context of alkali atoms we have to work with only a single electron.

Using the tools of perturbation theory, we can finally calculate the energy corrections due to the alkali atom-light interaction. In this example, the ground-state of the atom is described by an s-wave electronic orbital, and therefore the first-order correction to the energy vanishes; meanwhile the p-wave excited state, with an orbital angular momentum equal to one, gives rise to a nonzero transition matrix element for the dipole operator. The second-order correction therefore results in a potential for the atoms, given by

$$V^{\mathrm{ex}}(\mathbf{x}) = \frac{|\langle \mathrm{g}|\hat{\mathbf{d}} \cdot \boldsymbol{\varepsilon}|\mathrm{e}\rangle|^2}{4} \left(\frac{1}{E_{\mathrm{g}} - E_{\mathrm{e}} + \hbar\omega} + \frac{1}{E_{\mathrm{g}} - E_{\mathrm{e}} - \hbar\omega} \right) E^2(\mathbf{x}) \tag{3.6}$$

The first term on the right-hand side of (3.6) physically represents the stimulated absorption of a photon, while the second term corresponds to the stimulated emission of a photon. The expectation value $\langle \mathrm{g}|\hat{\mathbf{d}} \cdot \boldsymbol{\varepsilon}|\mathrm{e}\rangle$ depends on the specific atom and the polarization of the light, but can be written conveniently in terms of a specific angular frequency, known as Rabi angular frequency Ω.[5] Similarly, by defining the detuning from resonance as $\delta = \omega - (E_{\mathrm{e}} - E_{\mathrm{g}})/\hbar$, follows that when the detuning is small, the first term in (3.6) is much bigger than the second and the latter can thus be neglected. This leads to

$$V^{\mathrm{ex}}(\mathbf{x}) = \frac{\Omega^2}{\delta} \cos^2(2\pi z/\lambda) \exp\left\{ -\frac{x^2 + y^2}{w^2} \right\} \tag{3.7}$$

where we see that the potential can indeed be attractive or repulsive, depending on the sign of the detuning. When the detuning is negative, the atoms are attracted to the maxima of the laser intensity, where the potential energy of the atoms is minimal. In this case, the Gaussian profile of the laser beam (said to be red-tuned) automatically traps the atoms in the radial direction. When the detuning is positive, the atoms are attracted to the minima of laser intensity, where the potential energy of the atoms is also minimal. In this case, the Gaussian profile of the laser beam (said to be blue-tuned) repels the atoms in the radial direction, so that an additional trapping mechanism has to be provided (either with a magnetic potential or by adding a second red-tuned laser beam).

3.2 Bloch waves and Wannier functions

In order to derive the Bose-Hubbard model within the context of ultracold atoms trapped in optical lattices, a qualitative study of the single-site wavefunctions is needed. Being the atoms noninteracting and under the influence of a periodic optical-lattice potential, the relevant wavefunctions are Bloch waves

$$\chi_{\mathbf{n},\mathbf{k}}(\mathbf{x}) = \mathrm{e}^{\mathbf{i}\mathbf{k}\cdot\mathbf{x}} u_{\mathbf{n},\mathbf{k}}(\mathbf{x}) \tag{3.8}$$

namely, can be written as the product of a plane wave and a function $u_{\mathbf{n},\mathbf{k}}$ that is periodic with the lattice period [7]. Accordingly, the dispersion relation[6] now develops gaps at specific locations determined by the lattice structure: similarly to what happens for crystals, when the momentum approaches the boundary of the first Brillouin zone at $k_z = \pm 2\pi/\lambda$, with λ the wavelength of the laser light, the dispersion starts to deviate from the quadratic result. If

[3] Indeed, since Alkali atoms present only one valence electron, they do not follow Bose-Einstein statistics. Despite this fact, our arguments are general and will not be affected.

[4] The dipole operator is defined as $\hat{\mathbf{d}} = -e\sum_i \hat{\mathbf{r}}_i$, where $-e$ is the electron charge and $\hat{\mathbf{r}}_i$ are the position operators of the electrons relative to the nucleus of the atom.

[5] The Rabi angular frequency for a single laser is defined as $\hbar\Omega = |\langle \mathrm{g}|\hat{\mathbf{d}} \cdot \boldsymbol{\varepsilon}|\mathrm{e}\rangle| E_0$, where E_0 is the maximum amplitude of the electric field as in (3.1).

[6] The wavefunction of a free atom is a plane wave $\mathrm{e}^{\mathbf{i}\mathbf{k}\cdot\mathbf{x}}/\sqrt{V}$ and has an energy dispersion relation $\varepsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2\mathrm{m}$.

the momentum is increased past the boundary of the first Brillouin zone, the dispersion has a discontinuity and the difference in energy is the band gap.[7]

Within the context of an optical lattice with potential minima located at the lattice sites $\mathbf{x}_i$, it can be shown that for each band n_z a set of Wannier functions $w_{\mathbf{n}}(\mathbf{x}- \mathbf{x}_i)$ exists, such that the exact Bloch wavefunctions can be written as

$$\chi_{\mathbf{n},\mathbf{k}}(\mathbf{x}) = \sum_i \mathrm{e}^{\mathbf{i}\mathbf{k}\cdot\mathbf{x}_i} w_{\mathbf{n}}\left(\mathbf{x}-\mathbf{x}_i\right) \tag{3.9}$$

The Wannier functions are orthogonal for different bands n_z as well as for different sites i. For deep optical lattices we can use the tight-binding limit, in which we approximate the lattice potential near each site $\mathbf{x}_i$ with a harmonic potential. Then, the exact Wannier functions $w_{\mathbf{n}}\left(\mathbf{x}-\mathbf{x}_i\right)$ are actually to a very good approximation given by the harmonic oscillator wavefunctions $\chi_{\mathbf{n}}\left(\mathbf{x}-\mathbf{x}_i\right)$.

3.3 Hubbard models

The **Hubbard model**, originally developed to describe electron behavior in solids, models the transition between conducting and insulating states. It is based on the **tight-binding model**, which describes electrons that are tightly bound to their respective atoms with minimal interaction with nearby atoms. In the tight-binding model, the Hamiltonian accounts only for kinetic energy (hopping terms) and interactions with lattice atoms (atomic potential). The Hubbard model extends this by adding short-range interactions between electrons.

This model can also be applied to particles in strong periodic potentials, such as optical lattices, where the dynamics are simpler than in solid-state systems due to the absence of atomic interactions. In these scenarios, the Hubbard model serves as a useful approximation for particles in periodic potentials at low temperatures, assuming they occupy the lowest Bloch band and that long-range interactions are negligible.

In the tight-binding approximation, the Hubbard Hamiltonian is expressed using Wannier states, which are localized at each lattice site and coupled with neighboring sites, allowing particles to hop between them. This coupling strength is quantified by the hopping integral between nearby sites. As we will see, the Hubbard model's behaviour is influenced by the balance between the strength of the hopping integral, which characterizes the system's kinetic energy, and the strength of the interaction term. The system is said to be in the tight-binding limit when hopping integrals decrease rapidly with distance. However, when the interactions are strong, the behaviour of the Hubbard model can significantly differ from the standard tight-binding model.

Bose-Hubbard model. The Bose–Hubbard model, firstly introduced by Gersch and Knollman [4] in the context of granular superconductors, is the bosonic analogue of the Hubbard model for electrons. The Bose-Hubbard model efficiently describes the physics of interacting spinless bosons on an optical lattice, as it captures the essential properties of the system, while maintaining simplicity. The main goal of this section is to derive the Bose-Hubbard Hamiltonian from the following general imaginary-time action

$$\begin{aligned} S\left[\psi^*,\psi\right] = &\int_0^{\hbar\beta} \mathrm{d}\tau \int \mathrm{d}\mathbf{x}\ \psi^*(\mathbf{x},\tau)\left[\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\nabla^2}{2m} + V^{\mathrm{ex}}(\mathbf{x})\right]\psi(\mathbf{x},\tau) \\ &+ \frac{1}{2}\int_0^{\hbar\beta} \mathrm{d}\tau \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{x}'\ \psi^*(\mathbf{x},\tau)\,\psi^*\left(\mathbf{x}',\tau\right) V\left(\mathbf{x}-\mathbf{x}'\right)\psi\left(\mathbf{x}',\tau\right)\ \psi(\mathbf{x},\tau) \end{aligned} \tag{3.10}$$

which describes a gas of weakly interacting spinless bosons in a periodic potential. Here, because we are working in the spatial representation, the dependency is upon field operators (or better, their eigenvalues), and the isotropic optical-lattice potential is described by (3.7). By using the Wannier functions introduced in the previous section, we can expand the field operator eigenvalues as

$$\psi(\mathbf{x},\tau) = \textstyle\sum_{\mathbf{n},i} a_{\mathbf{n},i}(\tau)\, w_{\mathbf{n}}\left(\mathbf{x}-\mathbf{x}_i\right) \tag{3.11}$$

where the expansion coefficients $a^*_{\mathbf{n},i}(\tau)$ and $a_{\mathbf{n},i}(\tau)$ correspond to the eigenvalues of the creation and the annihilation operator respectively of an atom in the Wannier state $w_{\mathbf{n}}\left(\mathbf{x}-\mathbf{x}_i\right)$ at site i. Starting from this action, in order to derive the Bose-Hubbard Hamiltonian it is necessary to impose the right approximations to the system, as every Hubbard model in intrinsically an approximate model. *Firstly*, we will suppose to work with sufficiently low temperatures and for sufficiently small interaction energies, therefore with atoms occupying the lowest $\mathbf{n} = \mathbf{0}$ state of the lattice. As a result, we find the following lattice action[8] which can be seen as the sum of a non-interacting part $S_0\left[a^*, a\right]$ and of an

[7] That being said, we can specify the wavefunction by a band index n_z and a momentum k_z that takes on values within the first Brillouin zone only. That is exactly what we did in (3.8).

[8] Thanks to this first approximation, the band index $\mathbf{n}$ is now redundant.

interacting part $S_{\text{int}}[a^*, a]$.

$$S[a^*,a] = \int_0^{\hbar\beta} \mathrm{d}\tau \left\{ \sum_{\boldsymbol{ij}} a_i^*(\tau)\, \hbar \frac{\partial a_j(\tau)}{\partial \tau} \int \mathrm{d}\mathbf{x}\, w_{\mathbf{0}}^*(\mathbf{x}-\mathbf{x}_i) w_{\mathbf{0}}(\mathbf{x}-\mathbf{x}_j) \right.$$
$$+ \sum_{\boldsymbol{ij}} a_i^*(\tau) a_j(\tau) \int \mathrm{d}\mathbf{x}\, w_{\mathbf{0}}^*(\mathbf{x}-\mathbf{x}_i) \left[-\frac{\hbar^2\nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu \right] w_{\mathbf{0}}(\mathbf{x}-\mathbf{x}_j)$$
$$\left. + \tfrac{1}{2} \sum_{\boldsymbol{ii'jj'}} a_i^*(\tau) a_{i'}^*(\tau) a_j(\tau) a_{j'}(\tau) \iint \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}'\, w_{\mathbf{0}}^*(\mathbf{x}-\mathbf{x}_i)\, w_{\mathbf{0}}^*(\mathbf{x}'-\mathbf{x}_{i'})\, V(\mathbf{x}-\mathbf{x}')\, w_{\mathbf{0}}(\mathbf{x}'-\mathbf{x}_j)\, w_{\mathbf{0}}(\mathbf{x}-\mathbf{x}_{j'}) \right\}$$

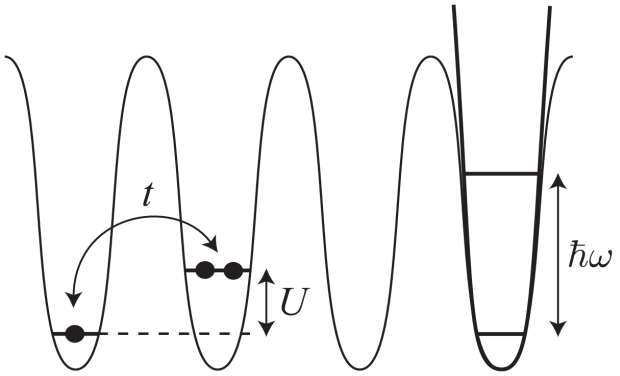

Figure 3.1: Picture taken from [17]. In the Bose-Hubbard model, two bosons on the same site have an interaction energy $\boldsymbol{U}$, while the probability to tunnel to a neighboring site is given by the hopping parameter $\boldsymbol{t}$. A typical optical lattice is well approximated by a harmonic potential of strength $\hbar\omega$ for its lowest-lying quantum states.

The non-interacting action $S_0[a^*, a]$ can be rewritten effectively by using the orthonormality of Wannier functions in the same band[9] and by introducing three new quantities, namely the **on-site energy** $\boldsymbol{\varepsilon_i}$, the **tunnelling amplitude** $\boldsymbol{t_{i,j}}$ between sites i and j and the **chemical potential** $\boldsymbol{\mu}$

$$S_0[a^*,a] = \int_0^{\hbar\beta} \mathrm{d}\tau \left[\sum_i a_i^*(\tau) \left(\hbar\frac{\partial}{\partial\tau} + \boldsymbol{\varepsilon_i} - \boldsymbol{\mu} \right) a_i(\tau) - \sum_{i\neq j} a_i^*(\tau)\, \boldsymbol{t_{i,j}}\, a_j(\tau) \right] \tag{3.12}$$

$$\boldsymbol{\varepsilon_i} = \int \mathrm{d}\mathbf{x}\, w_{\mathbf{0}}^*(\mathbf{x}-\mathbf{x}_i) \left[-\frac{\hbar^2\nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) \right] w_{\mathbf{0}}(\mathbf{x}-\mathbf{x}_i) \tag{3.13}$$

$$\boldsymbol{t_{i,j}} = -\int \mathrm{d}\mathbf{x}\, w_{\mathbf{0}}^*(\mathbf{x}-\mathbf{x}_i) \left[-\frac{\hbar^2\nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) \right] w_{\mathbf{0}}(\mathbf{x}-\mathbf{x}_j) \tag{3.14}$$

Changing the value of $\boldsymbol{\mu}$ changes the total number of bosons. Depending upon the physical conditions, a given system can either be constrained to be at a fixed chemical potential (the grand canonical ensemble) or have a fixed total number of bosons (the canonical ensemble).

The double summation in the tunnelling or hopping term is over all combinations i, j for which $i \neq j$. For a deep lattice, which will be our *second* assumption, the hopping energy $\boldsymbol{t_{i,j}}$ will be exponentially suppressed for all sites that are not nearest neighbors. Therefore we will restrict the summation to nearest neighbors only, while keeping the hopping amplitude constantly equal to $\boldsymbol{t}$.

Focusing now on the interaction part $S[a^*, a]$, the interactions between the atoms not only include on-site interactions but also interactions between atoms that are on remote sites. However, the latter interactions are typically exponentially suppressed, and for practical purposes it usually suffices to take only the on-site interactions into account. This ultimately consists in our *third* and last approximation.[10] As a result, by introducing the **on-site interaction strength** $\boldsymbol{U}$, we can efficiently rewrite the interaction action as

$$S_{\text{int}}[a^*,a] = \int_0^{\hbar\beta} \mathrm{d}\tau \frac{\boldsymbol{U}}{2} \sum_i a_i^*(\tau) a_i^*(\tau) a_i(\tau) a_i(\tau) \tag{3.15}$$

$$\boldsymbol{U} = \iint \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{x}'\, w_{\mathbf{0}}^*(\mathbf{x}-\mathbf{x}_i)\, w_{\mathbf{0}}^*(\mathbf{x}'-\mathbf{x}_i)\, V(\mathbf{x}-\mathbf{x}')\, w_{\mathbf{0}}(\mathbf{x}'-\mathbf{x}_i)\, w_{\mathbf{0}}(\mathbf{x}-\mathbf{x}_i) \tag{3.16}$$

[9] Namely, the condition $\int \mathrm{d}\mathbf{x}\, w_0^*(\mathbf{x}-\mathbf{x}_i)\, w_0(\mathbf{x}-\mathbf{x}_j) = \delta_{i,j}$

[10] The approximations we have introduced, collectively recreate the tight-binding approximation typical of an Hubbard model.

where $\boldsymbol{U > 0}$, representing the simplest possible repulsive interaction between on-site bosons. Finally, the Hamiltonian of the Bose-Hubbard model results to be

$$\hat{H} = -\frac{\boldsymbol{t}}{2} \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \hat{a}_i \hat{a}_j^\dagger + \sum_i (\boldsymbol{\varepsilon_i} - \boldsymbol{\mu}) \, \hat{a}_i^\dagger \hat{a}_i + \frac{\boldsymbol{U}}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i \tag{3.17}$$

As it will be clear in the next section, the above Hamiltonian also describes a system of interacting bosons on a **disordered lattice**. Indeed, the on-site energies can be tuned to be randomly and uniformly distributed between two energy values, e.g. $\boldsymbol{\varepsilon_i} \in [-\Delta, \Delta]$ with Δ being the excitation gap.

Parameter control and disorder. As seen in previous sections, the main parameters of an optical lattice are its potential well depth and its periodicity. The potential depth is adjusted by changing the laser power, while periodicity can be modified by altering the laser wavelength or the angle between the beams. As we will now show, this tunability allows precise control over the fundamental parameters of the Bose-Hubbard model, enabling the exploration of various configurations and the introduction of disorder into the system.

If we consider the tight-binding limit, therefore by working in a deep-lattice configuration, the optical-lattice potential (3.7) may be approximated accordingly in order to explicitly determine the parameters of interest in the Bose-Hubbard model. Indeed, by approximating (3.7) with its second-order expansion around a lattice site, with coefficient $\hbar\omega$, we can exactly solve the single-particle Schrödinger equation and estimate the hopping strength $\boldsymbol{t}$, as in [12]

$$\boldsymbol{t} = \frac{4 E_\mathrm{r}^{1/4} V_0^{3/4}}{\sqrt{\pi}} \, \mathrm{e}^{-\left(\frac{4V_0}{E_\mathrm{r}}\right)^{1/2}} \tag{3.18}$$

with $E_\mathrm{r} = 2\pi^2\hbar^2/m\lambda^2$ being the recoil energy.[11] In addition, having defined $\boldsymbol{\varepsilon_i}$ as the on-site case of $\boldsymbol{t_{i,j}}$, it inherits the same lattice-potential dependence. In a similar fashion, we can determine the on-site interaction strength $\boldsymbol{U}$ by approximating (3.7) with a pseudopotential[12] and by substituting into (3.15). Esplicitly:

$$V(\mathbf{x}-\mathbf{x}') = \frac{4\pi a \hbar^2}{m} \, \delta(\mathbf{x}-\mathbf{x}') \quad \xrightarrow[\text{in (3.15)}]{\text{by substituting}} \quad \boldsymbol{U} = \frac{2\hbar\omega a}{l\sqrt{2\pi}} \quad \text{with} \quad l = \sqrt{\frac{\hbar}{m\omega}} = \frac{\lambda}{4\pi} \left(\frac{E_\mathrm{r}}{V_0}\right)^{1/4} \tag{3.19}$$

where λ is the wavelength of the laser light that is used to create the optical lattice, a is the s-wave scattering length, and l is the harmonic oscillator length. Because we are evaluating the integrals in the tight-binding limit, the Wannier functions have been approximated by the harmonic-oscillator wavefunctions.

From this, we explicitly see that all the fundamental parameters of the Bose-Hubbard model depend on the optical lattice settings, namely its potential and its laser wavelength.[13] The impact of ultracold atomic and molecular quantum gases on present-day physics is linked to the extraordinary degree of control that such systems offer. Such tuning capability permits us to investigate the fundamental behavior of quantum matter under various conditions, one of which is on-site disorder.

[11] The recoil energy gives the kinetic energy of an atom initially at rest after the absorption of a single photon.

[12] This will be important in Landau's theory of phase transitions, when we will introduce the Bogoliubov approximation.

[13] For completeness, it is important to mention another important technique for tuning the interaction term, namely the *Feshbach's resonance technique* [15].

4 Phase Diagram

As we have shown in the previous chapter, ultracold bosonic atoms trapped in an optical lattice are efficiently described by the Bose-Hubbard model. Working in the zero-temperature limit, the resulting trapped Bose-Einstein condensate manifests unique quantum configurations depending on the model parameters and on the eventual disorder of the system. Specifically, the Bose-Hubbard model predicts three different quantum phases of matter: the **Mott-insulator phase**, which occurs when interactions are strong and particle density is commensurate; the **superfluid phase**, stable under weak interactions; and the **Bose glass** phase, which arises in the presence of disorder.

Here we observe such **quantum phase transitions** in a Bose-Einstein condensate with repulsive interactions, held in a two-dimensional optical lattice potential. By changing the parameters of the Bose-Hubbard model - and therefore by tuning the optical lattice configuration - we will explore the zero-temperature phase diagrams of both its ordered and disordered configurations. In the ordered case, the model undergoes a direct quantum phase transition from the superfluid phase to the Mott-insulator state. In the disordered case, we argue that a gapless, insulating Bose glass phase with nonzero compressibility must always intervene between the Mott and superfluid phases. The main references for this chapter are [1] and [17].

4.1 Quantum phase transitions

When a physical system crosses the boundary between two phases, its properties change fundamentally, driven by microscopic fluctuations.[1] When the temperature of the system approaches zero, all thermal fluctuations die out, preventing phase transitions in classical systems at zero temperature, as their opportunity to change has vanished. However, their quantum mechanical counterparts can show fundamentally different behaviour. In a quantum system, fluctuations are present even at zero temperature, due to *Heisenberg's uncertainty relation*. These microscopic quantum fluctuations may be strong enough to drive a phase transition in the ground state of a many-body system, bringing out a macroscopic change, when the relative strength of two competing energy terms is varied across a critical value.

Landau's theory of phase transitions. A phase transition is the phenomenon that a many-body system may suddenly change its properties in a rather drastic way due to the change of an externally controllable variable. Most phase transitions[2], despite covering a wide phenomenology, can be described with an appropriate **order parameter**. An order parameter essentially consists in a measure of the order before and after a phase transition, and therefore is able to discriminate between the two phases involved.[3] Such a transition, when the parameter describing the order in the system is discontinuous, is said to be of the *first-order*; on the contrary, when the order parameter changes from zero to a nonzero value in a continuous way, the transition is said to be of the *first-order*.

Consider a system that breaks some symmetries under a phase transition, which may be described by the variation of the order parameter $\boldsymbol{\eta}$. In the Landau approach to phase transitions, the central role is played by the **Landau free-energy functional** $\mathcal{F}_L[\boldsymbol{\eta}]$, which corresponds to an effective Hamiltonian that describes the system on a macroscopic scale after the microscopic fluctuations have been integrated out[4]

$$Z = \exp\{-\beta\mathcal{F}\} = \mathrm{Tr}\left[\int \mathrm{d}[\boldsymbol{\eta}]\ \delta\left[\boldsymbol{\eta}(\mathbf{x}) - \hat{\boldsymbol{n}}(\mathbf{x})\right]\ \mathrm{e}^{-\beta\hat{H}}\right] = \int \mathrm{d}[\boldsymbol{\eta}]\ \exp\left\{\frac{-\mathcal{F}_L[\boldsymbol{\eta}]}{k_B T}\right\} \approx \exp\left\{-\frac{\mathcal{F}_L[\langle\boldsymbol{\eta}\rangle]}{k_B T}\right\} \tag{4.1}$$

Obtaining an explicit form for the Landau free-energy is, however, generally prohibitive. As a result, phenomenological approaches and approximations are typically used to determine the correct form of the Landau free energy functional. A notable example is the **mean-field approximation**, which only takes into account the largest contribution to the partition function Z, obtained by minimizing the Landau free-energy functional with respect to the order parameter.[5]

Landau's approach to phase transitions is therefore based on an expansion of the **Landau free-energy functional** $\mathcal{F}_L[\boldsymbol{\eta}]$ in terms of an order parameter. In many systems with certain symmetries - and also in our case - the free

[1] In a classical example, it may melt or freeze.

[2] A rare exception to this rule is found in the *Kosterlitz-Thouless transition*.

[3] An important example of this can be found in the *Ising model* for magnetism. In this context, the ferromagnetic phase and the paramagnetic phase are distinguished by the value of the magnetization $\langle M\rangle$, which therefore represents the order parameter of the phase transition.

[4] Here $\hat{\boldsymbol{n}}$ is any continuous operator density describing the microscopic quantity of interest in the system, which may be defined as $\hat{\boldsymbol{n}} = \sum_i \delta(\mathbf{x} - \mathbf{x}_i)\hat{N}_i$. In the Ising model it is typically the spin density, while in the context of the Bose-Hubbard model it will be the bosonic occupation number. Moreover, the Dirac delta functional satisfies $\hat{1} = \int \mathrm{d}[\boldsymbol{\eta}]\ \delta\left[\boldsymbol{\eta}(\mathbf{x}) - \hat{\boldsymbol{n}}(\mathbf{x})\right]$

[5] It is worth to mention its evident similarity with the *stationary-phase approximation*, introduced in the context of the path-integral formulation of quantum mechanics.

energy depends only on even powers of the order parameter.[6] The goal is to find the value of such $\langle \boldsymbol{\eta} \rangle$ that minimizes the free-energy:

$$\mathcal{F}_L[\boldsymbol{\eta}] = V f_L[\boldsymbol{\eta}] = \frac{V}{2}\left[\alpha(T)\boldsymbol{\eta}^2 + \frac{\beta(T)}{2}\boldsymbol{\eta}^4 + \frac{\delta(T)}{3}\boldsymbol{\eta}^6 + \dots\right] \tag{4.2}$$

with V the volume of the system and $f_L[\boldsymbol{\eta}]$ the Landau free-energy density. Typically, despite the presence of higher order terms in the free energy, it is a reasonable to consider the expansion only up to the sextic order in the order parameter, as long as the order parameter is small. For the system to be thermodynamically stable - that is, the system does not seek an infinite order parameter to minimize the energy - the coefficient of the highest even power must be positive, so $\delta(T) > 0$.

Landau theory is essentially a mean-field theory, as it neglects microscopic fluctuations or correlations between different regions of the system, resulting in a uniform order parameter. While this approach is effective for systems where these assumptions apply, there are cases with long-range correlations where these assumptions fail. In such systems, Landau theory needs to be refined to properly describe their phase transitions.

Bose-Einstein condensation. Bose-Einstein condensation corresponds to a macroscopic occupation of the same single-particle quantum state, where macroscopic means that the density $\langle N_{\mathbf{0}} \rangle / V$ does not go to zero in the thermodynamic limit.[7] For a homogeneous ideal Bose gas, the average number of particles in the grand-canonical ensemble

$$\begin{aligned}\langle N \rangle &= -\frac{\partial \Omega}{\partial \mu} = \sum_{\mathbf{k}} N_{\mathrm{BE}}\left(\varepsilon_{\mathbf{k}}\right) = \sum_{\mathbf{k}} \frac{1}{\exp\left\{\beta\left(\varepsilon_{\mathbf{k}} - \mu\right)\right\} - 1} \\ &= \langle N_{\mathbf{0}} \rangle + \langle N' \rangle = \frac{1}{\exp\{-\beta\mu\} - 1} + \sum_{\mathbf{k}\neq\mathbf{0}} \frac{1}{\exp\left\{\beta\left(\varepsilon_{\mathbf{k}} - \mu\right)\right\} - 1}\end{aligned} \tag{4.3}$$

where Ω is the thermodynamic potential[8] and $N_{\mathrm{BE}}\left(\varepsilon_{\mathbf{k}}\right)$ is the average occupation number for bosons in the state $|\mathbf{k}\rangle$, which should therefore be larger or equal to zero. As a result, imposing such condition for the state with $\mathbf{k} = \mathbf{0}$, we find that $\mu \leq 0$.

Consider now an average number of particles $\langle N \rangle$, that we keep fixed. Upon lowering the temperature, we see from (4.3) that we have to increase the chemical potential to keep the number of particles constant, which can only be done until μ reaches zero. Such extreme condition ultimately defines the critical temperature for a free Bose gas. If we lower the temperature even further, then we can only keep the particle number constant by *macroscopically* occupying the ground state. The macroscopic occupation of the single-particle state with $\mathbf{k} = \mathbf{0}$ is called **Bose-Einstein condensation**.

As a result, we expect a Bose-Einstein condensed gas to develop strong correlations over the size of the system, or equivalently an off-diagonal long-range order. Formally, this can be made explicit by considering the one-particle density matrix, written in terms of the field operators

$$n\left(\mathbf{x}, \mathbf{x}'\right) = \langle \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}\left(\mathbf{x}'\right) \rangle \tag{4.4}$$

which tells us whether or not the presence of a particle at position $\mathbf{x}'$ is correlated with the presence of a particle at position $\mathbf{x}$. In order to understand the meaning of an off-diagonal long-range order, let us consider the density matrix near T_{C}, when the chemical potential is slightly below or equal zero. Since it depends only on the difference in the coordinates, the system is evidently translationally invariant and can be easily studied in the momentum representation:

$$\begin{aligned}\langle \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}\left(\mathbf{x}'\right) \rangle &= \tfrac{1}{V}\textstyle\sum_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\left(\mathbf{x}-\mathbf{x}'\right)} \langle \hat{\psi}^\dagger_{\mathbf{k}} \hat{\psi}_{\mathbf{k}} \rangle = \tfrac{\langle \hat{\psi}^\dagger_{\mathbf{0}} \hat{\psi}_{\mathbf{0}} \rangle}{V} + \int \tfrac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \tfrac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\left(\mathbf{x}-\mathbf{x}'\right)}}{\mathrm{e}^{\beta\left(\varepsilon_{\mathbf{k}}-\mu\right)}-1} \\ &\simeq \tfrac{\langle \hat{\psi}^\dagger_{\mathbf{0}} \hat{\psi}_{\mathbf{0}} \rangle}{V} + \tfrac{1}{\beta}\int \tfrac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \tfrac{\mathrm{e}^{-i\mathbf{k}\cdot\left(\mathbf{x}-\mathbf{x}'\right)}}{\varepsilon_{\mathbf{k}}-\mu} \\ &\simeq \tfrac{\langle \hat{\psi}^\dagger_{\mathbf{0}} \hat{\psi}_{\mathbf{0}} \rangle}{V} + \tfrac{m k_{\mathrm{B}} T}{2\pi|\mathbf{x}-\mathbf{x}'|}\mathrm{e}^{-\sqrt{2m|\mu||\mathbf{x}-\mathbf{x}'|/\hbar}}\end{aligned} \tag{4.5}$$

where in the first step we moved to the integral form, and inserted the Bose distribution. Since we are particularly interested in the limit $|\mathbf{x} - \mathbf{x}'| \to \infty$, we focus in the second step on the low-momentum or long-wavelength modes for

[6] This property holds, notoriously, for the Ising model, thanks to the spin reversal symmetry. As we will show, it is also the case for the Bose-Hubbard model.

[7] The thermodynamic limit of a system is the limit for a large number N of particles where the volume V is taken to grow in proportion with the number of particles.

[8] The *grand-canonical* thermodynamic potential Ω can be found by a proper manipulation of the partition function. For bosons, we find

$$\Omega = k_{\mathrm{B}} T \textstyle\sum_{\mathbf{k}} \log\left(1 - \mathrm{e}^{-\beta\left(\varepsilon_{\mathbf{k}}-\mu\right)}\right)$$

which $\beta(\varepsilon_{\mathbf{k}}-\mu)$ is small. As the chemical potential becomes zero and the occupation of the ground state becomes macroscopic, we have that $\langle\hat{\psi}_0^\dagger\hat{\psi}_0\rangle/V = \langle N_0\rangle/V$ is nonzero in the thermodynamic limit. Then, we find from (4.5) that the first term, which physically describes the constant nonzero density of Bose-Einstein condensed atoms, does not vanish at large separations $|\mathbf{x}-\mathbf{x}'|$. This is the off-diagonal long-range order in the single-particle density matrix. As a result, the one-particle density matrix seems to be the order parameter of the phase transition.

Bogoliubov approximation. Bose-Einstein condensation manifests strong correlations over the size of the system, resulting in a macroscopic occupation of the ground state. In order to properly describe the phase transition, it is therefore necessary to go beyond Landau's mean-field theory and include long-range correlations, which are naturally enclosed within the definition of the order parameter $n(\mathbf{x},\mathbf{x}')$. This procedure ultimately leads to the Landau-Ginzburg theory of phase transitions, which improves upon Landau's mean-field theory by incorporating spatial variations and fluctuations of the order parameter up to quadratic order in the free-energy expansion. In order to deal analytically with the resulting action, it is necessary to make approximations that take the dominant physics into account. An example of this, within the context of field-theory, is the **Bogoliubov approximation** of the order parameter.

Let us start by considering the zero-temperature limit of a Bose interacting gas, whose ground state wavefunction is in general a complicated linear superposition of states $|N_{\mathbf{0}},\cdots\rangle$. Here the occupation number of the zero-momentum state $N_{\mathbf{0}}$ fluctuates around the average value $\langle N_{\mathbf{0}}\rangle$, but is always a substantial fraction of the total number of atoms. As a result, within the subspace of these relevant states, we can consider the following approximation of the field operators

$$\hat{\psi}_0^\dagger\hat{\psi}_0\,|N_{\mathbf{0}},\cdots\rangle \approx \hat{\psi}_0\hat{\psi}_0^\dagger\,|N_{\mathbf{0}},\cdots\rangle \approx \langle N_{\mathbf{0}}\rangle\,|N_{\mathbf{0}},\cdots\rangle \tag{4.6}$$

which indeed suggests the possibility of replacing them by ordinary complex numbers, resulting in the **Bogoliubov substitution**. This implies that the field operators obtain a nonzero expectation value in the Bose-Einstein condensed phase, namely $\langle\hat{\psi}_{\mathbf{0}}\rangle = \sqrt{\langle N_0\rangle}e^{i\theta}$ or $\langle\hat{\psi}(\mathbf{x})\rangle = \sqrt{\langle n_0\rangle}e^{i\theta}$, which shows that we may use $\langle\hat{\psi}(\mathbf{x})\rangle$ as new the order parameter for the phase transition. To be precise, it is common to define the order parameter as $\langle\hat{\psi}(\mathbf{x})\rangle \equiv \psi_{\mathbf{0}}(\mathbf{x})$ followed by its normalization relation, thanks to which $\psi_{\mathbf{0}}(\mathbf{x})$ is also known as the **macroscopic wavefunction** of the Bose-Einstein condensate

$$\int \mathrm{d}\mathbf{x}\,|\psi_{\mathbf{0}}(\mathbf{x})|^2 = \langle N_{\mathbf{0}}\rangle \tag{4.7}$$

Within the language of field theory, since a generic quantum field must also depend on time (real or imaginary), the order parameter for Bose-Einstein condensation is defined by $\langle\psi(\mathbf{x},\tau)\rangle \equiv \psi_0(\mathbf{x})$. Using this information, we note that for time-independent fields the action (3.10) leads to the following Landau free-energy

$$\mathscr{F}_{\mathrm{L}}[\psi^*,\psi] = \int \mathrm{d}\mathbf{x}\left[\frac{\hbar^2}{2m}|\nabla\psi(\mathbf{x})|^2 + \left(V^{\mathrm{ex}}(\mathbf{x})-\boldsymbol{\mu}\right)|\psi(\mathbf{x})|^2 + \frac{\boldsymbol{U}}{2}|\psi(\mathbf{x})|^4\right] \tag{4.8}$$

where we replaced the interaction potential with a pseudopotential $V(\mathbf{x}-\mathbf{x}') = \boldsymbol{U}\delta(\mathbf{x}-\mathbf{x}')$, in agreement with the tight-binding limit assumption. Despite the evident simplification, it seems that we lost touch with any spatial correlation within the system, which must play a role. According to Bogoliubov theory, in order to restore the effect of correlations, we can perform a fluctuation expansion in the order parameter[9]

$$\psi(\mathbf{x},\tau) = \psi_{\mathbf{0}}(\mathbf{x}) + \psi'(\mathbf{x},\tau) \qquad \text{where} \qquad \int \mathrm{d}\mathbf{x}\,[\psi_{\mathbf{0}}^*(\mathbf{x})\psi'(\mathbf{x},\tau) + \psi_{\mathbf{0}}(\mathbf{x})\psi'^*(\mathbf{x},\tau)] = 0$$

which is the field theory equivalent of the Bogoliubov substitution. In replacing the fluctuation expansion within the action (3.10), we may neglect all the terms that are higher than second-order in the fluctuations, which amounts to the Bogoliubov approximation.[10] In order to understand the role of fluctuations within the system, let us go back to the correlation particle density $n(\mathbf{x},\mathbf{x}')$, now written within the context of Bogoliubov theory

$$n(\mathbf{x}) = \langle\psi(\mathbf{x},\tau)\psi^*\left(\mathbf{x},\tau^+\right)\rangle = |\psi_{\mathbf{0}}(\mathbf{x})|^2 + \langle\psi'(\mathbf{x},\tau)\psi'^*\left(\mathbf{x},\tau^+\right)\rangle$$

From here, it thus follows that $\langle N_{\mathbf{0}}\rangle$ is typically smaller than the total number of atoms $\langle N\rangle$ due to the presence of fluctuations. Note that the average $\langle\psi'(\mathbf{x},\tau)\psi'^*\left(\mathbf{x},\tau^+\right)\rangle$ not only describes the depletion of the condensate due to the thermal occupation of excited states, which happens already for the ideal Bose gas, but also the depletion due to interaction effects. Indeed, due to the presence of interactions the average $\langle\psi'(\mathbf{x},\tau)\psi'^*\left(\mathbf{x},\tau^+\right)\rangle$ is **nonzero** even at **zero temperature**. This depletion clearly cannot be caused by thermal fluctuations, and is thus entirely caused by quantum fluctuations. As we will see, these quantum fluctuations can even drive phase transitions at zero temperature, just like thermal fluctuations drive phase transitions at nonzero temperature. These kinds of phase transitions are therefore appropriately called *quantum phase transitions*.

[9] The condition is to consistently define the fluctuations $\psi'(\mathbf{x},\tau)$ such they contain all configurations that are orthogonal to the condensate $\psi_0(\mathbf{x}) \equiv \langle\psi(\mathbf{x},\tau)\rangle$.

[10] This thus means that we simply ignore $\mathcal{S}_{\mathrm{int}}[\psi'^*,\psi']$, which consists of the third and fourth-order terms.

4.2 Superfluid-to-Mott Insulator transition

The Bose-Hubbard model with no on-site disorder, described by the Hamiltonian (3.17), is predicted to manifest a *direct quantum phase transition* between its superfluid and Mott-insulator states at zero temperature. By considering integer and non-integer values for the average density of bosons per lattice site, and by taking the limiting cases of the model parameters, we can qualitatively determine the phase diagram of such transition.

- $\langle \hat{\boldsymbol{n}}_{\boldsymbol{i}} \rangle = \boldsymbol{n_0} \in \mathbb{N}$. Let us assume that there is an equal integer number of particles at each lattice site i. By considering the limit $t/U \to 0$, the strong repulsive interaction between the particles will make it energetically unfavorable for a boson to move from one site to another. As a result, there is also a nonzero energy penalty to create an excitation, and the system is incompressible. In this situation the gas is said to be in the **Mott-insulator phase**. In the opposite limit $U/t \to 0$, the interactions are so negligibly small that the particles can move without resistance through the system, minimizing their energy by hybridizing over the optical lattice. The (nearly) ideal Bose gas then Bose-Einstein condenses in the lowest momentum state of the lowest Bloch band and becomes **superfluid**. Thus, while keeping the average number of bosons fixed to an integer value, as the ratio t/U increases we expect a phase transition between the Mott-insulating ground state and the superfluid ground state.
- $\langle \hat{\boldsymbol{n}}_{\boldsymbol{i}} \rangle = \boldsymbol{n_0} + \boldsymbol{\delta n}$. Suppose we are in the **Mott-insulating phase** with an equal integer filling number of bosons per lattice site. If we now add one particle to the system, the average density of bosons per lattice site slightly deviates from the previous integer value. Since every lattice site is already occupied, this excess boson also minimizes its energy by delocalizing, being its interaction energy the same on each site. For this reason a gas which has, on average, a non integer number of bosons at each site, is expected to always be in a **superfluid phase** at zero temperature.

Decoupling approximation. As it turns out, despite the refinement to Landau theory, Bogoliubov theory cannot describe large depletions of the condensate and therefore fails to predict the superfluid-to-Mott insulator phase transition. The reason for this is that the Bogoliubov approach only approximately treats the interactions.[11] Nevertheless the main ideas of Bogoliubov theory, namely the fluctuation expansion, may be applied in the formulation of a different mean-field theory which treats the interactions exactly and approximates the kinetic energy of the atoms in the optical lattice.

Let us suppose that the system is initially in the **Mott-insulating state**[12] at zero temperature. In analogy to the Bogoliubov approach, we introduce the superfluid order parameter $\phi = \langle \hat{a}_i \rangle \in \mathbb{C}$ and assume it amounts to a small non-zero constant for all the sites of the lattice. By performing a fluctuation expansion of the order parameter around its expectation value, namely $a_i = \phi + \delta a_i$, we can manipulate the hopping term in the grandcanonical Hamiltonian (3.17) and separate correlations between sites

$$\begin{aligned} \hat{a}_i^\dagger \hat{a}_j &= \left(\hat{a}_i^\dagger - \langle \hat{a}_i^\dagger \rangle\right)\left(\hat{a}_j - \langle \hat{a}_j \rangle\right) + \langle \hat{a}_i^\dagger \rangle \hat{a}_j + \hat{a}_i^\dagger \langle \hat{a}_j \rangle - \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_j \rangle \\ &\approx \langle \hat{a}_i^\dagger \rangle \hat{a}_j + \hat{a}_i^\dagger \langle \hat{a}_j \rangle - \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_j \rangle = \hat{a}_j \phi^* + \hat{a}_i^\dagger \phi - |\phi|^2 \end{aligned} \tag{4.9}$$

where we have neglected the term involving the product of these fluctuations, as they are taken to be small. This leads to a **mean field decoupling** of the hopping term, which results to a diagonal Hamiltonian with respect to each site i

$$\begin{aligned} \hat{H}_{\text{eff}} &= \sum_i \left[\frac{\boldsymbol{U}}{2} \hat{n}_i \left(\hat{n}_i - 1\right) - \boldsymbol{\mu} \hat{n}_i \right] - \boldsymbol{t} \sum_{\langle i,j \rangle} \left[\hat{a}_i^\dagger \phi + \hat{a}_j \phi^* - |\phi|^2 \right] \\ &= \sum_i \left[\frac{\boldsymbol{U}}{2} \hat{n}_i \left(\hat{n}_i - 1\right) - \boldsymbol{\mu} \hat{n}_i + \boldsymbol{t} z |\phi|^2 \right] - \boldsymbol{t} z \sum_i \left[\hat{a}_i^\dagger \phi + \hat{a}_i \phi^* \right] \\ &\equiv \sum_i \left[\hat{H}_i + \hat{V}_i^{\mathbf{t}} \right] \qquad \xrightarrow[\text{Hamiltonian}]{\text{effective on-site}} \qquad \hat{H}_{\text{loc}} = \hat{H}^{(\mathbf{0})} + \hat{V}^{\mathbf{t}} \end{aligned} \tag{4.10}$$

where z is the **coordination number**, counting the number of next nearest neighbors. As a result, since the decoupled Hamiltonian is now local, we may focus on the effective on-site Hamiltonian, therefore dropping the subscript i. From here, in order to analytically determine the phase diagram, we may treat $\hat{V}^{\mathbf{t}}$ as a weak perturbation and rely on second-order perturbation theory.

As said in our qualitative description, the Mott-insulating phase is characterized by an integer boson density and a nonzero energy gap for all excitations. As a result, Mott insulators are also incompressible, since their filling density does not change under variations of the chemical potential $\boldsymbol{\mu}$. To show this, let us focus on the local unperturbed

[11] Indeed, Bogoliubov theory would describe the transition between a normal gas and the superfluid state.
[12] Namely, the system presents an equal integer filling number of bosons per lattice site and it is considered in the limit $\boldsymbol{U} >> \boldsymbol{t} > 0$.

Hamiltonian $\hat{H}^{\mathbf{0}}$. If we denote the unperturbed eigenenergies of the state with exactly n particles by $E_n^{(\mathbf{0})}$, we find that the unperturbed ground-state energy is simply the solution of a minimization problem

$$E_n^{(\mathbf{0})} = \frac{\boldsymbol{U}}{2} n\,(n-1) - \boldsymbol{\mu} n + \boldsymbol{t} z |\phi|^2 \qquad \xrightarrow[\text{energy}]{\text{ground-state}} \qquad E_{n_0}^{(\mathbf{0})} = \left\{ E_n^{(\mathbf{0})} \mid n = 0, 1, 2, \ldots \right\}_{\min} \tag{4.11}$$

from which the ground state $|n_0^{(\mathbf{0})}\rangle$ is straightforwardly defined. Since the eigenenergies depend on system's parameters, we also expect the energy-minimizing local occupation number to be a function of them. Indeed, if we suppose to be in the system's ground state, we can determine the local occupation number $n_0(\mu, U)$ by calculating the energy cost to add or remove one particle from the system[13]

$$E_{n_0+1}^{(\mathbf{0})} = \frac{\boldsymbol{U}}{2}\,(n_0{+}1)\,n_0 - \boldsymbol{\mu}\,(n_0{+}1) + \boldsymbol{t} z |\phi|^2 = E_{n_0}^{(\mathbf{0})} + \boldsymbol{U} n_0 - \boldsymbol{\mu} > E_{n_0}^{(\mathbf{0})} \quad \xrightarrow{\text{resulting in}} \quad n_0 > \frac{\mu}{U}$$

$$E_{n_0-1}^{(\mathbf{0})} = \frac{\boldsymbol{U}}{2}\,(n_0{-}1)\,(n_0{-}2) - \boldsymbol{\mu}\,(n_0-1) + \boldsymbol{t} z |\phi|^2 = E_{n_0}^{(\mathbf{0})} + \boldsymbol{U}\,(1-n_0) + \boldsymbol{\mu} > E_{n_0}^{(\mathbf{0})} \quad \xrightarrow{\text{resulting in}} \quad \frac{\mu}{U} > n_0 - 1$$

By iterating the reasoning above, we determine the ground state occupation number as a function of μ/U.[14] The corresponding ground state therefore consists in a Fock state with the same number of particles n_0 (occupancy for minimal energy) on each site of the lattice. In a similar fashion, it is straightforward to present another characteristic property of Mott insulators, namely their non-vanishing excitation gap Δ_0, defined as the sum of the energy cost needed to add and to remove one particle from the system.

$$n_0(\boldsymbol{\mu}/\boldsymbol{U}) = \begin{cases} 0 & \text{for } \boldsymbol{\mu}/\boldsymbol{U} < 0 \\ 1 & \text{for } 0 < \boldsymbol{\mu}/\boldsymbol{U} < 1 \\ 2 & \text{for } 1 < \boldsymbol{\mu}/\boldsymbol{U} < 2 \\ \vdots & \\ n & \text{for } n-1 < \boldsymbol{\mu}/\boldsymbol{U} < n \end{cases} \qquad \begin{aligned} |n_0^{(\mathbf{0})}\rangle &= \prod_{i=1}^{N} \frac{1}{\sqrt{n_0}} \left(a_i^\dagger\right)^{n_0} |\mathbf{0}\rangle \\ \Delta_0 &= (E_{n_0+1} - E_{n_0}) + (E_{n_0-1} - E_{n_0}) = \boldsymbol{U} \end{aligned}$$

As we can see, the states where μ/U takes an integer value are doubly degenerate on every site: this results in a 2^N fold degeneracy on the whole lattice, which will be broken by a non-zero $\boldsymbol{t}$.

That being said, the next step is to apply the principles of perturbation theory and compute the energy and state corrections.[15] Due to the fact that the perturbation $\hat{V}^{\mathbf{t}}$ is linear in the creation and annihilation operators, all corrections of an odd order to the energy will vanish in the occupation number basis. Since, as it will turn out, the sum of the energy corrections ultimately results in an expansion in the order parameter ϕ, we may apply Landau's theory of phase transitions to argue where the phase transition appears. Consequently, following Landau's approach, we will determine energy corrections up fourth order

$$\begin{aligned} E_n^{(\mathbf{0})} &= \frac{U}{2} n\,(n{-}1) {-} \mu + t z |\phi|^2 & E_{n_0}^{(\mathbf{1})} &= 0 \\ E_{n_0}^{(\mathbf{2})} &= (tz)^2 \left[\frac{n_0+1}{\mu - U n_0} + \frac{n_0}{U\,(n_0-1) - \mu} \right] |\phi|^2 & E_{n_0}^{(\mathbf{3})} &= 0 \end{aligned}$$

$$E_{n_0}^{(\mathbf{4})} = (tz)^4 |\phi|^4 \left[\frac{(n_0+1)(n_0+2)}{(\mu - n_0 U)^2\,[2\mu - (2n_0{+}1)U]} - \frac{(\mu{+}U)\left[\frac{n_0}{(\mu - n_0 U + U)^2} + \frac{n_0+1}{(\mu - n_0 U)^2} \right]}{(\mu - n_0 U)(\mu - n_0 U + U)} - \frac{(n_0-1) n_0}{[2\mu + (3{-}2n_0)U]\,(\mu - n_0 U + U)^2} \right]$$

Now, if we assemble the resulting corrections factoring out the order parameter, the resulting energy of the perturbed system is

$$E\,[\phi, \phi^*] = a_0 + a_2 |\phi|^2 + a_4 |\phi|^4 + \mathcal{O}\big(|\phi|^6\big) \tag{4.12}$$

which can be identified as the expansion of a thermodynamic potential in powers of a order parameter. According to Landau's theory, the phase transition will happen when the expansion coefficient a_2 vanishes, *if* the coefficient a_4 is positive; otherwise $E\,[\phi, \phi^*]$ would be unbound from below. Indeed, as shown in [17], a_4 is positive and we can proceed in finding the right conditions for the parameters. Since the energy functional depends on two variables, let us differentiate with respect to ϕ^* and ϕ consecutively.[16] The solution that minimizes the energy is the one for which the second derivative is positive, and this will depend on the sign of a_2.

$$\begin{aligned} \frac{\partial E}{\partial \phi^*} &= a_2 \phi + 2 a_4 |\phi|^2 \phi \overset{!}{=} 0 \qquad \xrightarrow{\text{resulting in}} \qquad \phi_0 = 0 \quad \text{or} \quad |\phi_\pm|^2 = -\frac{a_2}{2a_4} \\ \frac{\partial^2 E}{\partial \phi \partial \phi^*} &= a_2 + 4 a_4 |\phi|^2 \overset{!}{>} 0 \qquad \xrightarrow{\text{resulting in}} \qquad |\phi| = \begin{cases} 0 & \text{for } a_2 > 0 \\ \sqrt{\frac{-a_2}{2a_4}} & \text{for } a_2 < 0 \end{cases} \end{aligned} \tag{4.13}$$

[13] If the ground state has no particles, namely $n_0 = 0$, we then obtain the condition $\mu/U < n_0 = 0$.

[14] This result may seem counter intuitive, since we have stated that Mott insulators are incompressible. In reality, the problem is only apparent. As we will show, in the Mott-insulating limit the ground state occupation number can only have **discrete** values depending on the model's parameters, among which the chemical potential $\boldsymbol{\mu}$. This ultimately results in a vanishing compressibility.

[15] To ease the notation, we will denote the unperturbed state as $|n_0^{(\mathbf{0})}\rangle \equiv |n_0\rangle$.

[16] The order of partial differentiation does not matter, since $E\,[\phi, \phi^*]$ can be thought as arbitrarily smooth.

where the solution for $a_2 < 0$ corresponds to a continuum of points, namely the boundary of a circle with radius of $r_\phi \equiv \sqrt{-a_2/2a_4}$. Since the order parameter ϕ is non-zero for $a_2 < 0$ and zero for $a_2 > 0$, there must be a **second-order phase transition** at $a_2 = 0$. The order parameter ϕ characterizes the superfluid phase, indicating that the Mott-insulating phase is stable for $a_2 > 0$, while the superfluid phase occurs for $a_2 < 0$. Now, let us examine the system right at the transition line, namely when $a_2 = 0$. In order to simplify the notation, similarly to [18], we introduce the variables $\tilde{\mu} \equiv \mu/U$ and $w \equiv tz/U$

$$a_2 = tz + (tz)^2 \left[\frac{n_0+1}{\mu - Un_0} + \frac{n_0}{U(n_0-1)-\mu}\right] = wU\left[1 + w\left(\frac{n_0+1}{\tilde{\mu}-n_0} + \frac{n_0}{n_0-1-\tilde{\mu}}\right)\right] \stackrel{!}{=} 0$$

$$\xrightarrow{\text{solving for } w} \quad \boxed{w = \frac{(n_0-\tilde{\mu})\left[\tilde{\mu}-(n_0-1)\right]}{\tilde{\mu}+1}} \tag{4.14}$$

This equation defines the boundary of the **superfluid-to-Mott insulator transition**, which is shown in figure 4.1. In order to analytically describe the transition line, let us start by solving (4.14) for $\tilde{\mu}$. The resulting quadratic equation admits two solutions

$$\tilde{\mu}^2 - \tilde{\mu}(2n_0 - 1 - w) + w + n_0(n_0-1) = 0 \quad \xrightarrow{\text{resulting in}} \quad \begin{cases} \tilde{\mu}_+ = n_0 - \frac{1}{2} - \frac{w}{2} + \sqrt{w^2 - 4w(n_0+1/2)+1} \\ \tilde{\mu}_- = n_0 - \frac{1}{2} - \frac{w}{2} - \sqrt{w^2 - 4w(n_0+1/2)+1} \end{cases} \tag{4.15}$$

for given values of n_0, provided that the radicand is positive. These solutions, in fact, provide the cartesian description of the phase transition curve as $\tilde{\mu}_\pm(w)$ corresponds to the upper and lower branches of the lobes in figure 4.1, also known as **Mott lobes**. Every lobe, and therefore every pair of branches, is built around a given integer value of n_0. The solutions merge at the tips of the Mott lobes, where $w^2 - 4w(n_0+1/2)+1 = 0$, resulting in the critical values for w and $\tilde{\mu}$

$$\begin{aligned} w_c &= 2n_0 + 1 - 2\sqrt{n_0^2 + n_0} \\ \tilde{\mu}_c &= n_0 - 1/2 - w_c/2 = -1 + \sqrt{n_0^2 + n_0} \end{aligned} \tag{4.16}$$

In addition, at the specific points where $\mu = Un_0$ or $\mu = U(n_0 - 1)$, the ground energy is degenerate and $w = 0$. These points correspond, in our new representation, to the intersections of the Mott lobes with the $\tilde{\mu}$-axis. This ultimately means the phase boundary extends down to $t = 0$, right at the intersection points. On the other hand, for any $t > 0$ the system will inevitably in the superfluid state, for every U.[17]

As a conclusion of our analytical description of the phase transition, let us come back to the average number of bosons per lattice site and on the compressibility of both phases. Since the perturbed energy (4.12) is recognized as the grandcanonical thermodinamic potential, the average particle number per lattice site may be determined through the classic thermodynamic relation in (4.3), which leads to the definition of compressibility κ

$$\langle n \rangle = -\frac{\partial E[\phi, \phi^*]}{\partial \mu} = n_0 - \frac{\partial}{\partial \mu}\left[a_2|\phi|^2 + a_4|\phi|^4\right] \qquad \xrightarrow[\text{we define}]{\text{from which}} \qquad \kappa \equiv \frac{1}{\langle n \rangle^2}\frac{\partial \langle n \rangle}{\partial \mu} \tag{4.17}$$

This results in two radically different scenarios, depending on the phase of the system:

- In the Mott-insulating phase, where $\boldsymbol{t} = 0$ and therefore $\phi = 0$, the average number of bosons per lattice site equals the value that minimizes the energy, namely $\langle n \rangle = n_0$. This holds within a Mott-lobe for a given n_0, confirming our previous results. Looking at the compressibility of the Mott-insulating phase, since the average number of bosons is constant, κ ultimately vanishes. As a result, the system is incompressible everywhere within a Mott-lobe, having it fixed average integer density.

- In the superfluid phase, where the order parameter shifts to the non-zero value of $\phi = r_\phi$, the average density can assume any real value resulting from

$$\langle n \rangle = n_0 + \frac{a_2}{2a_4}\frac{\partial a_2}{\partial \mu} - \frac{a_2^2}{4a_4^2}\frac{\partial a_4}{\partial \mu} \qquad \xrightarrow[\langle n \rangle = n_0 \text{ for}]{\text{where}} \qquad \frac{a_2}{2a_4}\frac{\partial a_2}{\partial \mu} - \frac{a_2^2}{4a_4^2}\frac{\partial a_4}{\partial \mu} = 0 \tag{4.18}$$

  where $\langle n \rangle = n_0$ if the second and third term are zero. Since the $\partial a_2/\partial \mu = 0$ is satisfied at the tip of every Mott lobe, the phase transition at the tips happens with fixed constant integer density. On the other hand, anywhere else on the transition line, the transition is accompanied by a density change. Now, examining the superfluid compressibility, we see that it is indeed non-vanishing.

[17] Indeed, thanks within the new parametrization, $w = \frac{tz}{U} \to 0^+$ for $U \to \infty$.

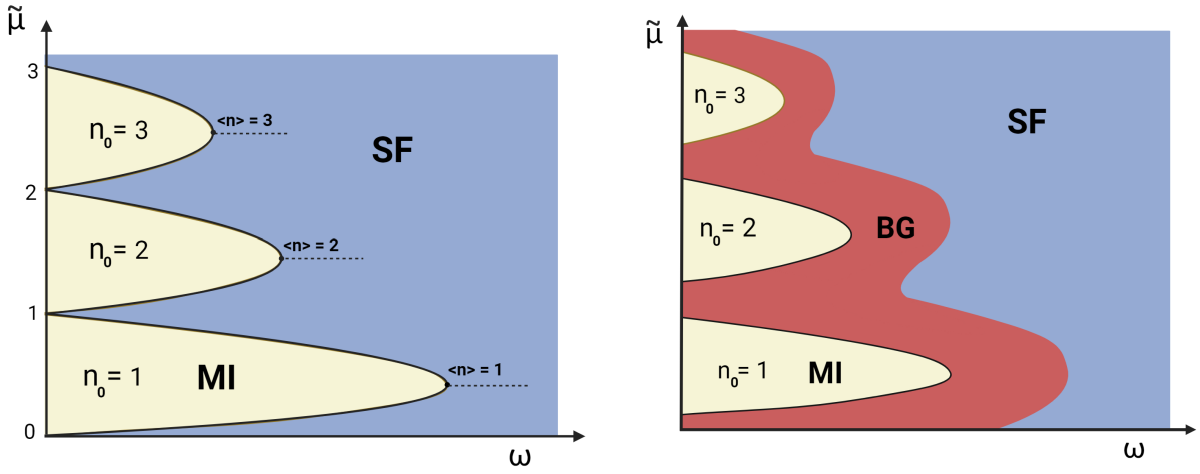

Figure 4.1: On the left, we present the resulting phase diagram of the Bose-Hubbard model with no disorder. As we can see, the system undergoes a direct quantum phase transition between the superfluid **SF** and the Mott-insulator **MI** phase. On the right, we propose a visualization of the phase diagram of the Bose-Hubbard model with on-site disorder. Indeed, the new Bose glass phase prevents a direct **MI-SF** quantum phase transition.

4.3 Bounded disorder

The interplay between disorder and interactions is one of the most intriguing and long-standing challenges in condensed matter physics, leading to numerous controversial theoretical and experimental findings. While the pure system is well understood, the disordered Bose-Hubbard model remains debated, even at a qualitative level. A key issue is the effect of arbitrarily weak disorder near the superfluid-to-Mott insulator quantum critical point of the pure system. Based on one-dimensional results by Giamarchi and Schulz [9], Fisher et al. [10] proposed the existence of a Bose glass phase in the disordered Bose-Hubbard model across all dimensions.

The Bose glass can be seen as a Mott insulator with isolated superfluid regions that do not connect, so the system remains insulating. These superfluid pockets notably alter the system's thermodynamics, leading to finite compressibility and the absence of a gap, despite the system remaining insulating.

Another important question is whether weak disorder affects the superfluid-insulator quantum phase transition at integer filling. Fisher et al. argued that a direct superfluid-to-Mott insulator transition is unlikely, though not entirely impossible. Interestingly, some numerical simulations and approximate methods have observed this rare outcome. Following the work of L. Pollet et al. [13], we introduce and prove the theorem of inclusions, which directly shows that a generic, bounded disorder prevents a direct superfluid-to-Mott insulator quantum phase transition.

Theorem [of Inclusions] *In presence of generic*[18]*, bounded disorder, there exist rare but arbitrarily large regions of the competing phase across a generic transition*[19] *line.*

Proof. The proof is straightforward if reducing the disorder bound enhances the superfluid phase [6]-[8]. In the opposite case, let us introduce a set of microscopic parameters $\vec{\xi}$ which control the shape and correlations of the disorder distribution. These parameters are considered alongside the disorder bound Δ and interaction U in the parameter space $(U, \Delta, \vec{\xi})$, where the critical hypersurface for the superfluid-insulator quantum phase transition is written as $\Delta = \Delta_c(U, \vec{\xi})$.

To simplify the analysis, without loss of generality, the interaction strength U is considered fixed and the system is examined as a function of changes in $\vec{\xi}$. The critical disorder threshold $\Delta_c(\vec{\xi})$ is assumed to be a continuous function of its microscopic parameters, and we consider a generic $\vec{\xi}$ that is not an extremum of Δ_c. Analyticity of $\Delta_c(\vec{\xi})$ can be expressed by a linear expansion

$$\Delta_c\left(\xi_i'\right) = \Delta_c\left(\xi_i\right) + A_i\left(\xi_i' - \xi_i\right)$$

for a particular component i. Given that disorder is inherently random, there are finite probabilities that arbitrarily large regions within the system will resemble disorder realizations corresponding to different parameter sets, denoted $\vec{\xi}_{\text{fluct}}$. These fluctuations lead to variations in the disorder threshold $\Delta_c(\vec{\xi})$, resulting in some regions where the disorder fluctuates away from the critical threshold.

In a sufficiently small neighborhood of the critical surface, due to the continuity of $\Delta_c(\vec{\xi})$, we can always find fluctuations $\vec{\xi}_{\text{fluct}}$ such that all points in the range

$$\mathcal{R}_\Delta = \left[\Delta_c(\vec{\xi}), \Delta_c(\vec{\xi}_{\text{fluct}})\right]$$

[18] By generic disorder we mean that any particular realization has a nonzero probability density to occur in a finite volume.
[19] By generic transition, we mean any first or second-order phase transition with an onset that is sensitive to all disorder characteristics.

remain within the superfluid region of the phase diagram. This is due to the fact that $\vec{\xi}$ is not an extremum. The deviation from the critical surface

$$\delta\Delta = \Delta_c(\vec{\xi}_{\text{fluct}}) - \Delta_c(\vec{\xi})$$

can be chosen small enough so that the fluctuation can compensate for disorder change. Thus, within a distance $|\delta\Delta|$ from the critical surface, the system develops arbitrarily large superfluid regions. These regions, being superfluid, manifest the absence of a gap due to the standard **Lifshitz tail** argument.

In a clean, ordered system, the energy spectrum tipically exhibits well-defined energy bands separated by gaps, in which no states exist. However, in a disordered system, random variations in the potential can create rare regions that resemble localized wells. These regions can host localized states at energies close to the band edges, effectively filling the gap. This phenomenon can be better understood by examining the density of states (**DOS**). Even though the **DOS** drops exponentially near the band edges, it never goes to zero in the presence of disorder, resulting in low but finite probability of states existing close to band edges, including inside the nominal gap region of the ordered system. The resulting extension of the **DOS** into what would otherwise be the gap is known as the Lifshitz tail.

In conclusion, the presence of these large superfluid domains prevents the system from undergoing a direct transition from superfluid to Mott insulator. Instead, a Bose Glass phase must emerge in between.

4.4 Superfluid-to-Bose Glass transition

Since the seminal works of Giamarchi and Schulz [9] and Fisher et al [10], the Hamiltonian (3.17) has been studied with a variety of techniques, mainly in one and two dimensions. In addition, highly sophisticated numerical simulations have been performed to uncover the full phase diagram of the disordered Bose-Hubbard model. In the following, our main purpose is not to compete with those simulations, but just to provide an interpretation of the phase diagram by means of a simple variational wavefunction.

Following the reasoning of [16], we will consider a two-dimensional Bose-Hubbard Hamiltonian in the presence of disorder and construct a trial many-body wavefunction by solving a single-particle problem for one boson at a time. Such wavefunction ultimately consists in a permanent of non-orthogonal single-particle wavefunctions, that are determined in a variational manner. More precisely, we will follow an Hartree-Fock-like variational approach to the problem of disordered and interacting bosons, that amounts to searching for the permanent that minimizes the total energy[20]. Since all coherence properties of the wavefunction are hidden in the single particle wavefunctions that build the permanent, we present a new criteria to investigate the superfluid-to-Bose glass transition, namely the **overlap matrix criterion**.

For now, let us assume that we have successfully found the optimal permanent for N particles, which can be written in terms of a set of single-particle wavefunctions ψ_α, with amplitude $\psi_{\alpha i}$ at site i

$$|\Psi\rangle = \prod_{\alpha=1}^{N} \left[\sum_i \psi_{\alpha i} a_i^\dagger\right] |\mathbf{0}\rangle \tag{4.19}$$

In order to validate the proposed criteria, we will check the presence of superfluidity by calculating the superfluid stiffness ρ_{sf}, defined through

$$\rho_{\text{sf}} \simeq \frac{L^2}{N} \frac{\partial^2 E_\theta}{\partial\theta^2}\bigg|_{\theta=0} \qquad \text{with} \qquad E_\theta = -\sum_{ij}\left[\tfrac{t_{ij}}{2} - \delta_{ij}\left(\epsilon_i - 2U\right)\right] C_{ij} + \tfrac{U}{2}\sum_i \left[\frac{\text{Per}(I_{iiii})}{\text{Per}(\Omega)} - 2\right] \tag{4.20}$$

where E_θ is the average value of the Hamiltonian (3.17), evalued in terms of permanents, with twisted boundary conditions.[21] As it will be clear in the proceeding, here $C_{ij} = \langle\Psi|a_i^\dagger a_j|\Psi\rangle$ is the density matrix, $\Omega_{\alpha\beta} = \sum_i \psi_{\alpha i}\psi^*_{\beta i}$ is the overlap matrix and $\text{Per}\left(I_{ijkl}\right) = \langle\Psi|a_i a_j a_k^\dagger a_l^\dagger|\Psi\rangle$.

Overlap matrix criterion. Since the wavefunctions that build a permanent need not be orthogonal to one another, we expect the overlap matrix $\Omega_{\alpha\beta} = \sum_i \psi_{\alpha i}\psi^*_{\beta i}$ to have non-zero off-diagonal elements[22]. In what follows we derive a simple criterion to detect an eventual superfluid phase of (4.19) based on the properties of the overlap matrix. Let us start by noting that the norm of (4.19) can be written as an integral over classical variables as [10]

$$\langle\Psi|\Psi\rangle = \int \prod_\alpha \frac{\mathrm{d}\xi_\alpha \mathrm{d}\xi_\alpha^*}{\pi} \mathrm{e}^{-\mathcal{S}(\xi,\xi^\dagger)} \qquad \text{with} \qquad \mathcal{S}\left(\xi,\xi^\dagger\right) = \xi^\dagger(\Omega - \mathbb{I})^{-1}\xi - \sum_\alpha \ln\left(1 + |\xi_\alpha|^2\right) \tag{4.21}$$

[20] Unlike conventional Hartree-Fock theory for fermions, such an approximation for bosons does not lead to significant simplifications with respect to exact numerical simulations because permanents are extremely difficult to handle.

[21] Such conditions can be considered along a given direction $\mathbf{x}$ or, equivalently, with the parameter for hopping between neighboring sites $t_{ij} = te^{\mathrm{i}\theta\vec{r}\cdot\vec{x}}$, where $\vec{r} = (\mathbf{R}_i - \mathbf{R}_j)/L$.

[22] For instance, if all bosons condense into a single state, then all ψ_α are equal and $\Omega_{\alpha\beta} = 1, \forall\alpha,\beta \in [1, N]$.

where $\mathcal{S}\left(\xi,\xi^\dagger\right)$ is the action describing the system, as proven in [16]. The main contribution to the integral comes from the saddle point,[23] which is the solution of

$$\xi_\alpha = \textstyle\sum_\beta \left(\Omega_{\alpha\beta}-\delta_{\alpha\beta}\right)\frac{1}{1+|\xi_\beta|^2}\xi_\beta \qquad \xrightarrow{\text{linearization}} \qquad \xi_\alpha = \textstyle\sum_\beta \left(\Omega_{\alpha\beta}-\delta_{\alpha\beta}\right)\xi_\beta \tag{4.22}$$

The above equation implies that finite values of ξ_α appear in groups, or equivalently that Ω is a block matrix. In the presence of disorder, this is suggestive of the existence of clusters occupied by bosons whose wavefunctions mutually overlap. By linearizing the equation, the condition for the appearance of a cluster translates into a block of Ω acquiring an eigenvalue $\Omega_{\alpha\beta}>2$.[24] In order to detect a long-range order within the system, in analogy to what we have found in (4.4), we resort to the definition of the density matrix[25]

$$C_{ij} = \langle\Psi|a_i^\dagger a_j|\Psi\rangle = \sum_{\alpha\beta}\psi_{i\alpha}^\dagger\,\langle\xi_\alpha\xi_\beta^\dagger\rangle\,\psi_{j\beta} \tag{4.23}$$

where we have rewritten C_{ij} within the path integral formulation, as shown in [16]. Here the average $\langle\xi_\alpha\xi_\beta^\dagger\rangle$ is weighted by $\exp\{-\mathcal{S}\}$, with the action $\mathcal{S}$ given by equation (4.19). It is important to notice that both classical variables ξ_α and ξ_β inherit a characteristic phase, which depends on the block to which the classical variable belongs and on its relative phase with respect to the block. As we will see, in order to correctly detect long-range order it is necessary to pay attention to such phases. Therefore let us define $\xi_i=\sum_\alpha\psi_{i\alpha}^\dagger\xi_\alpha$ and $\xi_j^\dagger=\sum_\beta\xi_\beta^\dagger\psi_{j\beta}$, through which the density matrix reads

$$C_{ij} = \sum_{\alpha\beta}\psi_{i\alpha}^\dagger\,\langle\xi_\alpha\xi_\beta^\dagger\rangle\,\psi_{\beta j} = \langle\xi_i\xi_j^\dagger\rangle \tag{4.24}$$

Thanks to the new parametrization, the linearized saddle point equation (4.22) becomes

$$\begin{gathered}\xi_\alpha = \textstyle\sum_\beta\left(\Omega_{\alpha\beta}-\delta_{\alpha\beta}\right)\xi_\beta = \sum_\beta\left[\sum_j\psi_{j\alpha}\psi_{j\beta}^\dagger\xi_\beta-\delta_{\alpha\beta}\xi_\beta\right] = \sum_j\psi_{j\alpha}\xi_j^\dagger-\xi_\alpha \\ \xrightarrow{\text{from which}} \qquad 2\textstyle\sum_\alpha\psi_{i\alpha}^\dagger\xi_\alpha = \sum_j\sum_\alpha\psi_{i\alpha}^\dagger\psi_{j\alpha}\xi_j^\dagger \\ 2\xi_i = \textstyle\sum_j\mathcal{O}_{ij}\xi_j^\dagger\end{gathered} \tag{4.25}$$

where in the last step we have introduced the matrix $\mathcal{O}_{ij}=\sum_\alpha\psi_{i\alpha}^\dagger\psi_{j\alpha}$, which represents the density matrix of the wavefunctions. From this reasoning, a criteria for detecting an extreme superfluid solution straightforwardly follows:

$$\mathcal{F} \equiv \frac{1}{N_\mathrm{s}}\sum_{ij}\mathcal{O}_{ij} \geq 2 \tag{4.26}$$

Iterative method. The Hartree-Fock simplified approach described in [16] consists in adding one boson at a time, with a wavefunction that is the ground state of a non-interacting Hamiltonian with a potential determined by the already added bosons. Specifically, we consider the non-normalized N-boson wavefunction

$$|\Psi_N\rangle = \prod_{\alpha=1}^{N}\left[\sum_j\chi_{\alpha j}a_j^\dagger\right]|\mathbf{0}\rangle \tag{4.27}$$

where $\chi_{\alpha j}$ with $j=1,\dots,N_\mathrm{s}$ are generically non-orthogonal single-particle wavefunctions. The first wavefunction χ_{1j} is the ground state of (3.17) with $\boldsymbol{U}=0$, as no bosons are present. Similarly, the $M+1$ wavefunction will be the ground state of the Hamiltonian

$$\hat{H}_\mathrm{app} = -\tfrac{\boldsymbol{t}}{2}\textstyle\sum_{ij}a_i^\dagger a_j+\sum_i\left[\boldsymbol{\epsilon_i}+\boldsymbol{U}\,\langle n_i\rangle\right]n_i \qquad \text{with} \qquad \langle n_i\rangle = \frac{\langle\Psi_M|a_i^\dagger a_i|\Psi_M\rangle}{\langle\Psi_M|\Psi_M\rangle} \tag{4.28}$$

where $\langle n_i\rangle$ is the average density of the previously added M bosons. In order to proceed algorithmically, it is important to translate our reasoning in terms of permanents. Let us start by defining the $M\times M$ overlap matrix $\Omega_{\alpha\beta}=\sum_{i=1}^{N_\mathrm{s}}\chi_{\alpha i}\chi_{\beta i}^\dagger$ with $\alpha,\beta=1,\dots,M$ and, for each couple of lattice sites (i,j), the $(M+1)\times(M+1)$ matrices D_{ij}

$$D_{ij} = \begin{pmatrix}\Omega & \hat{\chi}_i\\ \hat{\chi}_j^\dagger & \delta_{ij}\end{pmatrix} \qquad \text{where} \qquad \hat{\chi}_i=(\chi_{1i},\dots,\chi_{Mi})^t$$

By means of such definitions we can determine, for each iteration, the mean local density $\langle n_i\rangle$ and the intersite density matrix C_{ij} in terms of the wavefunction permanent

$$\langle n_i\rangle = \frac{\mathrm{Per}\left(D_{ii}\right)}{\mathrm{Per}(\Omega)}-1 \qquad C_{ij}\equiv\frac{\langle\Psi|a_i^\dagger a_j|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\mathrm{Per}\left(D_{ji}\right)}{\mathrm{Per}(\Omega)}-\delta_{ij} \qquad I_{ijkl} = \begin{pmatrix}\Omega & \hat{\chi}_i & \hat{\chi}_j\\ \hat{\chi}_k^\dagger & \delta_{ik} & \delta_{jk}\\ \hat{\chi}_l^\dagger & \delta_{il} & \delta_{jl}\end{pmatrix} \tag{4.29}$$

[23] As it will be clear, the saddle point approximation is rigorously valid only the emergent blocks of Ω are big enough.

[24] As remarked in [16], this is not the condition for superfluidity. The latter rather implies that an eigenvalue of Ω should grow with the number of bosons N, which means that several blocks should start to merge and overlap, until a percolating cluster emerges.

[25] Similarly to what we have seen in (4.4), off-diagonal long-range order implies that $C_{i,j}$ is finite for $|i-j|\to\infty$.

which enables us to investigate an eventual long-range off-diagonal order. This procedure is iterated until the desired number of N bosons is reached, resulting in the ground-state wavefunction of the bosonic system[26]. From here, as we stated, the superfluid properties of the model can be accessed by calculating the superfluid stiffness (4.20), for which the matrix I_{ijkl} now assumes the general form presented in (4.29). Upon repeating this calculation for several disorder configurations, we finally obtain the phase diagram[27] for our two-dimensional disordered Bose-Hubbard system.

As shown in figure 4.2, the phase transition is well described by examining the superfluid stiffness averaged over several on-site disorder strengths Δ, taken over different interaction energies U. Here the superfluid stiffness, represented through a contour plot, was set to zero in the regions of parameters where its variance was greater than its average.[28] Despite being an approximation, the superfluid stiffness well captures the qualitative behavior of the phase diagram: ρ_{sf} decreases with increasing disorder and, at fixed disorder, first increases with U and then diminishes.

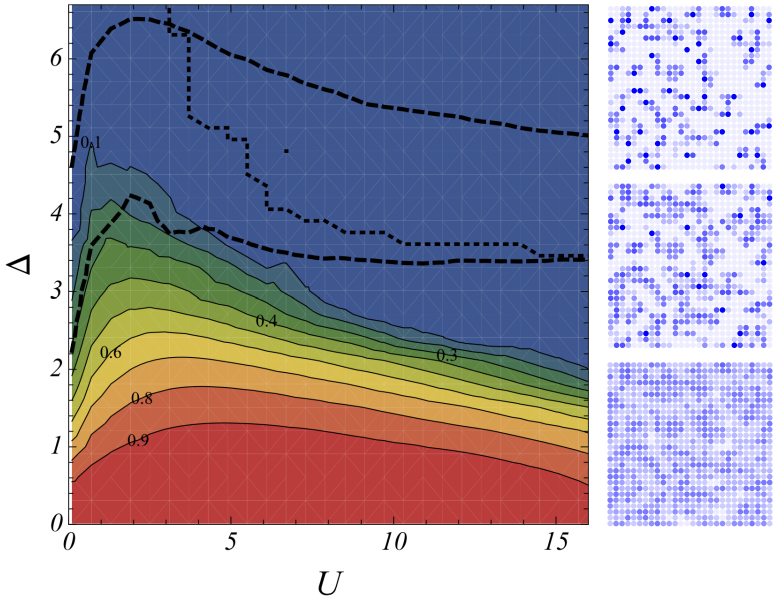

Figure 4.2: On the left, the contour plot of the superfluid stiffness ρ_{sf}, equation (4.20), for a 6×6 square lattice at filling $\nu = 1/4$, averaging over 400 disorder configurations. The two thick dashed lines and the dotted line show the border of the superfluid phase, obtained by looking at some indicators related to the overlap matrix, as discussed below. On the right, the contour plot of the particle density $\langle n_i\rangle$ on a 28×28 lattice with $N = 49$ bosons, i.e. filling $\nu = 1/16$, at $U = 10$ and for a single realization of disorder with $\Delta = 1, 2, 3$ from bottom to top (i.e. crossing the transition). The darker the sites, the higher the density. Here, in order to reach larger system sizes, the particle densities $\langle n_i\rangle$ have been determined through the simpler (4.30). ***Note:*** in both cases, the values of U and Δ are in units of t.

In the same figure, the conditions emerging from the overlap matrix criterion have been represented through the drawing of three dashed lines:[29]

- The thin dashed line represents the condition for which the saddle point linearized equation (4.22) always has nontrivial solutions, namely if Ω has eigenvalue 2. More explicitly, system's configurations *below* the thin dashed line are such that $(\Omega - 2\mathbb{I})$, or equivalently $(\mathcal{O} - 2\mathbb{I})$, has both positive and negative eigenvalues for any disorder, implying that the saddle point equation always has nontrivial solutions. *Above* the thin dotted line, instead, for some disorder configurations all the eigenvalues of Ω are smaller than 2.
- The two thick dashed lines correspond, instead, to specific values of the **superfluid parameter** $\mathcal{F}$ defined in (4.26). The *upper line* represents the condition $\overline{\mathcal{F}} = 2$, namely when the value of $\mathcal{F}$ averaged over several disorder configurations equals 2. The *lower line* represents the condition $\min(\mathcal{F}) = 2$, namely when the minimum value of $\mathcal{F}$ among the disorder configurations equals 2. Below those lines the corresponding quantities exceed the threshold value.

Thanks to figure 4.2, we can compare the superfluid-to-Bose glass transition obtained from the superfluid stiffness ρ_{sf} with that given by the overlap matrix criterion, and straightforwardly prove their agreement. Indeed, while a nontrivial solution of the saddle point equation occurs also for large disorder and weak interaction (the thin dashed line keeps on growing with decreasing U), the superfluid parameter $\mathcal{F}$, which detects the long-range order (thick dashed lines), follows correctly the stiffness behavior also for small interactions. As a result, we find that the superfluid

[26] As remarked in [16], the method can be easily extended to study excited states, as it is sufficient to select at any iteration not the ground state but an excited one. This would enable us to study the system at finite temperatures.

[27] Because in a finite system there cannot be a true gauge symmetry breaking, the phase diagram figure 4.2 consists in just an indication of what could happen in the thermodynamic limit.

[28] We are cutting off, therefore, the values of ρ_{sf} that are statistically undetermined.

[29] In this case, given the many-body wavefunction of equation (4.27), the overlap matrix is $\Omega_{\alpha\beta} = \sum_{i=1}^{N_{\text{s}}} \chi_{\alpha i}\chi^{\dagger}_{\beta i}$ with $\psi_{\alpha i} = \chi_{\alpha i}$. The action is given by equation (4.21) and the saddle point equation reads as in equation (4.22), which has nontrivial solution if Ω has eigenvalue 2.

properties of the many-body wavefunction (4.27) can be related to the matrix Ω of the overlaps between the single-particle wavefunctions $\chi_{\alpha i}$. In conclusion, the transition can be characterized, besides the vanishing stiffness, by the eigenvalues of the matrix of the overlaps between the singleparticle wavefunctions.

Finally, as we previously mentioned, a realistic view of a Bose glass is that of **disconnected droplets**. A way to confirm this idea is by plotting the average density, as shown in figure 4.2. Here, instead of equation (4.29), the average density has been defined as

$$\langle n_i \rangle \simeq \sum_{\alpha}^{N} |\chi_{\alpha i}|^2 \tag{4.30}$$

which is a good approximation for local densities, in order to computationally reach larger system sizes. We find that, at large disorder, bosons are indeed concentrated into droplets whose magnitude increases with decreasing disorder until a percolating cluster appears, which must presumably signal the onset of the superfluid phase. More generally, we could adopt this oversimplified approach in the iterative evaluation of the Hartree potential in equation (4.28), as if the already present M bosons were distinguishable. This approximation simplifies a lot the procedure for determining the single-particle wavefunctions, which can be pushed to very large system sizes. These single-particle wavefunctions can then be used to construct the permanent, whose superfluid properties can be assessed using the overlap matrix criterion. Even though such a procedure is hardly justifiable from the variational point of view, it provides a phase diagram that is qualitatively correct.

5 Conclusions

In this thesis, we have thoroughly examined the Disordered Bose-Hubbard Model, focusing on the effects of disorder on quantum phase transitions. One of the key results, grounded in the theorem of inclusions, is the finding that a direct transition from the superfluid to the Mott insulator phase is not possible in the presence of bounded disorder. Instead, the system undergoes a transition to an intermediate Bose Glass phase, characterized by finite compressibility, the absence of a gap, and localized insulating behavior.

To complement the theorem of inclusions, we introduced a variational method, the overlap matrix criterion, which provides an effective tool for analyzing phase transitions in the disordered system. Our results show that this method is consistent with the predictions of the theorem of inclusions, further reinforcing the stability of the Bose Glass phase in the presence of disorder.

The findings of this thesis are not only of theoretical significance but also have direct implications for experiments, particularly in systems such as ultracold atoms in optical lattices, where the Bose-Hubbard model can be realized with high precision. The variational method developed here can be extended to higher-dimensional systems and applied to study other forms of disorder, making it a versatile tool for understanding complex quantum systems.

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